Supporting Information for “State estimation and prediction using clustered particle filter”

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Particle adjustment matrix A

We describe how to find the adjustment matrix A of Eq. (9). As each observation $y_j, j = 1, 2, ..., N_{obs}$ updates only one cluster C_j, we suppress the observation and cluster indices for simplicity. Note that we consider update of $\mathbf{x}_k$ which is in the sub-state $\mathbb{R}^{N_{state}/N_{obs}}$.

From the prior particles $\{\mathbf{x}_k^f, k = 1, 2, ..., K\}$ and weight $\{\omega_k^f > 0, k = 1, 2, ..., K\}$, we first compute the prior mean

$$\mathbf{x}^f = \sum_k \omega_k \mathbf{x}_k^f \tag{1}$$

and covariance

$$R^f = \sum_k \omega_k (\mathbf{x}_k^f - \mathbf{x}^f)(\mathbf{x}_k^f - \mathbf{x}^f)^T = UU^T \tag{2}$$

where $U \in \mathbb{R}^{\frac{N_{state}}{N_{obs}} \times K}$ is the perturbation matrix whose k-th column is given by

$$\sqrt{\omega_k}(\mathbf{x}_k^f - \mathbf{x}^f) \tag{3}$$

Now our goal is to find a matrix A such that the posterior covariance R^a can be represented by

$$R^a = AR^f A^T = AUUA^T$$

so that the adjusted particles

$$\mathbf{x}_k^a = \mathbf{x}^a + A(\mathbf{x}_k^f - \mathbf{x}) \tag{4}$$

satisfies the posterior mean and covariance from the Kalman update formula.

First of all, using the particle perturbation matrix U, the Kalman gain Gcan be represented as follows

$$\begin{aligned} G &= R^f H^T (HR^f H^T + R_o)^{-1} \\ &= R^f H^T (HUU^T H^T + R_o)^{-1} \\ &= UU^T H^T (HUU^T H^T + R_o)^{-1} \\ &= U(I + U^T H^T (R_o)^{-1} HU)^{-1} U^T H^T R_o^{-1}. \end{aligned} \tag{5}$$

Now we use this representation of G for the posterior covariance

$$
\begin{aligned}
R^a &= (I - GH)R^f \\
&= \left(I - U(I + U^T H^T R_o^{-1} HU)^{-1} U^T H^T R_o^{-1}\right) UU^T \quad \text{from (5)} \\
&= U(I - (I + U^T H^T R_o^{-1} HU)^{-1} U^T H^T R_o^{-1} U)U^T \\
&= U(I + U^T H^T R_o^{-1} HU)^{-1} U^T \\
&= \left((R^f)^{-1} + H^T R_o^{-1} H\right)^{-1}
\end{aligned}
\tag{6}
$$

As the prior covariance and observation covariance matrices are symmetric and positive definite, we have the following eigenvalue decomposition

$$R^f = V\Sigma^2 V^T \tag{7}$$

and the following matrix

$$\Sigma V^T H^T R_o^{-1} HV\Sigma = WDW^T \tag{8}$$

with unitary matrices V and W and diagonal matrices Σ and D. Using V, W, Σ and D, the posterior covariance is further represented by

$$
\begin{aligned}
R^a &= V\Sigma W W^T \Sigma^{-1} V^T \left((R^f)^{-1} + H^T R_o^{-1} H\right)^{-1} A\Sigma^{-1} W W^T \Sigma V^T \\
&= V\Sigma W \left(W^T \Sigma V^T (R^f)^{-1} V\Sigma W + W^T \Sigma V^T H^T R_o^{-1} HV\Sigma W\right)^{-1} W^T \Sigma V^T \\
&= V\Sigma W \, (I + D)^{-1} \, W^T \Sigma V^T \\
&= V\Sigma W \, (I + D)^{-1/2} \, (I + D)^{-1/2} \, W^T \Sigma V^T \\
&= V\Sigma W \, (I + D)^{-1/2} \, \Sigma^{-1} V^T R^f V \Sigma^{-1} \, (I + D)^{-1/2} \, W^T \Sigma V^T \\
&= AUU^T A = \sum_k \omega_k A(\mathbf{x}_k^f - \mathbf{x}^f)(\mathbf{x}_k^f - \mathbf{x}^f)^T A^T
\end{aligned}
\tag{9}
$$

where $A = V\Sigma W \, (I + D)^{-1/2} \, \Sigma^{-1} V^T$ is the adjustment matrix for particles.

Soft threshold version clustered particle filter

In addition to the hard threshold version, we can also use a soft threshold clustered particle filter using innovation statistics. The soft version uses the statistics of the innovation $\{H\mathbf{x}_{C_j}^f - y_j\}$ which are the difference between the predicted observations and real observation. The innovation statistics are widely used to avoid catastrophic filter divergence of ensemble based methods (31) and increase filter accuracy (32) by adaptively inflating the prior covariance. In the soft version clustered particle filter, the innovation statistics are used to determine the tigger of the particle adjustment. The criterion used for the soft version clustered particle filter is to check the innovation error, that is, the distance between the predicted observation $H\mathbf{x}^f_{C_j}$ and the real observation y_j and trigger the particle adjustment if the innovation error is larger than a threshold value $\alpha\sqrt{r_o}, \alpha \geq 1$.

Soft version criterion for particle adjustment :

$$|H\mathbf{x}^f_{C_j} - y_j| \geq \alpha\sqrt{r_o}, \quad \alpha \geq 1 \tag{10}$$

In addition to the new criterion for the particle adjustment, the soft version clustered particle filter uses a multiplicative covariance inflation

$$\mathbf{x}^f_k \leftarrow \mathbf{x}^f_k + (1+\lambda)(\mathbf{x}^f_k - \mathbf{x}^f), \quad \lambda \geq 0 \tag{11}$$

before the assimilation step to account for variance underestimation, sampling errors and rank deficiency. As we use covariance inflation, we do not add the additional noise after resampling in our soft version. See Fig. S2 for the results of the hard and soft threshold version clustered particle filters applied for the 40-dim Lorenz 96 with $F = 8$ and 10 observations.

Soft Threshold Version Clustered Particle Filter Algorithm - one step assimilation

Given :
1) N_{obs} observations $\{y_1, y_2, ..., y_{N_obs}\}$
2) prior K particles $\{\mathbf{x}^f_{C_j,k}, k = 1, 2, ..., K\}$ and weight vectors $\{\omega^f_{l,k}, k = 1, 2, ..., K\}$ for each cluster $C_l, l = 1, 2, .., N_{obs}$
For y_j from $j = 1$ to N_{obs}
Inflate the prior covariance Eq. (11)
If The soft threshold criterion Eq. (10) is satisfied.
Update the prior particles using Eq. (9) to satisfy the Kalman update Eq. (10) and Eq. (11)
Else Use particle filtering
Update $\{\omega^f_{j,k}\}$ using Eq. (8)
If $K_{eff} = \frac{1}{\sum_k (\omega^a_{l,k})^2} < \frac{K}{2}$
Do resampling
End If
End If
End For

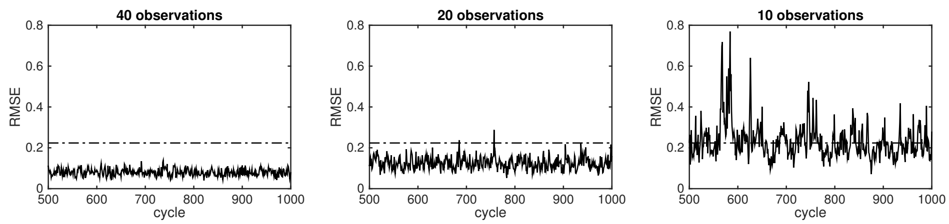

Fig. S1: Lorenz 96 F=8. Time series of RMS errors of EAKF using tuned parameters. Localization radius is 8 and covariance is 20%. Dash-dot line is observation error 0.22. 50 ensemble members are used.

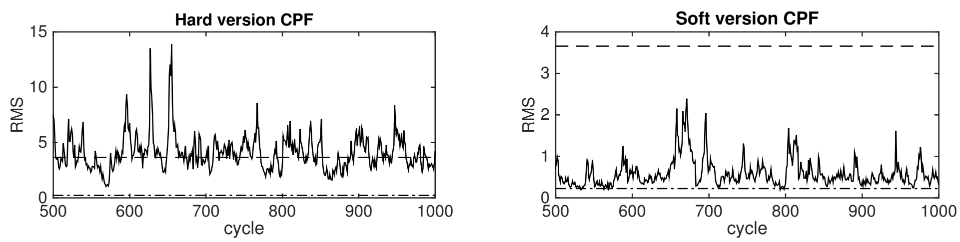

Fig. S2: Lorenz 96 F=8 with 10 observations. Time series of RMS errors of the hard and soft version clustered particle filters. Dash-dot line is observation error 0.22 and dash line is the climatological error 3.64. 200 ensemble members and particles are used. The hard version particle filter does not show any filtering skill with RMS errors comparable to or larger than the climatological error. The soft version clustered particle filter, which uses innovation statistics, has significantly improved skill with RMS errors smaller than the climatological error.

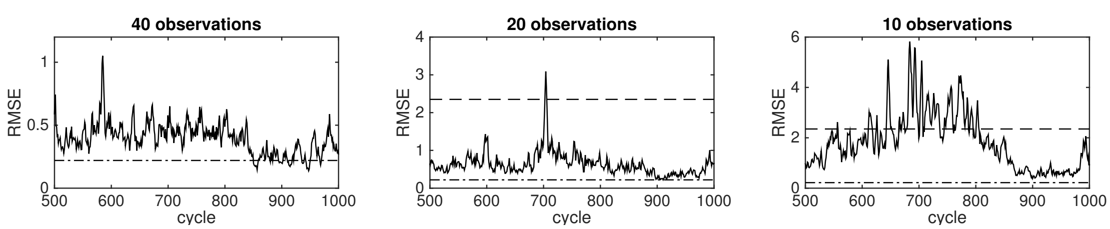

Fig. S3: Lorenz 96 F=5. Time series of RMS errors of the localized particle filter (LocPF). Dash-dot line is the observation error 0.22 and dash line is the climatological error 2.35.

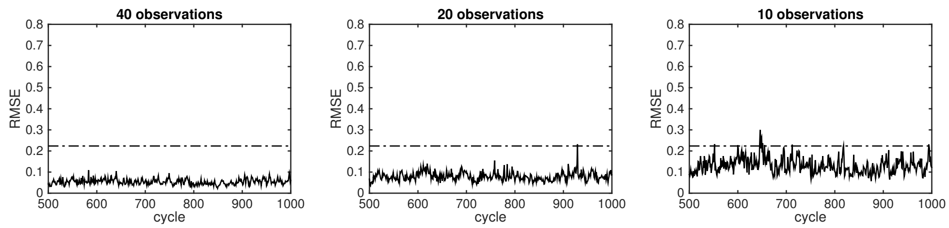

Fig. S4: Lorenz 96 F=5. Time series of RMS errors of EAKF using tuned parameters. Localization radius is 6 and covariance is 20%. Dash-dot line is the observation error 0.22. 50 ensemble members are used.

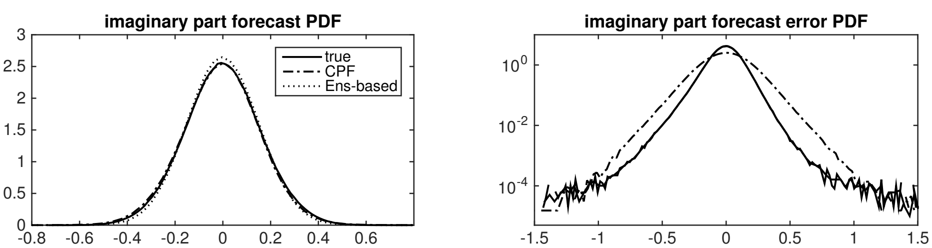

Fig. S5: MMT. Large-scale imaginary part forecast PDF (left) and forecast error PDF (right) using 64 observations.