Ensemble Kalman Filtering with One-Step-Ahead Smoothing

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ABSTRACT
The ensemble Kalman filter (EnKF) is widely used for sequential data assimilation. It operates as a succession of forecast and analysis steps. In realistic large-scale applications, EnKFs are implemented with small ensembles and poorly known model error statistics. This limits their representativeness of the background error covariances and, thus, their performance. This work explores the efficiency of the one-step-ahead (OSA) smoothing formulation of the Bayesian filtering problem to enhance the data assimilation performance of EnKFs. Filtering with OSA smoothing introduces an updated step with future observations, conditioning the ensemble sampling with more information. This should provide an improved background ensemble in the analysis step, which may help to mitigate the suboptimal character of EnKF-based methods. Here, the authors demonstrate the efficiency of a stochastic EnKF with OSA smoothing for state estimation. They then introduce a deterministic-like EnKF-OSA based on the singular evolutive interpolated ensemble Kalman (SEIK) filter. The authors show that the proposed SEIK-OSA outperforms both SEIK, as it efficiently exploits the data twice, and the stochastic EnKF-OSA, as it avoids observational error undersampling. They present extensive assimilation results from numerical experiments conducted with the Lorenz-96 model to demonstrate SEIK-OSA’s capabilities.

1. Introduction
Data assimilation (DA) is the process by which available observations are combined with dynamical models to constrain model predictions and determine the best possible estimate of a system’s state (Ghil and Malanotte-Rizzoli 1991). DA methods are generally grouped into two categories: 1) variational methods that aspire to fit the model’s trajectory to available observations through adjustments of a well-chosen set of control parameters (Le Dimet and Talagrand 1986) and 2) sequential methods that follow a probabilistic framework to split the Bayesian estimation problem into cycles of alternating forecast steps, to advance the distribution of the system state with the model, and analysis steps, to compute the posterior distribution based on incoming observations (Todling 1999).

The ensemble Kalman filter (EnKF) was introduced by Evensen (1994) as a Monte Carlo implementation of the Kalman filter (KF) (Kalman 1960) to tackle large-scale, sequential, nonlinear DA problems. It approximates the distribution of the system state by a collection of random realizations, or ensemble members, whose mean is the state estimate and sample covariance is the associated error covariance (Hoteit et al. 2015). The EnKF integrates the (analysis) ensemble members forward with the model in the forecast step and then updates them in the analysis step with incoming observations using a Kalman-like (best linear unbiased estimation) correction. Because of its reasonable computational cost, robust performance, and nonintrusive formulation, the EnKF has seen widespread use in many geophysical applications (Reichle et al. 2002; Carton and Giese 2008; Anderson et al. 2009; Hoteit et al. 2013; Nævdal et al. 2005; Triantafyllou et al. 2013).

The EnKF perturbs observations with random noise sampled from the observational error distribution before assimilation, such that its error covariance asymptotically matches that of the KF (Burgers et al. 1998). Later, this scheme became known as the stochastic EnKF (Tippett et al. 2003). This perturbation, however, introduces an additional source of sampling error and often underestimates the analysis error covariance, especially when the filter is implemented with small ensembles (Whitaker and Hamill 2002; Hoteit et al. 2015). Several deterministic EnKFs were proposed to update the ensemble’s sample mean and covariance without
perturbing the observations, exactly as in the KF (Tippett et al. 2003), and then to resample a new ensemble to proceed with the next forecast step. Among these, we cite the ensemble transform Kalman filter (ETKF) (Bishop et al. 2001), the ensemble adjustment Kalman filter (EAKF) (Anderson 2001), and the ensemble square root Kalman filter (EnSRF) (Whitaker and Hamill 2002), which performs the ensemble resampling implicitly using different deterministic square root transformations. This method of resampling contrasts with the explicit stochastic resampling of the singular evolutive interpolated Kalman (SEIK) filter (Pham et al. 1998; Hoteit et al. 2002), which is based on orthogonal random transformations.

Accurate estimates of the forecast error covariances, also known as background covariances, are crucial to EnKF-like filters. In real-world, large-scale applications, however, EnKFs are implemented with relatively small ensembles to limit computational cost and with poor model error statistics (Song et al. 2010). This limits the representativeness of EnKFs’ backgrounds and, thus, the filters’ performance. Various auxiliary techniques have been proposed to mitigate this background limitation, such as inflation (Anderson 2001), localization (Houtekamer and Mitchell 1998), hybrid (Hamill and Snyder 2000) and adaptive formulations (Song et al. 2010), and robust filtering (Luo and Hoteit 2011). Here, we follow a different approach that exploits information in (future) observations to compute improved backgrounds in EnKFs. The idea is to follow the one-step-ahead (OSA) smoothing formulation of the Bayesian filtering problem (Desbouvries et al. 2011), which first applies a smoothing step with the future observation before integrating the resulting “smoothed” state with the model to compute the background, all within a fully Bayesian-consistent framework. This approach has been recently used by Ait-El-Fquih et al. (2016) to derive a Bayesian framework for state-parameter estimation for the well-known dual EnKF (Moradkhani et al. 2005). In the resulting EnKF-OSA scheme, the observation is exploited twice: first to constrain the sampling of the forecast ensemble with the future observation, and next to update the resulting ensemble with the data. This additional OSA-smoothing step provides an improved background for the next analysis cycle and is, thus, expected to enhance EnKFs’ results. Indeed, when implemented under challenging situations, such as strong nonlinearities, sparse observation networks, or large assimilation windows, the ensembles’ perturbations estimated by standard EnKFs may not well represent the uncertainties of the prior state, thereby limiting the impact of the observation. Conditioning the forecast ensemble by the observations through a smoothing step should provide more accurate estimates of the background uncertainties for better exploitation of the observation in the analysis step.

A very similar idea, known as “running in place” (RIP), was proposed in Kalnay and Yang (2010) as a heuristic way to accelerate the spinup of the ETKF. It iteratively applies the two-stage update step based on criteria that ensure a reasonable fit to the data. Using the observations more than once in each assimilation window during spinup is justified by the need to maximize the initial extraction of information (Kalnay and Yang 2010). The RIP iterations may be interpreted as some kind of iterations on the OSA-smoothing step to deal with the nonlinear character of this step—a very common approach in the subsurface community (Emerick and Reynolds 2013; Luo et al. 2015; Ma et al. 2017; Chen and Oliver 2013). This method was successfully tested with a series of realistic models (Penny et al. 2013; Yang et al. 2013). By ignoring the underlying criteria, we found that RIP with one iteration is very similar to the proposed OSA-smoothing-based filtering scheme. This means that RIP with one iteration is Bayesian consistent and, thus, not heuristic, as has been suggested.

The goal of our work is twofold. Realizing the benefit of an improved background covariance for state estimation with the EnKF, we first demonstrate the relevance of the OSA-smoothing-based approach for state estimation. The performance of EnKF-like methods is known to level off after enough members are used (about the rank of the covariance matrices) (e.g., Hoteit et al. 2002; Evensen 2003). The idea here is to better exploit the observations in order to enhance the (approximate) ensemble background using future information. We then derive a new deterministic OSA-smoothing-like ensemble filter, the SEIK-OSA, which is suitable for data assimilation into large-scale oceanic and atmospheric models. This should improve the filtering results, compared to the EnKF-OSA, when the ensemble size is small, compared to the number of assimilated observations, a common scenario in geophysical applications (Hoteit et al. 2015). We demonstrate the efficiency of the SEIK-OSA with extensive numerical experiments with the strongly nonlinear Lorenz-96 (L96) model under various assimilation settings and scenarios.

The remainder of this paper is organized as follows. Section 2 describes the concept of the filtering problem with OSA smoothing and presents a (stochastic) EnKF-based solution for general nonlinear systems. The SEIK-OSA algorithm is derived in section 3. Results of numerical experiments with the Lorenz-96 model are then analyzed in section 4. The main conclusions are summarized and discussed in section 5.
2. OSA-smoothing-based filtering

a. Problem formulation

Consider the following discrete-time dynamical system:

\[
\begin{align*}
\mathbf{x}_n &= \mathcal{M}_{n-1}(\mathbf{x}_{n-1}) + \mathbf{\eta}_{n-1}, \\
\mathbf{y}_n &= \mathbf{H}_n \mathbf{x}_n + \mathbf{\varepsilon}_n,
\end{align*}
\]

(1)

where \( \mathbf{x}_n \in \mathbb{R}^{N_x} \) is the \( N_x \)-dimensional system state at time \( t_n \), \( \mathbf{y}_n \in \mathbb{R}^{N_y} \) is the corresponding observation, \( \mathcal{M}_{n-1} \) is a (nonlinear) operator integrating the system state from time \( t_{n-1} \) to \( t_n \), and \( \mathbf{H}_n \) is the observation operator that projects \( \mathbf{x}_n \) from the state space onto the observation space. Here, we assume that \( \mathbf{H}_n \) is linear to simplify the presentation of the filtering algorithms. The case of a nonlinear \( \mathbf{H}_n \) could be treated as usual in EnKFs; see, for example, Liu et al. (2016). The model and the observation process noise, \( \mathbf{\eta} = \{\mathbf{\eta}_n\}_{n \in \mathbb{N}} \) and \( \mathbf{\varepsilon} = \{\mathbf{\varepsilon}_n\}_{n \in \mathbb{N}} \), respectively, are assumed to be Gaussian with zero means and covariances \( \mathbf{Q}_n \) and \( \mathbf{R}_n \), respectively; \( \mathbf{\eta} \) and \( \mathbf{\varepsilon} \) are also assumed to be independent, jointly independent, and independent of the initial state \( \mathbf{x}_0 \).

The filtering problem consists of estimating, at each time \( t_n \), the state \( \mathbf{x}_n \) from the previous observations \( \mathbf{y}_{0:n} \overset{\text{def}}{=} \{\mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_n\} \). The posterior mean (PM), which minimizes the mean squared error (MSE), is commonly taken as a standard solution for this problem (Ait-El-Fquih and Hoteit 2016). Classical filtering schemes involve a forecast step to move from the analysis estimate at time \( t_{n-1} \) to the analysis estimate at the next time \( t_n \). The OSA-smoothing formulation of the filtering problem is based on the idea that the aforementioned standard filtering path, which computes the analysis state at a given time from the analysis state at the previous time, is not unique (Desbouvries and Ait-El-Fquih 2008; Desbouvries et al. 2011). In a linear Gaussian estimation problem, the same analysis estimate can, indeed, be also obtained if one includes a smoothing step between the two successive analyses. This formulation introduces a new update step to the state, based on future observations (smoothing), without violating the Bayesian filtering framework. The resulting OSA-smoothing-based filters are said to be Bayesian consistent, as they are derived, under only the common Gaussian assumption, from a theoretically sound generic algorithm that involves two Bayesian updates with the same data [see Eqs. (21) and (24) in Ait-El-Fquih et al. (2016)]. Unlike iterative algorithms, using the data twice does not affect in any way the Bayesian character of the OSA-smoothing-based filtering schemes, as these data are used to update two different quantities, \( \mathbf{x}_{n-1} \) and \( \mathbf{x}_n \). Fig. 1 outlines the difference between the classical KF algorithm and the KF with OSA smoothing (called hereafter KF-OSA). Both schemes provide the same state analysis estimate in the linear Gaussian case. The OSA-smoothing-based formulation is, however, expected to enhance the filter’s performance when the filter is not implemented under ideal conditions, with the future observation providing more information to compute the background statistics.

Desbouvries and Ait-El-Fquih (2008) and Desbouvries et al. (2011) derived KF and particle filter (PF)-like algorithms based on the OSA-smoothing formulation [see also Pitt and Shephard (1999) and Luo et al. (2014), who introduced an auxiliary PF involving OSA-smoothing, but in a different way]. Lee and Farmer (2014) also followed a similar strategy and presented a number of algorithms for estimating both the state and system noise. More recently, EnKF-OSA schemes were also proposed by Ait-El-Fquih et al. (2016) and Gharamti et al. (2015) to derive a dual-filter-like algorithm for state-parameter estimation of large-scale nonlinear systems. It is important to realize that the OSA-smoothing-based schemes are not fixed-lag smoothers (see, e.g., Simon 2006; Anderson and Moore 1979). The main difference between an OSA-smoothing-based scheme and a fixed-lag scheme is in the computation of the analysis distribution. The former computes it from the OSA-smoothing distribution, while the fixed-lag scheme computes it from the forecast distribution, following exactly the standard filtering update. The smoothing distribution/estimate is the final goal of the fixed-lag algorithms, while in our OSA-smoothing-based scheme, this distribution is only used to compute the analysis distribution, which is our final solution. Below, we present the EnKF-OSA algorithm for state estimation based on Ait-El-Fquih et al. (2016).
b. The (stochastic) EnKF-OSA algorithm

Let \( \{x_{n,i,j}^f\}_{i=1}^{N_s} \), \( \{x_{n,i}^a\}_{i=1}^{N_s} \), and \( \{x_{n,i}^{f,i}\}_{i=1}^{N_s} \) denote the forecast, analysis, and OSA-smoothed ensembles, respectively. For the analysis ensemble (and, similarly, for the forecast and smoothing ones), let \( x_n^a \) denote its empirical mean and \( S_n^a \) the ensemble perturbation matrix, with the \( i \)th column defined as \( (1/\sqrt{N_s-1})(x_{n,i}^{f,i} - x_n^a) \). Starting from an analysis ensemble at time \( t_{n-1} \), the analysis ensemble at the next time \( t_n \) is obtained following two steps:

1) SMOOTHING STEP

The forecast ensemble and the corresponding observation forecast ensemble \( \{y_{n,i,j}^f\}_{i=1}^{N_s} \) are first computed as

\[
x_{n-1,i}^{f,i} = x_{n-1}^{a} + P_{x_{n-1,i}^{a}y_{n}^{f,i}}^{-1}(y_n - y_{n,i}^{f,i}),
\]

where \( y_{n,i}^{f,i} \sim \mathcal{N}(0, Q_n) \), and \( y_n \sim \mathcal{N}(0, R_n) \). These are then used along with the observation \( y_n \) to smooth the previous analysis ensemble with the “future” observation \( y_n \) as

\[
x_{n-1,i}^{a} = \mathcal{M}_{n-1}(x_{n-1,i}^{f,i}) + \eta_{n-1,i}^{a},
\]

where \( \eta_{n-1,i}^{a} \sim \mathcal{N}(0, Q_{n-1}) \), and \( \mathcal{M}_{n-1} \) is the model gain

\[
\mathcal{M}_{n-1} = P_{x_{n-1}^{a}y_{n}^{f,i}}^{-1}H_{n}P_{y_{n}^{f,i}y_{n}^{f,i}}^{-1}(y_{n} - y_{n}^{f,i}),
\]

with \( P_{x_{n-1}^{a}y_{n}^{f,i}} = P_{x_{n-1}^{a}y_{n}^{f,i}}^{-1}H_{n}P_{y_{n}^{f,i}y_{n}^{f,i}}^{-1} + R_{n} \).

Here, \( S_{n}^{f,i} \) is the observation forecast ensemble perturbation matrix, with the \( i \)th column defined as \( (1/\sqrt{N_s-1})(y_{n,i}^{f,i} - y_{n}^{f,i}) \), with \( y_{n}^{f,i} \) the observation forecast ensemble mean.

2) ANALYSIS STEP

The resulting smoothed ensemble is then integrated forward in time with the model to compute the pseudo-forecast ensemble \( \{x_{n,i}^{f,i}\}_{i=1}^{N_s} \), which, in turn, is updated based on \( y_{n} \) to obtain the analysis ensemble of interest at \( t_{n} \):

\[
x_{n,i}^{f,i} = \mathcal{M}_{n}(x_{n,i}^{f,i}) + \eta_{n,i}^{f,i},
\]

where \( \eta_{n,i}^{f,i} \sim \mathcal{N}(0, Q_{n}) \), and \( \mathcal{M}_{n} \) is the analysis gain

\[
\mathcal{M}_{n} = P_{x_{n,i}^{a}y_{n}^{f,i}}^{-1}H_{n}P_{y_{n}^{f,i}y_{n}^{f,i}}^{-1}(y_{n} - y_{n}^{f,i}),
\]

where \( S_{n}^{f,i} \) is defined in a similar way as \( S_{n}^{f,i} \), but using the pseudoforecast members. To better explain the difference between the EnKF-OSA and the standard EnKF, we write how the analysis members are computed, starting from their counterparts at the previous time:

\[
x_{n,i}^{f,i} = \mathcal{M}_{n}(x_{n-1,i}^{f,i} + P_{x_{n-1,i}^{a}y_{n}^{f,i}}^{-1}(y_{n} - y_{n}^{f,i})),
\]

Here, we ignored the model noise term for simplicity. To compute the analysis members \( x_{n,i}^{a} \), the standard EnKF updates the forecast members \( x_{n,i}^{f,i} \) resulting from the model integration of the previous analysis ensemble \( x_{n,i}^{a} \) using one Kalman-like correction. In contrast, EnKF-OSA updates the pseudoforecast ensemble \( x_{n,i}^{f,i} \), which is computed by model integration of the smoothed ensemble \( x_{n-1,i}^{a} \) using a second Kalman-like correction. This explains why the EnKF-OSA is expected to provide an improved background for the analysis step and, thus, enhanced state estimates.

3. A deterministic EnKF-OSA algorithm (SEIK-OSA)

To derive a deterministic EnKF-OSA, we first present the KF-OSA algorithm that was introduced by Desbois et al. (2011), based on which we then derive SEIK-OSA.
a. KF-OSA

In the linear Gaussian framework \( \mathcal{M}_{n-1}(\mathbf{x}_{n-1}) = \mathbf{M}_{n-1}\mathbf{x}_{n-1} \), the forecast, analysis, and smoothing probability density functions (pdfs) are Gaussian (Desbouvries et al. 2011). Without abuse of notation with respect to their EnKF counterparts, let \( \mathbf{x}_{n}^f \), \( \mathbf{x}_{n}^a \), and \( \mathbf{x}_{n}^s \), respectively, denote the forecast, analysis, and OSA-smoothed PM estimates, and let \( \mathbf{P}_{n}^f \), \( \mathbf{P}_{n}^a \), and \( \mathbf{P}_{n}^s \) denote their corresponding error covariances. The KF-OSA algorithm can be summarized as follows.

1) SMOOTHING STEP

Forecast estimate \( \mathbf{x}_{n}^f \) and error covariance \( \mathbf{P}_{n}^f \) are first computed as in the classical KF:

\[
\mathbf{x}_{n}^f = \mathbf{M}_{n-1}^{-1}\mathbf{x}_{n-1}, \tag{14}
\]

\[
\mathbf{P}_{n}^f = \mathbf{M}_{n-1}^{-1}\mathbf{P}_{n-1}\mathbf{M}_{n-1}^T + \mathbf{Q}_{n-1}. \tag{15}
\]

Once the observation \( \mathbf{y}_{n} \) is available, a smoothing Kalman gain \( \mathbf{K}_{n-1}^s \) is computed to smooth the previous analysis estimate at time \( t_{n-1} \) as follows:

\[
\mathbf{K}_{n-1}^s = \mathbf{P}_{n-1}^a \mathbf{M}_{n-1}^T \mathbf{H}_{n}^T (\mathbf{H}_{n}\mathbf{P}_{n}^a \mathbf{H}_{n}^T + \mathbf{R}_{n})^{-1}, \tag{16}
\]

\[
\mathbf{x}_{n}^s = \mathbf{x}_{n}^a + \mathbf{K}_{n-1}^s (\mathbf{y}_{n} - \mathbf{H}_{n}\mathbf{x}_{n}^f), \tag{17}
\]

\[
\mathbf{P}_{n}^s = \mathbf{P}_{n-1}^a - \mathbf{K}_{n-1}^s \mathbf{H}_{n} \mathbf{M}_{n-1} \mathbf{P}_{n-1}^a. \tag{18}
\]

2) ANALYSIS STEP

The smoothed state is integrated forward in time using the dynamical model to compute the pseudoforecast:

\[
\mathbf{x}_{n}^f = \mathbf{M}_{n-1}^{-1}\mathbf{x}_{n}^s. \tag{19}
\]

The observation \( \mathbf{y}_{n} \) is then reexploited to update the pseudoforecast and compute the analysis mean and covariance as follows:

\[
\mathbf{x}_{n}^a = \mathbf{x}_{n}^f + \mathbf{K}_{n}(\mathbf{y}_{n} - \mathbf{H}_{n}\mathbf{x}_{n}^f), \tag{20}
\]

\[
\mathbf{P}_{n}^a = \mathbf{M}_{n-1}^{-1} \mathbf{P}_{n-1}^f \mathbf{M}_{n-1}^T + \mathbf{Q}_{n-1}, \tag{21}
\]

where

\[
\mathbf{K}_{n} = \mathbf{Q}_{n-1} \mathbf{H}_{n}^T (\mathbf{H}_{n} \mathbf{Q}_{n-1} \mathbf{H}_{n}^T + \mathbf{R}_{n})^{-1}, \tag{22}
\]

\[
\mathbf{M}_{n-1} = (\mathbf{I} - \mathbf{K}_{n} \mathbf{H}_{n}) \mathbf{M}_{n-1}, \tag{23}
\]

\[
\mathbf{Q}_{n-1} = (\mathbf{I} - \mathbf{K}_{n} \mathbf{H}_{n}) \mathbf{Q}_{n-1}. \tag{24}
\]

In the EnKF-OSA algorithm presented above, the analysis step of the pseudoforecast ensemble is performed based on the analysis Kalman gain \( \mathbf{K}_{n}^a = \mathbf{P}_{n}^a \mathbf{H}_{n} \mathbf{P}_{n}^a \), estimated from the ensembles, while in the KF-OSA algorithm (Desbouvries et al. 2011), the analysis correction is performed using \( \mathbf{K}_{n}^a \). Here, we show that in the linear Gaussian case, these two expressions are identical (see appendix for the proof), that is,

\[
\mathbf{Q}_{n-1} \mathbf{H}_{n}^T (\mathbf{H}_{n} \mathbf{Q}_{n-1} \mathbf{H}_{n}^T + \mathbf{R}_{n})^{-1} = \mathbf{P}_{n}^a \mathbf{H}_{n} \mathbf{P}_{n}^a. \tag{25}
\]

In an ensemble setting, this alternative expression allows us to directly estimate the analysis Kalman gain from the filter ensembles and enables more flexible incorporation of the model error covariance, following the various approaches discussed above.

b. SEIK-OSA algorithm

We follow the formulation of the SEIK filter in Pham (2001) and Hoteit et al. (2002) to derive SEIK-OSA from the KF-OSA algorithm.

1) SMOOTHING STEP

As in the stochastic EnKF-OSA described above, the smoothing step of SEIK-OSA aims at computing an OSA-smoothed ensemble \( \{\mathbf{x}_{n}^{s,i}\}_{i=1}^{N_e} \) from an analysis ensemble \( \{\mathbf{x}_{n}^{a,i}\}_{i=1}^{N_e} \), but following a deterministic formulation (Tippett et al. 2003). Accounting for model errors in the forecast step of the SEIK filter would continuously increase the rank of the forecast error covariances, thereby limiting the usefulness of the low-rank approximation (Hoteit et al. 2007). Various approaches have been proposed to account for model errors in ensemble-based techniques by, for example, inflating the background error covariance (Pham et al. 1998), projecting the model error onto the ensemble subspace (Pham 2001), or perturbing the forecast ensemble runs (Hoteit et al. 2007). For the sake of simplicity, we apply inflation here, keeping in mind the other available techniques. The forecast members and the associated error covariance matrix are then given by

\[
\mathbf{x}_{n}^{f,i} = \mathcal{M}_{n-1}(\mathbf{x}_{n}^{a,i}), \tag{26}
\]

\[
\mathbf{P}_{n}^{f,i} = \mathbf{P}_{n}^{f,i} - \frac{1}{N_e - 1} \sum_{i=1}^{N_e} (\mathbf{x}_{n}^{f,i} - \mathbf{x}_{n}^{f,i})(\mathbf{x}_{n}^{f,i} - \mathbf{x}_{n}^{f,i})^T. \tag{27}
\]

Denote by \( \mathbf{X}_{n}^{f,i} = \begin{bmatrix} \mathbf{x}_{n}^{f,1,i}^T & \mathbf{x}_{n}^{f,2,i}^T & \cdots & \mathbf{x}_{n}^{f,N_e,i}^T \end{bmatrix}^T \) the matrix whose columns are the forecast members; similar notations hold for the analysis \( \mathbf{X}_{n}^{a,i} \), smoothing \( \mathbf{X}_{n}^{s,i} \), and pseudoforecast ensembles \( \mathbf{X}_{n}^{f,i} \). Following the formulation of the error covariances in SEIK (Pham 2001), we can factorize the forecast and analysis error covariances as

\[
\mathbf{P}_{n}^{f} = \mathbf{L}_{n}^{f} \mathbf{G}(\mathbf{L}_{n}^{f})^T, \tag{28}
\]

\[
\mathbf{P}_{n}^{a} = \mathbf{L}_{n-1}^{a} \mathbf{G}(\mathbf{L}_{n-1}^{a})^T, \tag{29}
\]
where $L_n^{s} = X_n^{s} T$, $L_{n-1}^{s} = X_{n-1}^{s} T$, $G = (N_e - 1)^{-1} (T^T T)^{-1}$, and $T$ is an $N_e \times (N_e - 1)$ full column-rank matrix with a zero-column sum. The smoothed estimate is computed using the smoothing Kalman gain $K_n^{e-1}$ given by Eq. (16). Given Eqs. (28), (29), and $L_n^{s} = M_{n-1} L_{n-1}^{s}$ (Hoteit et al. 2008), with $M_{n-1}$ the tangent linear model, $K_n^{e-1}$ can be decomposed as

$$K_n^{e-1} = L_n^{a} U_n^{a-1} (H_n L_n^{a})^T R_n^{-1}, \quad (30)$$
$$U_n^{a-1} = [G^{-1} + (H_n L_n^{a})^T R_n^{-1} (H_n L_n^{a})]^{-1}. \quad (31)$$

The smoothed state estimate and the associated error covariance can be respectively computed as

$$\hat{x}_{n-1} = x_n^{a-1} + L_n^{a} U_n^{a-1} (H_n L_n^{a})^T R_n^{-1} (y_n - H_n \hat{x}_n^{s}), \quad (32)$$
$$P_n^{a-1} = L_n^{a} U_n^{a-1} (L_n^{a})^T. \quad (33)$$

The OSA-smoothed ensemble is then sampled from these two moments using the resampling scheme of SEIK:

$$\hat{x}_{n-1}^{s} = x_n^{a-1} + \sqrt{N_e - 1 L_n^{a} [\Omega_{n} (C_n^{e-1})^T]} \right]^T, \quad (34)$$

where $C_n^{e-1}$ is a square root of the matrix $(U_n^{a-1})^{-1}$ satisfying $(U_n^{a-1})^{-1} = C_n^{e-1} (C_n^{e-1})^T$, $\Omega_n$ is an $N_e \times (N_e - 1)$ matrix with orthonormal columns and a zero-column sum, and $\Omega_{n,i}$ denotes the $i$th row of $\Omega_n$. An efficient procedure to generate the random matrices, $\Omega_n$, is described by Pham (2001) and Hoteit et al. (2002).

2) ANALYSIS STEP

The analysis step [Eqs. (20)–(24)] of KF-OSE involves the model error covariance matrix $Q_{n-1}$ and requires the computation of the matrices $K_n$ and $Q_{n-1}$. For the analysis Kalman gain, we use Eq. (25) and replace $K_n$ with $K_n^{a} = P_n^{a} H_n^{a T} P_n^{a-1}$, which can be directly estimated from the ensembles. This expression of the Kalman gain can be further written as

$$K_n^{a} = \mathbb{E}[e_n^{a} (e_n^{a})^T] \left[\mathbb{E}[e_n^{a} (e_n^{a})^T]\right]^{-1}, \quad (35)$$
$$ = (P_n^{a} H_n^{a T} + P_n^{a} s_n^{a} H_n^{a T}) \left(1 + H_n^{a T} P_n^{a} H_n^{a} + P_n^{a} s_n^{a} H_n^{a} \right)^{-1}, \quad (36)$$

where $e_n^{a} = x_n^{a} - x_n^{s}$ is the pseudoforecast error, $P_n^{a} = \mathbb{E}[e_n^{a} (e_n^{a})^T]$, $e_n^{a} = y_n - H_n \hat{x}_n^{s}$ is the pseudoinnovation, and $P_{n,a} = \mathbb{E}[a_n x_n^{a}]$ is the cross covariance between the observational error and the pseudoforecast error.

To factorize the analysis error covariance $P_n^{a}$ in a square root form, we express it directly in terms of the analysis error $e_n^{a} = x_n^{a} - x_n^{a}$ as $P_n^{a} = \mathbb{E}[e_n^{a} (e_n^{a})^T]$. Using (20) leads to

$$P_n^{a} = (I - K_n^{a} H_n) P_n^{a} + K_n^{a} (H_n P_n^{a} H_n^T + R_n) K_n^{a T}$$
$$ - P_n^{a} (K_n^{a} H_n) - K_n^{a} P_n^{a} s_n^{a} (I - K_n^{a} H_n) K_n^{a T}$$
$$ - (I - K_n^{a} H_n) P_n^{a} s_n^{a} (I - K_n^{a} H_n) K_n^{a T}. \quad (37)$$

Typically, one should expect (and this is often observed in practice) the analysis error $e_n^{a-1}$ to be weakly correlated with the observational error $e_n^{a-1}$ and, likewise, the smoothing error $e_n^{a-1}$ with the observational error at the next step, $e_n$. Integrating the smoothing error with a deterministic model with additive noise independent from the $e_n$ should result in a pseudoforecast error $e_n^{a}$ that is weakly correlated with $e_n$, which justifies the assumption that the pseudoforecast error should be weakly correlated with the observational error (i.e., $P_n^{a} s_n^{a} = 0$). This was further confirmed in our numerical experiments. Neglecting this cross-covariance term in (36) allows us to decompose $K_n^{a}$ as

$$K_n^{a} = L_n^{f} U_n^{f} (H_n L_n^{f})^T R_n^{-1}, \quad (38)$$

and, thus, $P_n^{a}$ as

$$P_n^{a} = (I - K_n^{a} H_n) P_n^{f}$$
$$ = L_n^{f} U_n^{f} (L_n^{f})^T, \quad (39)$$

where $U_n^{f} = [G^{-1} + (H_n L_n^{f})^T R_n^{-1} (H_n L_n^{f})]^{-1}$, $P_n^{f} = L_n^{f} G (L_n^{f})^T$, and $L_n^{f} = X_n^f T$. We finally insert (38) into (20) to obtain the analysis update of the pseudoforecast state:

$$\hat{x}_n^{a} = \hat{x}_n^{f} + L_n^{f} U_n^{f} (H_n L_n^{f})^T R_n^{-1} (y_n - H_n \hat{x}_n^{f}). \quad (41)$$

The analysis members are then generated as

$$\hat{x}_{n,i}^{a} = x_n^{a} + \sqrt{N_e - 1 L_n^{f} [\Omega_{n,i} (C_n^{a})^T]} \right]^T, \quad (42)$$

c. Summary of the SEIK-OSE algorithm

The SEIK-OSE algorithm can be summarized as follows, starting from a given analysis ensemble $\{\hat{x}_{n-1,i}^{s}\}_{i=1}^{N_s}$:

1) SMOOTHING STEP
- The forecast ensemble $\{\hat{x}_{n-1,i}^{f}\}_{i=1}^{N_f}$ is first computed by integrating $\hat{x}_{n-1,i}^{s}$ with the model to the time of the next available observation.
The forecast members $x_{f,i}^{n}$ are then used with the incoming observation $y_{n}$ to smooth the previous analysis mean using (32).

The new smoothed members $x_{s,i}^{n+1}$ are then generated using (34).

2) ANALYSIS STEP

- The pseudoforecast ensemble $\{x_{f,i}^{n}\}_{i=1}^{N_{x}}$ is computed by integrating the $x_{i}^{n}$ with the model.
- The resulting $x_{f,i}^{n}$ with the current observation $y_{n}$ are used to compute the analysis mean, as in (41).
- The new analysis members $x_{a,i}^{n}$ are sampled using (42).

The proposed SEIK-OSA scheme, therefore, involves two forecast steps with the model: one to compute the forecast ensemble and the other to compute the pseudoforecast ensemble. It further performs two update steps: one to smooth the previous analysis estimate and the corresponding error covariance matrix using the “future” observation and another to update the pseudoforecast estimate and its error covariance using the same observation. This is, therefore, roughly twice more computationally demanding than the standard SEIK. As we will demonstrate with the numerical experiments presented in the next section, however, exploiting the information in the observation more efficiently enhances the ensemble filter’s performance, even when implemented with only half the ensemble of the classical filtering scheme—a situation in which both schemes require comparable computational cost.

4. Numerical experiments

a. Experimental setting

Numerical experiments are performed with the strongly nonlinear Lorenz-96 model (Lorenz and Emanuel 1998). The model simulates the time evolution of an atmospheric quantity based on a set of differential equations:

$$\frac{dx_{i}}{dt} = (x_{i-1,j} - x_{i-2,j})x_{i-1,j} - x_{i-1,j} + F, \quad i = 1, \ldots, N_{x},$$

where $x_{i,j}$ denotes the $i$th element of the state at time $t$. The nonlinear (quadratic) terms represent advection, and the linear term simulates dissipation. L96 obeys the energy conservation law and is sensitive to the initial conditions and external forcing. In its most common form, the system dimension is $N_{x} = 40$, and the forcing term $F$ is set to 8. For this value of $F$, disturbances propagate from low to high indices (west to east), and the model exhibits chaotic behavior. Boundary conditions are periodic [i.e., $x_{i-1,j} = x_{i-39,j}$, $x_{i,0,j} = x_{i,40,j}$, and $x_{i,41,j} = x_{i,1,j}$].

L96 was discretized using the Runge–Kutta 4th-order scheme with a constant time step, $\Delta t = 0.05$ (which
corresponds to 6 h in real-world time). The trajectory of a reference run is taken as the “true” trajectory to which Gaussian noise of zero mean and unit variance is added to generate the observations. The mean of the initial ensemble is taken as the mean of the model trajectory over the first 5000 model time steps, and the initial ensemble is generated by perturbing it with Gaussian noise with zero mean and identity covariance. We implement all filters with the covariance inflation (Anderson and Anderson 1999) and localization techniques (Houtekamer and Mitchell 1998). We apply the standard local analysis approach by restricting the update of each grid point to only observations falling within some influence radius (Sakov and Bertino 2011). After a spinup period of roughly 20 days to remove any detrimental impact, the simulations are run for a period of 5 years in model time (i.e., 7300 model steps, unless otherwise mentioned). We evaluate the performance of the filters using the root-mean-square error (RMSE) between the reference states $x_{(i,n)}$ and the filters’ estimates $\hat{x}_{(i,n)}$, averaged over all variables and over the assimilation period of $N_a$ cycles:

$$\text{RMSE} = \frac{1}{N_a} \sum_{n=1}^{N_a} \left( \frac{1}{N_k} \sum_{i=1}^{N_k} (x_{(i,n)} - \hat{x}_{(i,n)})^2 \right)^{1/2}. \quad (44)$$

To reduce statistical fluctuations, we repeat each experiment independently 10 times, with a randomly generated initial ensemble and randomly generated observational errors. We took the average of the RMSEs over these multiple runs as the final result.

b. Results and discussion

To test the filters under realistic and challenging situations, we consider three observational scenarios: full (i.e., all model variables are observed), half (i.e., every second variable is observed), and quarter (i.e., every fourth variable is observed). In each scenario, a series of sensitivity experiments is performed with various ensemble sizes, spatial and temporal observation frequencies, and observational error variances. Results of these experiments are presented with two-dimensional plots of the RMSE as a function of the inflation factor and the localization radius, with asterisks indicating the minimum-averaged RMSE values. White boxes indicate divergence of the filter.
localization radius. The localization support radii vary from 2 (strong localization) to 40 (weak localization) grid points. The inflation varies from 1 to 1.3 when no bias is introduced in the forecast model and from 1 to 2.5 otherwise.

1) ON THE APPROXIMATION $P_{x|\phi, e_n}$

The SEIK-OSA algorithm was derived assuming that $P_{x|\phi, e_n} = 0$. To evaluate the order of this term in comparison with the other terms in the Kalman gain (36), we implement EnKF-OSA using an ensemble size of 1000 (without localization and inflation) to eliminate the covariance undersampling noise and assimilate all model variables every four model steps. The results at day 365 shown in Fig. 2 suggest that $P_{x|\phi, e_n}$ is more than 10 orders of magnitude smaller than $P_{e|\phi}H_n^T$. Accordingly, $H_nP_{x|\phi, e_n}H_n^T$ is much smaller than $H_nP_{e|\phi}H_n^T + R_n$. We found that in terms of RMSEs, neglecting this term or not in EnKF-OSA resulted in similar performances. With small ensembles, neglecting this term in the EnKF-OSA even improved its performance. This is because $P_{x|\phi, e_n}$ is undersampled in this case. Based on these results, we neglect this term in both EnKF-OSA and SEIK-OSA in all following experiments.

2) SENSITIVITY TO THE ENSEMBLE SIZE

We first examine the sensitivity of the filters to the ensemble size. In realistic large-scale applications, one would be restricted to small ensembles to avoid prohibitive computational burden. We conduct the experiments using five different ensemble sizes: $N_e = 10, 20, 40, 80,$ and $160$. For the last two sizes, we implement the filters without localization and assess only the effect of inflation. We assimilate the observations every day, that is, every four model steps. We then investigate the three observational scenarios in which all, half, and one-quarter of the observations are assimilated. Figures 3, 4, and 5 present the performance of EnKF, EnKF-OSA, SEIK, and SEIK-OSA in terms of RMSE for $N_e = 10, 20,$ and $40$, respectively. As expected, the deterministic EnKFs outperform the stochastic EnKFs when the number of observations is close to or larger than the ensemble’s size (Hoteit et al. 2015). As the ensemble size increases, the performances of SEIK and EnKF become more comparable, whether or not filtering is implemented based on OSA smoothing. We consider, for instance, the case in which half of the observations are assimilated. With only 10 members, SEIK achieves a lower
minimum RMSE (0.84) than EnKF (1.06), corresponding to an improvement of 20%. Similarly, SEIK-OSA reaches an RMSE minimum of 0.7 versus 0.87 for EnKF-OSA, which corresponds also to an improvement of roughly 20%, while with 40 members, the differences become less pronounced.

The OSA-smoothing-based filters clearly perform better than the standard filters; this becomes more and more pronounced when less data are assimilated and when the filters are implemented with small ensembles, as shown in Fig. 3, in which the filters used $N_e = 10$ members. The minimum RMSEs achieved by SEIK-OSA are 0.38, 0.7, and 1.18 when, respectively, all, half, and one-quarter of the observations are assimilated, compared to 0.44, 0.84, and 1.52 with the standard SEIK. The stochastic EnKF-based versions exhibit similar behavior. Moreover, with OSA smoothing, the robustness of both EnKF and SEIK is clearly enhanced, mainly when fewer observations are assimilated (divergences are indicated in the figure by white boxes). With relatively larger ensembles, both EnKF-OSA and SEIK-OSA still outperform EnKF and SEIK in all observational scenarios, but the resulting improvements become less significant as the number of members increases (see Figs. 4 and 5 for which $N_e = 20$ and 40, respectively). This is consistent with our expectation of the benefit of OSA smoothing, which should be more pronounced when the filter is not implemented in an ideal setting, highlighting how a better exploitation of the data could mitigate filtering deficiencies.

Figures 3–5 suggest that the overall performances of the different schemes are sensitive to the choice of the filtering parameters, such as inflation factor and localization radius. For instance, the SEIK-based algorithms seem to require less localization than the EnKF ones, mainly when the ensemble size is smaller than the number of observations, a case in which the stochastic perturbations in the EnKF may introduce noise in the filter error covariances. When the ensemble size is relatively large, compared to the number of observations (see, e.g., Fig. 5, bottom panels, where $N_e = 10$ and $N_y = 40$), SEIK and EnKF require similar localization radii. In general, SEIK-OSA seems to require less localization than SEIK, which is probably related to the improved ensemble resulting from its two-stage update. This is, however, true for the EnKF only when the ensemble size is larger than the number of observations. Although the OSA smoothing provides an improved background, the effect of undersampling becomes more
FIG. 6. Time evolution between days 366 and 395 of the true state (circles), observations (stars), mean of analysis ensemble members (green dashed line), and boxplots of 10 ensemble members for the observed model variable 19, as resulting from (a) SEIK forecast, (b) SEIK analysis, (c) SEIK-OSA forecast, (d) SEIK-OSA analysis, (e) SEIK-OSA pseudoforecast, and (f) SEIK-OSA smoothing.
Fig. 7. As in Fig. 6, but for the nonobserved model variable 20.
pronounced because of its two update steps. Overall, SEIK-OSA is (generally) the least demanding in terms of localization, as it exploits the benefits of both the OSA-smoothing update to improve the background and the SEIK update to avoid the observations’ perturbations.

In terms of inflation, OSA-smoothing-based schemes seem to require larger inflations in general, compared to the standard schemes, and this becomes more pronounced as less data are assimilated. OSA smoothing tends to decrease the ensemble spread because of its two-stage update, thereby requiring large inflation to preserve enough spread for the following assimilation cycle.

To investigate more closely the impact of the additional smoothing step, we plot in Figs. 6 and 7 the time evolution of two model variables (observed variable 19 and nonobserved variable 20) over a 30-day period (i.e., between days 366 and 395) as estimated by SEIK and SEIK-OSA, respectively. The EnKFs exhibit similar behavior and are, thus, not shown. We present the box plots in which the whiskers are set using 0 and 95th percentiles. The dashed green line represents the filter estimate (the mean of the ensembles), the stars are the observations, and the circles are the true state. Plots are shown for the challenging case with only 10 ensemble members and assimilation of one-quarter of the observations. We use a localization radius of 4 and an inflation factor of 1.15. Overall, the forecast and analysis of SEIK-OSA are closer to the reference states than those of SEIK. This is more pronounced for the nonobserved variable. Consider, for example, the period ranging from day 382 to 387 in Fig. 7, where SEIK fails to accurately recover the reference states. SEIK-OSA, on the other hand, better tracks the true trajectory. This confirms our expectations related to the effect of the smoothing step.
on the pseudoforecast ensemble. From a probabilistic point of view, the forecast members are, indeed, samples from the forecast distribution
\[ p(x_n|y_{0:n-1}) = \int p(x_n|x_{n-1})p(x_{n-1}|y_{0:n-1}) \, dx_{n-1}, \]
where \( p(x_n|x_{n-1}) \) and \( p(x_{n-1}|y_{0:n-1}) \) are, respectively, the analysis and forecast distributions, and \( p(x_n|x_{n-1}) \) is the state transition density represented by the dynamical model. On the other hand, the pseudoforecast ensemble can be sampled from the distribution
\[ P(x_n) \overset{\text{def}}{=} \int p(x_n|x_{n-1})p(x_{n-1}|y_{0:n}) \, dx_{n-1}. \]
Thus, the forecast and the pseudoforecast ensembles are both computed following the same mechanism [i.e., by sampling from \( p(x_n|x_{n-1}) \)], the only difference being that the pseudoforecast ensemble starts from a (smoothed) ensemble \( \{x_{n,i}\}_{i=1}^{N_e} \) produced by the dynamical model, which is already constrained by the observation. This conditioning on the observation explains the improved pseudoforecast uncertainties, compared with the original forecast uncertainties. This two-stage update also explains why SEIK-OSA tends to reduce the ensemble spread, compared with the classical SEIK. Exploiting the information more efficiently in the observations, thus, improves the representativeness of the background ensembles and reduces their spread. As a matter of fact, the averaged forecast ensemble spread for the observed variable 19 over

<table>
<thead>
<tr>
<th>( N_e/2N_e )</th>
<th>EnKF-OSA/EnKF</th>
<th>SEIK-OSA/SEIK</th>
</tr>
</thead>
<tbody>
<tr>
<td>All</td>
<td>10/20</td>
<td>20/40</td>
</tr>
<tr>
<td></td>
<td>4.08</td>
<td>1.98</td>
</tr>
<tr>
<td></td>
<td>4.64</td>
<td>7.01</td>
</tr>
<tr>
<td>Half</td>
<td>10/20</td>
<td>20/40</td>
</tr>
<tr>
<td></td>
<td>9.38</td>
<td>1.8</td>
</tr>
<tr>
<td></td>
<td>2.22</td>
<td>5.67</td>
</tr>
<tr>
<td>Quarter</td>
<td>10/20</td>
<td>20/40</td>
</tr>
<tr>
<td></td>
<td>10.94</td>
<td>1.63</td>
</tr>
<tr>
<td></td>
<td>0.01</td>
<td>1.13</td>
</tr>
</tbody>
</table>

Fig. 10. As in Fig. 4, but with assimilation of observations every model time step.
the whole simulation period reduces from 1.95 with SEIK to 1.17 with SEIK-OSA, about a 40% reduction. This further explains why the OSA-smoothing-based schemes generally require larger inflation values than the standard schemes, mainly for the cases with sparse observations.

Figure 8 presents bar plots of the minimum RMSEs resulting from the best configuration of each filter, including also results from 80 and 160 members, as a function of the ensemble size, for the full, half, and one-quarter observation scenarios. Overall, the OSA-smoothing-based filters outperform the standard ones for all ensemble sizes. Furthermore, as expected, for large enough ensembles ($N_e = 160$), the stochastic variant, EnKF-OSA, outperforms SEIK-OSA, mainly when less data are assimilated (Lei et al. 2010; Hoteit et al. 2015). We also see that the OSA-smoothing-based filters not only outperform the corresponding standard schemes for the same ensemble size, but also when they are implemented with only half the number of ensemble members—that is, when the standard and OSA-smoothing-based filters require similar computational costs. In the same context, Fig. 9 summarizes the run times of EnKF-OSA and SEIK-OSA and of their standard counterparts for different ensemble sizes. We implement all the filters without inflation and localization and report the computing times required by each of them (in seconds) when all the data are assimilated every four model steps. One can see that, as expected, the computing times of EnKF-OSA and SEIK-OSA are roughly doubled, compared with those of EnKF and SEIK, respectively, for a given ensemble size. Besides, we clearly notice that the computing times of EnKF-OSA and SEIK-OSA are practically the same as those of EnKF and SEIK when implemented with twice the number of ensemble members ($2N_e$).

Table 1 reports the percentage of improvements computed using the minimum average RMSEs resulting from EnKF-OSA and SEIK-OSA when implemented with only half of the number of members of EnKF and SEIK, respectively. SEIK-OSA outperforms the standard SEIK for all tested scenarios, while EnKF-OSA improves upon the classical EnKF starting at $N_e = 20/40$, when the undersampling errors are less pronounced, which could be more severe in the two-stage update step of the EnKF-OSA.

3) SENSITIVITY TO THE FREQUENCY OF OBSERVATIONS

In the second set of experiments, we fix the ensemble size to $N_e = 20$ and vary the frequency at which the observations are assimilated. We tolerate an increase or
decrease of 5 days in model time (i.e., 20 model steps) to ensure that the last model step coincides with the last filter step if it is not the case with the 5-yr simulation period. Figures 10 and 11 plot the results of these experiments when the data are assimilated every model step and every six model steps, respectively. These are compared with those in Fig. 4, in which the data are assimilated every four model steps.

When the observations are assimilated frequently in time (every model step), filtering with or without OSA smoothing leads to similar results. With small assimilation windows, the system is well constrained by the data, and the filters are implemented under favorable conditions, with a large enough ensemble and weakly nonlinear conditions. With fewer observations assimilated in time, a situation in which the model becomes more nonlinear within the forecast period, the accuracy of the background approximation degrades, and the benefit of the OSA smoothing becomes clearly pronounced. The OSA-smoothing-based schemes are found to be more robust and provide more accurate estimates, compared with those of EnKF and SEIK (Figs. 4, 11). When the observations are assimilated every six model time steps, EnKF-OSA leads to about 15%, 20%, and 16% improvement over EnKF when all, half, and one-quarter of the observations are assimilated, respectively, while SEIK-OSA leads to 18%, 22%, and 21% improvement over SEIK for the same observational scenarios.

Figure 12 illustrates the evolution of the minimum RMSEs for different frequencies of assimilated observations, ranging between every model step and every 20 model steps. The percentages of improvements resulting from the OSA-smoothing-based schemes with respect to the standard ones are also reported. As stated above, the benefit of the OSA-smoothing step becomes pronounced only when the data are not assimilated very frequently; the largest relative improvements generally correspond to an assimilation frequency of six or eight model steps. This is, however, true only up to a certain frequency (2 to 12 or 16, depending on the observational density), beyond which the performance of the OSA-smoothing-based schemes starts to converge toward that of the standard ones. For large assimilation windows, the model becomes strongly nonlinear, and the linear cross correlations become irrelevant to conducting the smoothing step (Song et al. 2013). One ad hoc way that might improve the results with large assimilation windows would be to apply the smoothing on the model state between the previous and current analysis times, as suggested by (Yang et al. 2013).

4) SENSITIVITY TO THE VARIANCE OF THE OBSERVATIONAL ERRORS

In this set of experiments, we fix the ensemble size to $N_e = 20$ and assimilate the observations every four model steps. Three new values of the variance of the observational error are tested: a small $\sigma^2 = 0.1$, a relatively large $\sigma^2 = 2$, and a large $\sigma^2 = 4$. Figures 13 and 14 present the results of the experiments with $\sigma^2 = 0.1$ and $\sigma^2 = 2$. Comparing these results with those of Fig. 4, where the observational error variance is set to 1, we can see that, as expected, the
filters’ performance degrades as the noise level in the observations increases. The standard and OSA-smoothing-based filters exhibit comparable performances in the case of small observational errors. However, additional experiments that we conducted, in which we designed the background to be less accurately estimated, compared with that of Fig. 13 using smaller ensemble sizes and larger assimilation windows, suggest that the OSA-smoothing-based filters outperform the standard schemes. For instance, repeating the same experiment of Fig. 13 but assimilating the observations every eight model steps (instead of every four), we found that OSA-smoothing-based schemes significantly outperform the standard ones, especially when the observations are sparse. The results, indeed, suggest that when only one-quarter of the observations are assimilated, SEIK and EnKF, respectively, reach minimum RMSEs of 1.58 and 1.45, compared to 0.90 and 0.84 with SEIK-OSA and EnKF-OSA. One can also see from Figs. 13 and 14 that as the noise level increases, EnKF-OSA and SEIK-OSA outperform EnKF and SEIK, respectively, in all observational scenarios.

Figure 15 plots the minimum RMSE values for all filtering schemes, considering the four tested values of observational error variances (0.1, 1, 2, and 4) along with the percentages of relative improvements resulting from the OSA-smoothing-based schemes with respect to the standard ones. Overall, OSA-smoothing-based filters always outperform the classical ones, particularly when the variance of the noise in the observations is larger than 1, suggesting better ability to filter out the noise in the data using the improved background. For instance, when the observational error variance is set to 2 (which is the case of Fig. 14), the estimates are improved by about 12%, 12%, and 8% when, respectively, all, half, and one-quarter of the observations are assimilated using EnKF-OSA, and 14%, 11%, and 9% using SEIK-OSA.

5) SENSITIVITY TO BIAS IN THE FORECAST MODEL

We test the filters’ performance with a biased forecast model. The L96 model is integrated with $F = 6$ in the filter’s forecast step, while the reference states are simulated using $F = 8$. Larger inflation-factor values, ranging from 1 to 2.5, are considered in this set of experiments. The ensemble size is set to 20, data are assimilated every four model steps, and the observational error variance is set to 1. As shown in Fig. 16, the results are consistent with those of the unbiased case (Fig. 4); that is, EnKF-OSA and SEIK-OSA still outperform EnKF and SEIK when the model is biased.

FIG. 13. As in Fig. 4, but for an observational error variance equal to 0.1.
and as the number of assimilated observations decreases, these improvements become more pronounced. Indeed, EnKF-OSA performs 3%, 10%, and 15% better, in terms of RMSE, than EnKF performs when, respectively, all, half, and one-quarter of the observations are assimilated, whereas SEIK-OSA is 4%, 10%, and 17% better than SEIK.

To eliminate the ensemble undersampling error and focus on background limitations due to the bias, we conducted an

![Diagram](image)

**Fig. 15.** (bottom) Minimum average RMSE for all tested filters as a function of the observational error variance and (top) percentages of relative improvements, respectively, brought by EnKF-OSA and SEIK-OSA with respect to EnKF and SEIK. (left) All, (middle) half, and (right) one-quarter of the observations were assimilated every four model steps using 20 ensemble members.
experiment using a large ensemble of 200 members without localization. We found that the EnKF-OSA estimates are 10%, 12%, and 13% more accurate than those of the standard EnKF when, respectively, all, half, and one-quarter of the observations are assimilated, whereas SEIK-OSA estimates are 13%, 13%, and 14% more accurate than those of SEIK for the same scenarios. This suggests that exploiting more the observations may also help to mitigate bias in the forecast model.

5. Discussion and summary

We investigated the relevance of an ensemble filtering strategy that replaces the classical filtering path, which involves a forecast step between two successive analyses, with an alternative path that exploits more information in the observations. The proposed filtering scheme, which introduces one-step-ahead smoothing of the state between two successive analyses, is an ensemble implementation of a fully Bayesian filtering approach. The new smoothing step involves more information in the estimation process, which provides more reliable background. This is shown to improve the ensemble filter’s performance when the filter is implemented under imperfect conditions. The resulting filters bear strong resemblance to the running in place ETKF scheme, which was introduced as a heuristic approach.

Our goals were to evaluate the relevance of the OSA-smoothing strategy and to propose a new deterministic ensemble variant that is suitable for data assimilation into large-scale oceanic and atmospheric models. We constructed such a filter based on the SEIK filter, which we called SEIK-OSA.

Numerical experiments with the Lorenz-96 model demonstrated the relevance of the proposed OSA-smoothing strategy. Even though OSA-smoothing-based ensemble filters are computationally about twice more demanding than are standard ensemble filtering schemes for the same ensemble size, these schemes generally lead to more accurate estimates using only half the ensemble size of the standard schemes. The assimilation results also suggested that the proposed OSA-smoothing-based filters are clearly more efficient and more robust than the standard filters under all tested experimental settings and scenarios. This was more pronounced particularly when the filters were implemented in the challenging situations of low spatial and temporal data coverage, large sampling errors, noisy observations, and biased forecast model.
The proposed ensemble-OSA schemes are straightforward to implement and require only a few modifications to an existing ensemble filtering code. They were further found particularly efficient in situations depicting realistic scenarios. Future work will focus on testing the new OSA-smoothing schemes with large-scale oceanic and atmospheric data assimilation problems. Another future direction we will take is to consider using an OSA-smoothing-based strategy in the context of nonlinear, non-Gaussian filtering, such as the particle and Gaussian mixture filters.

Acknowledgments. This work is supported by King Abdullah University of Science and Technology Award CRG3-2156.

APPENDIX

Proof of (25)

By inserting (17) in (19), we obtain

\[ x_n^{f_i} = x_n^{p_i} + K_n^{e_i}(y_n - H_n x_n^{f_i}), \]  

(A1)

where \( K_n^{e_i} = (P_n^{f_i} - Q_{n-1})H_n^T(H_n P_n^{f_i} H_n^T + R_n)^{-1} \). The errors \( e_n^{f_i} \) and \( e_n^{p_i} \), respectively, associated with the estimates \( x_n^{f_i} \) and \( y_n \) are given by

\[ e_n^{f_i} = (I - H_n^T K_n^e) (x_n - x_n^{f_i}) - K_n^{e_i} e_n^{p_i}, \]  

(A2)

\[ e_n^{p_i} = x_n^{f_i} e_n^{p_i} + e_n. \]  

(A3)

The cross covariance \( P_{x_n^{f_i}, x_n^{p_i}} \) can thus be expressed as

\[
P_{x_n^{f_i}, x_n^{p_i}} = \mathbb{E}[e_n^{f_i}(e_n^{p_i})^T],
\]

\[ = (I - K_n^e H_n^T) (I - K_n^e H_n^T)^T H_n^T - K_n^e R_n (I - H_n K_n^e)^T, \]

\[ = [P_n^{f_i} H_n^T - K_n^e (P_n^{f_i} H_n^T + R_n)](I - H_n K_n^e)^T, \]

\[ = Q_{n-1} H_n^T (I - H_n K_n^e)^T. \]  

(A4)

The covariance \( P_{y_n} \) can also be expressed as

\[
P_{y_n} = \mathbb{E}[H_n e_n^{p_i}(e_n^{p_i})^T],
\]

\[ = H_n P_{x_n^{f_i}, x_n^{p_i}} + \mathbb{E}[e_n^{p_i} H_n (I - K_n^e H_n) (x_n - x_n^{f_i})] + (I - H_n K_n^e) e_n^{p_i}^T, \]

\[ = (H_n Q_{n-1} H_n^T + R_n) (I - H_n K_n^e)^T. \]  

(A5)

We can then check that \( I - H_n K_n^e \) is invertible, as it can be expressed as

\[ I - H_n K_n^e = (H_n Q_{n-1} H_n^T + R_n) (H_n P_n^{f_i} H_n^T + R_n)^{-1}. \]  

(A6)

From (A4), (A5), and (A6), we readily obtain (25).

REFERENCES


