Adapting reduced-size control space in hybrid data assimilation

M. Krysta[1,2], E. Blayo[2], E. Cosme[1], J. Verron[1] and A. Vidard[3]

[1] LEGI, BP 53, 38041 Grenoble Cedex 9, France

[2] LJK, University of Grenoble, BP 53, 38041 Grenoble Cedex 9, France

[3] INRIA, Grenoble, France

Abstract

Observations may be abundant in nowadays oceanography but they are restricted to some components of the state vector only. Consequently, a need for some prior information on the unobserved variables arises. In the standard 4D-Var it is accounted for via regularising properties of the background error covariance matrix. On the other hand, feasibility requirements may result in reduction of the size of the control vector and confine data assimilation correction to a small-size subspace of the original state space. Hence the necessity of an appropriate definition of such a subspace which must be of a low dimension and, at the same time, preserve regularising properties of the background error covariance matrix.

The question addressed in this study goes even further and tackles the problem of adapting the form of the control subspace to account for additional information gained in the data assimilation procedure. The problem has been studied in the framework of a hybrid approach to data assimilation. Hybrid in this study refers to a method merging an incremental 4D-Var with an equivalent Kalman smoother, both in a reduced rank approximation. The skeleton of the hybrid is thus formed by the 4D-Var enriched with an admixture of the smoother delivering a recipe for the evolution of the error covariance matrix. Its update is made at each transition from one assimilation window to another, at both analysis and forecast step. The analysis update modifies the reduced size error covariance matrix accordingly to the quality of the measurements assimilated into the system. Following system's trajectory in the forecast step, the basis spanning the control subspace is also adjusted.

A series of OSSEs implementing the hybrid method into a shallow water model in a wind driven double-gyre configuration has been performed. It has been opted for a definition of the reduced-size control subspace reflecting the directions of the largest variability of the system. These directions have been obtained via principal component analysis of several different samples of model trajectory. A number of tests has been performed in various configurations of twin experiments and the circumstances where the hybrid outperforms the standard 4D-Var have been identified. The general conclusion inferred from this study indicates that the propagation of the basis spanning the control subspace is capable of compensating for imperfect initialisation of this subspace and the most pertinent examples are shown below.

Ingredients

• Incremental variational approach (4D-Var)

A transition from a background state to an analysis is ensured via a sequence $\{\mathbf{x}_0^{a,(k)}\}_{k=0}^{k=K}$ of intermediate states : $\mathbf{x}_0^{a,(k+1)} = \mathbf{x}_0^f + \delta\mathbf{x}_0^{(k+1)}$, defined in terms of increments $\delta\mathbf{x}_0^{(k+1)}$ which minimise a cost function

$$\mathcal{J}\left(\delta\mathbf{x}_0^{(k+1)}\right) \;=\; \frac{1}{2}\,\delta\mathbf{x}_0^{(k+1)^T}[\boldsymbol{B}]^{-1}\,\delta\mathbf{x}_0^{(k+1)} + \frac{1}{2}\left[\mathbf{H}'\mathbf{M}'.\boldsymbol{\delta}\mathbf{x}_0^{(k+1)} - \mathbf{d}^{(k)}\right]^T \mathbf{R}^{-1}\left[\mathbf{H}'\mathbf{M}'.\boldsymbol{\delta}\mathbf{x}_0^{(k+1)} - \mathbf{d}^{(k)}\right] \qquad (1)$$

where $\mathbf{M}'$ and $\mathbf{H}'$ stand for a linearised model M and observation operator H,

$$\mathbf{d}^{(k)} = \mathbf{y} - H(\mathcal{M}(\mathbf{x}_0^f + \delta\mathbf{x}_0^{(k)})) + \mathbf{H}'.\delta\mathbf{x}^{(k)}\,; \qquad \mathbf{y} = \begin{bmatrix}\mathbf{y}_1\\ \mathbf{y}_2\\ \vdots\\ \mathbf{y}_N\end{bmatrix}\,;\ \mathbf{M}' = \begin{bmatrix}\mathbf{M}'(t_0,t_1)\\ \mathbf{M}'(t_0,t_2)\\ \vdots\\ \mathbf{M}'(t_0,t_N)\end{bmatrix}\ \cdots$$

and $\boldsymbol{B}$ and $\mathbf{R}$ are background and observation error covariance matrices, respectively. As $\mathcal{J}\left(\delta\mathbf{x}_0^{(k+1)}\right)$ is a quadratic function, the analysis increment can be obtained analytically

$$\delta\mathbf{x}_0^{(k+1)} = \boldsymbol{B}\mathbf{M}'^T\mathbf{H}'^T\left[\mathbf{H}'\mathbf{M}'\boldsymbol{B}\mathbf{M}'^T\mathbf{H}'^T + \mathbf{R}\right]^{-1}.\mathbf{d}^{(k)} \qquad (2)$$

• Extended Kalman Smoother (EKS)

It acts globally on the entire assimilation window. Its counterpart to cost function minimisation consists in searching for an increment which corrects the background state and is imposed to be a linear function, represented by a gain matrix $\mathbf{K}$, of innovation $\mathbf{d}^{(k)}$

$$\boldsymbol{\delta}\mathbf{x}_0^{(k+1)} = \mathbf{x}_0^{a,(k+1)} - \mathbf{x}_0^f = \mathbf{K}.\mathbf{d}^{(k)}$$

Minimisation of the analysis error yields

$$\mathbf{K} = \mathbf{P}_0^f\mathbf{M}'^T\mathbf{H}'^T\left[\mathbf{H}'\mathbf{M}'\mathbf{P}_0^f\mathbf{M}'^T\mathbf{H}'^T + \mathbf{R}\right]^{-1}, \qquad \text{and consequently} \qquad \boldsymbol{\delta}\mathbf{x}_0^{(k+1)} = \mathbf{P}_0^f\mathbf{M}'^T\mathbf{H}'^T\left[\mathbf{H}'\mathbf{M}'\mathbf{P}_0^f\mathbf{M}'^T\mathbf{H}'^T + \mathbf{R}\right]^{-1}.\mathbf{d}^{(k)} \qquad (3)$$

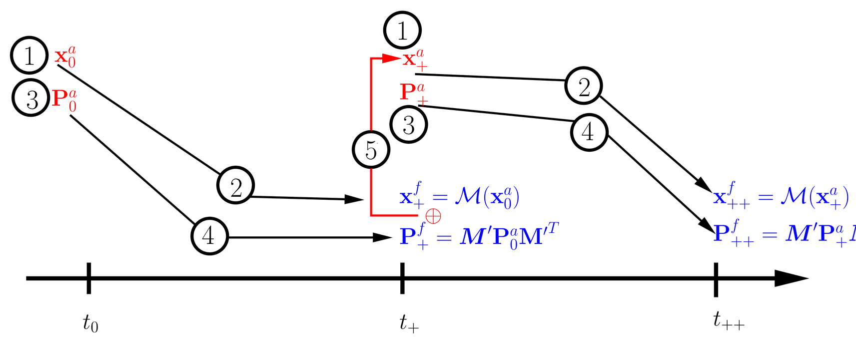
• Foundations of hybridisation

- Appropriate linearisation ensures equality of analyses, Eq.(2) and Eq.(3,) produced by both methods if $\boxed{\boldsymbol{B} = \mathbf{P}_0^f}$
- Additionally, the EKS provides the analysis error covariance matrix

$$\mathbf{P}_0^a \;=\; \left[[\mathbf{P}_0^f]^{-1} + \mathbf{M}'^T\mathbf{H}'^T\mathbf{R}^{-1}\mathbf{H}'\mathbf{M}'\right]^{-1} \qquad (4)$$

The increments being equal, the analysis error covariance matrix $\mathbf{P}_0^a$ also refers to the solution of the variational problem. It substitutes $\boldsymbol{B}$ in the cost function $\mathcal{J}(\delta\mathbf{x}_0^{(k+1)})$ at each assimilation window.

Hybrid algorithm



Full rank

1. $\mathbf{x}_0^a = \mathbf{x}_0^f + \boldsymbol{\delta}\mathbf{x}_0$ [via 4D-Var]
   A sequence of minima of cost functions $\{\mathcal{J}(\delta\mathbf{x}_0^{(k)})\}_{k=0}^{k=K}$ is computed on $[t_0, t_+]$
2. $\mathbf{x}_+^f = \mathcal{M}(\mathbf{x}_0^a)$
3. $\mathbf{P}_0^a$ [via smoother, Eq.(4)]
4. $\mathbf{P}_+^f = \boldsymbol{M}'\mathbf{P}_0^a\boldsymbol{M}'^T$
5. $\mathbf{P}_+^f$ injected into 4D-Var on $[t_+, t_{++}]$
6. $\mathbf{x}_+^a = \mathbf{x}_+^f + \boldsymbol{\delta}\mathbf{x}_+$ via 4D-Var on $[t_+, t_{++}]$
   which coincides with the first step of the algorithm

Reduced rank

Error covariance matrix based on a low-rank approximation (SEEK filter-alike) $\mathbf{P}_0^f = \mathbf{L}_0\mathbf{U}_-\mathbf{L}_0^T = \mathbf{L}_0\mathbf{W}_-\mathbf{W}_-^T\mathbf{L}_0^T$ where $\mathbf{L}_0 \in \mathbb{R}^{n\times r}$ and $\mathbb{R}^{r\times r} \ni \mathbf{U}_- = \mathbf{W}_-\mathbf{W}_-^T$ according to the Cholesky decomposition.

1. $\mathbf{x}_0^a = \mathbf{x}_0^f + \boldsymbol{\delta}\mathbf{x}_0 = \mathbf{x}_0^f + \mathbf{L}_0\mathbf{W}_-\boldsymbol{\chi}$ [via 4D-Var]
   where $\mathbb{R}^r \ni \boldsymbol{\chi}^{(k)} \longrightarrow \boldsymbol{\chi}$ arises from a series of cost functions of the form

$$\mathcal{J}(\boldsymbol{\chi}^{(k+1)}) = \frac{1}{2}\,\boldsymbol{\chi}^{(k+1)^T}\boldsymbol{\chi}^{(k+1)} + \frac{1}{2}\left[\mathbf{H}'\mathbf{M}'.\boldsymbol{\delta}\mathbf{x}_0^{(k+1)} - \mathbf{d}^{(k)}\right]^T\mathbf{R}^{-1}\left[\mathbf{H}'\mathbf{M}'.\boldsymbol{\delta}\mathbf{x}_0^{(k+1)} - \mathbf{d}^{(k)}\right]$$

2. $\mathbf{x}_+^f = \mathcal{M}(\mathbf{x}_0^a)$
3. **Analysis :** $\mathbf{P}_0^a = \mathbf{L}_0\mathbf{U}_0\mathbf{L}_0^T = \mathbf{L}_0\mathbf{W}_0\mathbf{W}_0^T\mathbf{L}_0^T$ where

$$\mathbf{U}_0^{-1} = \mathbf{U}_-^{-1} + \sum_i \mathbf{L}_0^T\boldsymbol{M}'^T\boldsymbol{H}'^T\mathbf{R}_i^{-1}\boldsymbol{H}'\boldsymbol{M}'\mathbf{L}_0 \qquad \text{low rank matrix modified}$$

   and the inverse exists since $\mathbf{U}_-$ is supposed to be symmetric, positive definite and the same argument holds for the second term. There is, however, new Cholesky decomposition to be made : $\mathbf{U}_0^{-1} = \mathbf{W}_0^{-T}\mathbf{W}_0^{-1}$ as required by the first step of the alogorithm
4. **Forecast :** $\mathbf{P}_+^f = \mathbf{L}_+\mathbf{U}_0\mathbf{L}_+^T = \mathbf{L}_+\mathbf{W}_0\mathbf{W}_0^T\mathbf{L}_+^T$ where

$$\mathbf{L}_+ = \boldsymbol{M}'\mathbf{L}_0 \qquad \text{basis of the control subspace modified}$$

5. $\mathbf{P}_+^f$ injected into 4D-Var on $[t_+, t_{++}]$
6. $\cdots$ coincides with the first step of the algorithm

OSSEs' configuration

Numerous OSSEs have been performed to test the hybrid method. Shallow water model in a wind driven double-gyre configuration has been employed to represent an ocean circulation model, $\mathcal{M}$, in our data assimilation experiments. The simulation begins with the system at rest. 5-year spin-up comes in the first place. It is directly followed by 10-year free simulation. Different sections of the resulting free trajectory are sampled with 2-day frequency in order to build various sets of the EOFs which are employed to initialise the subspace of control. Background state is issued immediately from this 10-year simulation. 4 years coming next define the period of data assimilation experiments and are split into 30-day assimilation windows. Yet another period of 4 years constitutes true trajectory of the system and is sampled with 10-day frequency to produce synthetic measurements of sea surface height. Some white noise is added to these measurements to account for observation error (5 cm).

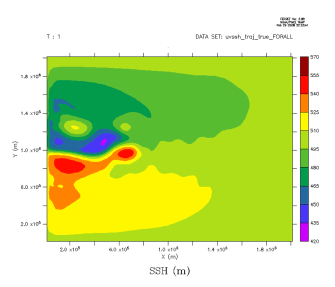
Shallow water model

$$\begin{aligned}
\partial_t u + u\partial_x u + v\partial_y u - fv + g^*\partial_x h &= \frac{\tau}{\rho_0 h} - ru + \nu\Delta u\\
\partial_t v + u\partial_x v + v\partial_y v + fu + g^*\partial_y h &= \frac{\tau}{\rho_0 h} - rv + \nu\Delta v\\
\partial_t h + \partial_x(hu) + \partial_y(hv) &= 0
\end{aligned}$$

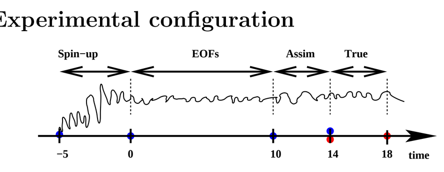
Forcing along the horizontal axis

$$\tau = \tau_0 \sin\left(\frac{2\pi}{L}\left(y - \frac{L}{4}\right)\right)$$

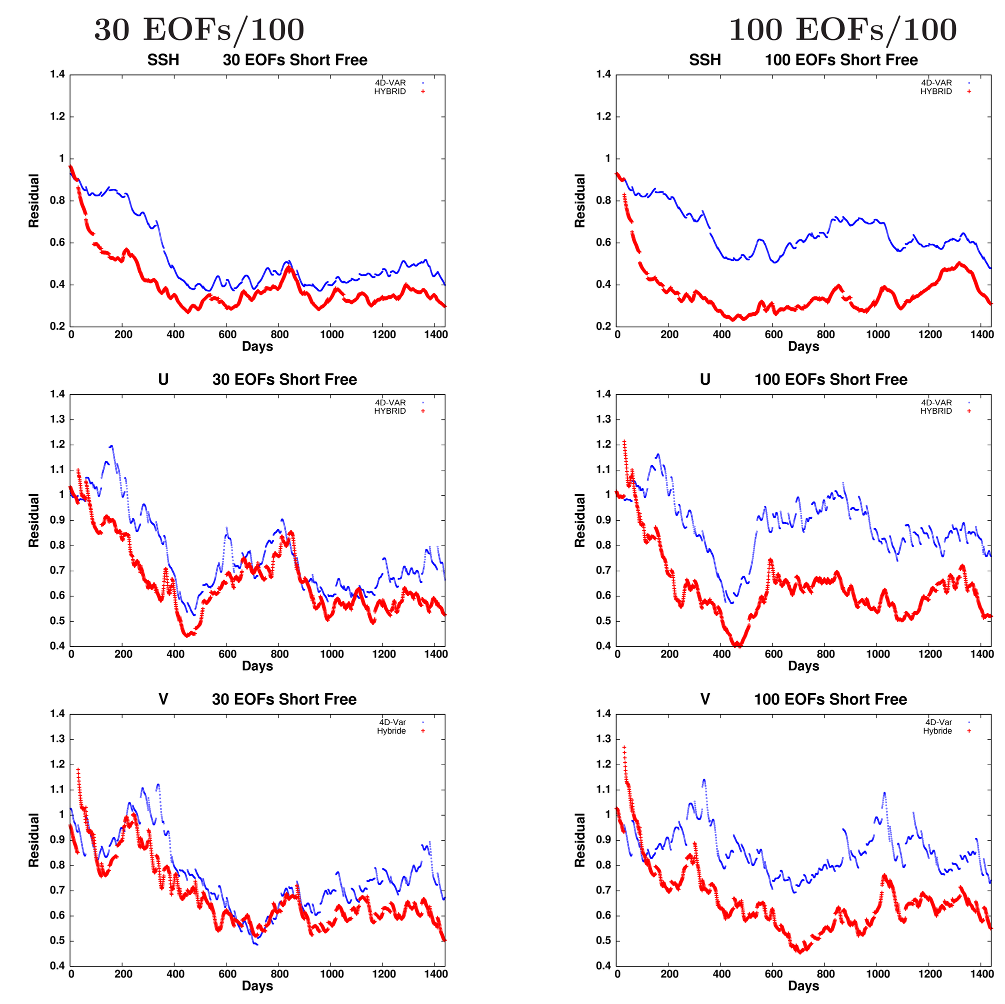
Simulation Snapshot



Experimental configuration



Numerical results



Residual of the analysis error as a function of time (4 years) for reduced rank data assimilation. Subspaces of control spanned by 30 (left) and 100 (right) vectors issued from short-term sampling of free trajectory. The results for both an observed variable (ssh) and the unobserved ones (u, v) are shown. Control subspace of dimension 100 defines a configuration where the hybrid approach (red) employing an evolving basis of control, and consequently background error covariance matrix, outperforms the standard 4D-Var (blue) which keeps the initial basis fixed.

• Initialising control subspace

Free model trajectory has been sampled with 2-day frequency over a period exceeding 6 months, considered to be short in comparison to a reference period of 10 years. The sample has been used to build a set of 100 EOFs. Two experiments employing the subspaces of control initialised by a subset of first 30 of them and the entire set of 100 have been performed. The results are shown on the left hand side.

• Evaluating control subspace

The information content of the vectors spanning the subspaces of control in our data assimilation experiments has been evaluated against full information contained in the system. Full information is hypothesised to be represented by state vectors issued from 10-year long true trajectory sampled with 2-day frequency. Consequently, a basis of the EOFs or a set of Fourier coefficients yielded from this sample are supposed to constitute full description of true system.

Firstly, we tackle the problem of a degree to which the subspaces of control represent the true system. The figures on the right hand side (top line) illustrate the projections of the full set of EOFs on the bases employed in data assimilation experiment in their initial (blue) and evolved (red) form.

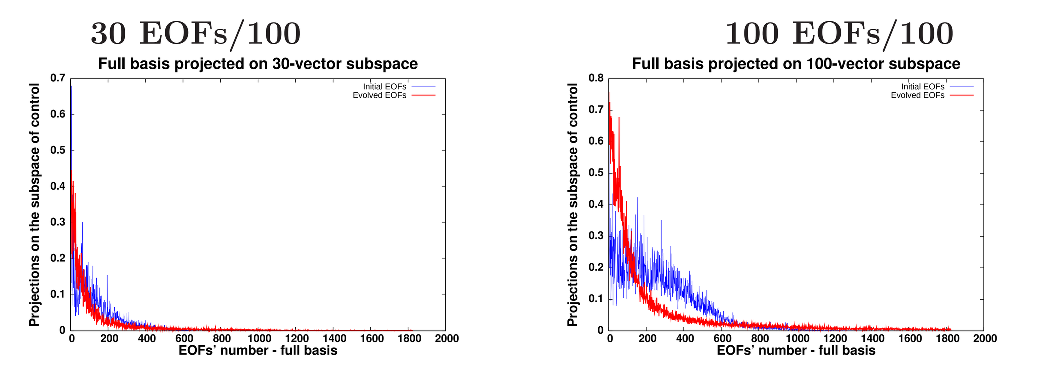
Secondly, bottom line, we show the projections of the first 100 Fourier coefficients representing full system information, again on the bases spanning the subspaces of control in their initial (blue) and final (red) forms.

• Discussion

It is noticeable that the hybrid method ensures considerable improvement with respect to the 4D-Var in case where the control subspace is spanned by 100 vectors. In contrast, an experiment employing only 30 of them shows weaker evidence of improvement due to basis evolution. Dramatic improvement of data assimilation results in the former case is to be associated with the ability of data assimilation system to acquire and retain information which is missing from the vectors spanning the control subspace at the initial stage.

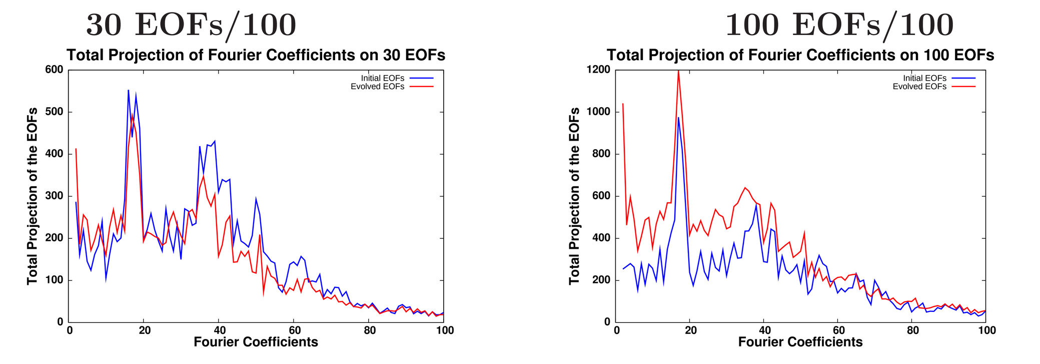
Two experiments presented here also illustrate the fact that the evolution of the first EOFs (high eigenvalues) has no significant impact on data assimilation performance. In contrast, evolution of those of the basis vectors which are initialised by the EOFs associated with smaller eigenvalues is responsible for considerable improvement of data assimilation results.

• Projections of the reference EOFs



Projections of the complete EOFs' basis on initial (blue) and final (red) subspaces of control. Results refer to the subspaces of dimension 30 (left) and 100 (right). In the second case a significant quantity of information has been accumulated in the vectors defining the subspace of control as a result of their evolution in data assimilation procedure.

• Projections of Fourier coefficients



Sum of the projections of the Fourier coefficients on all the vectors spanning the subspaces of control, 30 (left) and 100 (right) respectively. The evolving basis (red) accumulated some information missing from the basis initialised by a set of the EOFs at the beginning of data assimilation experiment. The phenomenon is far more pronounced in case where the subspace of control is spanned by 100 vectors.

Conclusions

- Hybrid method prescribes the evolution of the basis spanning the control subspace in reduced rank data assimilation. It may outperform the corresponding 4D-Var where the basis remains static. The configurations owing considerable improvement to the hybrid algorithm are the ones in which the EOFs initialising the subspace of control account exclusively for short-term characteristics of a modelled physical phenomenon.
- Evolving basis accumulates long term features of a model ensuring its transportation. The evidence of the presence of such supplementary information in a basis at the end of data assimilation experiment in comparison to its initial form has been shown in the figures illustrating the projections of full model characteristics (EOFs and Fourier coefficients) on the bases spanning the subspaces of control.
- Optimal configuration for reduced rank data assimilation employing the EOFs to define the subspace of control is as follows. The vectors initialised by the EOFs describing long term behaviour of the system may be kept static. The ones which are initialised by the EOFs representing short-term behaviour of the system should evolve. A clear cut between the two families of the EOFs is problem and configuration dependent and opens perspective for further investigations.