Update on KENDA (Kilometer-scale Ensemble-Based Data Assimilation System) and a Particle Filter

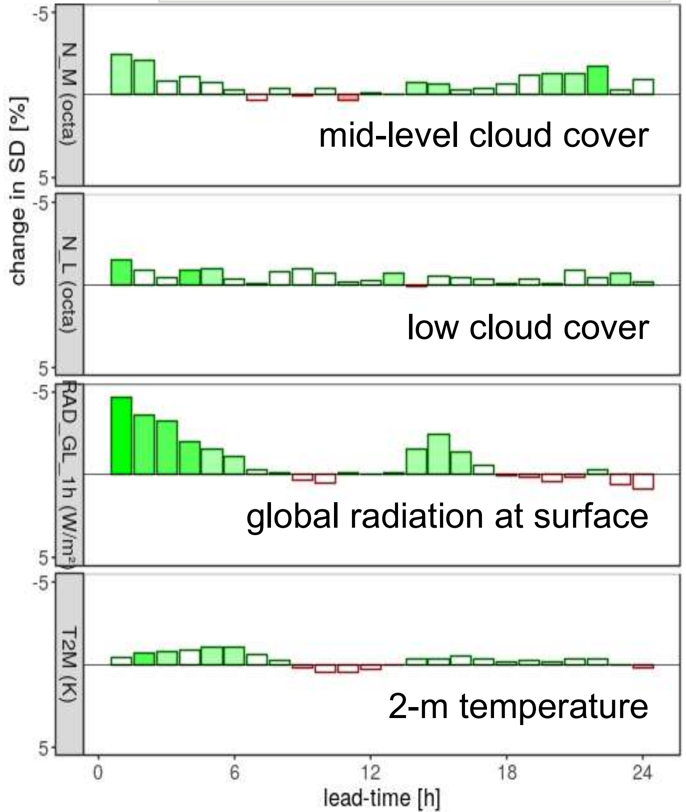
Christoph Schraff

- Update on KENDA (short selection)
- Localized Mixture Coefficients Particle Filter
  (Nora Schenk, Anne Walter, Roland Potthast, DWD)

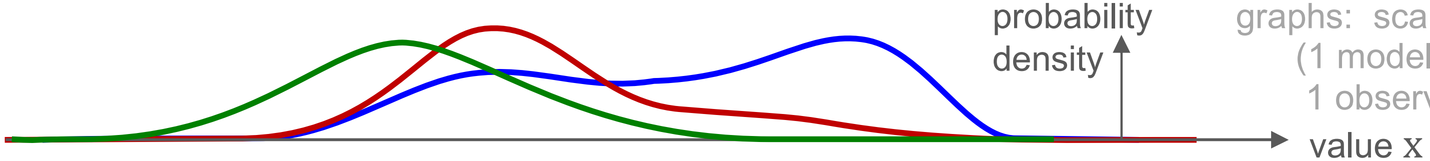
Update on KENDA
(short selection)

- 3 wind lidars + 1 MW radiometer (BT) operational at MeteoSwiss *(Claire Merker, Daniel Regenass Daniel Leuenberger a.o.)*
- latent heat nudging: major revision, only humidity updated now *(Klaus Stephan)*
- radar volume data *(Thomas Gastaldo; Klaus Stephan, Uli Blahak a.o.)*
  - radial winds (Italian stations) operational at ARPAE
  - EMVORADO can process radar Z + Vr from all neighbouring countries of DE
- SEVIRI VIS: technically ready for operations *(Lilo Bach a.o.)*
  - positive impacts, except precip due to model biases (too much cloud + humidity, too little convective precip)
  - → adjusting model parameters (model – DA interaction)
  - this winter: in ICON-D2 parallel routine
    in ICON-RUC 24/7 test system
- SEVIRI WV all-sky: clear positive impact, into parallel routines in 2023 *(Annika Schomburg a.o.)*

Synop verif. June 2021
06, 12, 18-UTC runs
change [%] of std. dev
due to SEVIRI VIS



Intro to the Particle Filter: Ensemble DA – analysis step



graphs: scalar case (1 model variable x, 1 observation y)

Bayes theorem

analysis pdf (posterior) → $p^a(\mathrm{x}|\mathrm{y}) \;\propto\; p(\mathrm{y}|\mathrm{x}) \cdot p^b(\mathrm{x})$ ← background pdf (prior)

↑ observation pdf (likelihood)

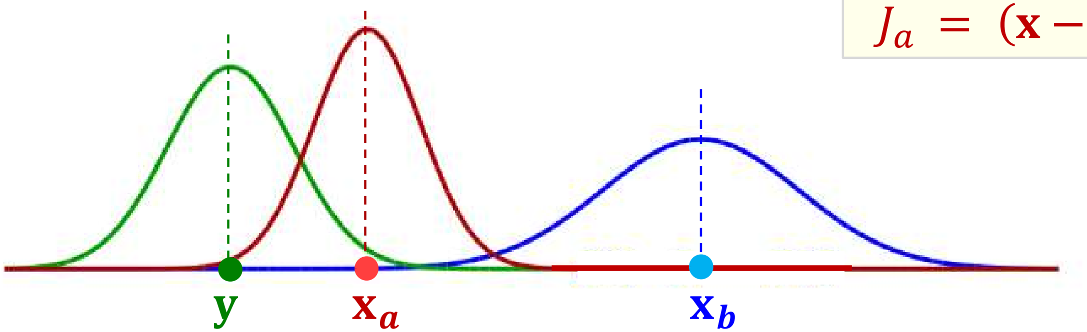
- pdf's assumed Gaussian

$$p^a(\mathbf{x}|\mathbf{y}) \;\propto\; e^{-½\, J_o(\mathbf{x},\mathbf{y})} \cdot e^{-½\, J_b(\mathbf{x})} \;=\; e^{-½\, J_a(\mathbf{x})}$$

$$J = J_o + J_b \;=\; (\mathbf{y}-H(\mathbf{x}))^T\mathbf{R}^{-1}\,(\mathbf{y}-H(\mathbf{x})) \;+\; (\mathbf{x}-\mathbf{x}_b)^T\mathbf{B}^{-1}\,(\mathbf{x}-\mathbf{x}_b)$$

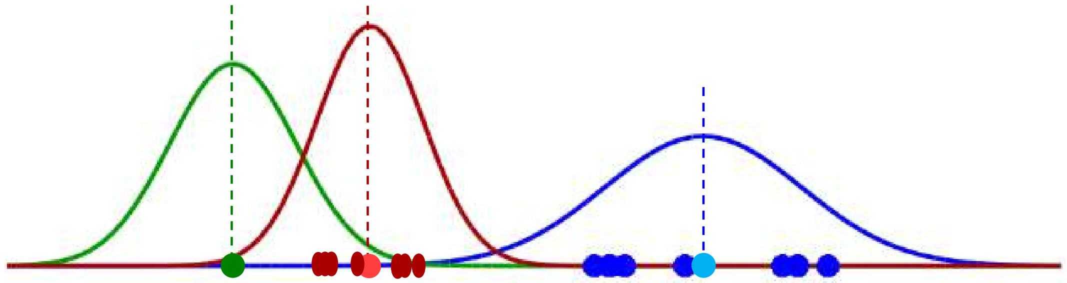
$$J_a \;=\; (\mathbf{x}-\mathbf{x}_a)^T\mathbf{A}^{-1}\,(\mathbf{x}-\mathbf{x}_a)$$

→ Kalman Filter for linear system



$$\mathbf{x}_a \;=\; \mathbf{x}_b \;+\mathbf{K}\,(\mathbf{y}-\mathbf{x}_b)$$
$$\mathbf{A} \;=\; (\mathbf{I}-\mathbf{KH})\,\mathbf{B}$$
$$\mathbf{K} \;=\; \mathbf{BH}^T\left(\mathbf{R}+\mathbf{HBH}^T\right)^{-1}$$

- (high-dimensional) non-linear system (NWP) : pdf's approximated by ensembles



→ **LETKF** (EnKF)

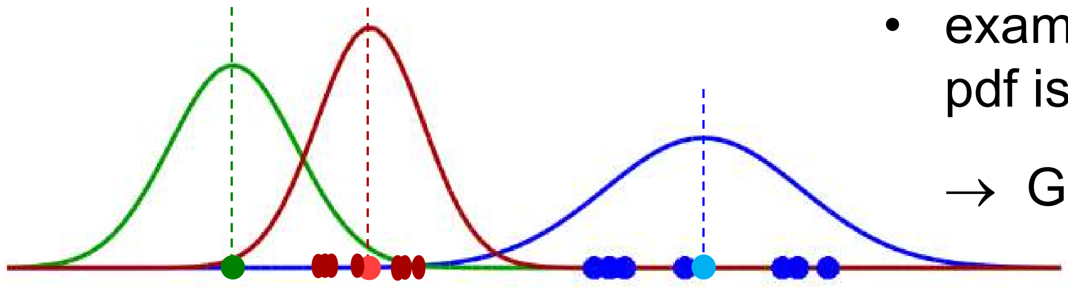
$$\mathbf{B} = \frac{1}{K-1}\mathbf{X}^b\left(\mathbf{X}^b\right)^T$$

$\boldsymbol{k}$-th column of $\mathbf{X}^b = \mathbf{x}_k^b - \bar{\mathbf{x}}^b$: 'ensemble perturbations' or 'ensemble deviations'

in the (K-1) -dimensional (!) sub-space S spanned by background ensemble perturbations :

$$\mathbf{x}_{(k)}^{(a)} = \bar{\mathbf{x}}^b + \mathbf{X}^b\,\mathbf{w}_{(k)}^{(a)}$$

set up cost function $J(\mathbf{w})$ in ensemble space,
explicit solution $\mathbf{w}_k^a$ for minimisation (Hunt et al., 2007)

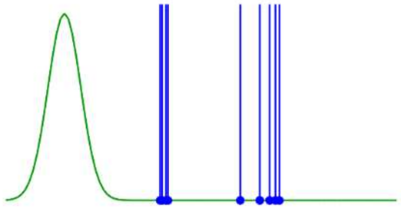


- example: background ensemble indicates pdf is non-Gaussian (slightly bi-modal)

  → Gaussian assumption by LETKF (EnKF) not fulfilled

- Particle Filter: no assumption on pdf; sequential importance resampling (SIR)

$$p^b(\mathrm{x}) := \frac{1}{K}\sum_{k=1}^{K}\delta(\mathbf{x}-\mathbf{x}_k^b)$$



⇩ Bayes

$$p^a(\mathbf{x}|\mathbf{y}) = \sum_k w_k\,\delta(\mathbf{x}-\mathbf{x}_k^b) \quad , \quad \sum_k w_k = 1$$

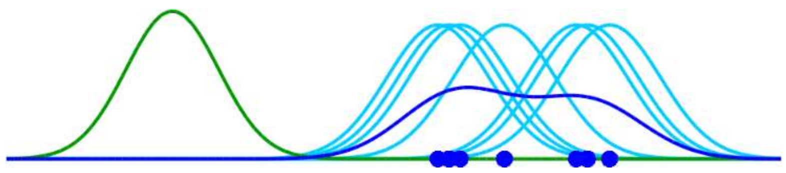
$$w_k \propto p(\mathbf{y}|\mathbf{x}_k^b) \propto e^{-\frac{1}{2}(\mathbf{y}-H(\mathbf{x}_k^b))^T\mathbf{R}^{-1}(\mathbf{y}-H(\mathbf{x}_k^b))}$$

↑ if Gaussian obs errors

→ resampling (particle drawn from analysis pdf by sampling with replacement; particles can be chosen multiple times)

→ for high-dim systems, many obs: only very few particle chosen, filter collapse

1 Background

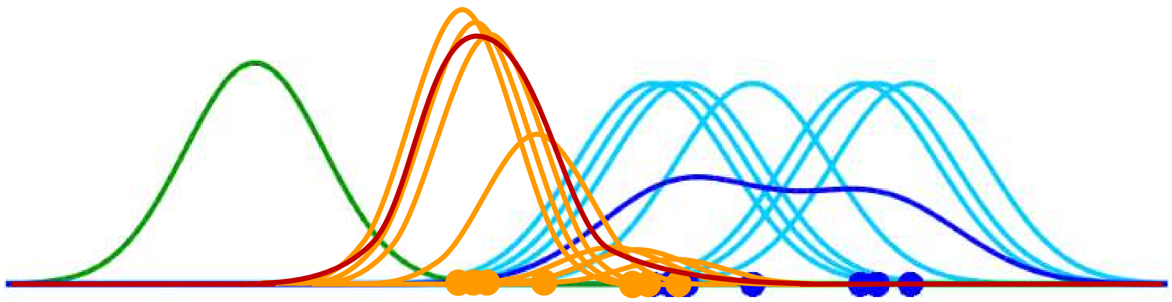


assumptions on background pdf:

1. Gaussian mixture
   (sum of Gaussians, i.e. non-Gaussian)

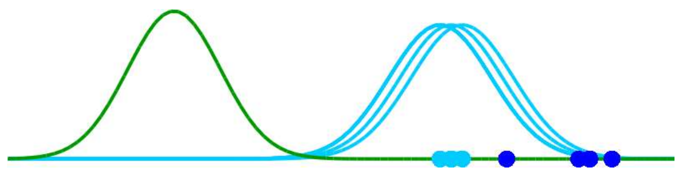
2. covariance $\mathbf{B}_k^p$ of each particle k : $\mathbf{B}_k^p := \mathbf{B}_{\boldsymbol{k}}^p$

$$\rightarrow \; p^a(\mathbf{x}|\mathbf{y}) \propto e^{-\frac{1}{2} J^o(\mathbf{x},\mathbf{y})} \cdot \sum_k e^{-\frac{1}{2} J_k^b(\mathbf{x})} = \sum_k e^{-\frac{1}{2} J_k^a(\mathbf{x})}$$

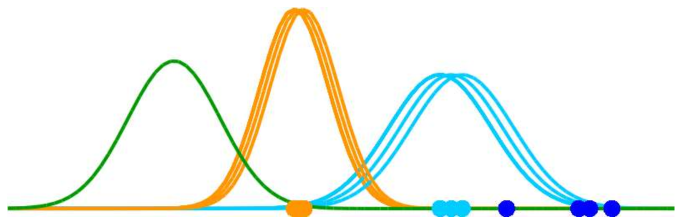


→ DA cycle, aim: describe $p^a(\mathbf{x}|\mathbf{y})$ by
k equally weighted members

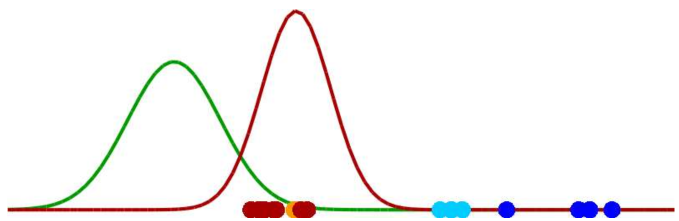
1 Resampling



2 Shift of Particles

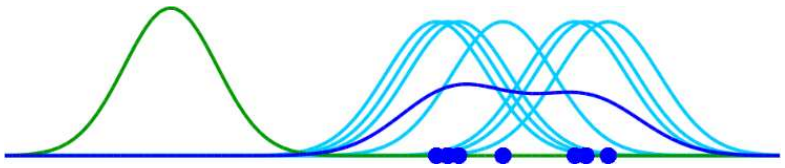


3 Gaussian Rejuvenation



Localized Mixture Coefficients Particle Filter LMCPF

1 Background



assumptions on background pdf:

1. Gaussian mixture
   (sum of Gaussians, i.e. non-Gaussian)

2. covariance $\mathbf{B}_k^p$ of each particle k

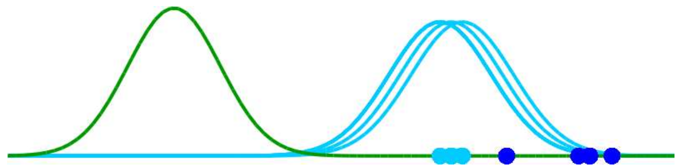
$$\mathbf{B}_k^p \;:=\; \mathbf{B}_{\boldsymbol{k}}^p := \kappa\,\mathbf{B}^{LETKF} = \kappa\,\frac{1}{K-1}\,\mathbf{X}^b\left(\mathbf{X}^b\right)^T$$

→ pdf / cost function in ensemble space

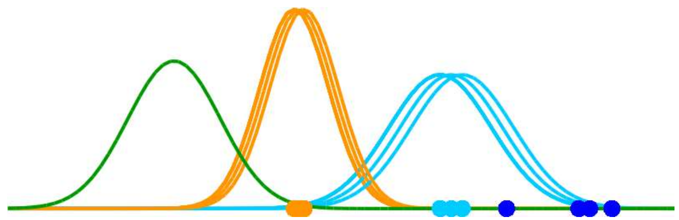
$$\mathbf{x}_{(k)}^{(a)} = \bar{\mathbf{x}}^b + \mathbf{X}^b\,\mathbf{w}_{(k)}^{(a)}$$

as in LETKF, but $\mathbf{w}_{(k)}^{a,\,LMCPF} \neq \mathbf{w}_{(k)}^{a,\,LETKF}$

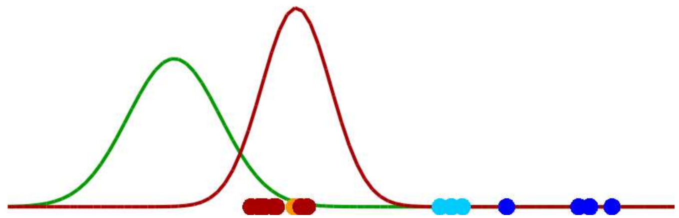
1 Resampling



2 Shift of Particles



3 Gaussian Rejuvenation



LMCPF: Resampling

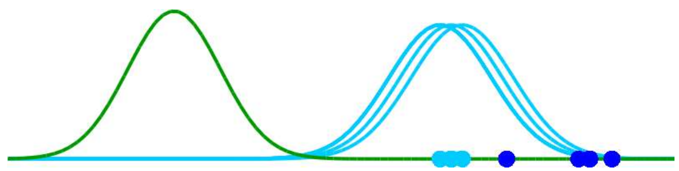
- compute relative weights of particles (members) acc. to their analysis pdf

$$w_k \;\propto\; e^{-\frac{1}{2}\left(\mathbf{y}-H(\mathbf{x}_k^b)\right)^T \left(\mathbf{R}+\mathbf{H}\mathbf{B}^p\mathbf{H}^T\right)^{-1}\left(\mathbf{y}-H(\mathbf{x}_k^b)\right)}$$

⇩ weights in ensemble space:

$$\widetilde{w}_k \;\propto\; e^{-\frac{1}{2}(\mathbf{C}-\mathbf{e}_k)^T\left(\mathbf{I}+\frac{K}{K-1}\widetilde{\mathbf{R}^{-1}}\right)^{-1}\widetilde{\mathbf{R}^{-1}}(\mathbf{C}-\mathbf{e}_k)}$$

1 Resampling



$\mathbf{Y}^b = \mathbf{H}\mathbf{X}^b$ ens. pert. in observation space

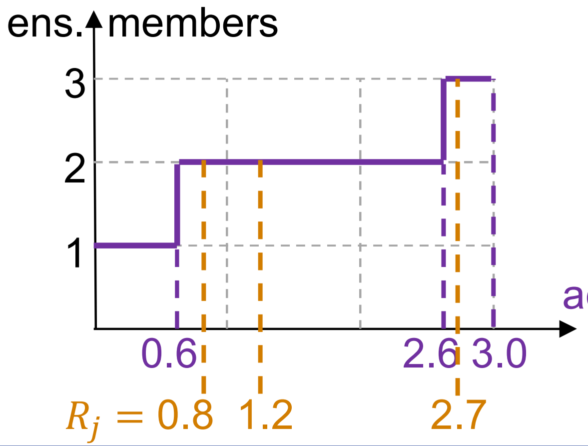
$\widetilde{\mathbf{R}^{-1}} := \mathbf{Y}^{b^T}\mathbf{R}^{-1}\mathbf{Y}^b$ inverse **R**-matrix (in ens. space)

$\mathbf{X}^b\,\mathbf{e}_k = \mathbf{x}_k^b - \bar{\mathbf{x}}^b$ e_k: k-th ensemble member (“)

$\mathbf{C} := \widetilde{\mathbf{R}^{-1}}^{-1}\mathbf{Y}^{b^T}\mathbf{R}^{-1}(\mathbf{y}-\bar{\mathbf{y}}^b)$ ens. mean innovation projected on ensemble space

- sampling with replacement, based on weights (scaled: $\Sigma_k \widetilde{w}_k^a = K$)

example: $K = 3;\;\; \widetilde{w}_1^a = 0.6,\;\; \widetilde{w}_2^a = 2.0,\;\; \widetilde{w}_3^a = 0.4$



- accumulated weights : $w_k^{ac} = w_{k-1}^{ac} + \widetilde{w}_k^a$
- draw K random numbers $r_j \sim U([0,1])$, e.g. $0.8, 0.2, 0.7$
  set $R_j = j - 1 + r_j$
- $\forall j$ select member k with $w_{k-1}^{ac} < R_j \leq w_k^{ac}$

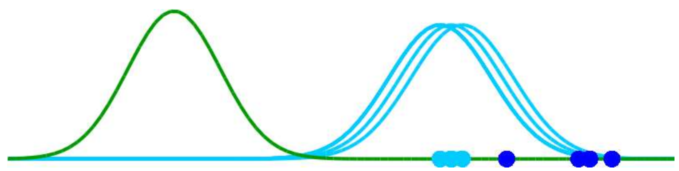
$$\breve{\mathbf{W}}\mathbf{e}_1 = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \mathbf{e}_2$$

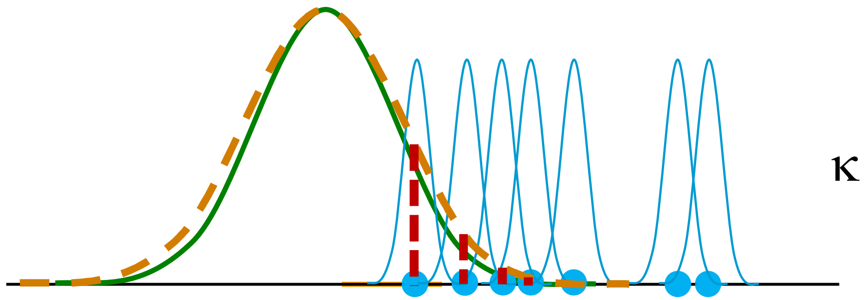
LMCPF: Resampling

$$w_f^a(\mathbf{x}) = e^{-\frac{1}{2}(\mathbf{y}-H(\mathbf{x}))^T\left(\mathbf{R}+\kappa\cdot\mathbf{HB}^{LETKF}\mathbf{H}^T\right)^{-1}(\mathbf{y}-H(\mathbf{x}))}$$

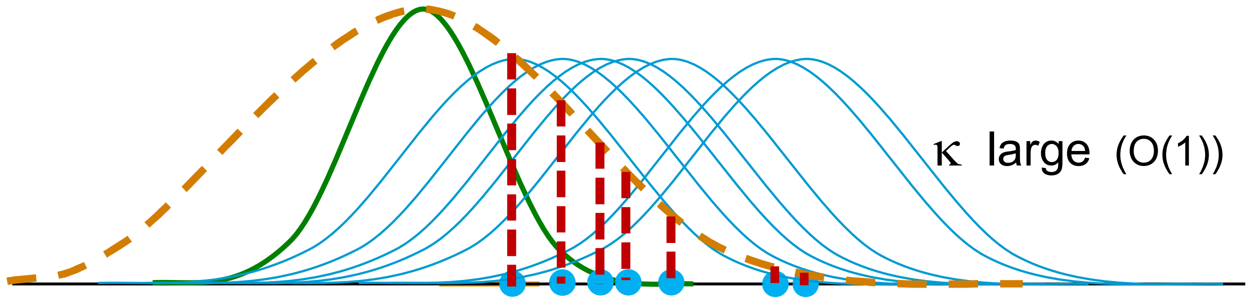
$$w_k^a \propto w_f^a\left(\mathbf{x}_k^b\right)$$

1 Resampling

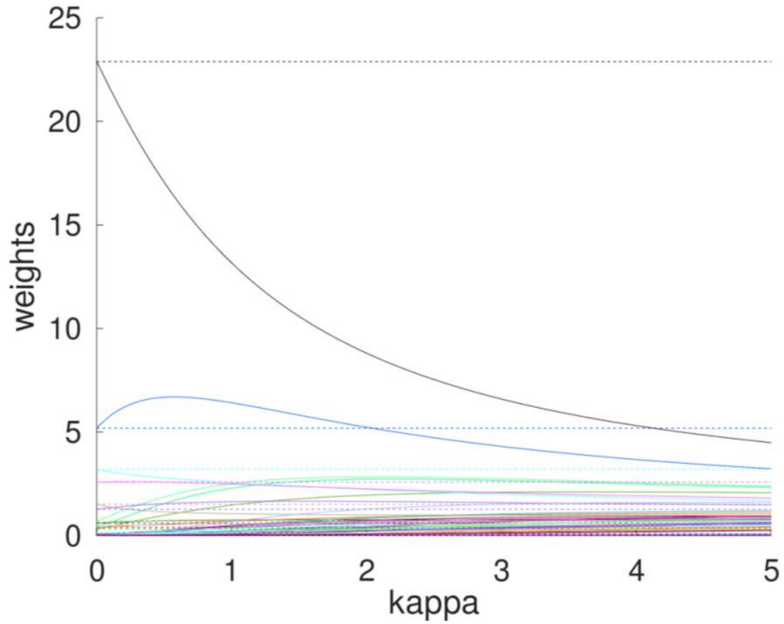




$\kappa \rightarrow 0$ (→ δ-funct.: SIRF)



κ large (O(1))



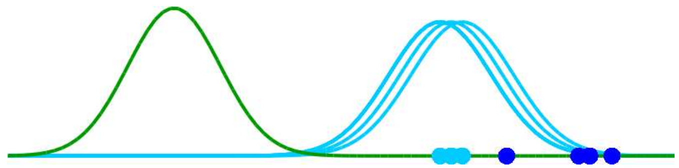
→ with increasing κ, resampling is less selective, i.e. more members are kept

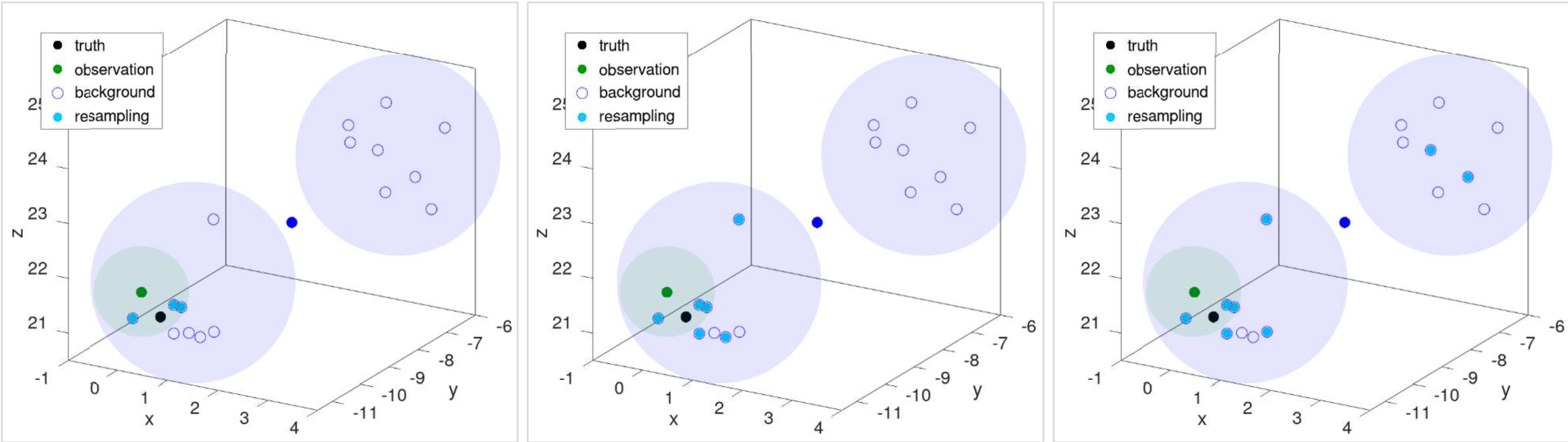
LMCPF: Resampling

$$w_f^a(\mathbf{x}) = e^{-\frac{1}{2}(\mathbf{y}-H(\mathbf{x}))^T\left(\mathbf{R}+\kappa\cdot\mathbf{HB}^{LETKF}\mathbf{H}^T\right)^{-1}(\mathbf{y}-H(\mathbf{x}))}$$

$$w_k^a \propto w_f^a\left(\mathbf{x}_k^b\right)$$

1 Resampling





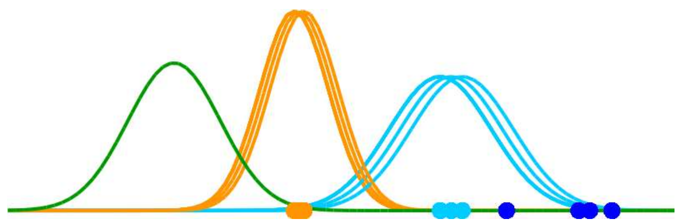
$\kappa = 0$ (particles = δ-funct.: SIRF) $\kappa = 0.5$ $\kappa = 1$

→ with increasing κ, resampling is less selective, i.e. more members are kept

LMCPF: Shift of Gaussian particles

2 Shift of Particles

analysis for each of the Gaussian particles:



$$\mathbf{x}_k^a = \mathbf{x}_k^b + \Delta\mathbf{x}_k = \mathbf{x}_k^b + \left(\left(\mathbf{B}_k^p\right)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\right)^{-1} \mathbf{H}^T\mathbf{R}^{-1}\left(\mathbf{y} - H\mathbf{x}_k^b\right)$$

⇩ in ensemble space, $\mathbf{B}_k^p = \kappa\, \mathbf{B}^{LETKF} = \kappa \frac{1}{K-1}\mathbf{X}^b\left(\mathbf{X}^b\right)^T$

$$\boldsymbol{\beta}_k^a = \mathbf{e}_k + \boldsymbol{\beta}_k^{shift} = \mathbf{e}_k + \frac{\kappa}{K-1}\left(\mathbf{I} + \frac{\kappa}{K-1}\widetilde{\mathbf{R}^{-1}}\right)^{-1}\widetilde{\mathbf{R}^{-1}}(\mathbf{C} - \mathbf{e}_k)$$

$$\mathbf{W}_k^{shift} := \left(\boldsymbol{\beta}_1^{shift}, \dots, \boldsymbol{\beta}_K^{shift}\right) \in \mathbb{R}^{K\times K}$$

$\mathbf{Y}^b = \mathbf{H}\mathbf{X}^b$ ens. pert. in observation space

$\widetilde{\mathbf{R}^{-1}} := \mathbf{Y}^{b^T}\mathbf{R}^{-1}\mathbf{Y}^b$ inverse **R**-matrix (in ens. space)

$\mathbf{X}^b\,\mathbf{e}_k = \mathbf{x}_k^b - \bar{\mathbf{x}}^b$ e_k: k-th ensemble member (")

$\mathbf{C} := \widetilde{\mathbf{R}^{-1}}^{-1}\mathbf{Y}^{b^T}\mathbf{R}^{-1}(\mathbf{y} - \bar{\mathbf{y}}^b)$ ens. mean innovation projected on ensemble space

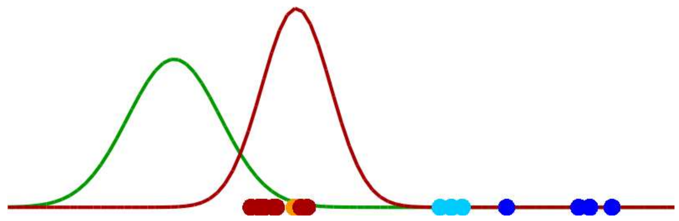
LMCPF:
Gaussian rejuvenation

Deutscher Wetterdienst

duplication and perturbation of selected particles:

3 Gaussian Rejuvenation

new particles are drawn from a Gaussian distribution around each selected and shifted particle, based on:



1) random matrix $\mathbf{N} \in \mathbb{R}^{K \times K}$ with standard-normal distributed entries

2) spread control factor $\sigma(\rho)$;

$$\rho = \frac{\mathbf{d}_{o-b}^T \, \mathbf{d}_{o-b} - \, trace(\mathbf{R})}{trace\,(\mathbf{HB}^{LETKF}\mathbf{H}^T)}$$

(multiplicative covariance inflation factor of LETKF, $\rho > 1$ if FG ensemble underdispersive)

3) analysis covariance matrix for (each) Gaussian particle in ensemble space

$$\mathbf{A}^p = (\mathbf{I} - \mathbf{K}^p\mathbf{H})\mathbf{B}^p$$

⇩ in ensemble space

$$\widetilde{\mathbf{A}}_k^p = \frac{\kappa}{K-1}\left(\mathbf{I} + \frac{\kappa}{K-1}\widetilde{\mathbf{R}^{-1}}\right)^{-1}$$

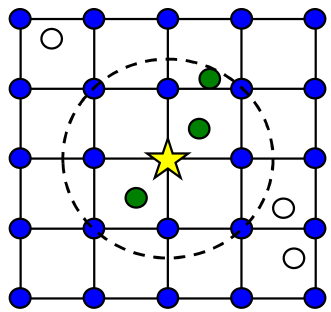
LMCPF: analysis ensemble

$\mathbf{x}_k^a = \bar{\mathbf{x}}^b + \mathbf{X}^b \, \mathbf{w}_k^{LMCPF}$

$\mathbf{w}_k^{LMCPF}$ = $\boldsymbol{k}$-th column of transform matrix $\mathbf{W}^{LMCPF}$

$$\mathbf{W}^{LMCPF} = \underbrace{\breve{\mathbf{W}}}_{\text{resampling}} + \underbrace{\mathbf{W}^{shift} \cdot \breve{\mathbf{W}}}_{\text{shift of particles}} + \underbrace{\sigma(\rho) \cdot (\widetilde{\mathbf{A}_k^p})^{\frac{1}{2}} \cdot \mathbf{N}}_{\text{Gaussian rejuvenation}}$$

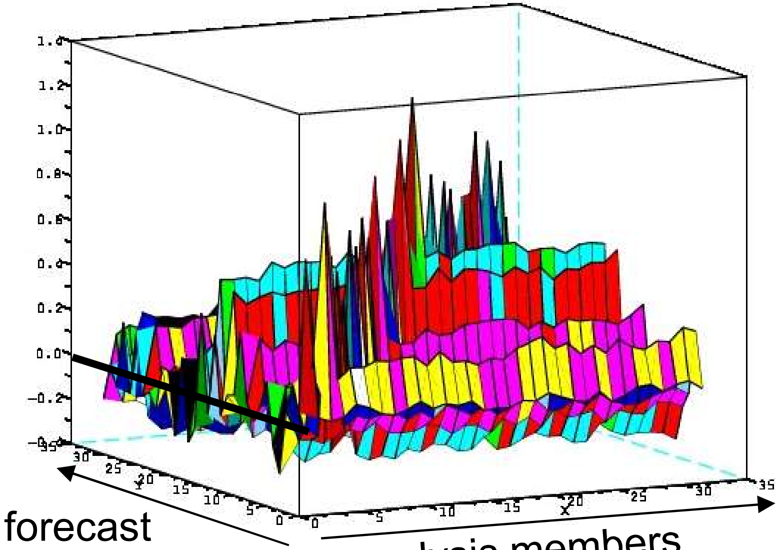
do analysis in the space of the ensemble deviations (as in LETKF)



- explicit localization in observation space:
  compute $\mathbf{W}_{loc}^{LMCPF}$ separately at every point of coarse analysis grid after scaling $\mathbf{R}^{-1}$ by Gaspari-Cohn (selects obs only in vicinity), interpolate $\mathbf{W}_{loc}^{LMCPF}$ to model grid and apply to $\mathbf{X}_k^b$

- computationally efficient,
  but also restricts analysis correction to
  local subspace spanned by the ensemble

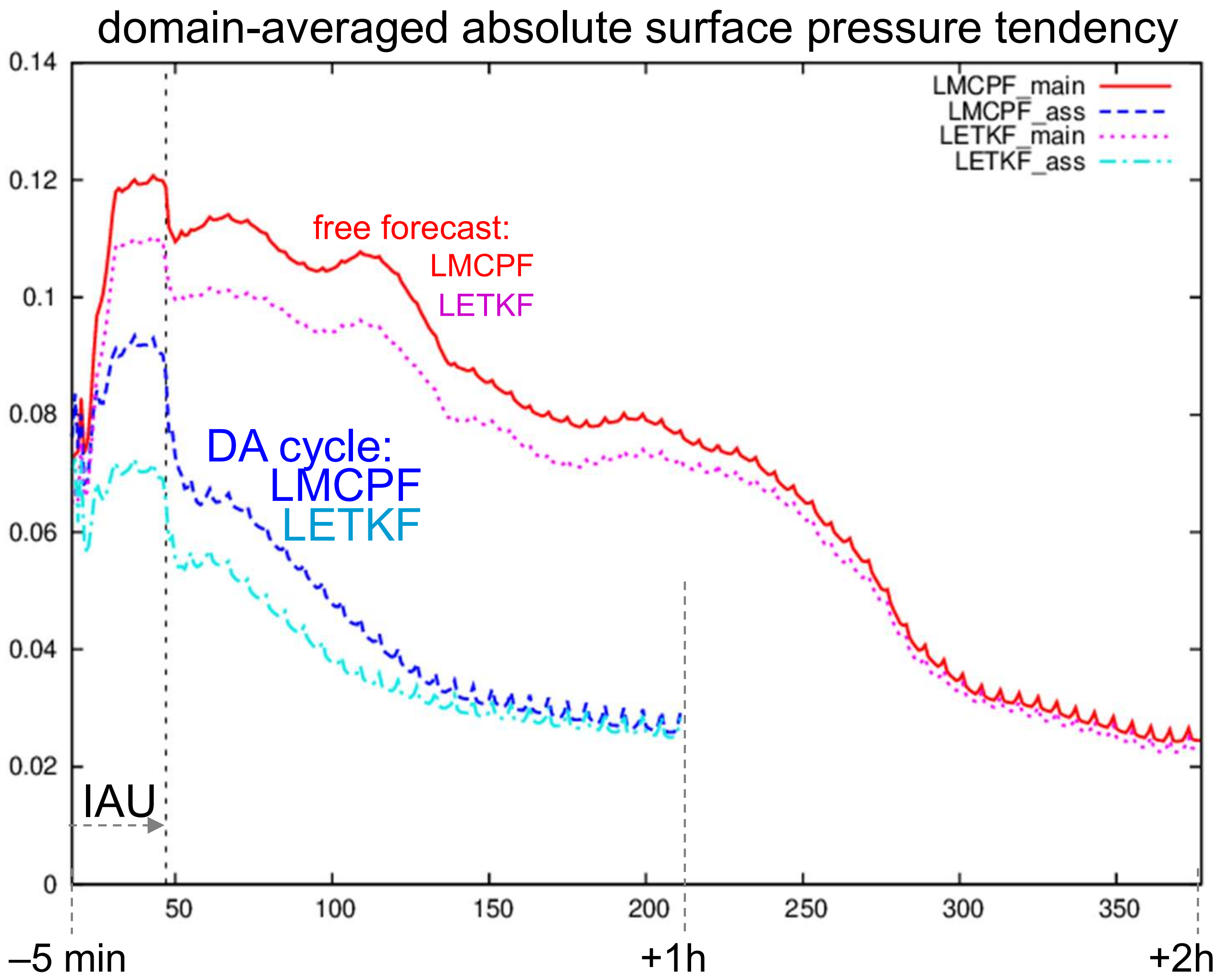
- analysis ensemble members
  are locally linear combinations
  of first guess ensemble members



LMCPF:
Application to ICON-D2

Deutscher Wetterdienst

localisation → strong spatial variations of transform matrix → strong imbalances ?



→ ICON-D2 with IAU: imbalances only moderately increased in LMCPF vs. LETKF

LMCPF
Application to ICON-global

Deutscher Wetterdienst

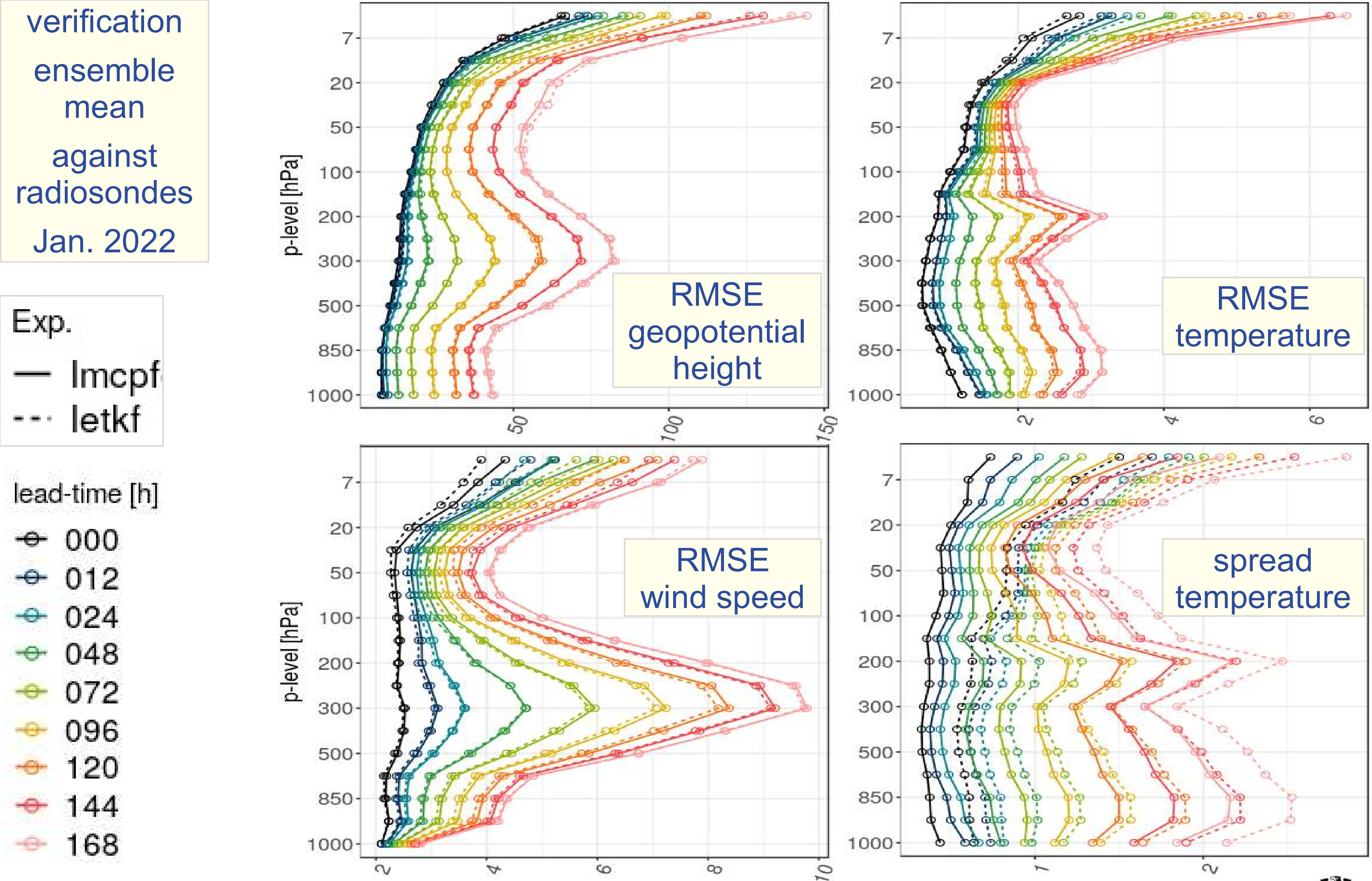
DWD

verification

ensemble mean

against radiosondes

Jan. 2022



- LMCPF able to show better results than LETKF for Lorenz 1996 model
- LMCPF runs stably for ICON-D2 (8 days), but FG rmse ~ 5 % larger than LETKF
- LMCPF runs stably for ICON-global (months), skill as good as LETKF (troposphere)
- LMCPF ensemble spread smaller than with LETKF

Outlook:

- automatic adjustment of particle uncertainty parameter κ
- limited HR ! (LMCPF yet to be considered experimental system for research)

➔ Potthast, R., A. Walter, A. Rhodin,2019. A localized adaptive particle filter within an operational NWP framework. Monthly Weather Review, 147(1):345–362.

➔ Walter A., N. Schenk, P. J. van Leeuwen, R. Potthast, 2022. Particle Filtering and Gaussian Mixtures - On a Localized Mixture Coefficients Particle Filter (LMCPF) for Global NWP. (Under review).

➔ Schenk N., R. Potthast, A. Walter, 2022. On Two Localized Particle Filter Methods for Lorenz 1963 and 1996 Models. Frontiers in Applied Mathematics and Statistics (Accepted).