Ensemble Kalman Filtering with One-Step-Ahead (OSA) smoothing: Application to State-Parameter Estimation and 1-Way Coupled Models

Naila Raboudi, Boujemaa Ait-El-Fquih, Ibrahim Hoteit

King Abdullah University of Science and Technology
Earth Science & Engineering
Applied Mathematics and Computational Sciences

January, 2019
Consider a discrete-time dynamical system

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

\[\eta_{n-1} \sim \mathcal{N}(0, \mathbf{Q}_{n-1})\]

\[\varepsilon_n \sim \mathcal{N}(0, \mathbf{R}_n)\]
Context and Motivation

- Consider a discrete-time dynamical system

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

- Ensemble Kalman Filters (EnKFs)
  - Robust performance
  - Reasonable computational cost
  - Non-intrusive formulation
  - Small ensembles in large scale applications
  - Poorly known model error statistics
  - Nonlinear dynamics

\( \Rightarrow \) Limit the representativeness of EnKFs background covariances.
Some auxiliary techniques

- Inflation (Anderson 2001)
- Localization (Houtekamer and Mitchell 1998)
- Hybrid formulation (Hamill and Snyder 2000)
- Adaptive formulation (Song et al. 2010)
Some auxiliary techniques
- Inflation (Anderson 2001)
- Localization (Houtekamer and Mitchell 1998)
- Hybrid formulation (Hamill and Snyder 2000)
- Adaptive formulation (Song et al. 2010)

Our approach: Improve the background through a more efficient use of the data:

Follow the One-Step-Ahead (OSA) smoothing formulation of the Bayesian filtering problem:

→ OSA adds a smoothing step with the future observation, within a Bayesian framework, to compute an ”improved” background
The standard filtering path, which involves the forecast pdf when moving from the analysis pdf at $n - 1$ to the analysis pdf at the next time $n$, is not unique.
Bayesian formulation of the OSA smoothing algorithm

- The standard filtering path, which involves the forecast pdf when moving from the analysis pdf at $n - 1$ to the analysis pdf at the next time $n$, is not unique

- Standard path

$$p(x_{n-1}|y_{0:n-1}) \xrightarrow{\text{Forecast}} p(x_n|y_{0:n-1}) \xrightarrow{\text{Analysis}} p(x_n|y_{0:n})$$

- OSA smoothing path

$$p(x_{n-1}|y_{0:n-1}) \xrightarrow{\text{Smoothing}} p(x_{n-1}|y_{0:n}) \xrightarrow{\text{Analysis}} p(x_n|y_{0:n})$$
The standard filtering path, which involves the forecast pdf when moving from the analysis pdf at $n - 1$ to the analysis pdf at the next time $n$, is not unique.

Standard path

$$p(x_{n-1}|y_{0:n-1}) \xrightarrow{\text{Forecast}} p(x_n|y_{0:n-1}) \xrightarrow{\text{Analysis}} p(x_n|y_{0:n})$$
The standard filtering path, which involves the forecast pdf when moving from the analysis pdf at \( n - 1 \) to the analysis pdf at the next time \( n \), is not unique.

**Standard path**

\[
p(x_{n-1}|y_{0:n-1}) \xrightarrow{\text{Forecast}} p(x_n|y_{0:n-1}) \xrightarrow{\text{Analysis}} p(x_n|y_{0:n})
\]

**Corresponding KF algorithm**

\[
x^a_{n-1}
\]
Bayesian formulation of the OSA smoothing algorithm

- The standard filtering path, which involves the forecast pdf when moving from the analysis pdf at \( n - 1 \) to the analysis pdf at the next time \( n \), is not unique.

- Standard path

\[
p(x_{n-1}|y_{0:n-1}) \xrightarrow{\text{Forecast}} p(x_n|y_{0:n-1}) \xrightarrow{\text{Analysis}} p(x_n|y_{0:n})
\]

- Corresponding KF algorithm

```
\[ x_a^{n-1} \xrightarrow{\text{Forecast (}M_{n-1}\text{)}} x_f^f \]
```
The standard filtering path, which involves the forecast pdf when moving from the analysis pdf at \( n - 1 \) to the analysis pdf at the next time \( n \), is not unique.

**Standard path**

\[
p(x_{n-1}|y_{0:n-1}) \xrightarrow{\text{Forecast}} p(x_n|y_{0:n-1}) \xrightarrow{\text{Analysis}} p(x_n|y_{0:n})
\]

**Corresponding KF algorithm**

\[
\begin{align*}
X^a_{n-1} & \xrightarrow{\text{Forecast (}M_{n-1}\text{)}} X^f_n \\
X^f_n & \xrightarrow{\text{Analysis (}y_n\text{)}} X^a_n
\end{align*}
\]
The standard filtering path, which involves the forecast pdf when moving from the analysis pdf at \( n - 1 \) to the analysis pdf at the next time \( n \), is not unique.

OSA smoothing path

\[
p(x_{n-1} | y_{0:n-1}) \xrightarrow{\text{Smoothing}} p(x_{n-1} | y_{0:n}) \xrightarrow{\text{Analysis}} p(x_n | y_{0:n})
\]
The standard filtering path, which involves the forecast pdf when moving from the analysis pdf at $n - 1$ to the analysis pdf at the next time $n$, is not unique.

**OSA smoothing path**

\[ p(x_{n-1}|y_{0:n-1}) \xrightarrow{\text{Smoothing}} p(x_{n-1}|y_{0:n}) \xrightarrow{\text{Analysis}} p(x_n|y_{0:n}) \]

**Corresponding KF-OSA algorithm**

\[
\begin{align*}
\text{Forecast:} & \quad x_{a,n-1} \\
\text{Reforecast:} & \quad x_{f_1,n-1} \\
\text{Analysis:} & \quad x_{a,n} \\
\text{Smoothing:} & \quad x_{a,n-1} \\
\end{align*}
\]
The standard filtering path, which involves the forecast pdf when moving from the analysis pdf at $n - 1$ to the analysis pdf at the next time $n$, is not unique.

**OSA smoothing path**

$$p(x_{n-1}|y_{0:n-1}) \xrightarrow{\text{Smoothing}} p(x_{n-1}|y_{0:n}) \xrightarrow{\text{Analysis}} p(x_n|y_{0:n})$$

**Corresponding KF-OSA algorithm**

- $x_{n-1}^a$ (Analysis)
  - Forecast ($M_{n-1}$)
  - $x_{n-1}^f$ (Forecast)
  - $x_n$ (Analysis)
The standard filtering path, which involves the forecast pdf when moving from the analysis pdf at $n - 1$ to the analysis pdf at the next time $n$, is not unique.

OSA smoothing path

$$p(x_{n-1}|y_{0:n-1}) \xrightarrow{\text{Smoothing}} p(x_{n-1}|y_{0:n}) \xrightarrow{\text{Analysis}} p(x_n|y_{0:n})$$

Corresponding KF-OSA algorithm
The standard filtering path, which involves the forecast pdf when moving from the analysis pdf at \( n - 1 \) to the analysis pdf at the next time \( n \), is not unique.

### OSA smoothing path

\[
p(x_{n-1} \mid y_{0:n-1}) \rightarrow \text{Smoothing} \rightarrow p(x_{n-1} \mid y_{0:n}) \rightarrow \text{Analysis} \rightarrow p(x_{n} \mid y_{0:n})
\]

### Corresponding KF-OSA algorithm

\[
x^{a}_{n-1} \rightarrow \text{Forecast} (\mathcal{M}_{n-1}) \rightarrow x^{f_1}_{n} \\
\quad \text{Smoothing} (y_{n}) \rightarrow x^{s}_{n-1} \\
\quad \text{Reforecast} (\mathcal{M}_{n-1}) \rightarrow x^{f_2}_{n} \\
\quad \text{Analysis} \rightarrow p(x_{n} \mid y_{0:n})
\]
Bayesian formulation of the OSA smoothing algorithm

- The standard filtering path, which involves the forecast pdf when moving from the analysis pdf at \( n - 1 \) to the analysis pdf at the next time \( n \), is not unique.

- OSA smoothing path

\[
p(x_{n-1} | y_{0:n-1}) \xrightarrow{\text{Smoothing}} p(x_{n-1} | y_{0:n}) \xrightarrow{\text{Analysis}} p(x_n | y_{0:n})
\]

- Corresponding KF-OSA algorithm
KF Vs KF-OSA algorithms

- KF and KF-OSA use different paths to compute same analysis/forecast
- KF applies 1 update and 1 forecast step while KF-OSA applies 2 "update" and 2 "forecast" steps
- KF-OSA uses the observation twice within a consistent Bayesian framework (for the RIP of Kalnay and Yang (2010))
Motivation behind EnKF-OSA

Why an EnKF-OSA would outperform a classical EnKF?
- Conditions the ensemble sampling with future information
- Provides an improved background which should help mitigating for the sub-optimal character of EnKFs
- This should be particularly expected when the filter is not implemented under ideal conditions

Stochastic EnKF-OSA update equations

**Smoothing:**

\[ x_{n-1}^{s,i} = x_{n-1}^{a,i} + P_{x_{n-1}^{a,i},y_{n}^{f_1,y_{n}^{f_1}}}^{-1} \left( y_{n}^{i} - H_{n} x_{n}^{f_1,i} \right) \]

**Analysis:**

\[ x_{n}^{a,i} = x_{n}^{f_2,i} + K_{n}^{a} \left( y_{n}^{i} - H_{n} x_{n}^{f_2,i} \right) \]

\[ K_{n}^{a} = Q_{n-1} H_{n}^{T} (H_{n} Q_{n-1} H_{n}^{T} + R_{n})^{-1} = P_{x_{n}^{f_2},y_{n}^{f_2},y_{n}^{f_2}}^{-1} \]
Analysis step of EnKF-OSA

- Should be related to the sampling step in the particle filter (PF) with optimal proposal density (Doucet et al., 2001; Desbovries et al., 2011)

Deriving a deterministic EnKF-OSA

- We derived SEIK-OSA by assuming uncorrelated pseudo-forecast and observational errors
Numerical experiments with Lorenz-96

- Governing equations (L-96)

\[
\frac{dx_i}{dt} = (x_{i+1} - x_{i-2})x_{i-1} - x_i + F
\]

- Experimental setup
  - Twin experiments
  - 5-years simulation period

- Compare EnKF, EnKF-OSA, SEIK and SEIK-OSA

- 3 different observational scenarios: all (40), half (20), and quarter (10) of the variables

- Data are assimilated every 4 model steps (1 day)

- Inflation and local analysis are used
Figure: Time-averaged RMSE as a function of the localization radius ($x$ axis) and inflation factor ($y$ axis) (20 members, DA every 4 model steps)
Numerical experiments with Lorenz-96

**Figure:** Percentages of relative improvement, in terms of RMSE, resulting from SEIK-OSA compared to SEIK using the same and half the ensemble size.
Numerical experiments with Lorenz-96

**Figure:** Percentages of relative improvement, in terms of RMSE, resulting from SEIK-OSA compared to SEIK using the same and half the ensemble size

- Benefit of OSA is more pronounced when
  - less data are assimilated
  - filter implemented with small ensembles, neglected model error
- EnKF-OSA outperformed EnKF even with half the ensemble size (i.e., similar computational cost)
Joint project with Clint Dawson (UT-Austin)

ADCIRC: ADvanced CIRCulation model

EnKF-OSA is tested with a realistic setting of ADCIRC configured for storm surge forecasting in the Gulf of Mexico during Hurricane Ike (2008)

Pseudo-observations of sea surface levels from a network of buoys are assimilated

Combine OSA with hybrid formulation for efficient implementation with small ensembles

Compare 4 EnKFs: ETKF, ETKF_{Hyb}, ETKF-OSA and ETKF_{Hyb}-OSA

Filters are tested under the same computational cost
Storm surge forecasting using ETKF-OSA

Figure: Coastal-averaged RMSEs [m] of maximum water elevation forecast errors for different LA radii and inflation factors
Main conclusions: OSA for ensemble state estimation

- OSA exploits the future observation, which provides improved background
- EnKF-OSAs outperformed the standard EnKFs for comparable computational costs
- The improvements are particularly pronounced when the filter is implemented under challenging conditions
- The hybrid formulation enables a more efficient implementation of the OSA formulation
- The smoothing window should not be too large so that the linear (correlation-based) updates remain relevant, *iterations may help*
EnKF-OSA scheme for state-parameter estimation
EnKF-OSA scheme for state-parameter estimation

\[
\left\{ x_{n-1}^{(i),a} \left( \theta_{n-1}^{(i)} \right) \right\}_{i=1}^{N_e}
\]
EnKF-OSA scheme for state-parameter estimation

\[
\begin{align*}
\{x_{n-1}^{a,(i)}(\theta^{(i)}|_{n-1})\}_{i=1}^{N_e} & \quad \mathcal{M}_{n-1} \\
\{x_{n}^{f_1,(i)}\}_{i=1}^{N_e}
\end{align*}
\]
EnKF-OSA scheme for state-parameter estimation

EnKF $\theta$

EnKF $\mathbf{x}$

\[
\begin{align*}
\left\{ \mathbf{x}_{n-1}^{a,(i)} \left( \theta^{(i)} \right|_{n-1} \right\}_{i=1}^{N_e} & \rightarrow \mathcal{M}_{n-1} \\
\left\{ \mathbf{x}_{n-1}^{s,(i)} \left( \theta^{(i)} \right|_{n} \right\}_{i=1}^{N_e} & \rightarrow \left\{ \mathbf{x}_n^{f_1,(i)} \right\}_{i=1}^{N_e}
\end{align*}
\]

Analysis $\theta$

Smoothing $\mathbf{x} \left( \mathbf{y}_n \right)$
State-parameter estimation with OSA

EnKF-OSA scheme for state-parameter estimation

EnKF $\theta$
EnKF $x$

Analysis $\theta$
Smoothing $x$ $(y_n)$

EnKF $\theta$
EnKF $x$

$\{x_{n-1}^a,(i) (\theta_{n-1}^{(i)}) \}_{i=1}^{N_e}$
$\mathcal{M}_{n-1}$
$\{x_{n}^{f_1,(i)}\}_{i=1}^{N_e}$

$\{x_{n-1}^s,(i) (\theta_{n}^{(i)}) \}_{i=1}^{N_e}$
$\mathcal{M}_{n-1}$
$\{x_{n}^{f_2,(i)}\}_{i=1}^{N_e}$
State-parameter estimation with OSA

EnKF-OSA scheme for state-parameter estimation

EnKF $\theta$

EnKF $x$

$\{x^{a,(i)}_{n-1}(\theta^{(i)}_{|n-1})\}_{i=1}^{N_e}$

$\mathcal{M}_{n-1}$

$\{x^{f_1,(i)}_{n}\}_{i=1}^{N_e}$

$\{x^{s,(i)}_{n-1}(\theta^{(i)}_{|n})\}_{i=1}^{N_e}$

$\mathcal{M}_{n-1}$

$\{x^{f_2,(i)}_{n}\}_{i=1}^{N_e}$

Analysis $\theta$

Smoothing $x$ ($y_n$)

Analysis $x$ ($y_n$)

EnKF-OSA scheme for state-parameter estimation

EnKF $\theta$

EnKF $x$

$\{x^{a,(i)}_{n-1}(\theta^{(i)}_{|n-1})\}_{i=1}^{N_e}$

$\mathcal{M}_{n-1}$

$\{x^{f_1,(i)}_{n}\}_{i=1}^{N_e}$

$\{x^{s,(i)}_{n-1}(\theta^{(i)}_{|n})\}_{i=1}^{N_e}$

$\mathcal{M}_{n-1}$

$\{x^{f_2,(i)}_{n}\}_{i=1}^{N_e}$

Analysis $\theta$

Smoothing $x$ ($y_n$)

Analysis $x$ ($y_n$)
EnKF-OSA scheme for state-parameter estimation

- Introduced by Gharamti et al. (2015) and Ait-El-Fquih et al. (2016) to derive a Bayesian framework for the "dual-EnKF" (Moradkhani et al. 2005)
- "Original" dual-EnKF missed the smoothing step of the state ($\mathbf{x}$)
Subsurface hydrology state-parameter estimation

We estimate the water head and the hydraulic conductivity

**Figure**: Mean average absolute errors (AAE) of log-hydraulic conductivity, \( \log(k) \), in terms of the observation frequency of hydraulic head data. Data are obtained from 9 wells, every 1, 3, 5, 10, 15 and 30 days using \( N_e = 100 \)
Subsurface hydrology state-parameter estimation

We estimate the water head and the hydraulic conductivity

Figure: Time series of AAE for hydraulic head (left) and conductivity (right). Data of hydraulic head are obtained from $p = 15, 25$ wells using $N_e = 100$

OSA improves the state and parameter estimation with EnKFs
Consider the discrete-time OWC dynamical system:

\[
\begin{align*}
\mathbf{x}_n &= \mathcal{M}^{x}_{n-1} \left( \mathbf{x}_{n-1} \right) + \eta^x_{n-1} \\
\mathbf{z}_n &= \mathcal{M}^{\tilde{z}}_{n-1} \left( \mathbf{z}_{n-1}, \mathbf{x}_{n-1} \right) + \eta^{\tilde{z}}_{n-1} \\
\mathbf{y}^x_n &= \mathbf{H}^x_n \mathbf{x}_n + \mathbf{v}^x_n \\
\mathbf{y}^{\tilde{z}}_n &= \mathbf{H}^{\tilde{z}}_n \mathbf{z}_n + \mathbf{v}^{\tilde{z}}_n
\end{align*}
\]
Consider the discrete-time OWC dynamical system:

\[
\begin{align*}
\mathbf{x}_n &= \mathcal{M}_{x_{n-1}}^x (\mathbf{x}_{n-1}) + \eta_{x_{n-1}}^x \\
\mathbf{z}_n &= \mathcal{M}_{z_{n-1}}^z (\mathbf{z}_{n-1}, \mathbf{x}_{n-1}) + \eta_{z_{n-1}}^z \\
\mathbf{y}_n^x &= \mathbf{H}_n^x \mathbf{x}_n + \mathbf{e}_n^x \\
\mathbf{y}_n^z &= \mathbf{H}_n^z \mathbf{z}_n + \mathbf{e}_n^z
\end{align*}
\]

- Two classical solutions
  - **Strong (Joint) formulation (EnKF-S):** Applies the filtering scheme on the augmented state \( \mathbf{X}_n = [\mathbf{x}_n^T \mathbf{z}_n^T]^T \)
    - Cross-correlations considered in the update
    - Cross-correlations may not be well estimated with small ensembles and not very representative in the presence of strong nonlinearities
  - **Weak formulation (EnKF-W)** Applies the filtering scheme on each component separately
    - Separate updates are more practical in real applications
    - Loss of information from neglecting cross-correlations
Strong EnKF-OSA (EnKF-S-OSA) introduces:

→ an extra smoothing step for both state components using the future observations of both variables (a joint smoothing update)

→ an analysis step of both states, each using its own observation

The "separate" analysis steps result from the uncorrelated model errors $\eta_n^x$ and $\eta_n^z$. 
Numerical experiments with OWC Lorenz-96

- Governing equations (Coupled L-96)

\[ \frac{dx_i}{dt} = (x_{i+1} - x_{i-2}) x_{i-1} - x_i + F - \frac{hc}{b} \sum_{j=1}^{K} z_{j,i}, \quad i = 1, \ldots, n_x = 8 \]

\[ \frac{dz_{j,i}}{dt} = (z_{j-1,i} - z_{j+2,i}) c b z_{j+1,i} - c z_{j,i} + \frac{hc}{b} x_i, \quad j = 1, \ldots, K = 16 \]
Numerical experiments with OWC Lorenz-96

- Governing equations (OWC L-96)

\[
\frac{dx_i}{dt} = (x_{i+1} - x_{i-2})x_{i-1} - x_i + F \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad i = 1, \ldots, n_x = 8
\]

\[
\frac{dz_{j,i}}{dt} = (z_{j-1,i} - z_{j+2,i})cbz_{j+1,i} - cz_{j,i} + \frac{hc}{b}x_i, \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad j = 1, \ldots, K = 16
\]

- Twin experiments \((8 + 1) \times 16 = 144\) variables
- 3-years simulation period
- Time step: 0.005
- Assimilation scenarios
  - Every second state variable (from each component) is observed every 4 model steps (1 day)
- We use covariance inflation and correlation-based localization to address the different spatial scales between components (Luo et al., 2017)
Numerical experiments with OWC Lorenz-96

- Governing equations (OWC L-96)

\[
\frac{dx_i}{dt} = (x_{i+1} - x_{i-2}) x_{i-1} - x_i + F \\
\frac{dz_{j,i}}{dt} = (z_{j-1,i} - z_{j+2,i}) cbz_{j+1,i} - cz_{j,i} + \frac{hc}{b} x_i, 
\]

\[i = 1, \cdots, n_x = 8\]

\[j = 1, \cdots, K = 16\]

- Twin experiments
  - \((8 + 1) \times 16 = 144\) variables
  - 3-years simulation period
  - Time step: 0.005

- Assimilation scenarios
  - Every second state variable (from each component) is observed every 4 model steps (1 day)
  - We use covariance inflation and correlation-based localization to address the different spatial scales between components (Luo et al., 2017)
Numerical experiments with OWC Lorenz-96

Figure: Time averaged RMSE as function of inflation factor, $N_e = 40$

- OSA formulation is beneficial
- With OSA, EnKF-S outperforms EnKF-W
- EnKF-S requires large enough ensembles to outperform EnKF-W
- OSA more robust to inflation values
Main conclusions: OSA for OWC systems

- OSA is beneficial for strong and weak OWC DA compared to the standard EnKF
- EnKF-W-OSA outperforms the other schemes with very small ensembles
- The benefit of EnKF-S-OSA is more pronounced with less data
- The smoothing window should not be too large so that the linear correlation-based updates remain relevant, *iterations may help*
Main conclusions: OSA for OWC systems

- OSA is beneficial for strong and weak OWC DA compared to the standard EnKF
- EnKF-W-OSA outperforms the other schemes with very small ensembles
- The benefit of EnKF-S-OSA is more pronounced with less data
- The smoothing window should not be too large so that the linear correlation-based updates remain relevant, *iterations may help*

- *We are working on implementing the EnKF-OSA within the Data Research Testbed (DART) to test it with a high resolution MIT general circulation model (MITgcm) of the Red Sea*
Thank you

References


