High-rank Ensemble Transform Kalman Filter (HETKF)

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Outline

- ❑ Background
- ❑ Methods
- ❑ Cycling Experiments
- ❑ Summary and Discussion

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Ensemble Kalman Filter (EnKF)

- A Monte Carlo approximation to the traditional Kalman Filter (KF) (Kalman and Bucy, 1961).

- Compared to 3DVar, EnKF estimates forecast errors in a flow-dependent fashion by running an ensemble of short-range forecasts.

- Different EnKF variants were developed for efficient implementation purposes.
  - EnKF with perturbed observations (Houtekamer and Mitchell 1998)
  - Ensemble Transform Kalman filter (ETKF, Bishop et al. 2001, Wang and Bishop 2003, Wang et al. 2004)
  - Local parallel ETKF (LETKF, Hunt et al. 2007)
  - Ensemble Adjustment Kalman Filter (EAKF, Anderson 2001)
  - Ensemble Square Root Filter (EnSRF, Whitaker and Hamill, 2002)

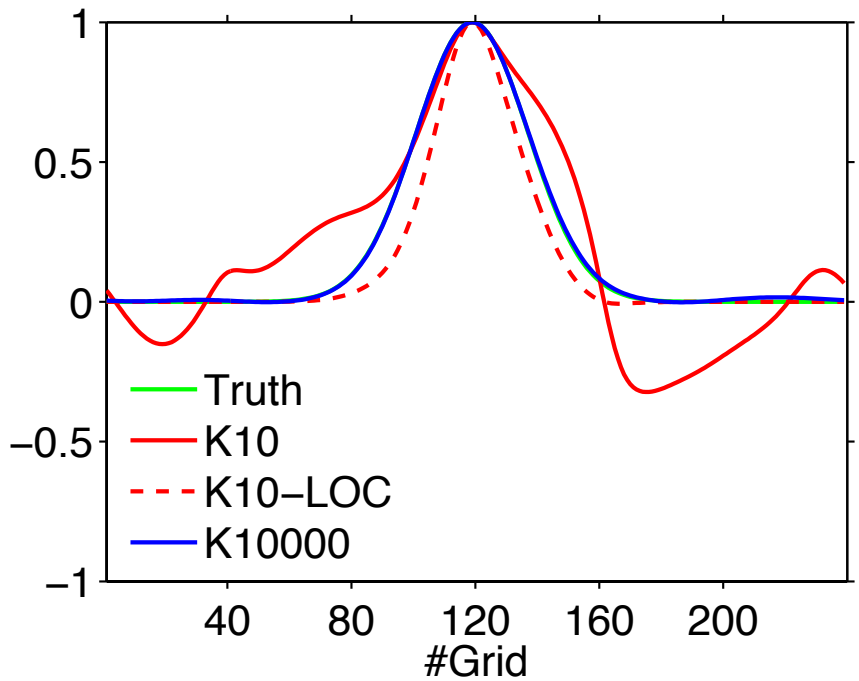
- Hybrid ensemble-variational (EnVar) method
  - A linear combination of the static background covariances and the covariances from an ensemble of short-range forecasts.
  - GSI-based hybrid 3DEnVar and 4DEnVar system (Wang et al. 2013; Wang and Lei 2014; Kleist and Ide 2015ab) became operational for NCEP GFS since 2012.

Sampling Errors in EnKF

- Caused by running a small-sized ensemble (~10^2) due to the computational constraints .
- Characterized by the spurious correlations in distant regions (solid red .vs. green).
- Cause noisy analysis increments or even the filter divergence (Hamill 2006).
- Alleviated by **<u>increasing the ensemble size</u>** (blue) or **<u>localization techniques</u>** (dashed red).

Table. 1 in Houtekamer and Zhang (2016)

Center	CMC	ECMWF	NCEP
Algorithm	Stochastic EnKF	LETKF	Deterministic EnSRF
Status	Operational	Research	Operational
N_{obs}	700 000	4 000 000	600 000
N_{ens}	256	100	80
N_{model}	96 000 000	370 000 000	213 000 192
N_{cores}	2304	2880	660



Localization Methods in EnKF

- **Homogeneous distance-dependent localization**
  - To remove the correlations between distant regions that are assumed to be physically small or spurious.
  - **B-localization** by applying a Schur product between the raw background error covariances and a predefined distance-dependent localization matrix (Houtekamer et al. 2001, 2005).
  - **R-localization** by inflating the observation variances with an increasing distance from the model state variable of interest (Hunt et al. 2007).

- **Adaptive localization** (Anderson 2007; Bishop and Hodyss 2007; Gasperoni and Wang 2015)

- **Spectral localization** (Buehner and Charron, 2007)

- **Variable Transformation/localization** (Kepert 2009)

- **Variable localization** (Kang et al. 2011)

- **etc**

Studies on B- and R-localizations

- **Miyoshi and Yamane (2007) and Greybush et al. (2011)**
  - With applying the same localization coefficients, B-localization produced stronger localization effect than R-localization in the assimilation of single observation.
  - Theoretical quantitative difference of B- and R-localizations was not straightforward to conclude in the assimilation of multiple observations.

- **Janjić et al. (2011) and Nerger et al. (2012)**
  - Within the Lorenz-96 model, B-localization outperformed R-localization especially when the observation errors were much smaller than the background errors.

- **Sakov and Bertino (2011)**
  - Both localization methods were supposed to yield similar results in the practical applications by comparing the structures of the Kalman gain with applying B- and R-localizations.

- **Greybush et al. (2011) and Holland and Wang (2013)**
  - Within simplified dynamical models, B- and R-localizations resulted in different amounts of imbalance, which, in turn, affected the analysis accuracy.

Objectives:

--- To further explore and understand the fundamental mathematical differences of B- and R-localizations

- The Kalman gain with applying B- and R-localizations is derived from the generic EnKF update equations and compared mathematically.
  - **For the same effective localization function that determines the correlations between different grid points, B-localization results in a higher-rank prior covariance matrix than R-localization.**
- High-rank ETKF (HETKF) is introduced by implementing B-localization method in the ensemble transform Kalman filter (ETKF) to distinguish from ETKF with R-localization.
- Examine if the higher-rank from B-localization can directly contribute to the improved analysis relative to the low-rank R-localization.

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Higher-rank of B-localization over R-localization

(Huang et al. 2018 to be submitted to MWR)

❑ EnKF

$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{K}[\mathbf{y}^o - H(\mathbf{x}^b)],$$

$$\mathbf{P}^b = \frac{1}{K-1}\mathbf{X}'^b(\mathbf{X}'^b)^{\mathrm{T}} = \mathbf{Z}^b(\mathbf{Z}^b)^{\mathrm{T}},$$

$$\mathbf{K}_i = (\mathbf{P}^b\mathbf{H}^{\mathrm{T}})_i(\mathbf{H}\mathbf{P}^b\mathbf{H}^{\mathrm{T}} + \mathbf{R})^{-1}.$$

❑ B-localization

$$\mathbf{P}^b_{\mathrm{Bloc}} = \mathbf{P}^b \circ \mathbf{L}.$$

$$(\mathbf{K}_{\mathrm{Bloc}})_i = (\mathbf{P}^b_{\mathrm{Bloc}}\mathbf{H}^{\mathrm{T}})_i(\mathbf{H}\mathbf{P}^b_{\mathrm{Bloc}}\mathbf{H}^{\mathrm{T}} + \mathbf{R})^{-1}.$$

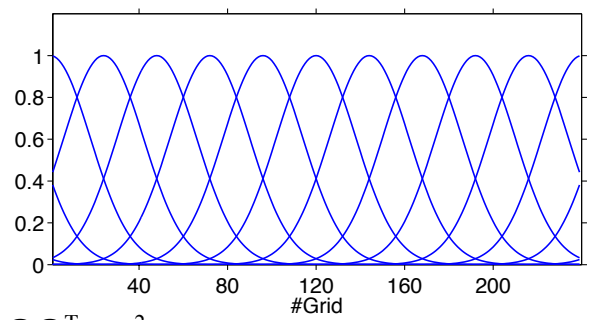
❑ R-localization

$$\mathbf{R}^i_{\mathrm{Rloc}} = [\mathrm{diag}(\mathbf{g}_i)]^{-1}\mathbf{R}[\mathrm{diag}(\mathbf{g}_i)]^{-1},$$

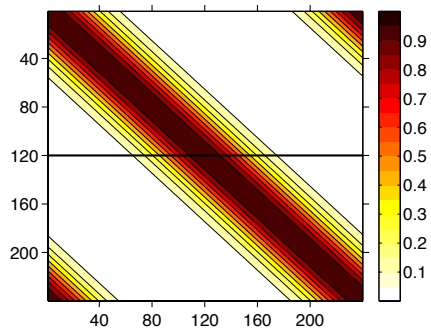
$$(\mathbf{K}_{\mathrm{Rloc}})_i = (\mathbf{P}^b\mathbf{H}^{\mathrm{T}})_i(\mathbf{H}\mathbf{P}^b\mathbf{H}^{\mathrm{T}} + \mathbf{R}^i_{\mathrm{Rloc}})^{-1}.$$

- Effects of R-localization can be realized by a Schur product of P^b and $(\mathbf{g}_i\mathbf{g}_i^{\mathrm{T}})$

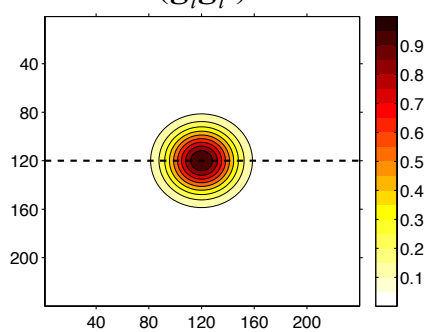
$\mathbf{G} = [\mathbf{g}_1, \mathbf{g}_2, \ldots, \mathbf{g}_n].$

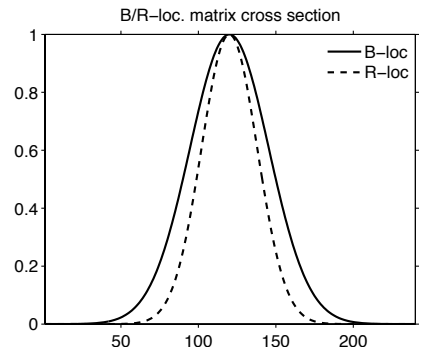


$\mathbf{L} = \mathbf{G}\mathbf{G}^{\mathrm{T}} / w^2$

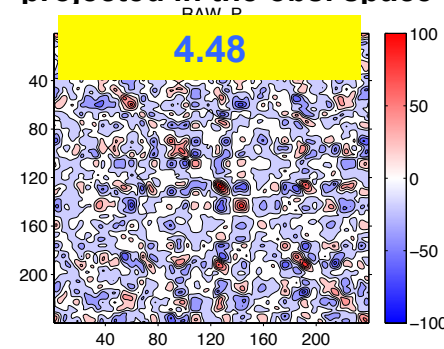


$(\mathbf{g}_i\mathbf{g}_i^{\mathrm{T}})$

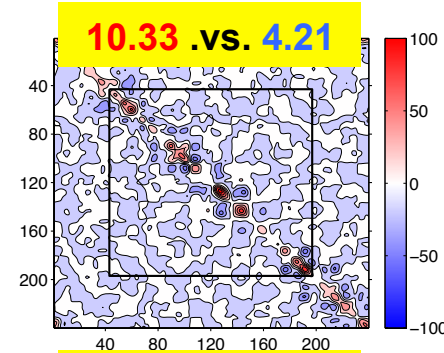




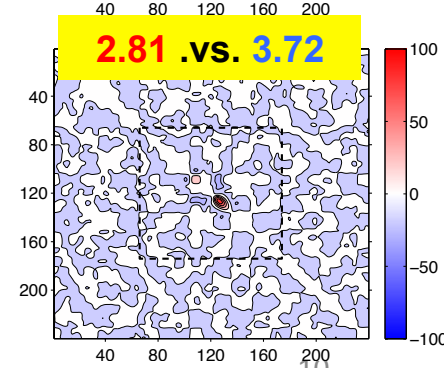
- $\mathbf{P}^b$ projected in the obs. space



$\mathbf{P}^b \circ \mathbf{L}$



$\mathbf{P}^b \circ (\mathbf{g}_i\mathbf{g}_i^{\mathrm{T}})$



- **B-localized P^b shows the largest E-dimension (Patil et al. 2001).**

ETKF with R-localization

- The background ensemble perturbations are transformed to the analysis ensemble perturbations on the ensemble subspace by a transformation matrix **T** (Bishop et al. 2001; Wang and Bishop 2003; Wang et al. 2004).

$$\mathbf{Z}^a = \mathbf{Z}^b\mathbf{T}, \quad \mathbf{Z}^b = \mathbf{X}'^b \Big/ \sqrt{K-1}$$

- The transformation matrix **T** is solved so that the analysis ensemble covaraince are updated by following the optimal data assimilation theory.

$$\mathbf{P}^a = (\mathbf{I}-\mathbf{KH})\mathbf{P}^b,$$

$$\mathbf{A} = (\mathbf{HZ}^b)^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{HZ}^b) = \mathbf{C}\Gamma\mathbf{C}^{\mathrm{T}},$$

$$\mathbf{T} = \mathbf{C}(\Gamma+\mathbf{I})^{-1/2}\mathbf{C}^{\mathrm{T}}.$$

- The background ensemble mean is updated by,

$$\overline{\mathbf{x}}^a = \overline{\mathbf{x}}^b + \mathbf{Z}^b[\mathbf{C}(\Gamma+\mathbf{I})^{-1}\mathbf{C}^{\mathrm{T}}](\mathbf{HZ}^b)^{\mathrm{T}}\mathbf{R}^{-1}[\mathbf{y}^o - \overline{H(\mathbf{x}^b)}].$$

- R-localization is generally applied in ETKF (Hunt et al. 2007).

$$\mathbf{R}^i_{\mathrm{Rloc}} = [\mathrm{diag}(\mathbf{g}_i)]^{-1}\mathbf{R}[\mathrm{diag}(\mathbf{g}_i)]^{-1},$$

High-rank Ensemble Transform Kalman Filter (HETKF)

- HETKF is introduced to realize B-localization within the ETKF algorithm by extending and ***M***odulating the raw ensemble ***P***erturbations (**MP-localization**, following Bishop and Hodyss 2009)

- The extended modulated ensemble perturbations are directly input to ETKF algorithms to update the ensemble mean and ensemble perturbations.

- "HETKF" is used given the higher-rank of ETKF with B-localization relative to ETKF with R-localization.

MP-localization in HETKF

- Calculate the eigenvalues **Λ** (large→small) and eigenvectors **E** of the original B-localization matrix **L**.

$$\mathbf{L} = \mathbf{E}\boldsymbol{\Lambda}\mathbf{E}^{\mathrm{T}} = (\mathbf{E}\boldsymbol{\Lambda}^{1/2})(\mathbf{E}\boldsymbol{\Lambda}^{1/2})^{\mathrm{T}}.$$

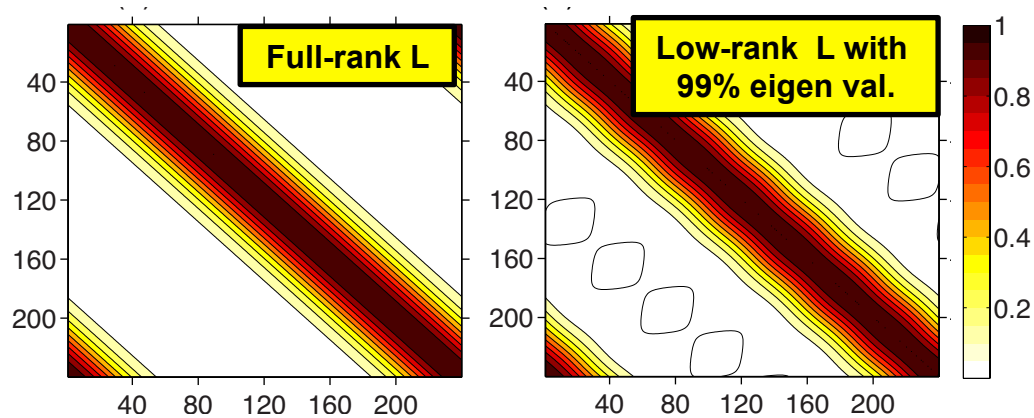
- Generate the modulation matrix $\hat{\mathbf{G}}$ and a low-rank B-localization matrix $\mathbf{L}_{\text{low\_rank}}$ by selecting the first *M* leading eigenvectors (**<u>99% of the sum of all the eigenvalues</u>**)

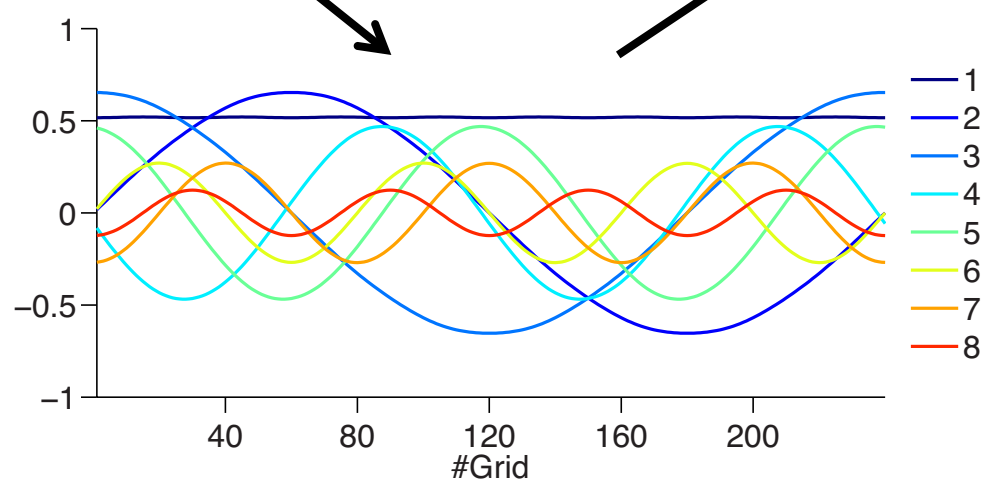
$$\mathbf{L}_{1\sim M} = (\mathbf{E}\boldsymbol{\Lambda}^{1/2})_{1\sim M}(\mathbf{E}\boldsymbol{\Lambda}^{1/2})^{\mathrm{T}}_{1\sim M},$$

$$\hat{\mathbf{G}} = \{[\mathrm{diag}(\mathbf{L}_{1\sim M})]^{-1/2}\left[(\mathbf{E}\boldsymbol{\Lambda}^{1/2})\right]_{1\sim M}\}$$

$$= [\hat{\mathbf{g}}_1, \hat{\mathbf{g}}_2, \ldots, \hat{\mathbf{g}}_M]$$

$$\mathbf{L}_{\text{low-rank}} = \hat{\mathbf{G}}\hat{\mathbf{G}}^{\mathrm{T}}.$$





- **The first modulation function is a constant.**
- **Similar structures of Full and Low-rank L.**

MP-localization in HETKF

- Generate the modulated background ensemble perturbation matrix $\hat{\mathbf{X}}'^b$ with ***MK*** members by a Schur product of each raw ensemble perturbation vector with each column of the modulation matrix $\hat{\mathbf{G}}$.

$$\hat{\mathbf{X}}'^b = \sqrt{\frac{MK-M}{K-1}}[\mathrm{diag}(\hat{\mathbf{g}}_1)\mathbf{X}'^b, \mathrm{diag}(\hat{\mathbf{g}}_2)\mathbf{X}'^b, \ldots, \mathrm{diag}(\hat{\mathbf{g}}_M)\mathbf{X}'^b]$$

$$\textit{where},\ \mathrm{diag}(\hat{\mathbf{g}}_j)\mathbf{X}'^b = [\hat{\mathbf{g}}_j \circ \mathbf{x}'^b_1,\ \hat{\mathbf{g}}_j \circ \mathbf{x}'^b_2,\ \ldots,\ \hat{\mathbf{g}}_j \circ \mathbf{x}'^b_K]$$

and $\circ$ denotes the Schur or elementwise product.

$$\hat{\mathbf{Z}}^b = \frac{\hat{\mathbf{X}}'^b}{\sqrt{MK-M}}.$$

- The size of the modulated ensemble perturbation matrix is increased from ***K*** to ***MK***.
- The ensemble covariances estimated from $\hat{\mathbf{X}}'^b$ with ***MK*** members are equivalent to the original B-localized background ensemble covariances.

$$\frac{\hat{\mathbf{X}}'^b(\hat{\mathbf{X}}'^b)^{\mathrm{T}}}{MK-M} \cong \frac{\mathbf{X}'^b(\mathbf{X}'^b)^{\mathrm{T}}}{K-1} \circ \mathbf{L}.$$

B-localization is implicitly realized in HETKF by modulating the raw ensemble perturbation matrix.

Ensemble Mean Update in HETKF

- The ensemble mean in HETKF will be updated by replacing $\mathbf{Z}^b$ of $n \times K$ dimension with $\hat{\mathbf{Z}}^b$ of $n \times (MK)$ dimension in ETKF.

$$\mathbf{A} = (\mathbf{H}\hat{\mathbf{Z}}^b)^{\mathrm{T}} \mathbf{R}^{-1} (\mathbf{H}\hat{\mathbf{Z}}^b) = \mathbf{C}\boldsymbol{\Gamma}\mathbf{C}^{\mathrm{T}},$$

$$\mathbf{T} = \mathbf{C}(\boldsymbol{\Gamma} + \mathbf{I})^{-1/2}\mathbf{C}^{\mathrm{T}},$$

$$\overline{\mathbf{x}}^a = \overline{\mathbf{x}}^b + \hat{\mathbf{Z}}^b[\mathbf{C}(\boldsymbol{\Gamma} + \mathbf{I})^{-1}\mathbf{C}^{\mathrm{T}}](\mathbf{H}\hat{\mathbf{Z}}^b)^{\mathrm{T}}\mathbf{R}^{-1}[\mathbf{y}^o - \overline{H(\mathbf{x}^b)}].$$

Ensemble Perturbation Update in HETKF

--- To select *K* members from the *MK*-member analysis perturbations

- Extended modulated *MK*-member background perturbations in HETKF will produce *MK*-member analysis perturbations by directly using ETKF algorithm.

$$\hat{\mathbf{Z}}^a = \hat{\mathbf{Z}}^b \mathbf{T}.$$

- The stochastic and deterministic filter formulas are examined to provide a robust comparison between R- and B/MP-localizations in ETKF.

Stochastic filter (R-S .vs. MP-S)	Each member is updated by the ensemble mean update equation of ETKF algorithm and different set of perturbed observations, thus avoiding the selection issue in HETKF.
Deterministic filter (R-D .vs. MP-D)	Ensemble mean and perturbations are updated by ETKF algorithm. Afterwards, in HETKF, the first *K*-member posterior perturbations are selected and demodulated by an element-wise product with the inverse of the first modulation function (**which is a constant**) and divided by the square-root ratio, i.e., $\hat{\mathbf{Z}}^a_{\mathrm{MP-D}} = \{[\mathrm{diag}(\hat{\mathbf{g}}_1)]^{-1}\hat{\mathbf{z}}^a_1, [\mathrm{diag}(\hat{\mathbf{g}}_1)]^{-1}\hat{\mathbf{z}}^a_2, \ldots, [\mathrm{diag}(\hat{\mathbf{g}}_1)]^{-1}\hat{\mathbf{z}}^a_K\} \Big/ \sqrt{\frac{MK-M}{K-1}}.$

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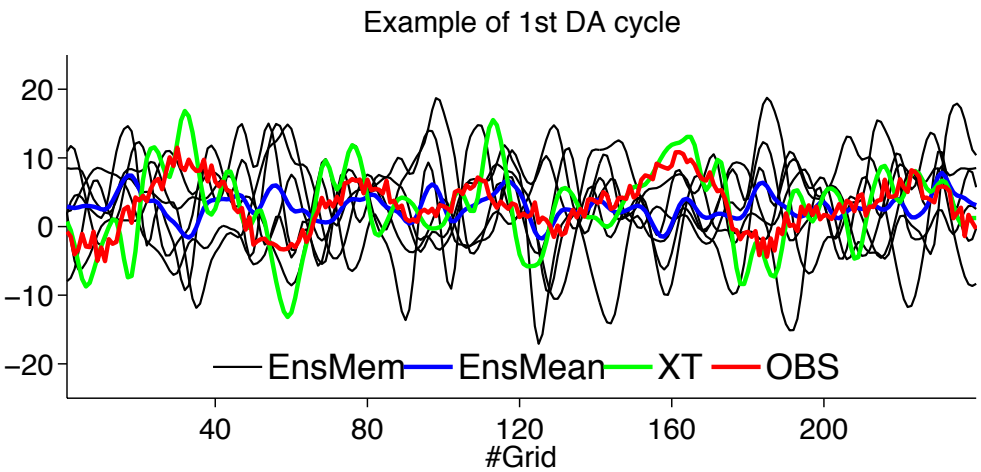
Experiment Design

- Lorenz Model II (Lorenz, 2005; n=240).
- Integral-type observations are simulated by averaging the model variables at grids [*i*-10, *i*+10] for *i* th grid and adding random error (*N*(0,1.32)).

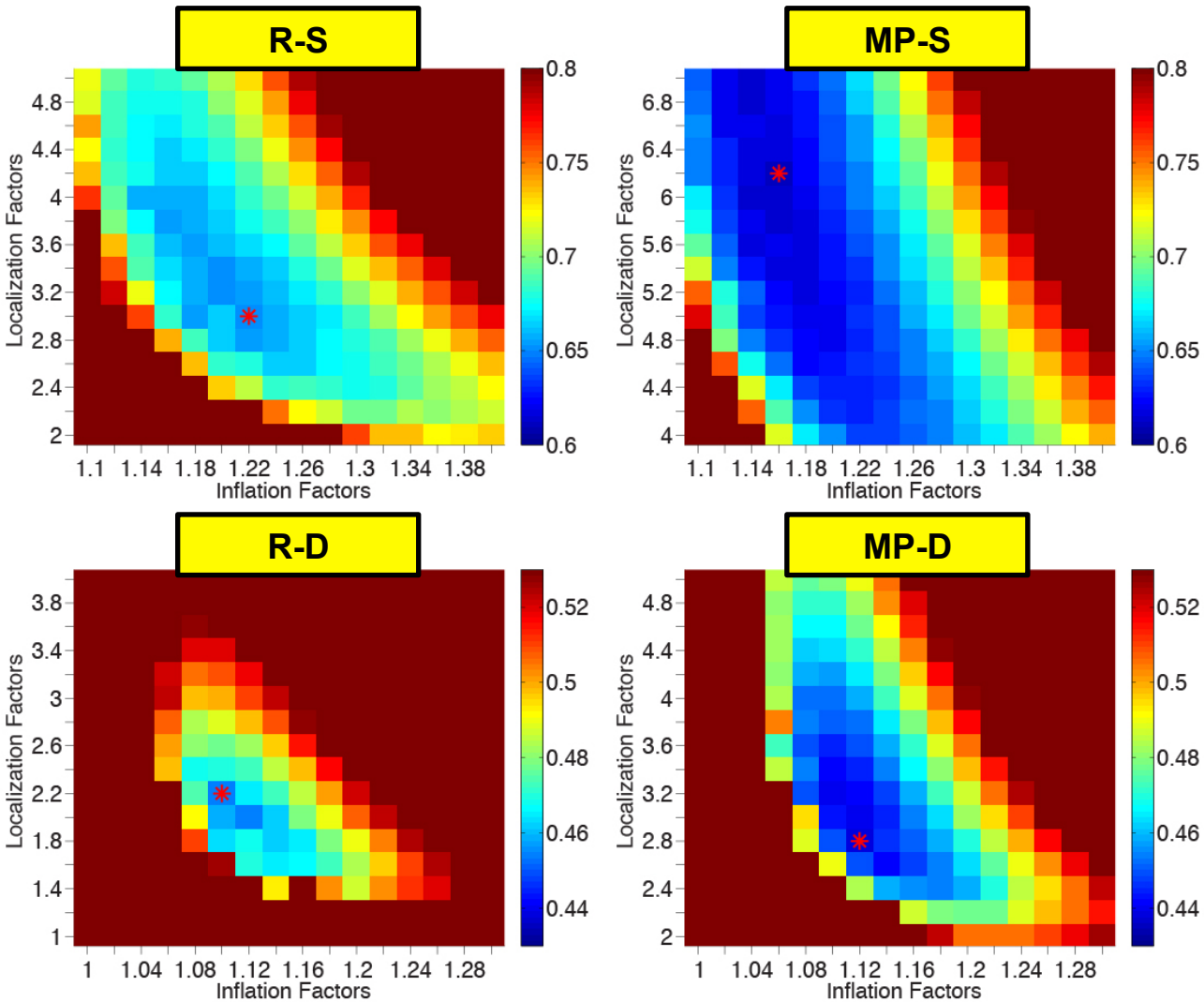


- Two scenarios are examined.
  - **K6PX** (fixed ensemble size but increased observation numbers X=30/60/120/240)
  - **KYP240** (fixed observation number but increased ensemble sizes Y=3/6/9)
- Each experiment is repeated eight times with both localization and inflation tuned.
- RMSE is calculated between the analysis and the "truth" and averaged over the last 8,000 cycles(total 10,000 cycles) in each experiment.
- Percentage of RMSE reduction (PRR) of MP-localization over R-localization,

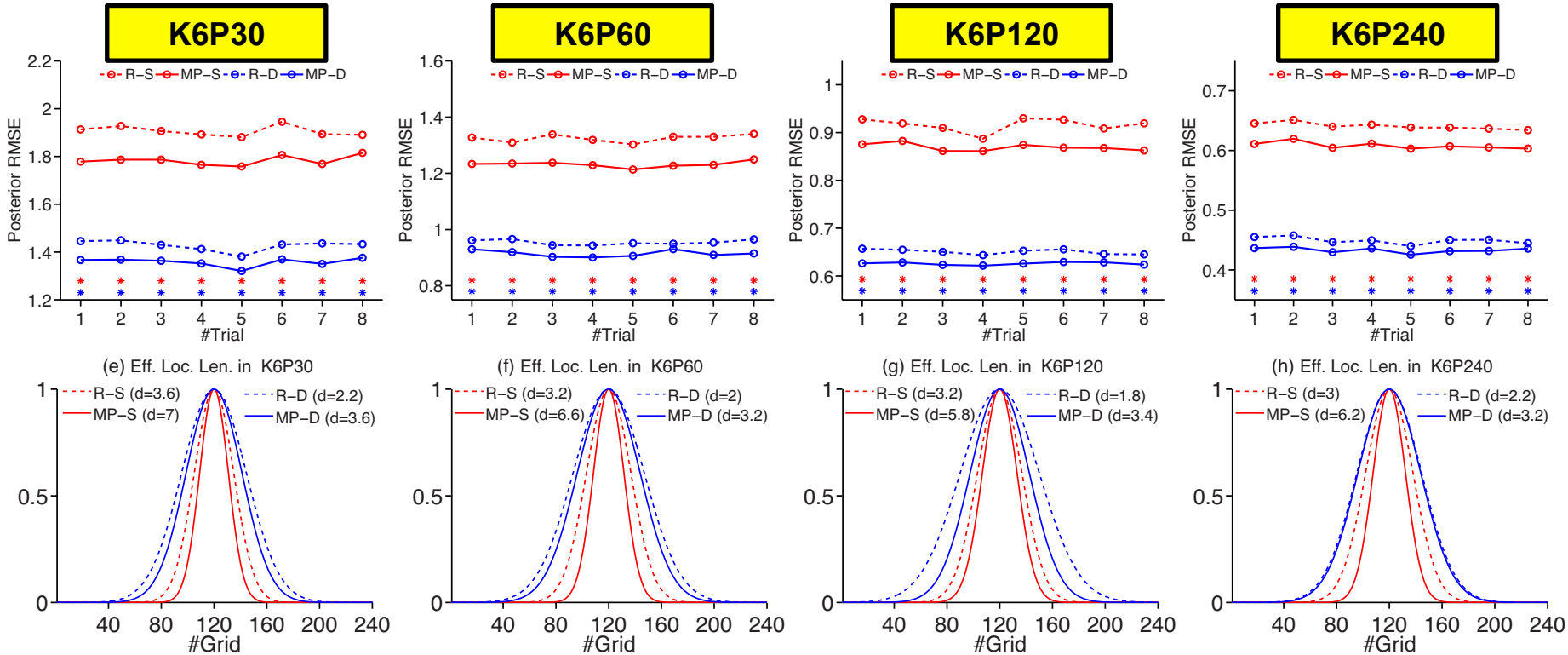
$$PRR = \frac{\mathrm{RMSE(R\text{-}loc)} - \mathrm{RMSE(MP\text{-}loc)}}{\mathrm{RMSE(R\text{-}loc)}} \times 100\%.$$

Localization and Inflation Tuning in K6P240

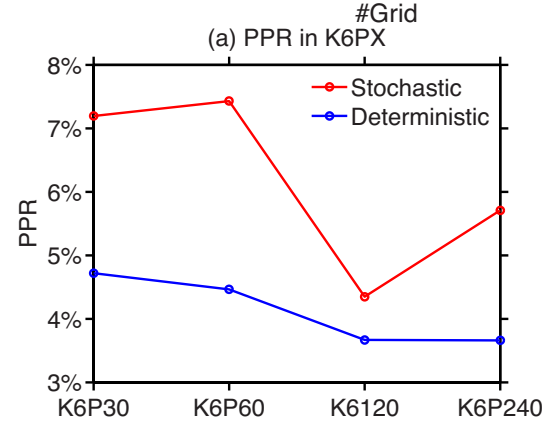
- HETKF with MP-loc outperforms ETKF with R-loc with best-tuned localization and inflation factors (red star).
- Det. method shows smaller errors than Sto. Method.
- The deterministic HETKF with MP-loc shows the most accurate analysis.
- HETKF with MP-loc is less sensitive to localization & inflation factors (broader blue areas).



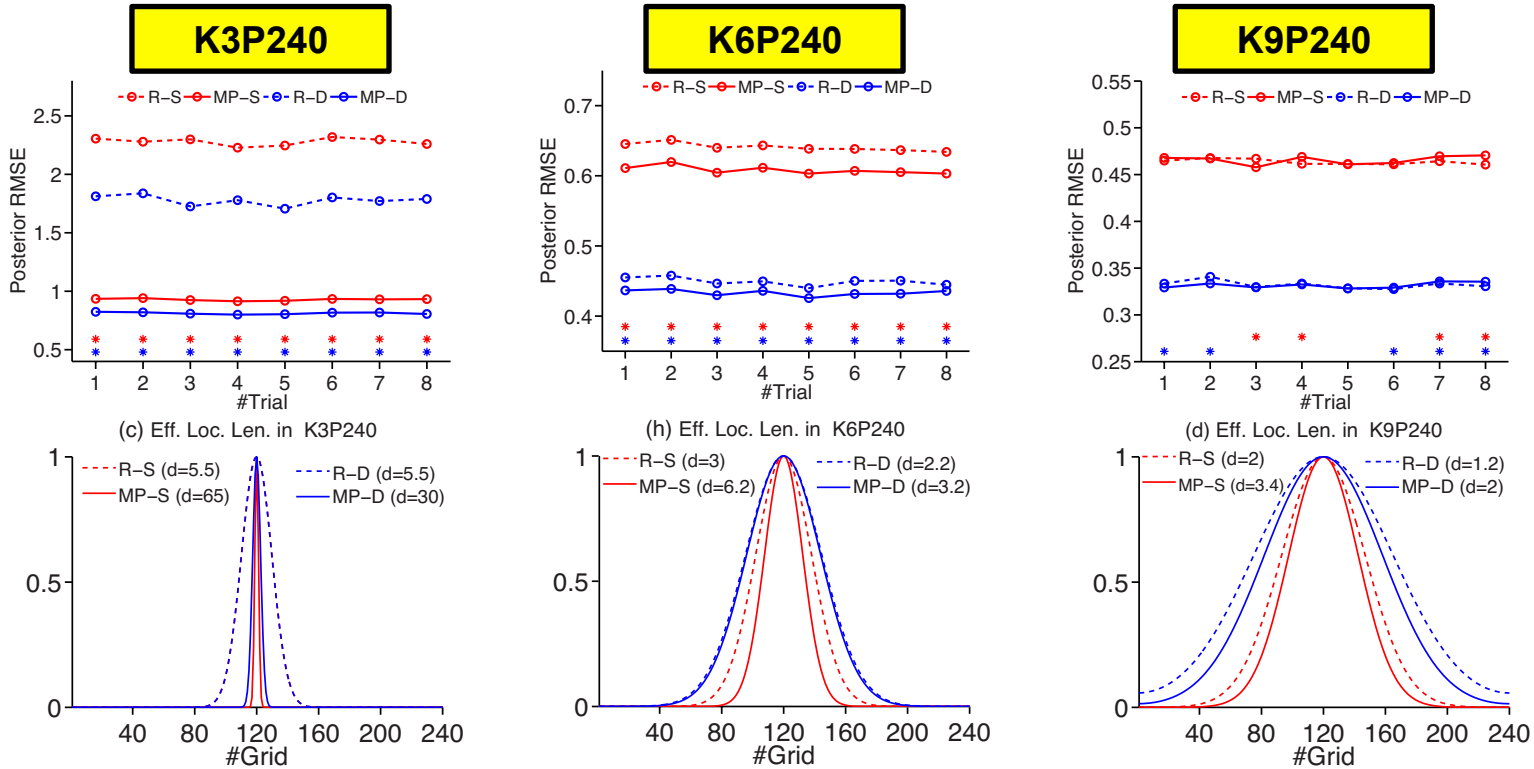
Comparison of fixed ensemble size but increased observation numbers (K6PX)



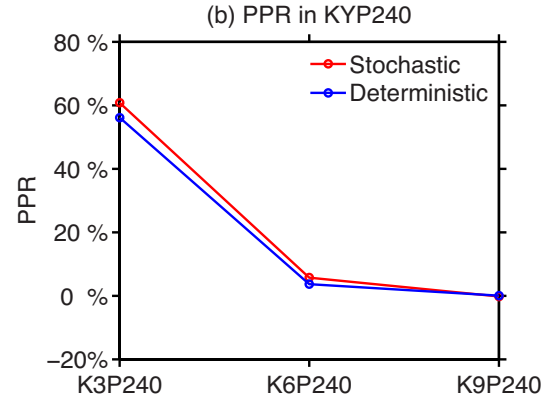
- HETKF with MP-loc shows smaller errors and shorter effective localization length scale than ETKF with R-loc.
- Det. method shows smaller errors and requires less localization than Sto. method.
- With more observations assimilated, the advantage of HETKF with MP-loc over ETKF with R-loc tends to be reduced.



Comparison of fixed observation number but increased ensemble size (KYP240)



- With increased ensemble size, the superiority of HETKF with MP-loc over ETKF with R-loc is reduced.
- The effective localization length scale is increased with increased ensemble size.



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Summary and Discussion

- Theoretical derivations (details not shown here) show that for the same effective localization function that determines the correlations at different grid points, B-localization results in a higher-rank prior covariance matrix than R-localization.
- High-rank ETKF with MP-localization is introduced to implicitly realize B-localization in ETKF.
- The superiority of higher-rank of B/MP-localization over R-localization is demonstrated within Lorenz Model II.
  - HEKTF with MP-loc outperforms ETKF with R-loc especially for smaller ensemble size, consistent with that the higher-rank from B- /MP-localization is expected to contribute more for small ensemble size .
  - With increased observation densities, the advantage of HETKF with MP-loc over ETKF with R-loc tends to be slightly reduced, possibly due to the enhanced overall improvement by assimilating larger number of observations.
  - HETKF with MP-loc is less sensitive to the localization and inflation factors. The best-tuned effective localization length scale of HETKF with MP-loc is smaller than that of ETKF with R-loc, this is excepted for the higher-rank in B/MP-localization.
  - In both HETKF with MP-loc and ETKF with R-loc, the deterministic method shows smaller errors and requires less localization than the stochastic method, this could be caused by the sampling errors associated to the perturbed observations in the stochastic method (Whitaker and Hamill 2002).

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Thanks!