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Hybridization of the 4D-Var with a SEEK smoother in view of oceanic applications

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1. Introduction

Two main approaches, variational and sequential, coexist in geophysical data assimilation applications. In the variational approach, a cost function embracing all the observations accumulated within a given time interval is minimized. Some external knowledge on the system is generally introduced in a regularization term, namely a background \mathbf{x}^b (known as \mathbf{x}^f in the sequential approach), and the corresponding background error covariance matrix \mathbf{B} (whose sequential counterpart is the forecast error covariance matrix \mathbf{P}^f). There exists several approaches to model \mathbf{B} , either purely statistical (e.g. Derber and Bouttier, 1999; Wu and Purser, 2002; Buehner, 2005; Bannister, 2008a,b and references herein), or parameterizations based on physical, physical/statistical or empirical considerations (e.g. Weaver and Ricci, 2004; Weaver *et al.*, 2005). Nevertheless, in the standard 4D-Var, once \mathbf{B} has been specified it remains static over the entire duration of a data assimilation experiment.

Contrary to variational assimilation, sequential assimilation provides estimates of the covariance matrices of the forecast and analysis errors at each step of the assimilation process. Kalman smoothers (KS) (e.g. Cohn *et al.*, 1994; Evensen and Van Leeuwen, 2000; Cosme *et al.*, 2009) generalize the Kalman filter (KF) analysis by using data within the entire time span under consideration. In practice, the KF/KS and their variants are easier to implement than 4D-Var, but are unable to handle the large size system state vectors that are met in realistic geophysical problems. Various forms of adaptation have been developed aiming at reducing the computational burden, among which one can cite the Ensemble Kalman filter (EnKF) (Evensen, 1994) and the Singular Evolutive Extended Kalman filter (SEEK) (Pham *et al.*, 1998; Brasseur and Verron, 2006).

Many efforts have been made towards understanding the connections between variational and sequential methods and to open new research avenues based on their complementarities. An analysis of equivalences and differences between 4D-Var and KF prompts to combine both approaches to draw practical benefits of each and to provide more powerful algorithms. The first idea to advance is clearly to take advantage of the natural complementarity of 4D-Var and KF/KS with regard to \mathbf{B} , that is to use 4D-Var for updating the state and KF/KS to update \mathbf{B} . Building such a strategy results in practical atmospheric and oceanic applications to deal with some form of order reduction for the KF/KS, and therefore for the 4D-Var too. Reduced-order 4D-Var has already been explored with some success by Blayo *et al.* (1999) and Robert *et al.* (2005) in particular. It is therefore tempting to explore a fully consistent scheme for hybridization between 4D-Var and a reduced-order KF/KS approach. Note that a hybridization between the 4D-Var and the SEEK filter has already been investigated in an oceanic case by Robert *et al.* (2006a). For atmospheric applications, Liu *et al.* (2008, 2009) explored a coupling between 4D-Var and the EnKF. In a similar framework, Zhang *et al.* (2009) have privileged a linear combination of a static and dynamically estimated error

covariance matrix, as put forward by Hamill and Snieder (2000).

The objective of this work is to derive a consistent hybridization between an incremental 4D-Var and a SEEK smoother (issued from the SEEK filter), under a perfect-model hypothesis. The skeleton of the hybrid formalism is thus formed by the incremental 4D-Var, and the error covariance matrix update is made according to the smoother, whenever a transition between two adjacent assimilation windows occurs. This work is in the line of full theoretical consistency for the hybridization scheme developed by Veersé (2000), but pushes significantly forward the applicative demonstration. It differs from the work by Liu *et al.* (2008, 2009) and Zhang *et al.* (2009) in the sense of scheme's consistency owing to the use of the SEEK smoother instead of the Ensemble Kalman filter. Section 2 presents the mathematical development for the hybrid formulation. Section 3 presents a reference example with a simple shallow-water model. Section 4 further discusses results based on alternative assumptions that could be chosen for the experiments, and attempts to assess the context where hybridization should no longer be beneficial.

2. Hybrid variational-smoothing algorithm

Notations In this section, we only need to consider a single assimilation window $[t_0, t_N]$. It holds N instants t_1, \dots, t_N , where observations $\mathbf{y}_1^o, \dots, \mathbf{y}_N^o$ are available, with error covariance matrices $\mathbf{R}_1, \dots, \mathbf{R}_N$. $\mathbf{y}^o = [\mathbf{y}_1^{oT}, \dots, \mathbf{y}_N^{oT}]^T$ is the concatenated observation vector (T in exponent stands for transposition) and \mathbf{R} the \mathbf{R}_i -block diagonal observation error covariance matrix. \mathbf{x}_0 is the state vector at t_0 , and $\mathbf{x} = [\mathbf{x}_1^T, \dots, \mathbf{x}_N^T]^T$ is a concatenated state vector, where $\mathbf{x}_i = \mathcal{M}_{0 \rightarrow i}(\mathbf{x}_0)$ is the solution of the dynamical model integration from t_0 to t_i . The corresponding linearized model is called $\mathbf{M}'_{0 \rightarrow i}(\cdot)$ where (\cdot) stands for the trajectory around which linearization takes place. The concatenated linearized model is $\mathbf{M}'(\cdot) = [\mathbf{M}'_{0 \rightarrow 1}(\cdot)^T \dots \mathbf{M}'_{0 \rightarrow N}(\cdot)^T]^T$. Finally, the observation operator is denoted $\mathcal{H}(\mathbf{x}) = [\mathcal{H}_1(\mathbf{x}_1)^T, \dots, \mathcal{H}_N(\mathbf{x}_N)^T]^T$ and the linearized operator $\mathbf{H}'(\mathbf{x})$. It is defined as a block diagonal matrix formed with the single time linearized operators $\mathbf{H}'_i(\mathbf{x}_i)$.

Reduced order incremental 4D-Var In the incremental 4D-Var, the cost function is formulated in terms of an increment $\delta\mathbf{x}_0$ to be added to the initial condition at t_0 . The transition from a background state \mathbf{x}_0^b towards an analysis \mathbf{x}_0^a occurs via the sequential computation of K intermediate increments $\delta\mathbf{x}_0^{(k)}$ and analyses $\mathbf{x}_0^{a,(k)} = \mathbf{x}_0^b + \delta\mathbf{x}_0^{(k)}$. These increments are obtained through the minimization of a sequence of cost functions:

$$\begin{aligned} \mathcal{J}(\delta\mathbf{x}_0^{(k+1)}) &= \frac{1}{2} \delta\mathbf{x}_0^{(k+1)T} \mathbf{B}_0^{-1} \delta\mathbf{x}_0^{(k+1)} \\ &+ \frac{1}{2} \left[\mathbf{H}'(\mathbf{x}^{a,(k)}) \cdot \mathbf{M}'(\mathbf{x}_0^{a,(k)}) \cdot \delta\mathbf{x}_0^{(k+1)} - \mathbf{d}^{(k)} \right]^T \mathbf{R}^{-1} \left[\mathbf{H}'(\mathbf{x}^{a,(k)}) \cdot \mathbf{M}'(\mathbf{x}_0^{a,(k)}) \cdot \delta\mathbf{x}_0^{(k+1)} - \mathbf{d}^{(k)} \right] \end{aligned} \quad (1)$$

where \mathbf{B}_0 is the background error covariance matrix, and the innovation $\mathbf{d}^{(k)}$ is given by

$$\mathbf{d}^{(k)} = \mathbf{y}^o - \mathcal{H}(\mathbf{x}^{a,(k)}) + \mathbf{H}'(\mathbf{x}^{a,(k)}) \cdot \mathbf{M}'(\mathbf{x}_0^{a,(k)}) \cdot \delta\mathbf{x}_0^{(k)} \quad (2)$$

The benefit of the incremental formulation lies in the use of linearized operators, which do not depend any more on the unknown variables, i.e. on the increments $\delta\mathbf{x}_0$. Thus the functions to be minimized at each step are quadratic in $\delta\mathbf{x}_0$, and the solution for a given iteration k can be computed analytically:

$$\delta\mathbf{x}_0^{(k+1),\text{VAR}} = \mathbf{B}_0 \mathbf{M}'^T \mathbf{H}'^T \left[\mathbf{H}' \mathbf{M}' \mathbf{B}_0 \mathbf{M}'^T \mathbf{H}'^T + \mathbf{R} \right]^{-1} \mathbf{d}^{(k)} \quad (3)$$

To keep the formulas concise we have skipped here the explicit dependence on the trajectory around which the operators have been linearized. One must bear in mind, however, that the linearization must be repeated each time we pass from k^{th} to $(k + 1)^{\text{th}}$ cost function. Once the 4D-Var analysis is done, the state is transported from t_0 to $t_0 + T$ with the nonlinear model, thus providing a background state for the next 4D-Var batch.

In geophysical applications, the 4D-Var problem is generally ill-conditioned, and the use of a preconditioning technique is required. Formally, this can be brought with an eigendecomposition of the background error covariance matrix

$$\mathbf{B}_0 = \mathbf{L}_0 \mathbf{U}_0^b \mathbf{L}_0^T \quad (4)$$

All eigenvalues being positive, the square root of \mathbf{U}_0^b can be defined and easily computed. With the change of control variable $\delta \mathbf{x}_0^{(k+1)} = (\mathbf{L}_0 \mathbf{U}_0^{b1/2}) \chi^{(k+1)}$, the cost function is rewritten :

$$\mathcal{J}(\chi^{(k+1)}) = \frac{1}{2} \chi^{(k+1)T} \chi^{(k+1)} + \frac{1}{2} \left[\mathbf{H}' \cdot \mathbf{M}' \cdot \delta \mathbf{x}_0^{(k+1)} - \mathbf{d}^{(k)} \right]^T \mathbf{R}^{-1} \left[\mathbf{H}' \cdot \mathbf{M}' \cdot \delta \mathbf{x}_0^{(k+1)} - \mathbf{d}^{(k)} \right] \quad (5)$$

The decomposition of the background error covariance matrix not only allows preconditioning, but also rank reduction (Blayo *et al.*, 1999; Robert *et al.*, 2006b). It consists in reducing the dimension of \mathbf{U}_0^b to only a few, preserving exclusively the largest eigenvalues. \mathbf{L}_0 must also be modified to exclude the eigenvectors corresponding to the discarded eigenvalues.

Equivalent fixed-interval smoother The second ingredient of the hybrid method is an (incremental) extended Kalman smoother, built so that the equivalence with the previous incremental 4D-Var can be ensured (Veersé, 2000). Hence, the analysis is computed at the beginning of the assimilation window for both the state and the covariance matrix. The incremental aspect makes it different from other fixed-lag smoothers (Ménard and Daley, 1996; Evensen and Van Leeuwen, 2000; Li and Navon, 2001). The smoother computes a series of incremental analyses with respect to a background state. Let us suppose that $\delta \mathbf{x}_0^{(k)}$ has already been found. The $(k + 1)^{\text{th}}$ analysis is imposed to be a linear function of $\mathbf{d}^{(k)}$:

$$\delta \mathbf{x}_0^{(k+1), \text{EKS}} \equiv \mathbf{x}_0^{a, (k+1)} - \mathbf{x}_0^b = \mathbf{K}^{(k+1)} \mathbf{d}^{(k)} \quad (6)$$

The gain matrix $\mathbf{K}^{(k+1)}$ is determined by minimizing the trace of the analysis error covariance matrix $\mathbf{P}_0^{a(k+1)}$: $\mathbf{K}^{(k+1)} = \mathbf{B}_0 \mathbf{M}'^T \mathbf{H}'^T \left[\mathbf{H}' \mathbf{M}' \mathbf{B}_0 \mathbf{M}'^T \mathbf{H}'^T + \mathbf{R} \right]^{-1}$. One should keep in mind that the reference to the trajectory around which linearization takes place (here, $\mathbf{x}^{a, (k)}$) have been skipped, since it is the only factor accounting for the differences between the gain matrix at successive iterations k . Once $\mathbf{K}^{(k+1)}$ has been reported into (6), it can be easily noticed that the increment coincides with the one given by (3) and obtained in the variational approach. In addition the EKS provides an increment to the covariance matrix:

$$\delta \mathbf{P}_0^{(k+1)} \equiv \mathbf{P}_0^{a(k+1)} - \mathbf{B}_0 = -\mathbf{K}^{(k+1)} \mathbf{H}' \mathbf{M}' \mathbf{B}_0 \quad (7)$$

This increment is worth being computed only after the state analysis is found, to obtain the final analysis covariance matrix \mathbf{P}_0^a (intermediate matrices are not used). Once the smoother analysis performed, the analyzed state at t_0 can be transported to $t_0 + T$ with the nonlinear model, providing the background state for the next time interval. The analysis error covariance matrix can also be propagated to yield the corresponding covariance matrix:

$$\mathbf{B}_N = \mathbf{M}'_{0 \rightarrow N} \mathbf{P}_0^a \mathbf{M}'_{0 \rightarrow N}^T \quad (8)$$

Rank reduction is common in the Kalman filtering approach, and different algorithms have been presented in the literature (Evensen, 94; Verlaan and Heemink, 1998; Pham *et al.*, 1998). In the SEEK filter, the background covariance matrix is factorized following (4). As with the 4D-Var previously, rank reduction consists in reducing the dimension of \mathbf{U}_0^b to only a few eigenvalues. From (7), it can be shown that the analysis error covariance matrix at iteration k reads:

$$\mathbf{P}_0^{a(k+1)} = \mathbf{L}_0 \mathbf{U}_0^{a(k+1)} \mathbf{L}_0^T \quad (9)$$

$$\text{with } (\mathbf{U}_0^{a(k+1)})^{-1} = \mathbf{U}_0^{b-1} + \mathbf{L}_0^T \mathbf{M}'^T \mathbf{H}'^T \mathbf{R}^{-1} \mathbf{H}' \mathbf{M}' \mathbf{L}_0 \quad (10)$$

where, again, the dependence of the last term on the intermediate analysis $\mathbf{x}^{a,(k)}$ is not explicit. As with the full rank smoother, computing the intermediate matrices $\mathbf{U}_0^{a(k+1)}$ is superfluous and may be avoided. The final analysis matrix computed at the last iteration can be propagated over the assimilation window. Should we define

$$\mathbf{L}_N = \mathbf{M}'(\mathbf{x}_0^a) \mathbf{L}_0 \quad (11)$$

then the error covariance matrix at the end of the interval reads: $\mathbf{B}_N = \mathbf{L}_N \mathbf{U}_0^a \mathbf{L}_N^T$

Hybridization We have shown that the increments computed by the incremental 4D-Var and by an appropriate fixed-interval smoother were theoretically identical, provided the same ingredients are used in other respects. The smoother also offers the opportunity to update and propagate the background error covariance matrix from one batch to the next. Combining the incremental 4D-Var cycle (for the state vector) with the smoother cycle (for the covariance matrix) results in a perfectly consistent hybrid 4D-Var/smoother. Moreover the eigenvalue decomposition of the background covariance matrix does not spoil the consistency. To summarize, the hybrid 4D-Var/SEEK smoother proceeds as follows:

1. A sequence of 4D-Var analysis to compute a state increment (minimization of (5), k running from 1 to K);
2. the 4D-Var analyzed state is transported with the dynamical model: $\mathbf{x}_N^b = \mathcal{M}_{0 \rightarrow N}(\mathbf{x}_0^a)$;
3. SEEK smoother analysis for the reduced covariance matrix ((10), where the model is linearized around the analysis trajectory computed with 4D-Var, \mathbf{x}_0^a);
4. the reduced error basis is transported following (11).

3. A first demonstrative numerical implementation

We present here a first implementation of the hybrid method, in a simple ocean model. The aim is to demonstrate that hybrid can significantly improve the performance of assimilation with regard to the 4D-Var approach with \mathbf{B} kept static. We choose a case where the background error statistics are only partly known, which is the case of most applications.

The experimental framework is extensively described in Krysta *et al.* (2009). We use a reduced gravity shallow water model mimicking wind-driven mid-latitude circulation. Although rather simple, this model is able to develop strongly nonlinear dynamics, with a meandering zonal jet and associated eddies (Fig.1a). Once the model stabilized, a 10-year simulation has been performed. Given the present model limited dynamics, almost its whole range of variability has been explored during this 10-year period. A complete set of 1865 reference EOFs, denoted \mathbf{L}^{ref} has been constructed from a 2-day sampling of this trajectory, which is regarded as a comprehensive representation of the model variability. Note that the

first 100 reference EOFs retain 75.7% of the total variability. Another 10-year simulation has been performed following the previous one. The 15th – 18th year period has been selected to represent "true" trajectory of the system, from which measurements are extracted. The observations have been chosen to be the water height h only, every 10 days, everywhere in the domain, with the addition of a white noise. The two other variables (velocity (u, v)) are unobserved. The length of the assimilation windows is 30 days. The background value for the initial condition of the first assimilation window has been chosen fully decorrelated from the true state, and the background error covariance matrix \mathbf{P}_1^f used in the first assimilation window has been defined consistently, using 100 EOFs corresponding to a 2-day sampling of the 200 days preceding this initial condition. This corresponds to a context where one has only partial knowledge of the variability of the system. Then, two 4-year data assimilation experiments have been conducted, the first one with standard incremental 4D-Var keeping the background error covariance matrix constant, and the second one employing the hybrid method. We have compared their results to a so-called *free run* (a simulation without assimilation starting from the background value of the initial condition) by computing a relative error, defined as $\|\mathbf{x}^a - \mathbf{x}^t\| / \|\mathbf{x}^{free} - \mathbf{x}^t\|$.

This relative error is decreased by roughly 50% for the observed variable, and 25% for the unobserved ones (Fig.2), which indicates a significantly better performance of the hybrid method with regard to the 4D-Var. The reason might be that the EOFs spanning the initial subspace of control are issued from a sample which is not long enough to define a \mathbf{B} matrix of sufficient quality. Hence, keeping this matrix unchanged does not allow for a fully accurate correction of the model state by the 4D-Var, while making this initial basis evolve ensures a significant improvement of data assimilation results. These results can be interpreted from the point of view of the quantity of information contained in the bases spanning control subspaces, or in other words a degree to which these subspaces represent the true error directions. The 1865 reference EOFs, which contain almost full information on the variability of the model, have been projected on the control subspaces employed in our hybrid experiments, both in their initial and final forms (Fig.1b). While the basis \mathbf{L}_1 spanning the initial control subspace is distributed over the first 400-500 reference EOFs, the basis \mathbf{L}_{48} at the end of the 4-year assimilation experiment is much more focused on the first reference EOFs, which are the ones containing relevant information. To be more specific, the quantity of information contained in a given basis \mathbf{L} can be defined as $Q(\mathbf{L}) = \sum_{i=1}^{1865} \lambda_i^{ref} p_i^{\mathbf{L}} / \sum_{i=1}^{1865} \lambda_i^{ref}$ where λ_i^{ref} is the eigenvalue corresponding to the i -th reference EOF, and $p_i^{\mathbf{L}}$ is the projection of this EOF on \mathbf{L} (i.e. the value displayed along the y -axis for \mathbf{L}_1 and \mathbf{L}_{48} in Fig.1b). The ideal value for Q when dealing with a basis of 100 vectors is $Q(L_1^{ref}, \dots, L_{100}^{ref}) = 0.757$. In the present experiment, the initial information content is $Q(\mathbf{L}_1) = 0.24$, and grows up to $Q(\mathbf{L}_{48}) = 0.46$, which illustrates the positive effect of the evolution of the background error covariance matrix as ensured by the hybrid method.

4. Discussion

A large- and meso-scale ocean circulation system is commonly described as a dynamical system with an attractor. Therefore most of the variability of the system can be described by a basis \mathbf{A} of low dimension. A challenge for a reduced order assimilation method is then to make the control subspace $Span(\mathbf{L})$ contain the largest possible fraction of the variability

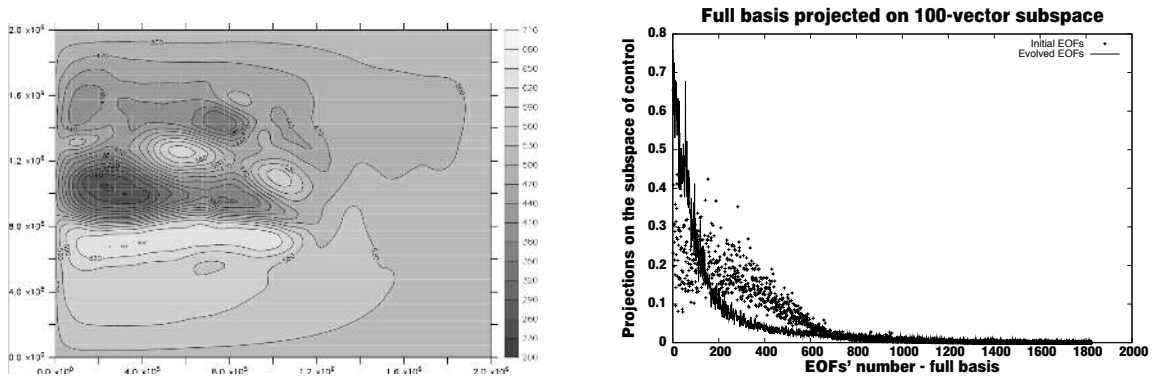


Figure 1: a) Left: Snapshot of the water height field simulated with the shallow water model. b) Right: Projection of the 1865 reference EOFs on the subspace of control at the beginning (crosses) and at the end (solid line) of the assimilation period.

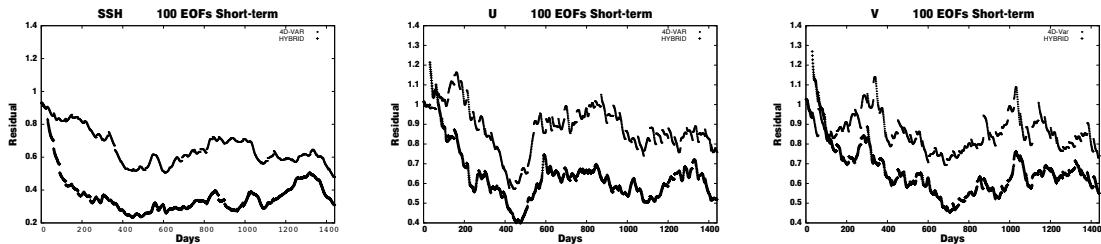


Figure 2: Relative error as a function of time for h (left), u (middle) and v (right), for the 4D-Var (thin line) and hybrid (thick line) 4-year data assimilation experiments.

subspace $Span(\mathbf{A})$ at each assimilation time window. We may identify two important factors in this regard: the initialization of \mathbf{x}^b and \mathbf{L} , and the ability of the system to make \mathbf{L} evolve correctly so that $Span(\mathbf{L})$ significantly intersects $Span(\mathbf{A})$ at each assimilation window. Additional numerical experiments have been performed, which try to identify the conditions in which the hybrid method can or cannot improve the assimilation results.

In a first testcase, \mathbf{L} has been initialized by the 100 first reference EOFs, which holds 75% of the system variability spectrum. It is almost a perfect initialization in the sense that $Span(\mathbf{A}) \subset Span(\mathbf{L})$. Consequently, \mathbf{L} enables corrections to the background state in all the possible directions of the true system variability. By construction of the basis, this property holds true for the whole assimilation period. Hence 4D-Var performs strikingly well over the entire assimilation period (Fig.3, top panel). Making \mathbf{L} evolve in this context should not bring improvements. It is indeed the case: we observe no significant differences in performance between 4D-Var and hybrid for about 6 initial assimilation cycles (200 days); then the use of the tangent linear approximation to transport \mathbf{L} leads to a gradual deterioration of the results with respect to the static case.

This almost perfect initialization can be partly deteriorated, and we can consider a case where the initial basis \mathbf{L} correctly represents the short-term variability of the system, but not the full system characteristics. In this case $Span(\mathbf{A})$ and $Span(\mathbf{L})$ partly overlap. Such an initial configuration is exactly the one illustrated by the test case described in section 3, with the dimension of the error subspace basis equal to 100, which is high enough to possibly

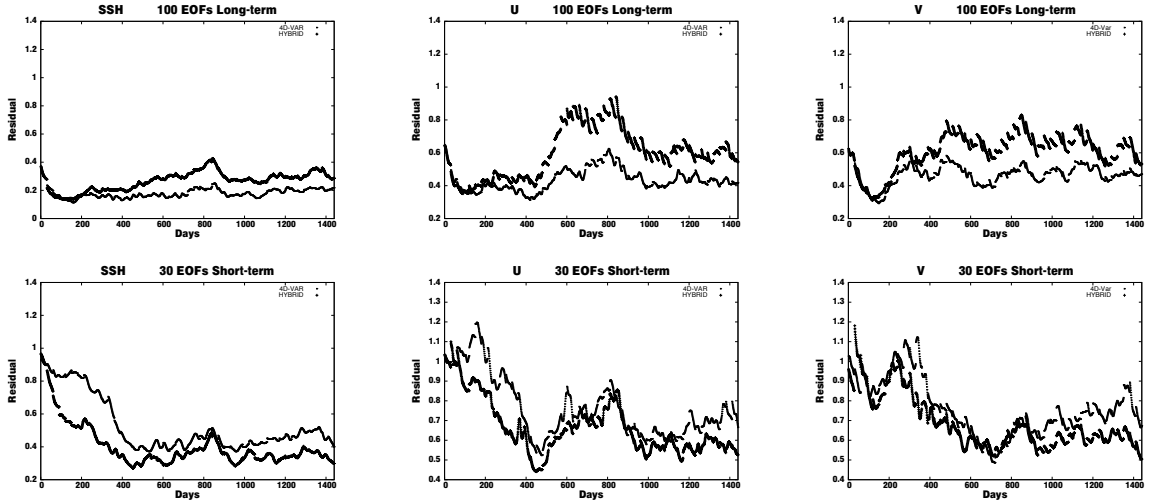


Figure 3: Same as Fig.2, but for an initial subspace \mathbf{L}_1 constituted by the 100 first reference EOFs (top) or the 30 first EOFs (bottom).

represent a large part of full system's variability in our present case. As the initial basis \mathbf{L} is representative mostly of the short term variability of the system, the performance of 4D-Var with a fixed \mathbf{L} is somewhat poor. With the hybrid method, however, the (linearized) model proves to be able to make \mathbf{L} evolve in a way leading to improved results.

The initialization of \mathbf{L} can be further deteriorated by limiting its size to a number of vectors which is insufficient to possibly represent a significant part of the full system's variability. Fig.3 (bottom panel) shows the results for an example of such a configuration, with the initial basis formed by only the first 30 EOFs. The hybrid performs better than 4D-Var, although not as clearly as with 100 EOFs. Actually the difference between the two lies mostly in the 4D-Var results. In case of 30 EOFs, 4D-Var produces smaller error residuals than with 100 EOFs (Fig.2), possibly due to a non optimal finding of the minimizer in the latter case. Hybrid's results, however, are rather similar, slightly better in the case of 100 EOFs.

These different experiments tends to lead to the conclusion that the configurations owing considerable improvement to the hybrid algorithm are the ones in which the EOFs account exclusively for short-term characteristics of a physical phenomenon. If the long-term ones are present, then basis evolution has no positive impact on data assimilation results and can even deteriorate them. An optimal configuration for reduced rank data assimilation employing the EOFs to define the subspace of control would hence possibly be as follows. The vectors initialized by the EOFs describing long-term behavior of the system may be kept static. The ones which are initialized by the EOFs representing short-term behavior 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. These conclusions echo the studies undertaken with the background error covariance matrix built as a linear combination of a static and dynamically updated term.

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