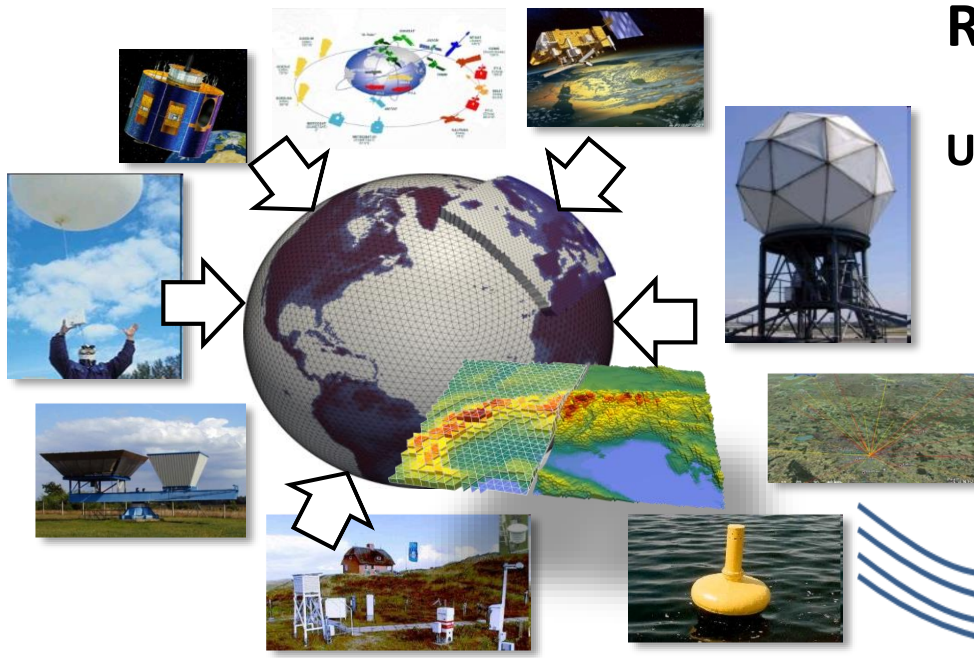
Deutscher Wetterdienst
Wetter und Klima aus einer Hand

Ensemble Data Assimilation and Particle Filters for NWP

Roland Potthast
NWP @ DWD & University of Reading



With the help of many people, in particular:

Anne Walter,
Andreas Rhodin
Harald Anlauf,
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Olaf Stiller,
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Martin Lange,
Stefanie Hollborn,
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Christoph Schraff,
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Klaus Stephan
Ulrich Blahak

Partners include:
P.-J van Leeuwen
Sebastian Reich
Dan Crisan
H.R. Künsch
Amos Lawless
S. Dance
Nancy Nichols

Heinz-Werner Bitzer, Annika Schomburg, Silke May, Marc Pondrom, Kristin Raykova, Thomas Rösch, Michael Bender, Christian Welzbacher, Lilo Bach, Lisa Neef, Zoi Paschalidi, Walter Acevedo, Axel Hutt, Daniel Egerer, Gerhard Paul, Ana Fernandez, Stefan Declair

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Why Distributions , Risk, Uncertainty?

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Extreme Weather Even... triggered by ... threaten ...ure and economy!

Lightning, C... precipitatio... impact the life of inc...viduals ans the society.

...es:s	Level
	Moderate
...-10)	Strong
...ainfall (10-25mm/h)	Strong
Storm Force Gusts, Heavy Rainfall	Strong
Storm Force Gusts, Heavy Rainfall, Hail	Strong

Protect Lifes!

Protect Property!

Protect Society and Business

We need Uncertainty Estimates for Risk Prediction!

NOW, 5min, 30min, … 1h, 2h, 6h, 24h, 72h, …

Why Distributions , Risk, Unc nty?

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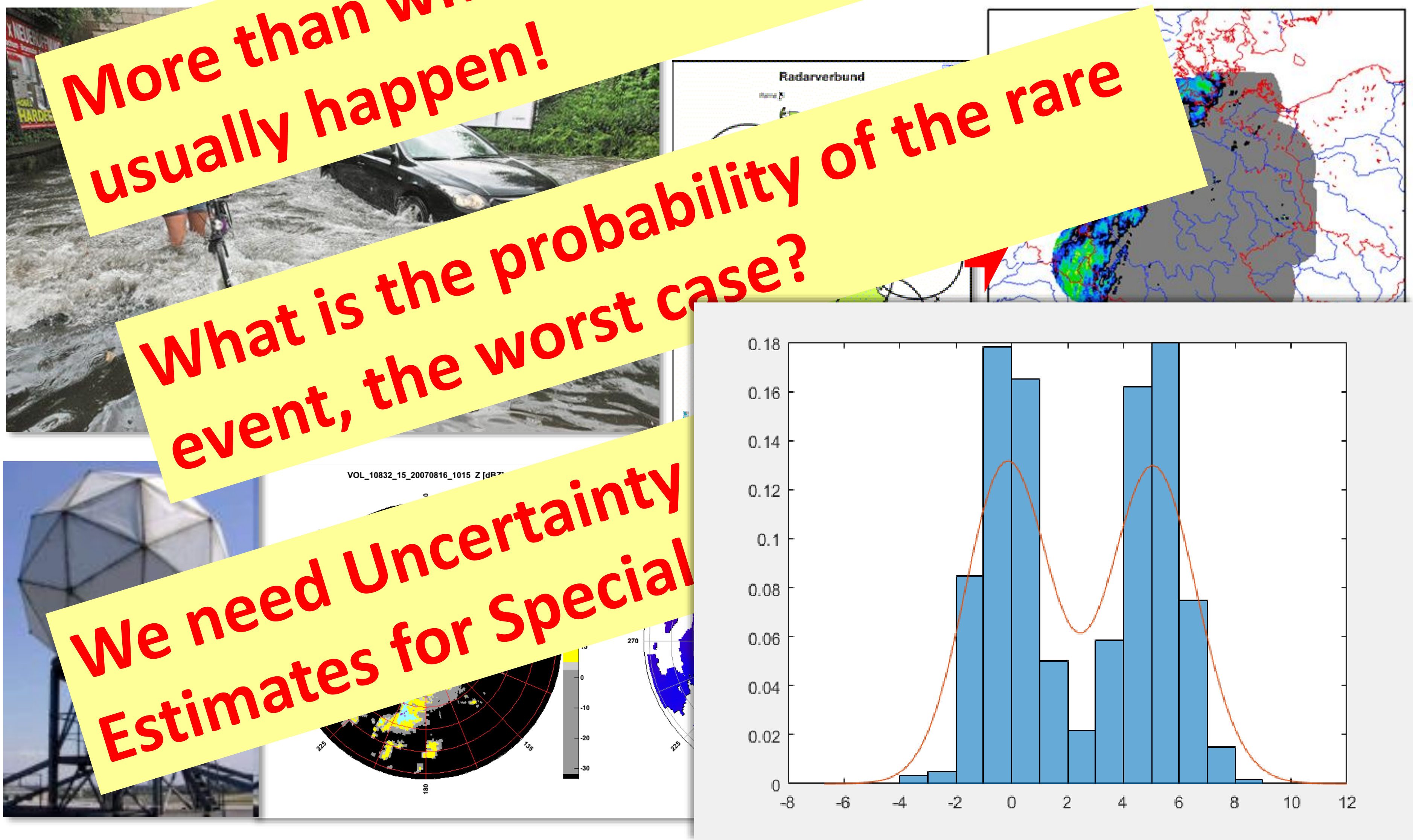
More than what would usually happen!

What is the probability of the rare event, the worst case?

We need Uncertainty Estimates for Special



Why Distributions , Risk, Uncertainty?

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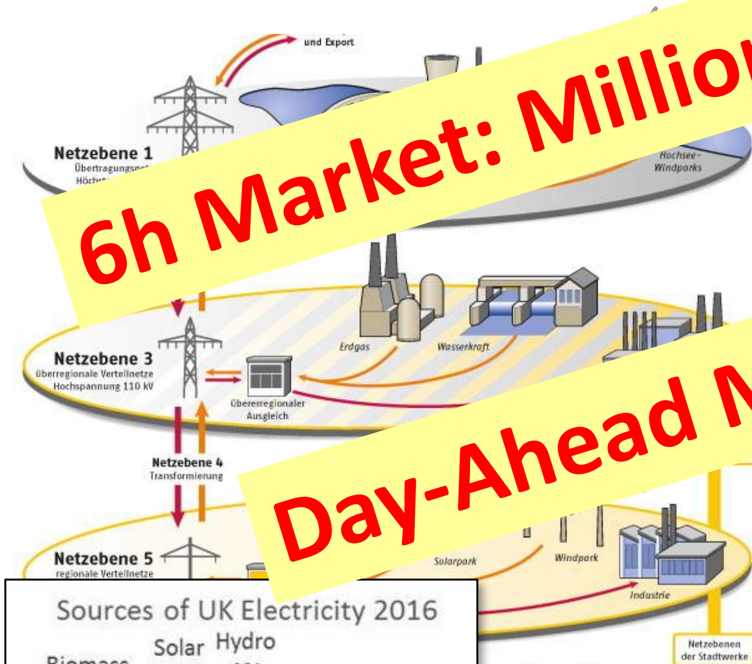

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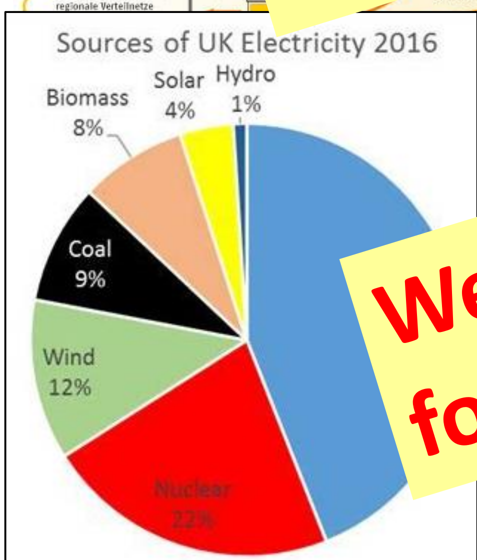
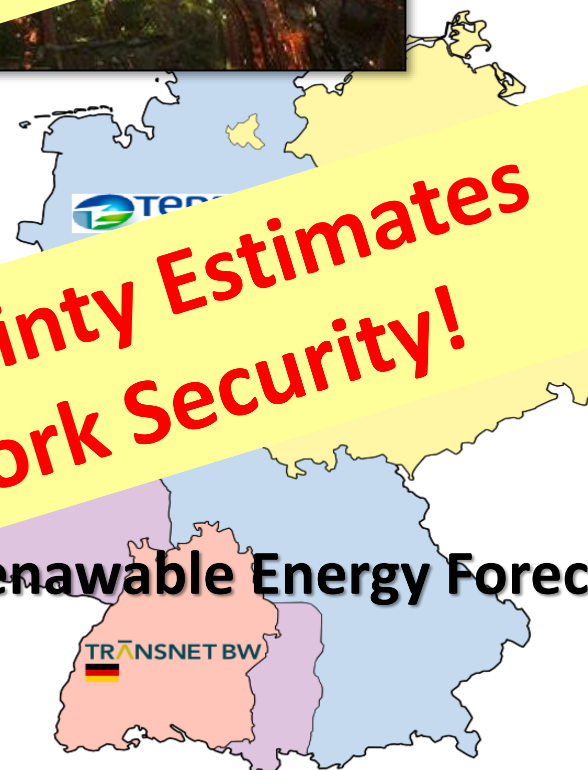




6h Market: Millions

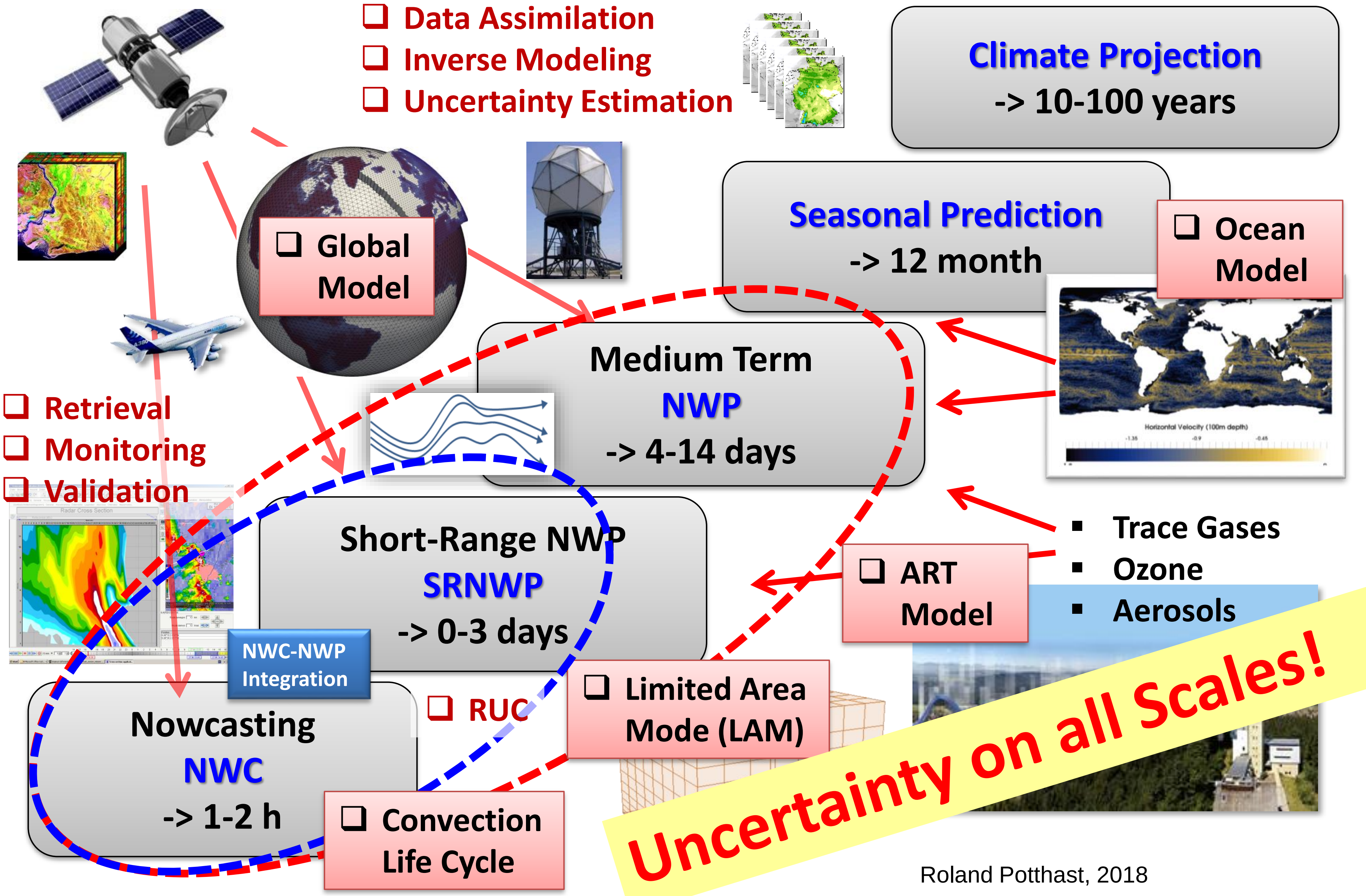
Day-Ahead Market: Billions!

We need Uncertainty Estimates for Energy Network Security!

Renawable Energy Forecasting

Bildquelle: https://de.wikipedia.org/wiki/%C3%9Cbertragungsnetzbetreiber

Framework Numerical Weather Prediction

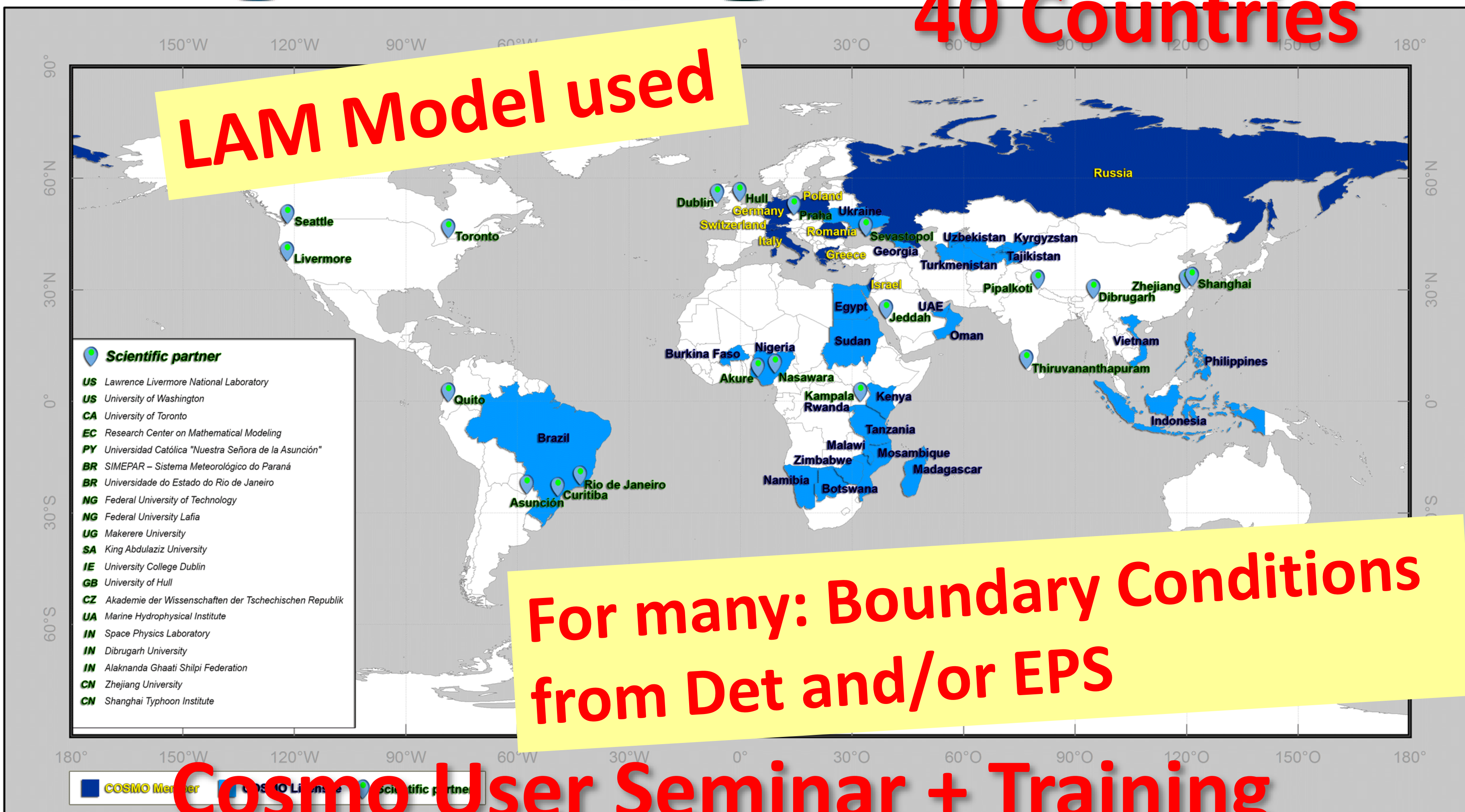


CONSORTIUM FOR SMALL SCALE MODELING

COSMO

40 Countries

LAM Model used



For many: Boundary Conditions from Det and/or EPS

Cosmo User Seminar + Training Course + Symposium

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Data Assimilation Methods

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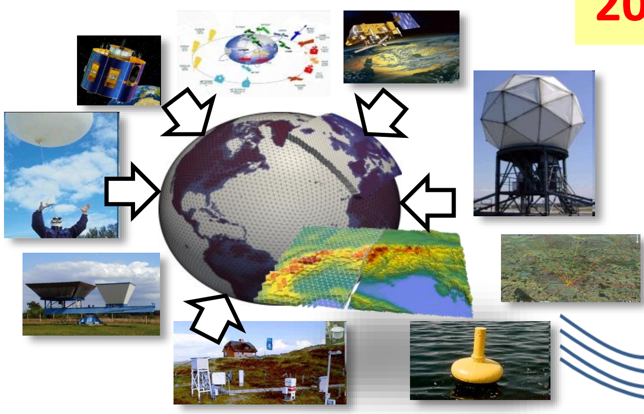
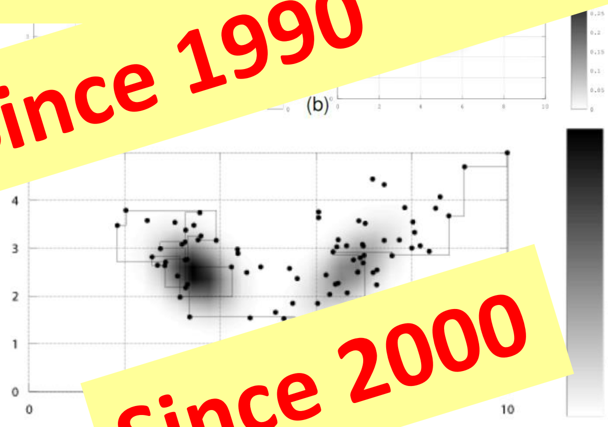
- Why **variational** Data Assimilation (3D/4D-VAR)?

20 years 4D-VAR at ECMWF





Since 1990

- Why **Ensemble** Data Assimilation (EDA)?

Since 2000

- Why **Hybrid** Methods? (3D/4D-EnVAR)

Since 2010

- Why Particle **Filters**? (PF,GPF,ETPF,LAPF,LMCPF)

Since 2020

☺

Variational Analysis (3D/4D-VAR)

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Recall where we came from …

The minimization of

Obs Operator

$$J(x) = \|x - x^b\|^2_{B^{-1}} + \|y - Hx\|^2_{R^{-1}}$$

leads to the **analysis**

Climatological covariances

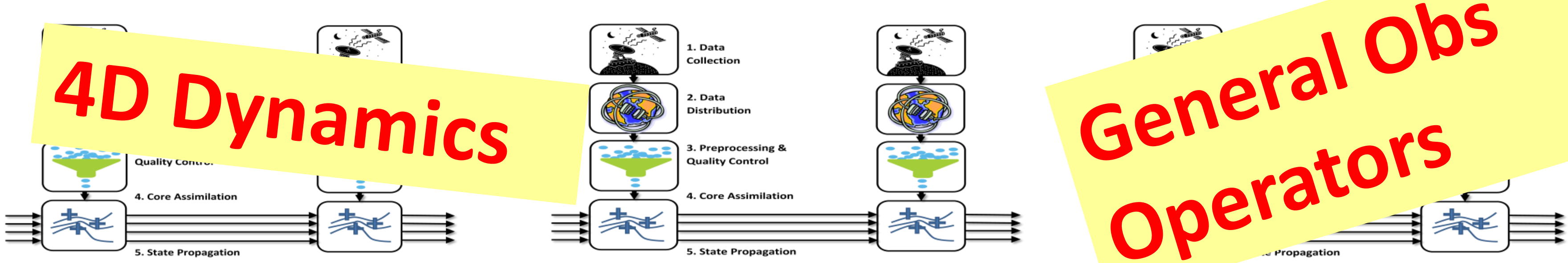
Minimization

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

This is the mother of all data assimilation formulas

4D Dynamics

General Obs Operators



Stochastic View ⇔ Minimization

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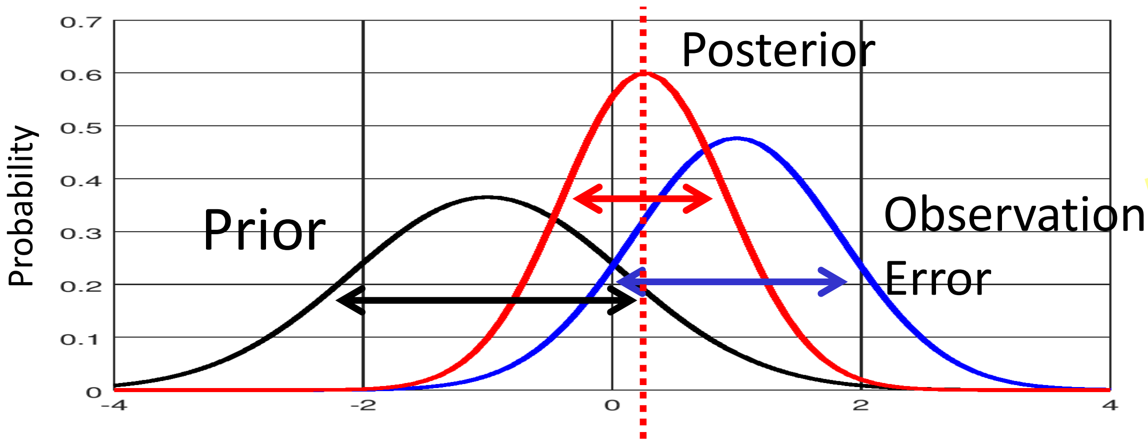


Var == Mean/ ML estimator!

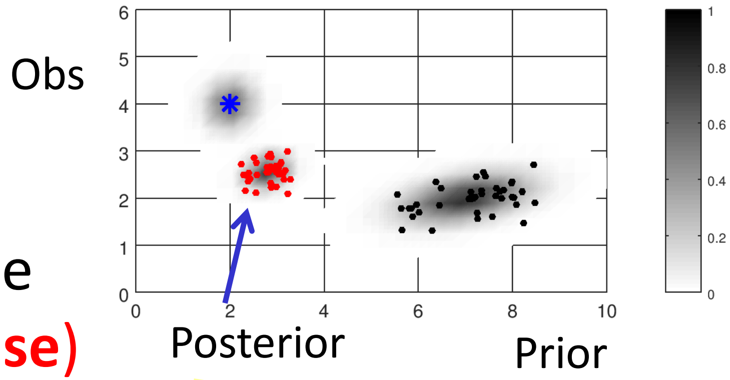
- **Gaussian Prior** $$p(x) = e^{-\frac{1}{2}(x-x^b)^T B^{-1}(x-x^b)}$$
- **Gaussian Data Error** $$p(y|x) = e^{-\frac{1}{2}(y-Hx)^T R^{-1}(y-Hx)}$$
- **Gaussian Posterior**

Maximum Likelyhood Estimator = Minimization of Functional = 3/4DVar

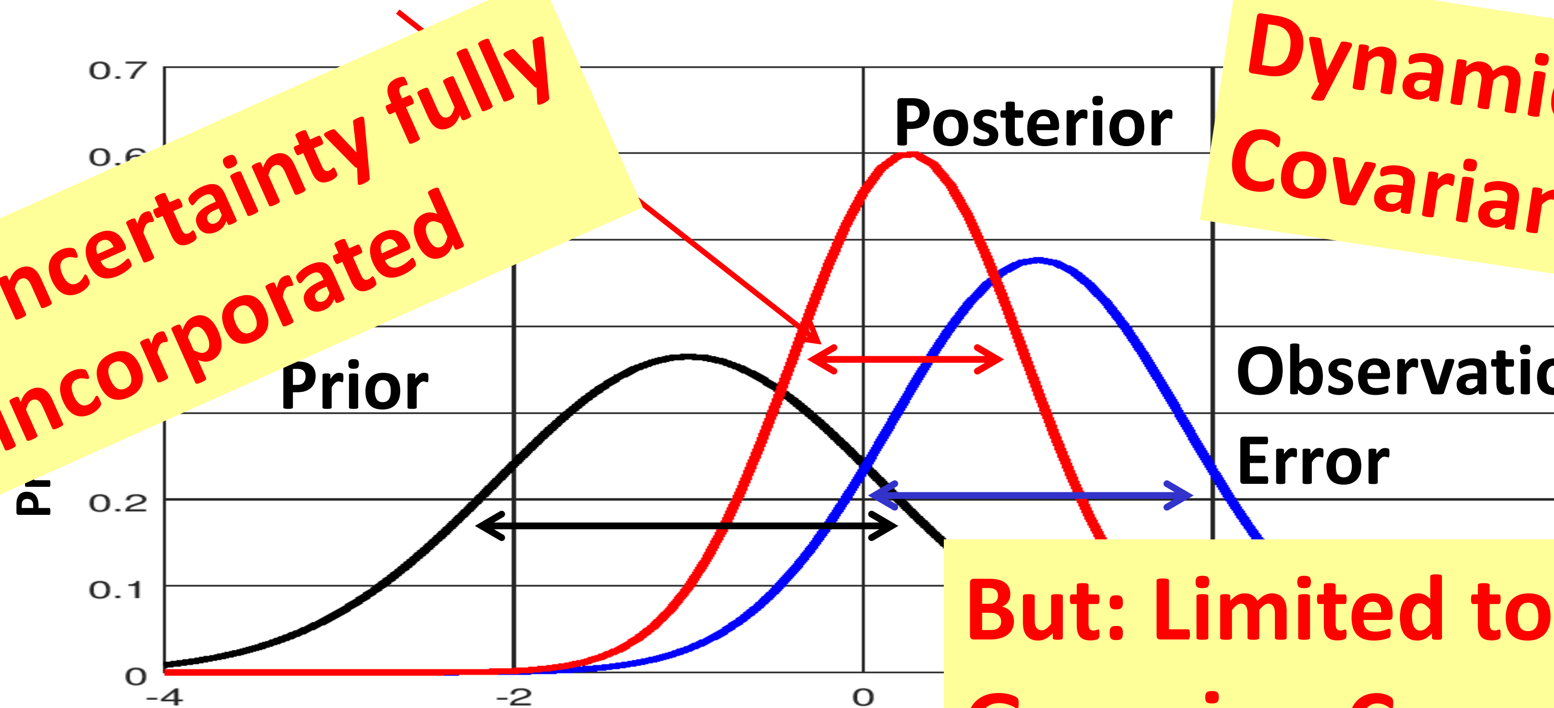
$$p(x|y) = c\, e^{-\frac{1}{2}\left\{\overbrace{(x-x^b)^T B^{-1}(x-x^b)+(y-Hx)^T R^{-1}(y-Hx)}\right\}}$$

Kalman Filter & Uncertainty Estimation

Basic Idea of the Kalman Filter



- **Sequentiel** Assimilation of Data
- Do not only adapt the mean, but also the **Covariance B (Uncertainty, Gaussian Case)**



Uncertainty fully incorporated

Dynamical Covariances

But: Limited to the Gaussian Case

EDA: Ensemble Kalman Filter (EnKF)

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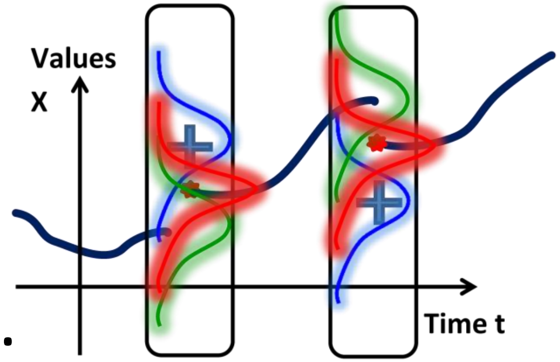
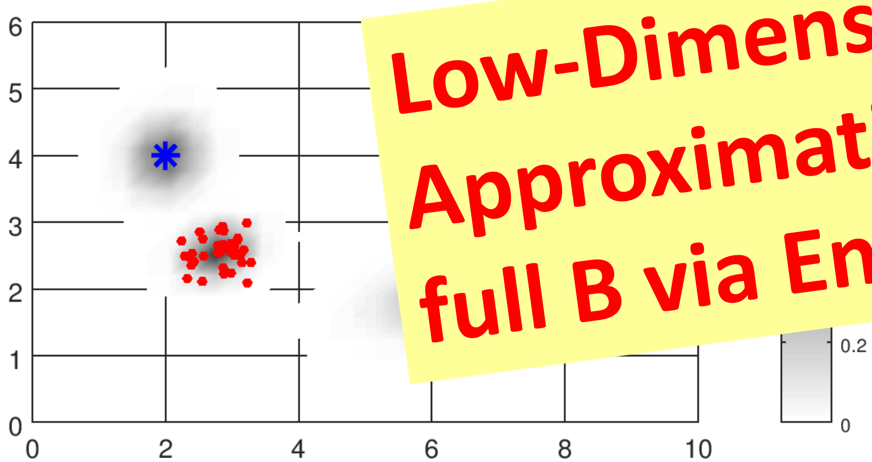
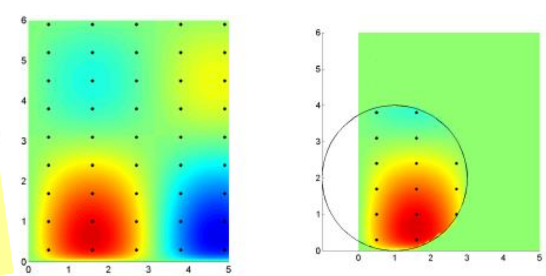
- Kalman Filter needs B update => **expensive**!
- **Estimate** B based on an ensemble of forecasted states (**stochastic estimator**).



B will be **flow-dependent** and variable, depending on the **model dynamics** and on the **observations**



Low-Dimensional Approximation to full B via Ensemble!



Needs Localization

Localized: LETKF

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Global NWP Modelling: Det + EPS

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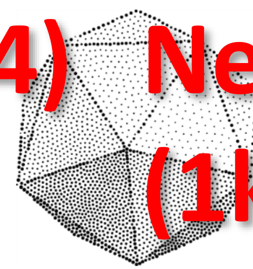
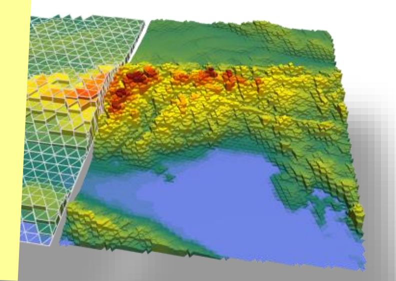


1) ICON Model 13km
2) Nest over Europe (6.5km; 2-way)
3) ICON-LAM D2
4) Nest over Germany (1km; 2-way) D1
5) NWC Ensemble

- 3h cycles global+Europe: 180h fc
- 1h ana cycle LAM, 3h fc cycle: 27h fc
- RUC cycle 1h: 6-12h fc



Full Observation System

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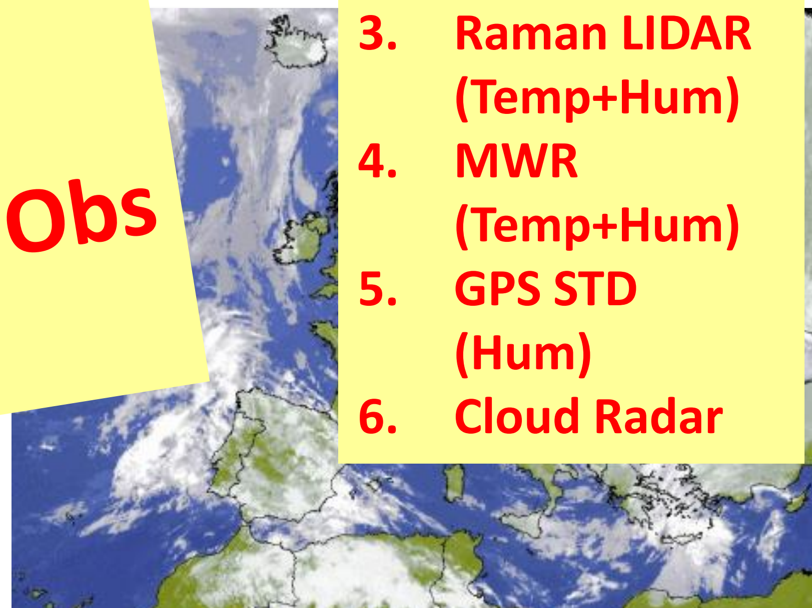
Conventional and Remote Sensing

Exploring Pilot Stations for Boundary Layer Remote Sensing Obs 2019-2025

1. Doppler-LIDAR (Wind)
2. DIAL (Humidity)
3. Raman LIDAR (Temp+Hum)
4. MWR (Temp+Hum)
5. GPS STD (Hum)
6. Cloud Radar



Conventional Synop + Airplanes

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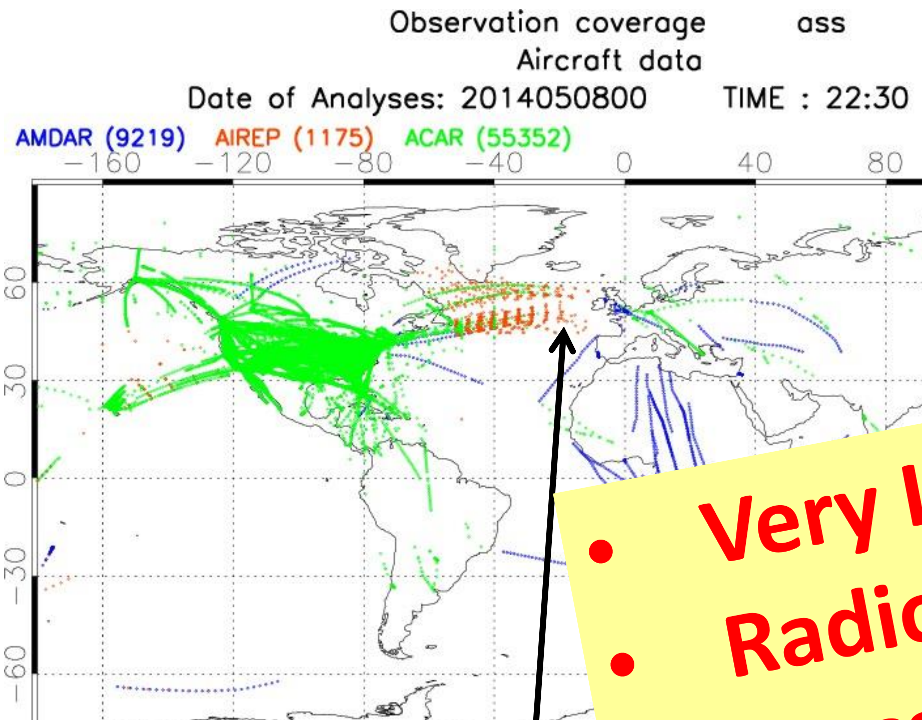
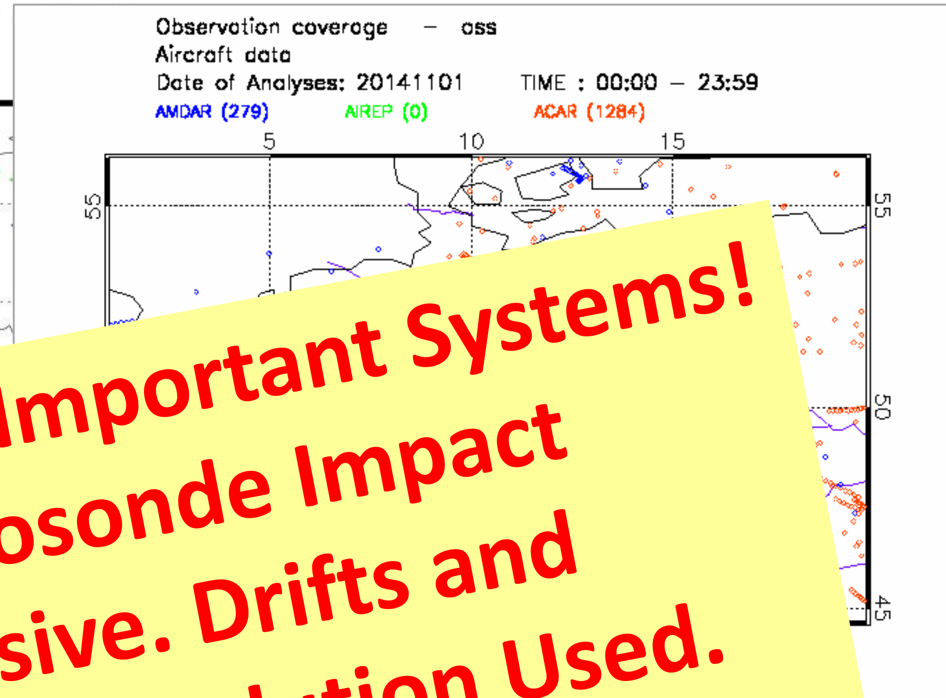
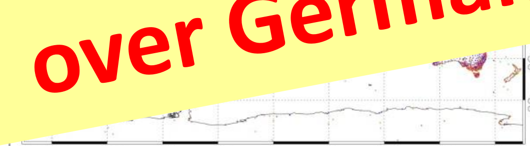
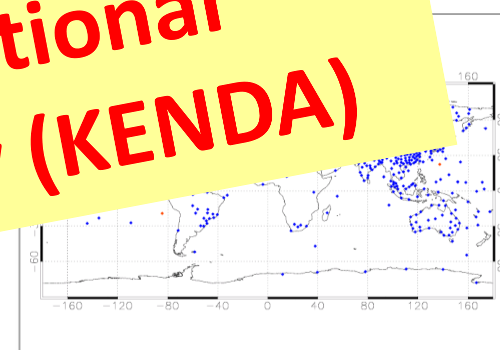








- Very Important Systems!
- Radiosonde Impact massive. Drifts and High-Resolution Used.
- Mode-S Operational over Germany (KENDA)

Observations: Geostationary Satellites

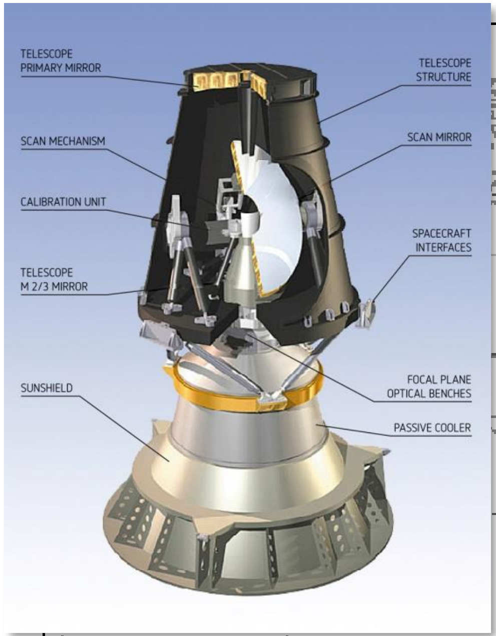
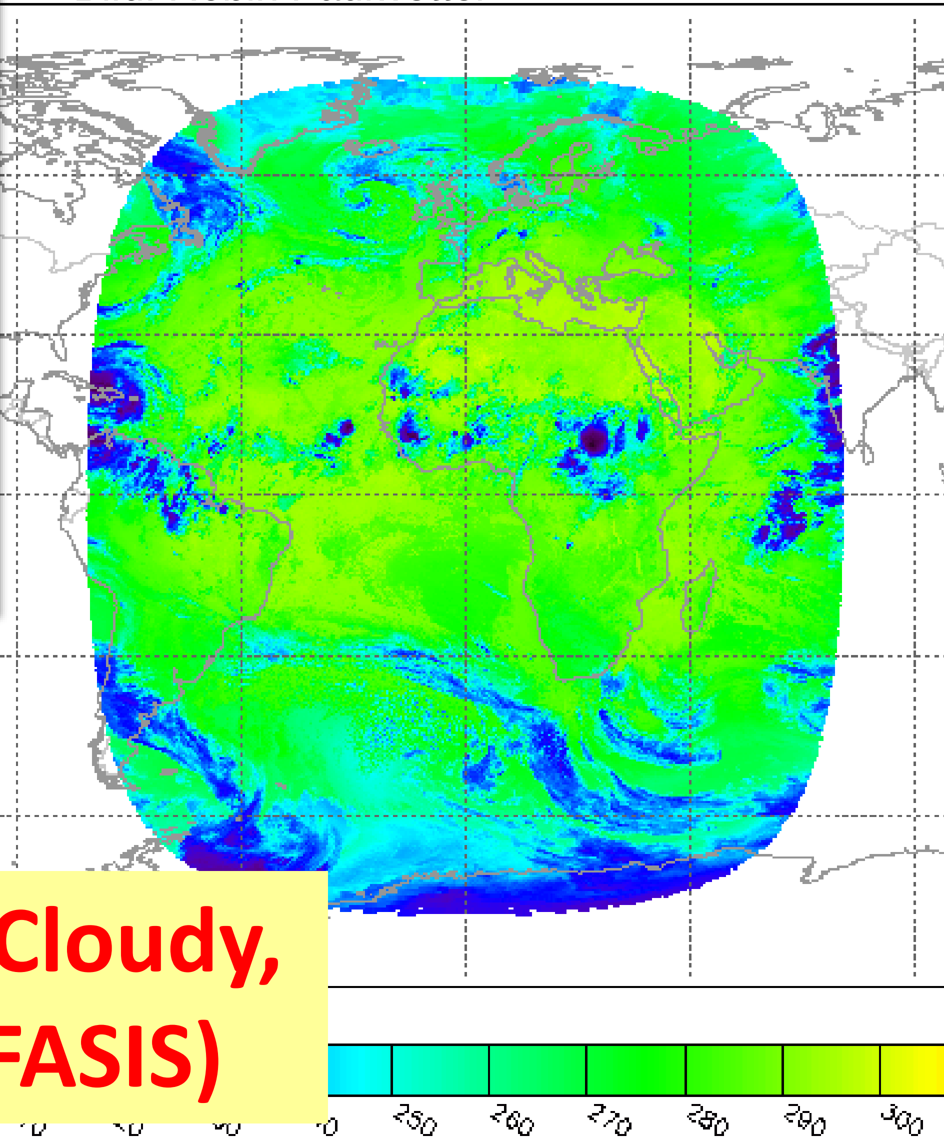
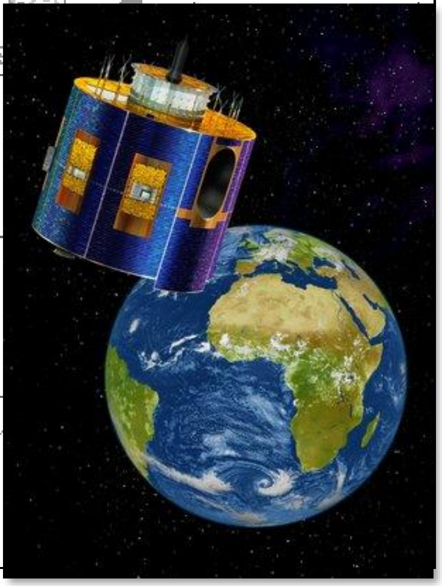


Bild: Robin Faulwetter



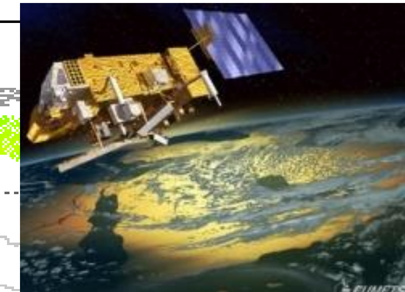
SEVIRI
Visible,
Near Infrared,
Infrared

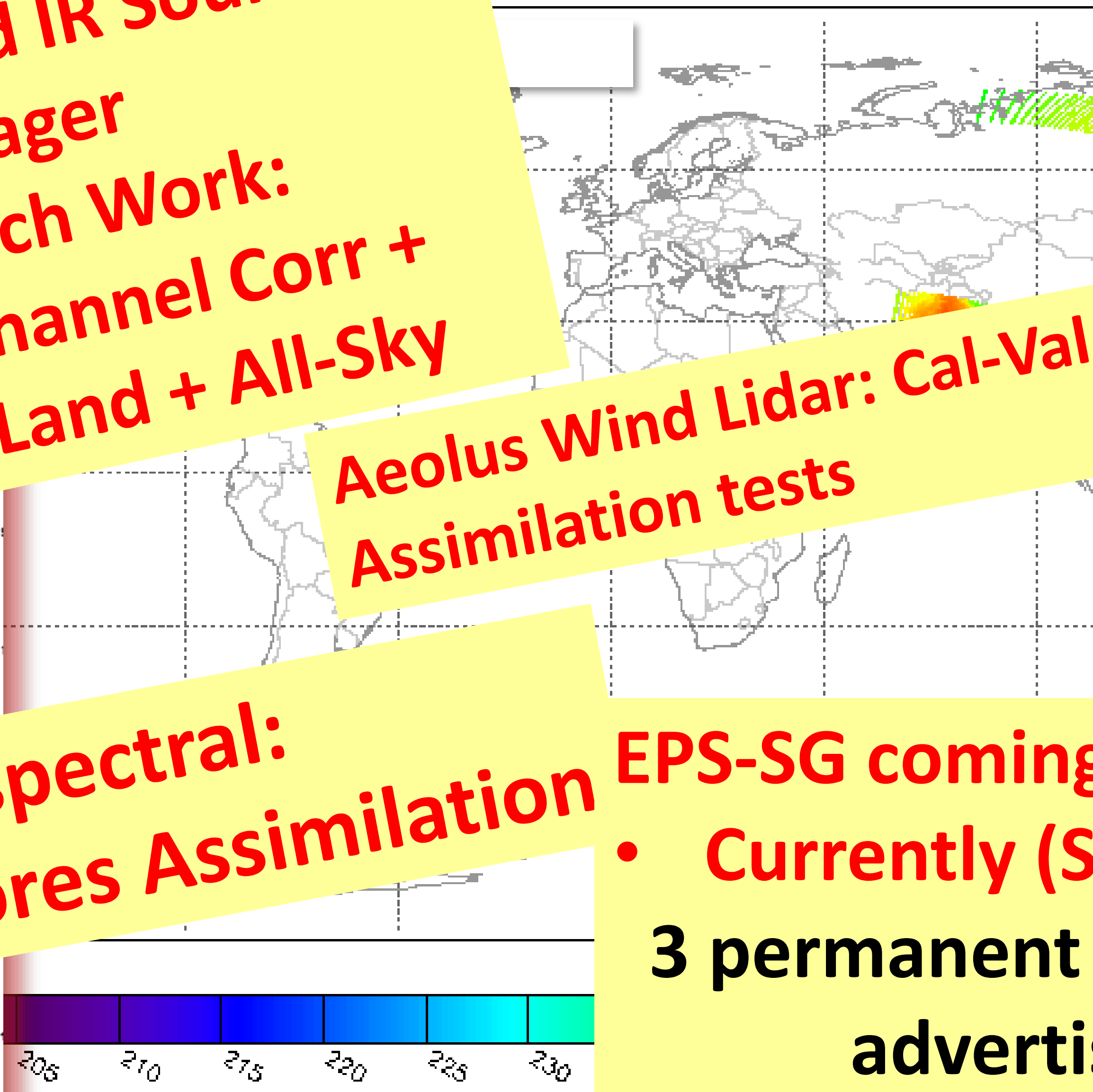


Clear and Cloudy,
IR, VIS (MFASIS)

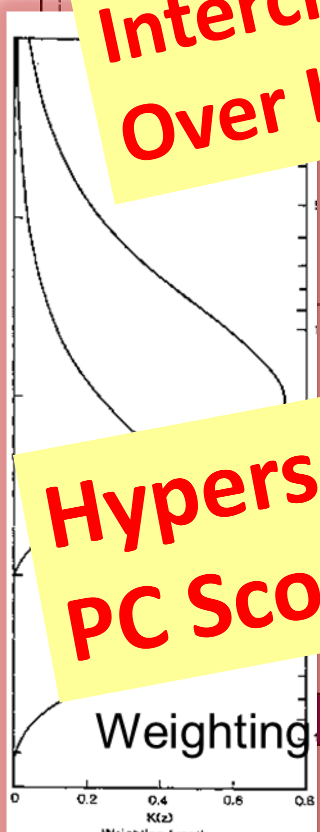
Observations: Polar Orbiting Satellites

MW and IR Sounder and Imager Research Work: Interchannel Corr + Over Land + All-Sky





Aeolus Wind Lidar: Cal-Val + Assimilation tests



Hyperspectral: PC Scores Assimilation

EPS-SG coming …

- Currently (Sept 2018):

3 permanent positions advertised

Ensemble Datenassimilation EnVar

Operational since January 2016

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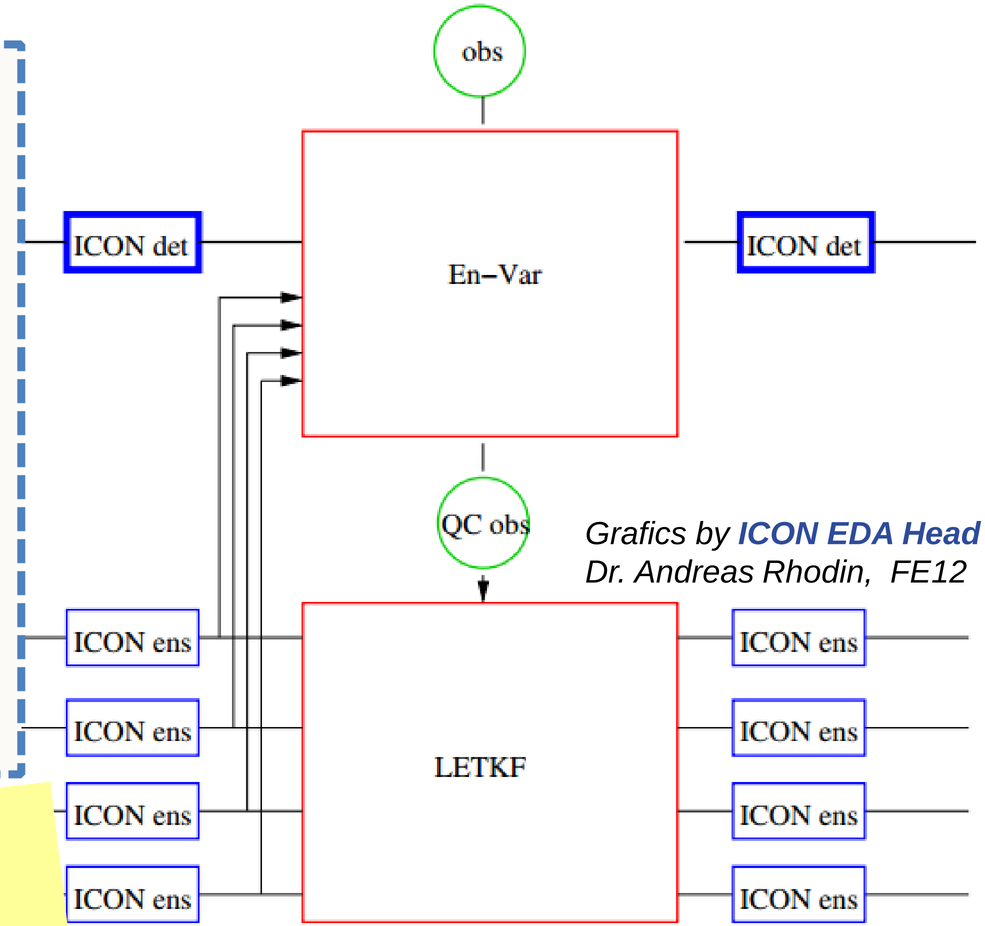
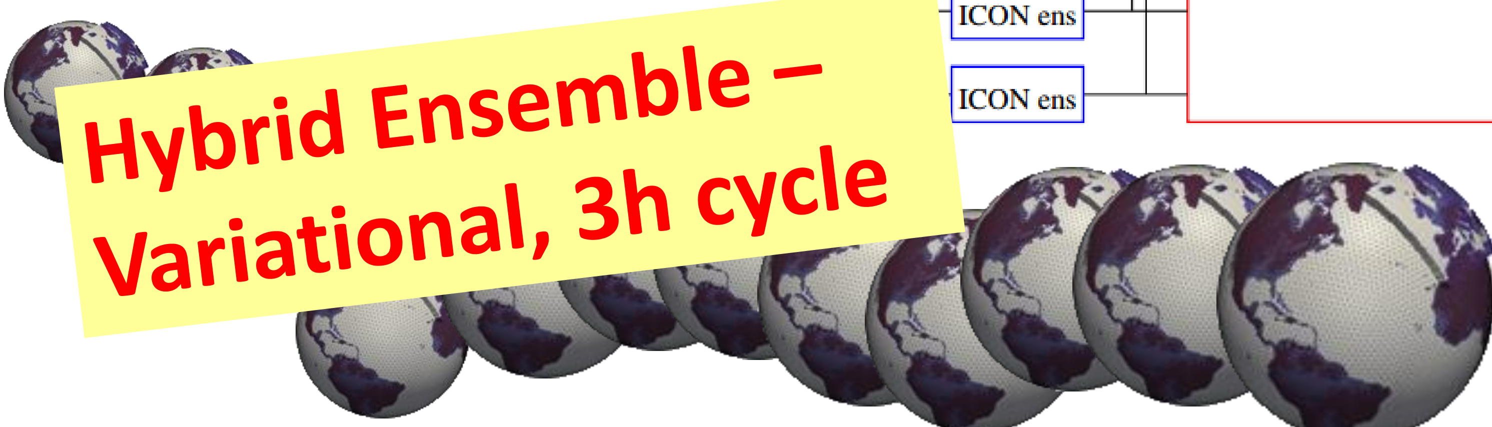
We are running **ICON EDA** in our Routine since *Jan 2016*

- 40 Members each with 40km global resolution and 20km NEST over Europe
- 1 deterministic 13km/6.5km
- **EPS forecasts** 40 Members 7 Days + 1 Deterministic
- Output for convective-scale EDA/EPS
- **Hybrid System**

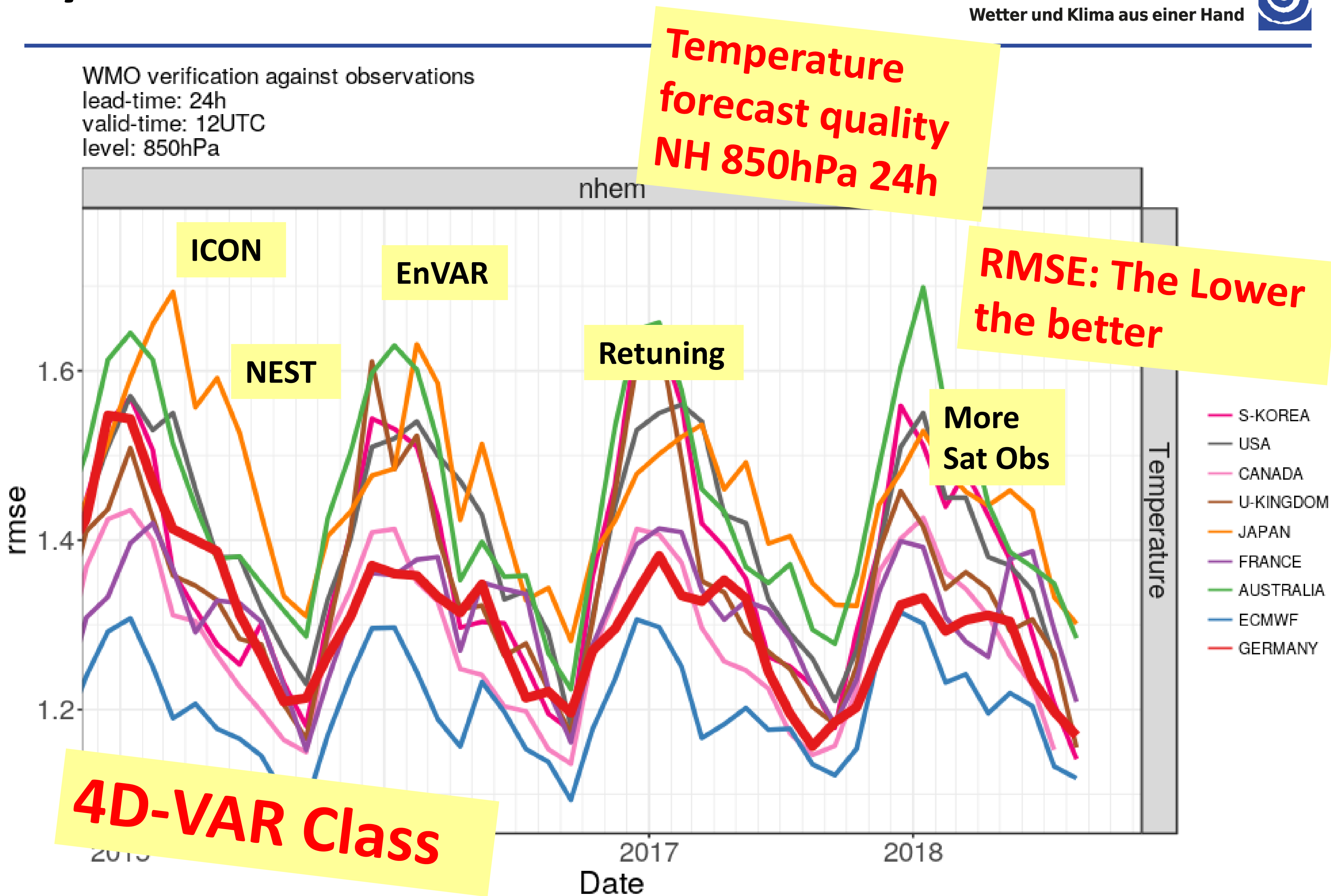


*Grafics by **ICON EDA Head***
Dr. Andreas Rhodin, FE12



Hybrid Ensemble – Variational, 3h cycle

Hybrid Methods: EnVAR Scores



Hybrid Methods: EnVAR Scores

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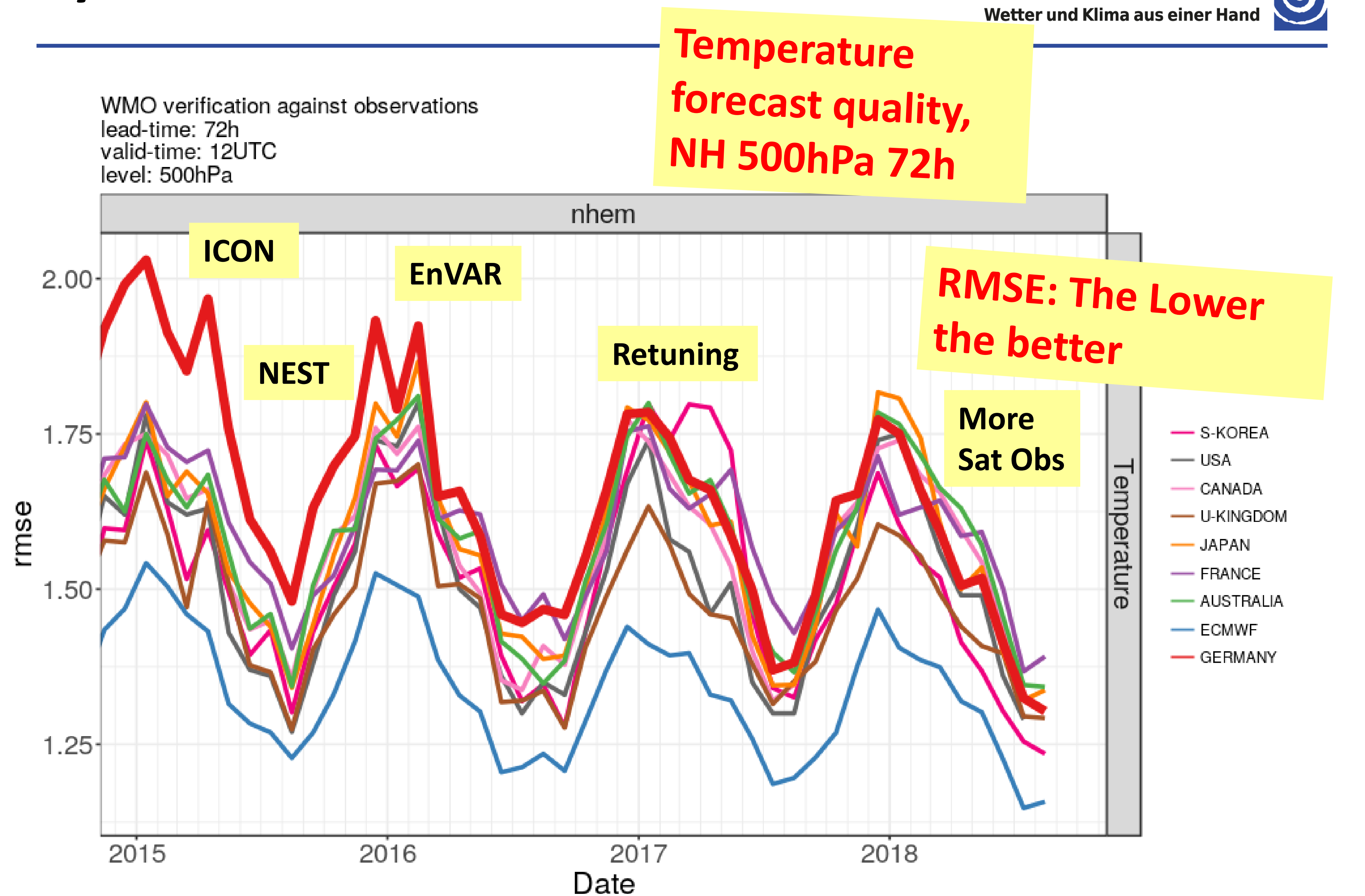

Roland Potthast

Hybrid Methods: EnVAR Scores

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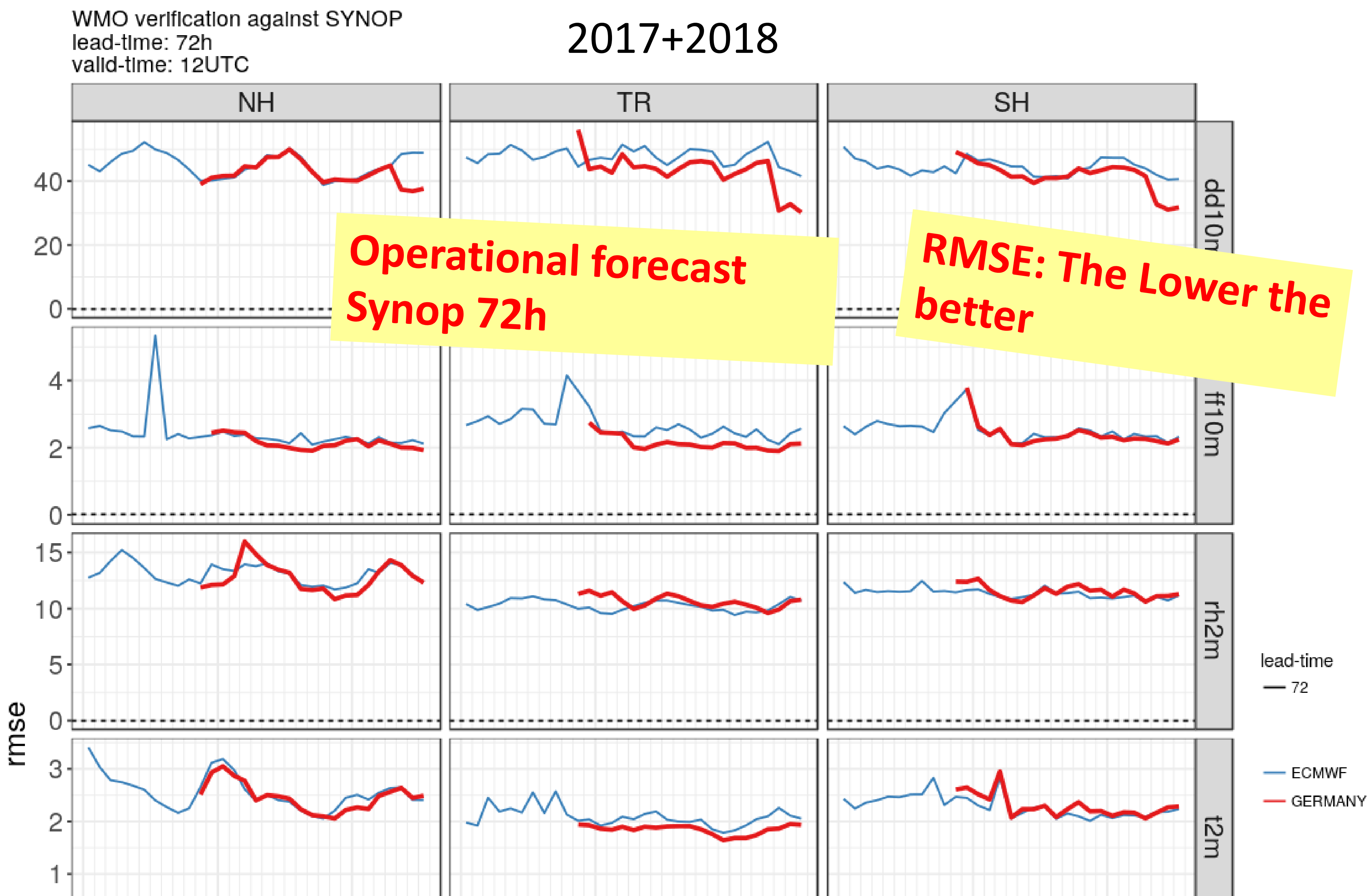
2017+2018



Hybrid Methods: EnVAR Scores

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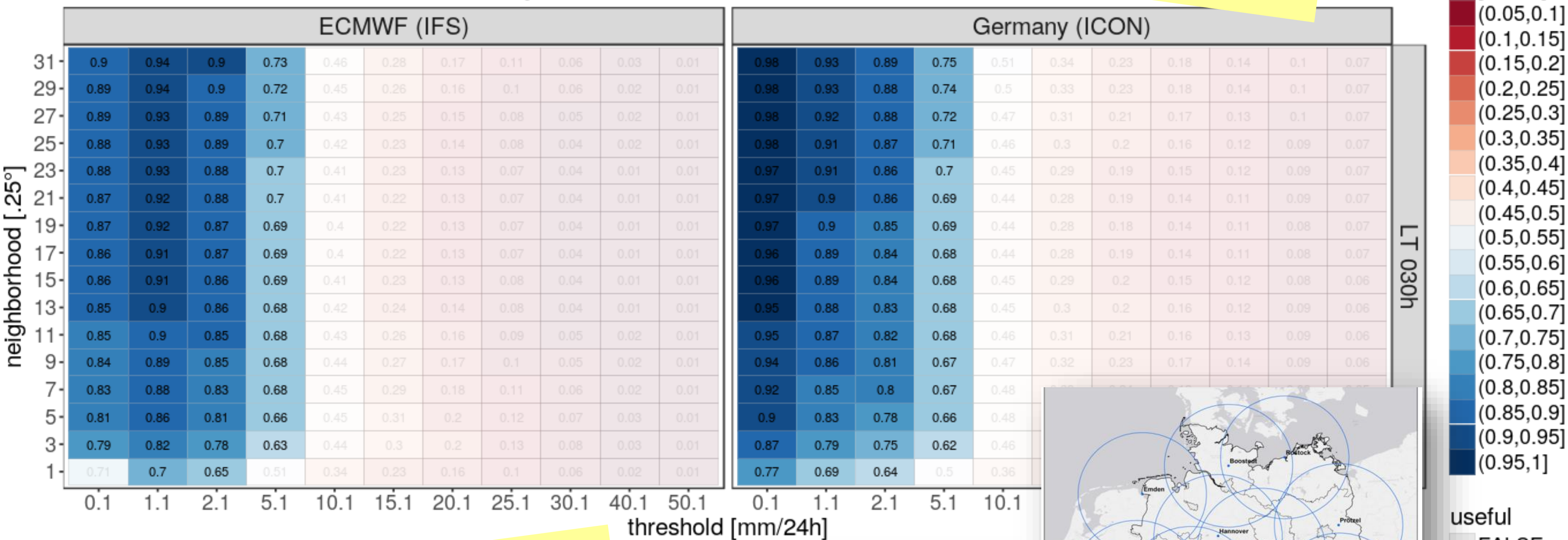
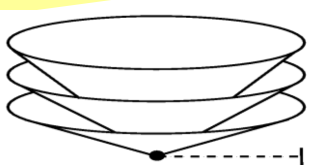
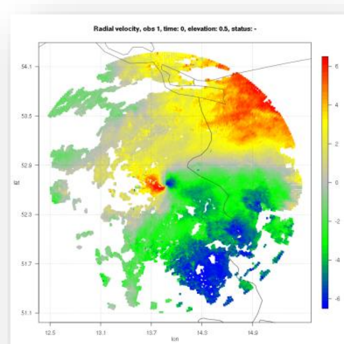
FSS: the higher the better

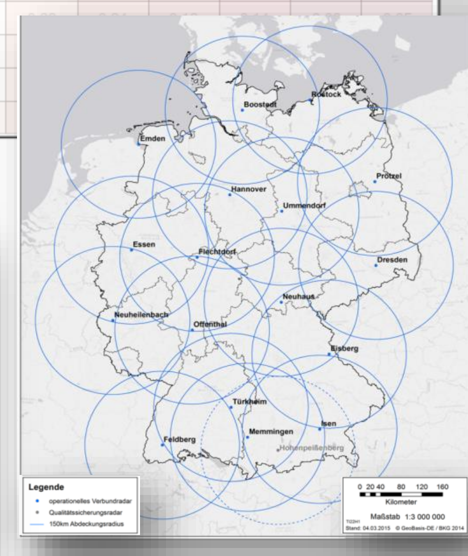
OBS: german radar (rw) 06UTC-06UTC
PRED: rr_24h (0.25°)
INI: 00UTC
CASES: ECMWF (IFS) 90, Germany (ICON) 90



Operational forecast Precipitation vs RADAR







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BAYES Data Assimilation

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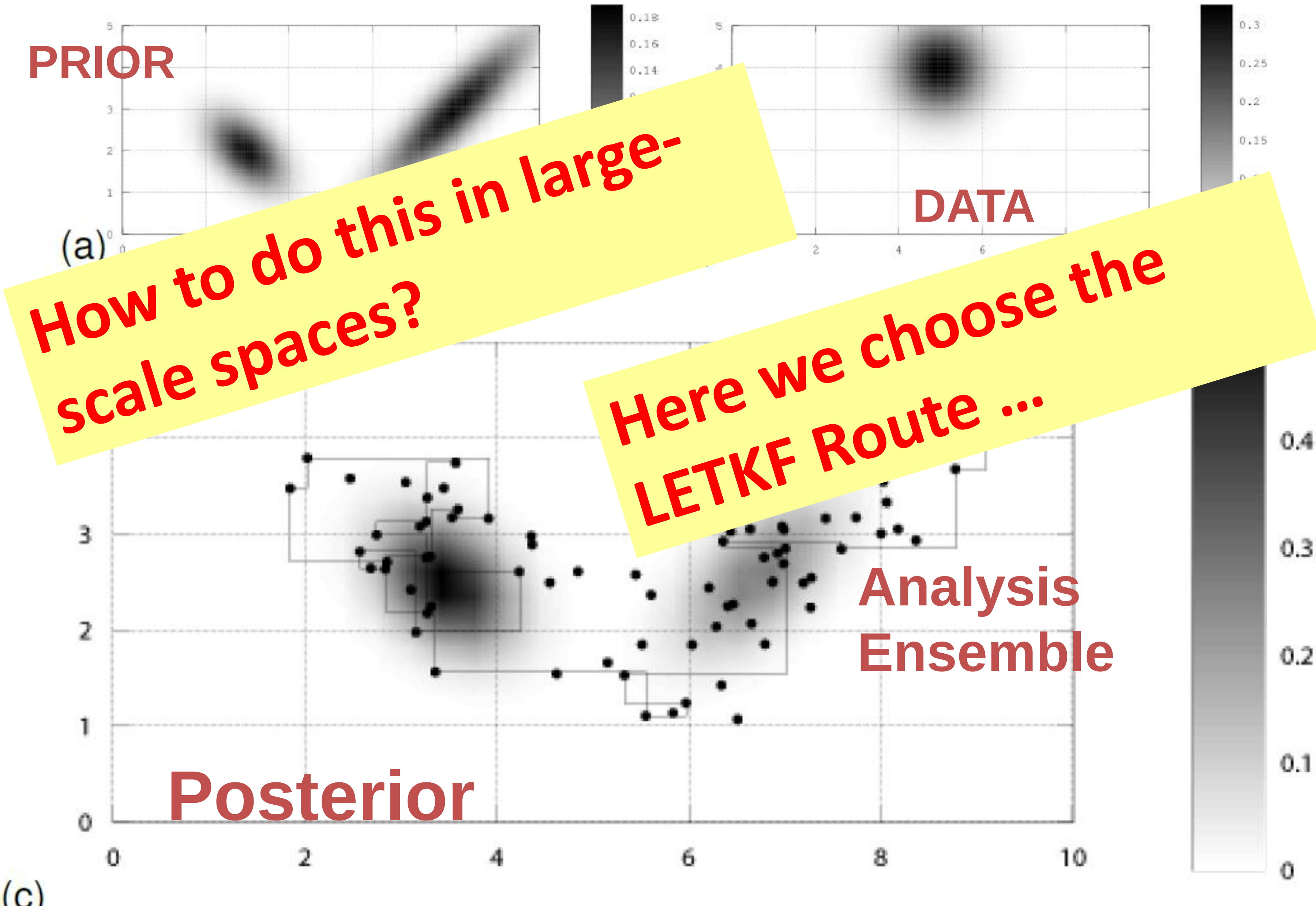

How to do this in large-scale spaces?

Here we choose the LETKF Route …

Bayesian Filtering via PF

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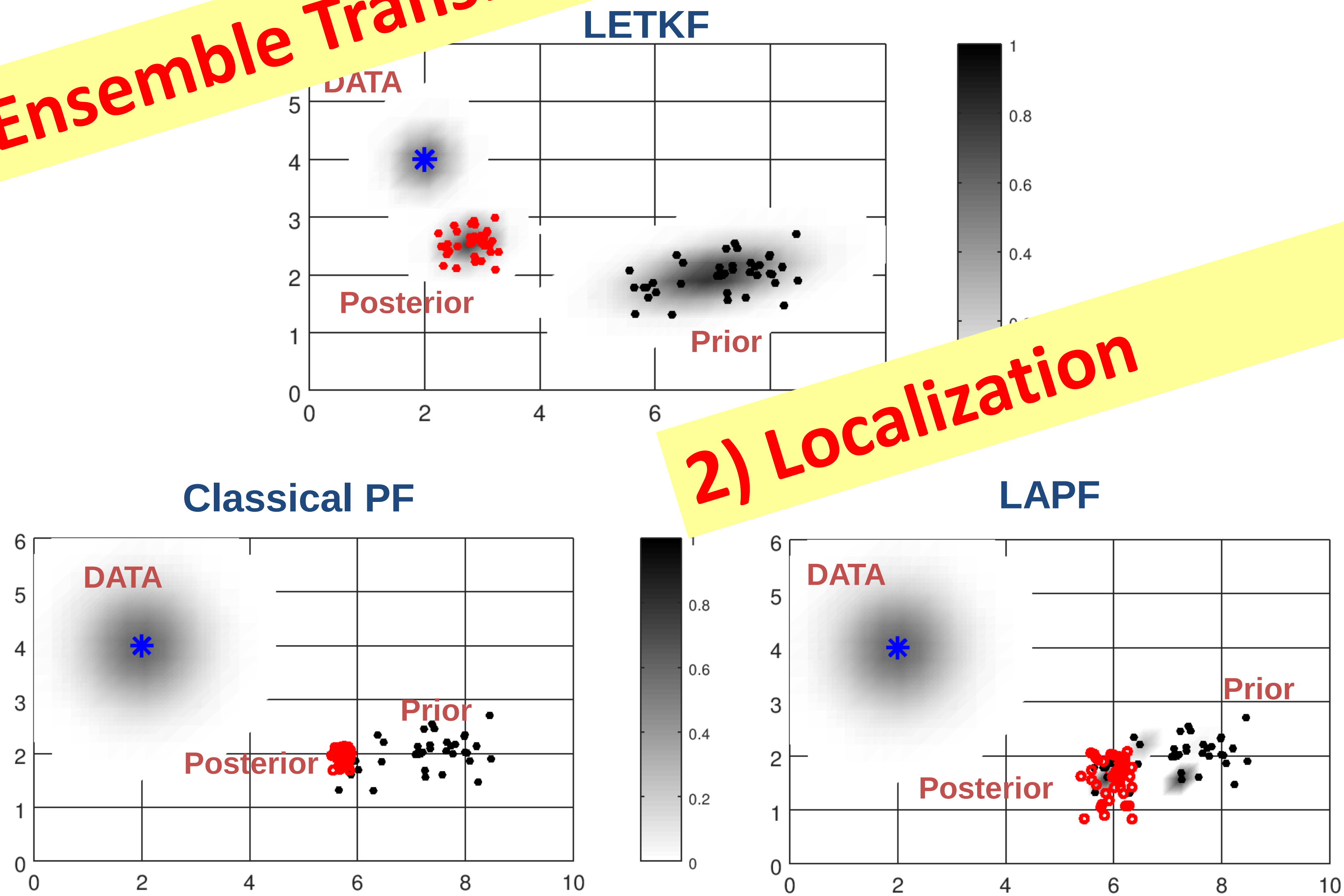
1) Ensemble Transform

2) Localization



Bayesian Filtering via PF

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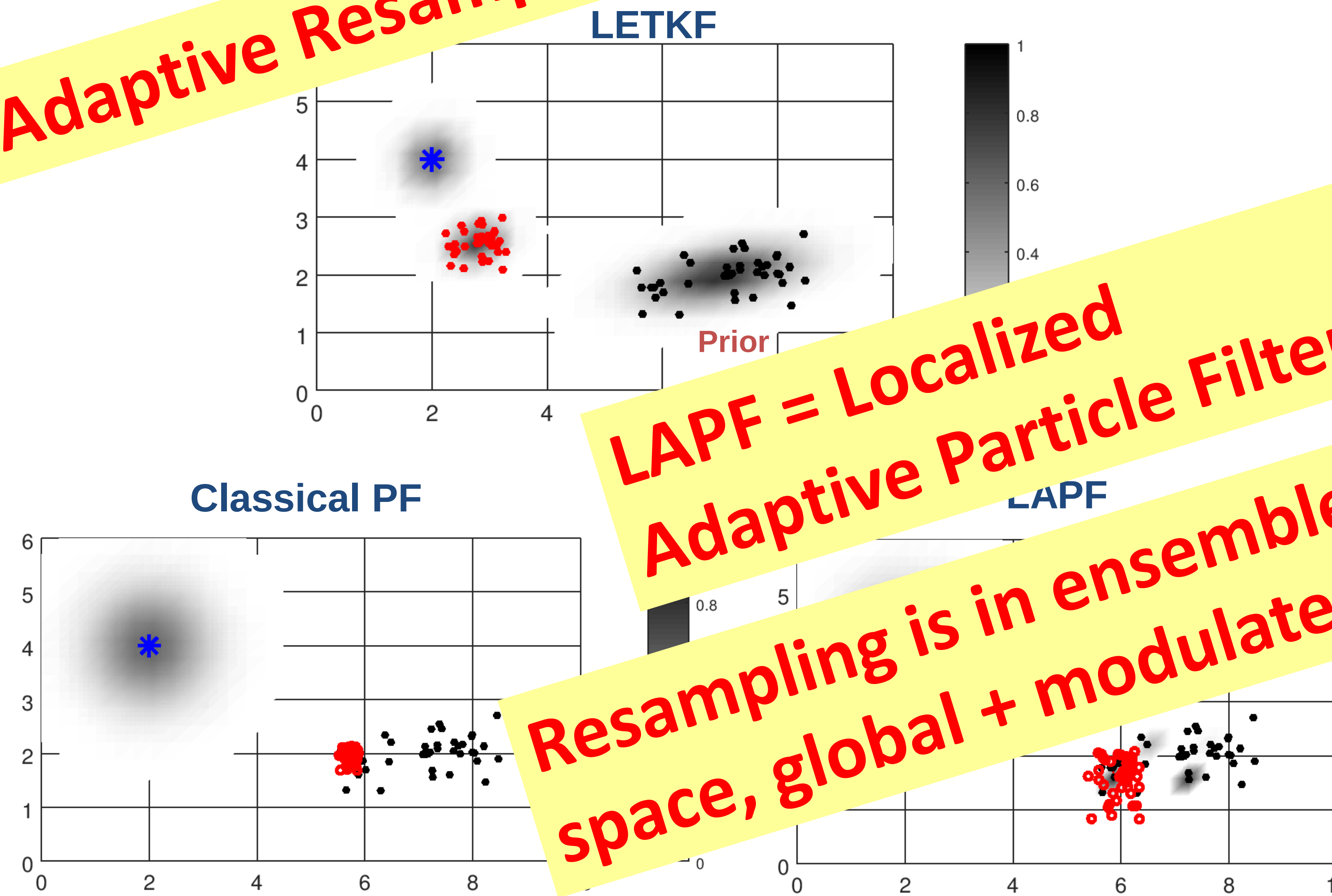
3) Adaptive Resampling



LAPF = Localized Adaptive Particle Filter

Resampling is in ensemble space, global + modulated

LAPF = Transform, Localization, Adaptivity with **global modulated Resampling**

First Step: The Classical Particle Filter

- **Bayes formula** to calculate new analysis distribution

$$p_k^{(a)}(x) := p(x|y_k) = c\, p(y_k|x) p_k^{(b)}(x), \qquad x \in \mathbb{R}^n$$

c is a normalization factor: $\int_X \; p_k^{(a)}(x) dx = 1$

Classical PF Approach

- To carry out the analysis step at time t_k **aposteriori weights** $p_k^{(a)}$ are calculated

$$p_{k,l}^{(a)} = c\, e^{-\frac{1}{2}\left(y-Hx^{(l)}\right)^T R^{-1}\left(y-Hx^{(l)}\right)}$$

c is chosen such that $\sum_{l=1}^{L} p_{k,l}^{(a)} = L$

Second Step: Classical Resampling

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- **Accumulated weights** w_{ac} are defined:

$$w_{ac_0} = 0$$
$$w_{ac_i} = w_{ac_{i-1}} + p_i^a, \qquad i = 1, \ldots, L$$

  where L denotes the ensemble size

- Drawing $r_j \sim U([0,1]), j = 1, \ldots, L$, set $R_j = j - 1 + r_j$ and define **transform matrix *W*** for the particles by:

$$W_{i,j} = \begin{cases} 1 & if\ R_j \in \left(w_{ac_{i-1}}, w_{ac_i}\right], \\ 0 & otherwise, \end{cases}$$

  $i, j = 1, \ldots, L$ with $W \in \mathbb{R}^{LxL}$, $(s, t]$ denotes the interval of values $s < \eta \leq t$.

Resampling

Third Step: Spread Control

Adaptivity based on o-b statistics

- Based on the adaptive multiplicative **inflation factor ρ** determined by the LETKF

$$\rho = \frac{\mathrm{E}\left[\boldsymbol{d}_{o-b}^{T}\boldsymbol{d}_{o-b}\right] - \mathrm{Tr}(\mathbf{R})}{Tr(\boldsymbol{H}\boldsymbol{P}^{b}\boldsymbol{H}^{T})}$$

- **Weighting factor α** has been chosen, due to the small ensemble size ($L = 40$)

$$\rho_k = \alpha\tilde{\rho}_k + (1-\alpha)\rho_{k-1}$$

Third Step: Spread Control

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- **Pertubation factor σ** is used to add spread to the system

$$\sigma = \begin{cases} c_0, & \rho < \rho^{(0)} \\ c_0 + (c_1 - c_0) * \dfrac{\rho - \rho^{(0)}}{\rho^{(1)} - \rho^{(0)}}, & \rho^{(0)} \leq \rho \leq \rho^{(1)} \\ c_1, & \rho > \rho^{(1)} \end{cases}$$

where $c_0 = 0.02$, $c_1 = 0.2$,

$\rho^{(0)} = 1.0$ and $\rho^{(1)} = 1.4$, with

$\sigma = c_1$ if $\rho \geq \rho^{(1)}$ and

$\sigma = c_0$ if $\rho \leq \rho^{(0)}$

Enforce the desired spread!

Fourth Step: Gaussian Resampling

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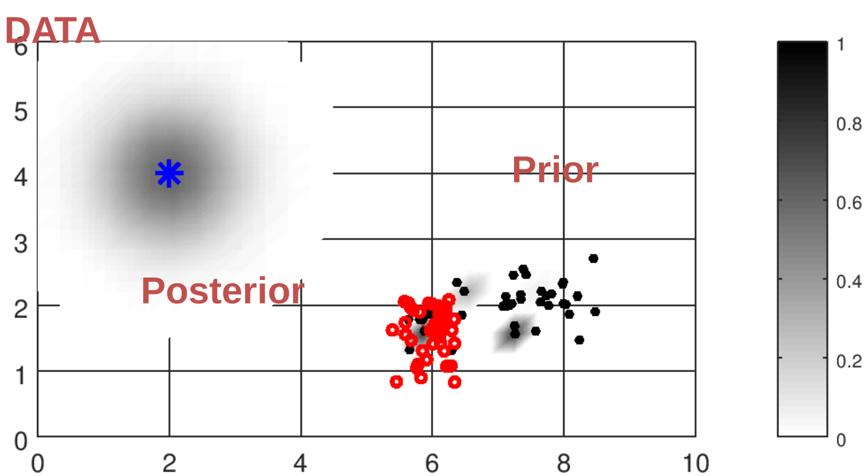
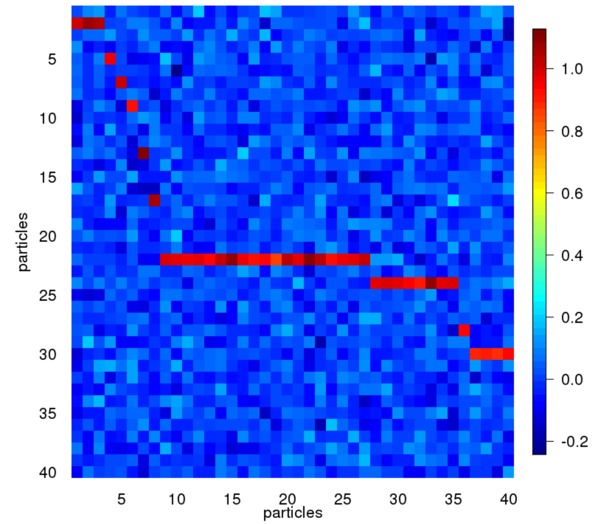
- **Weights *W*** are modified by applying the **pertubation factor σ**

$$W = W + R_{nd} * \sigma$$

with R_{nd} normally distributed random numbers



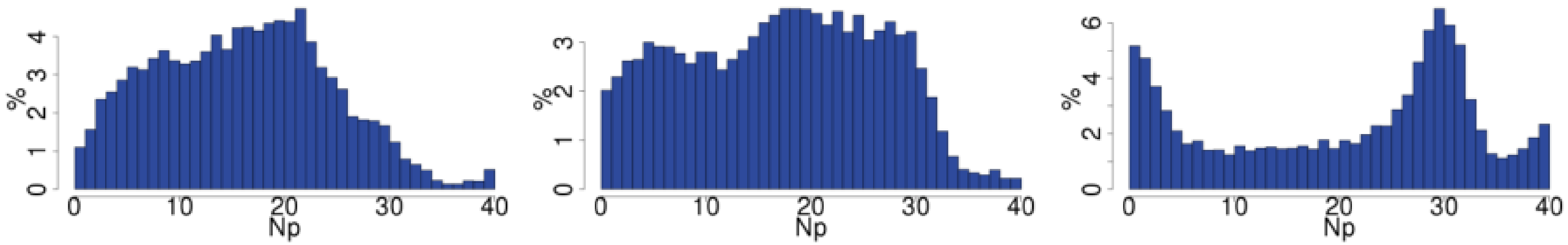


An example for a W-Matrix after applying σ determined wit… for 60… are chosen

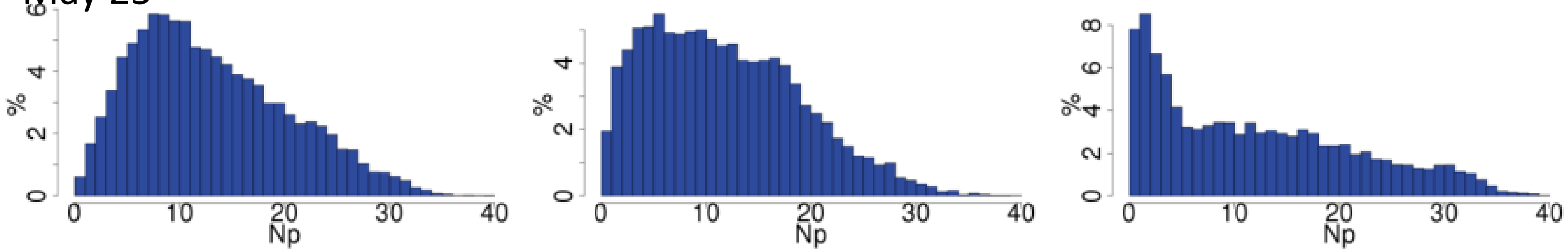
Enforce the desired spread!

Effective Ensemble Size Distributions

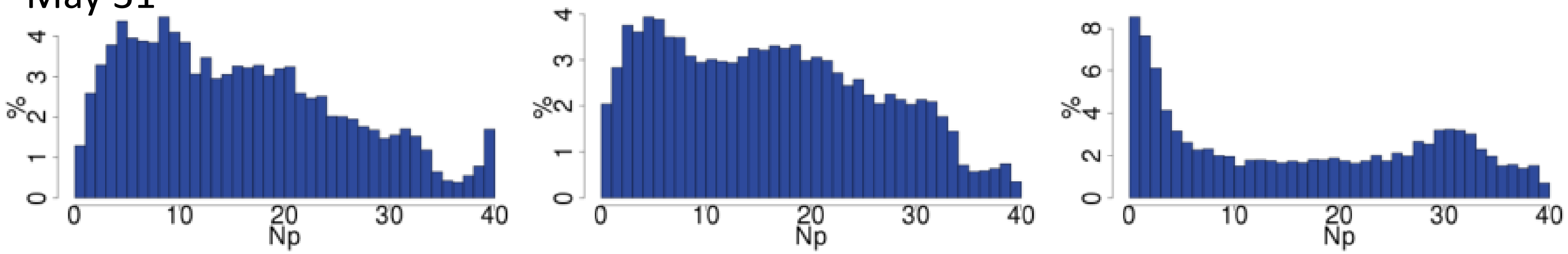
May 20



May 25



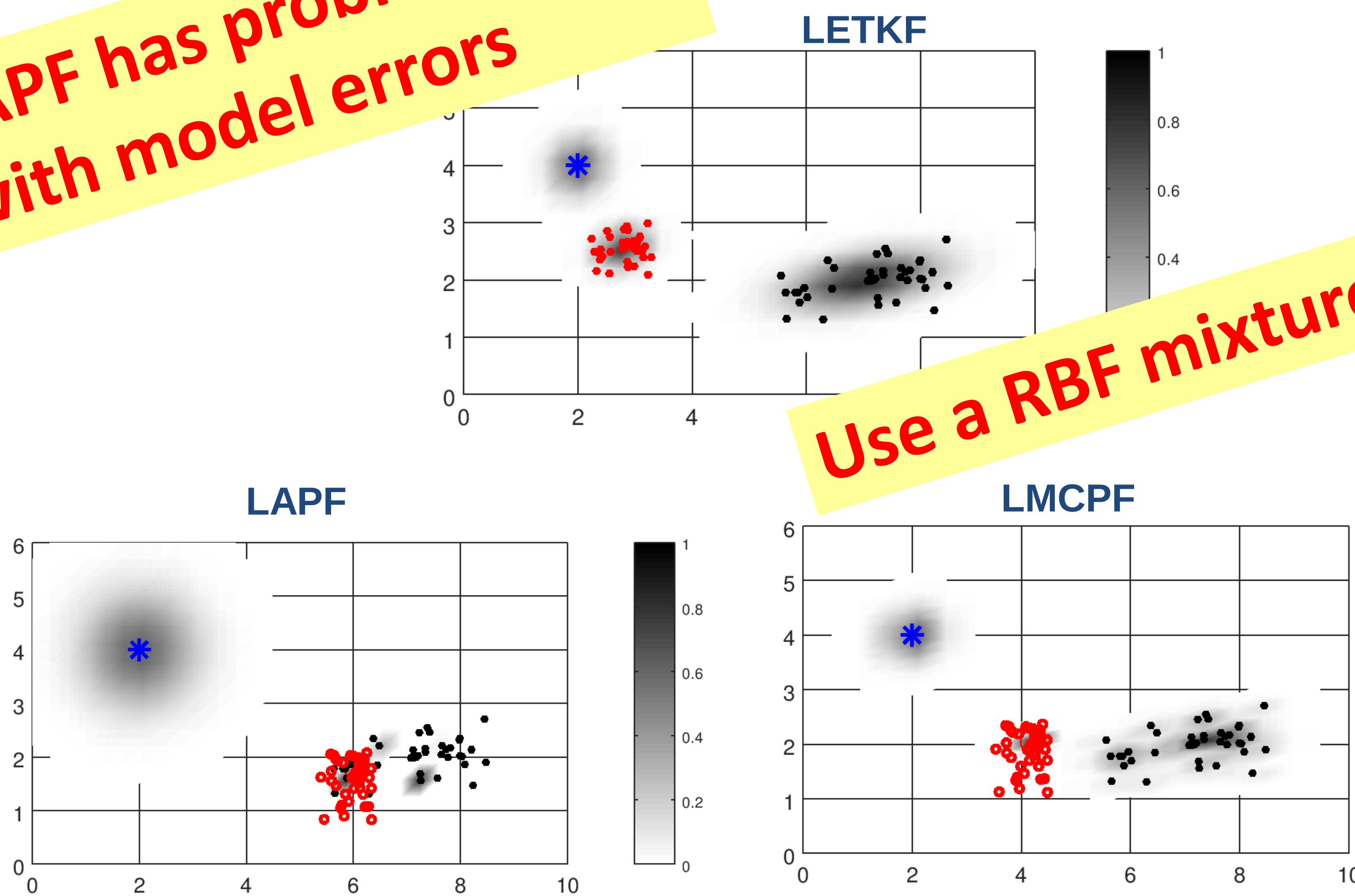
May 31



100 hPa | 500 hPa | 1000 hPa

LAPF versus LMCPF

LAPF has problems with model errors



Use a RBF mixture

LMCPF = Transform, Localization, RBF mixture, Adaptivity

LMCPF Basics

- **Kalman Filter**

$$x^{(a)} = x^{(b)} + BH^T(R + HBH^T)^{-1}(y - Hx^{(b)})$$

$$K = BH^T(R + HBH^T)^{-1} \qquad \tilde{B} = (I - KH)B$$

- **Ensemble B Estimator**

$$\bar{x} := \frac{1}{L}\sum_{\ell=1}^{L} x^{(\ell)}$$

$$\boxed{B = \frac{1}{L-1} X X^T}$$

$$X = \left(x^{(1)} - \bar{x}, \ldots, x^{(L)} - \bar{x}\right) \quad \in \mathbb{R}^{n \times L}.$$

LMCPF Basics: B Posterior

$$\boxed{Y := HX}$$

$$\begin{aligned}
\tilde{B} &= (I - KH)B \\
&= (I - BH^T(R + HBH^T)^{-1}H)B \\
&= \Big(I - \gamma X \boxed{X^T H^T}(R + \gamma \boxed{HX}\boxed{X^T H^T})^{-1}H\Big)\gamma X X^T \\
&= X\Big(I - \gamma Y^T(R + \gamma Y Y^T)^{-1} Y\Big)\gamma X^T \\
&= X\Big(I - \gamma\boxed{(I + \gamma Y^T R^{-1} Y)^{-1} Y^T R^{-1}} Y\Big)\gamma X^T \\
&= X\Big((I + \gamma Y^T R^{-1} Y)^{-1}(\boxed{I + \gamma Y^T R^{-1} Y} - \gamma Y^T R^{-1} Y\Big)\gamma X^T \\
&= X(I + \gamma Y^T R^{-1} Y)^{-1}\gamma X^T \\
&= X(\frac{1}{\gamma} I + Y^T R^{-1} Y)^{-1} X^T
\end{aligned}$$

$$\boxed{Y^T(R + \gamma Y Y^T)^{-1} = (I + \gamma Y^T R^{-1} Y)^{-1} Y^T R^{-1}}$$

RBF Basis Function in Ensemble Space

LMCPF Basics: Bayes Formula

Gaussian Mixture Case

$$
\begin{aligned}
p(x|y) &= cp(y|x) \cdot p(x) \\
&= ce^{-\frac{1}{2}(y-Hx)^T R^{-1}(y-Hx)} \sum_{\ell=1}^{L} p_G(x - x^{(\ell)}) \\
&= c \sum_{\ell=1}^{L} e^{-\frac{1}{2}(y-Hx)^T R^{-1}(y-Hx)} p_G(x - x^{(\ell)}),
\end{aligned}
$$

$$
p_G(x - x^{(\ell)}) = \tilde{c} e^{-\frac{1}{2}(x-x^{(\ell)})^T G^{-1}(x-x^{(\ell)})}
$$

Explicit Calculations possible for each term

We need a selection based on relative weights!

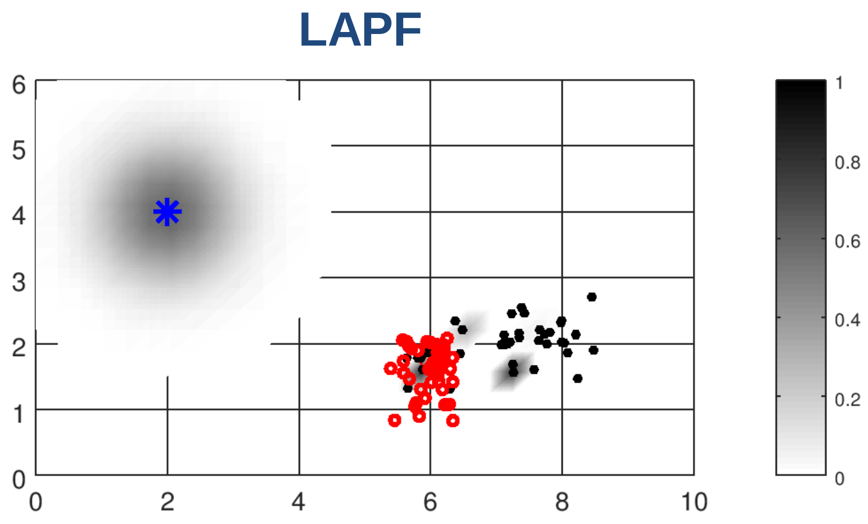
LMCPF Basics: Relative Weights

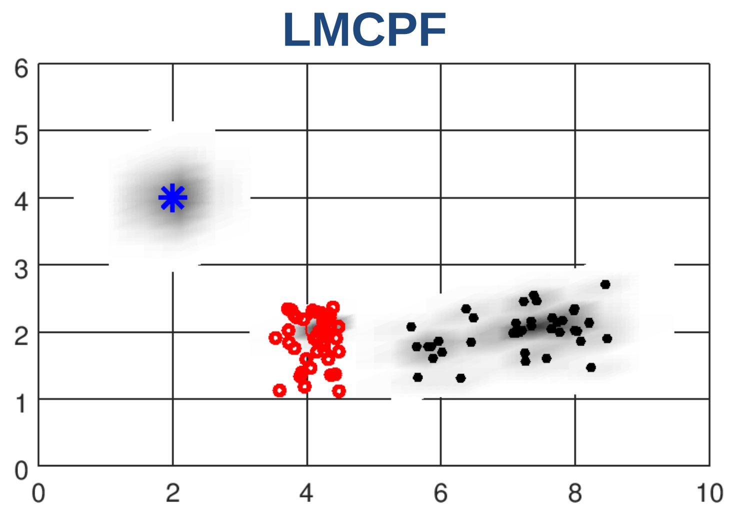
Deutscher Wetterdienst
Wetter und Klima aus einer Hand

$$w_\ell := e^{-\frac{1}{2}(y-Hx^{(\ell)})^T R^{-1}(y-Hx^{(\ell)})}, \quad \ell = 1, ..., L$$

$$w_{tot} := \sum_{\ell=1}^{L} w_\ell.$$

We need a selection based on relative weights!





LAPF and LMCPF Weights

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Projection onto Ensemble Space

Abbreviating $A := \mathbf{Y}^T\mathbf{R}^{-1}\mathbf{Y}$ and $C := A^{-1}\mathbf{Y}^T\mathbf{R}^{-1}(\mathbf{y}^o - \overline{\mathbf{y}}^b)$

Projection Operator

$$P(\mathbf{y}^o - \overline{\mathbf{y}}^b) = \mathbf{Y}(\mathbf{Y}^T\mathbf{R}^{-1}\mathbf{Y})^{-1}\mathbf{Y}^T\mathbf{R}^{-1}(\mathbf{y}^o - \overline{\mathbf{y}}^b),$$

Projected discrepancy

$$\begin{aligned} P(\mathbf{y}^o - H\mathbf{x}^{(\ell)}) &= \mathbf{Y}A^{-1}\mathbf{Y}^T\mathbf{R}^{-1}((\mathbf{y}^o - \overline{\mathbf{y}}^b) - \mathbf{Y}e_\ell) \\ &= \mathbf{Y}(C - e_\ell), \;\; \ell = 1, \ldots, L. \end{aligned}$$

Exponent

$$P(\mathbf{y}^o - H\mathbf{x}^{(\ell)})]^T\mathbf{R}^{-1}P(\mathbf{y}^o - H\mathbf{x}^{(\ell)}) = [C - e_\ell]^T A[C - e_\ell], \;\; \ell = 1, \ldots, L,$$

Weight

$$\boxed{w_{k,\ell} = ce^{-\frac{1}{2}[C-e_\ell]^T A[C-e_\ell]}, \;\; \ell = 1, \ldots, L.}$$

LAPF and LMCPF Weights

Deutscher Wetterdienst
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Classical versus projected weights

$$
\begin{aligned}
w_{k,\ell}^{classical} &= e^{-\frac{1}{2}[(\mathbf{y}^o - H\mathbf{x}^{(\ell)})]^T \mathbf{R}^{-1}[(\mathbf{y}^o - H\mathbf{x}^{(\ell)})]} \\
&= e^{-\frac{1}{2}[\left(P+(I-P)\right)(\mathbf{y}^o - H\mathbf{x}^{(\ell)})]^T \mathbf{R}^{-1}[\left(P+(I-P)\right)(\mathbf{y}^o - H\mathbf{x}^{(\ell)})]} \\
&= e^{-\frac{1}{2}[P(\mathbf{y}^o - H\mathbf{x}^{(\ell)})]^T \mathbf{R}^{-1}[P(\mathbf{y}^o - H\mathbf{x}^{(\ell)})]} \cdot \underbrace{e^{-\frac{1}{2}[(I-P)(\mathbf{y}^o - H\mathbf{x}^{(\ell)})]^T \mathbf{R}^{-1}[(I-P)(\mathbf{y}^o - H\mathbf{x}^{(\ell)})]}}_{=\tilde{c}},
\end{aligned}
$$

Factor is a constant term, since we have

$$
\begin{aligned}
(I-P)(\mathbf{y}^o - Hx^{(\ell)}) &= (I-P)(\mathbf{y}^o - \overline{\mathbf{y}}^b + \mathbf{Y}e_\ell) \\
&= (I-P)(\mathbf{y}^o - \overline{\mathbf{y}}^b) - \underbrace{(I-P)\mathbf{Y}e_\ell}_{=0}.
\end{aligned}
$$

Projected particle filter weights and classical particle filter weights are <u>equivalent theoretically</u>, but numerically <u>remove a very small common factor</u>

Fourth Step: Gaussian Resampling

Deutscher Wetterdienst
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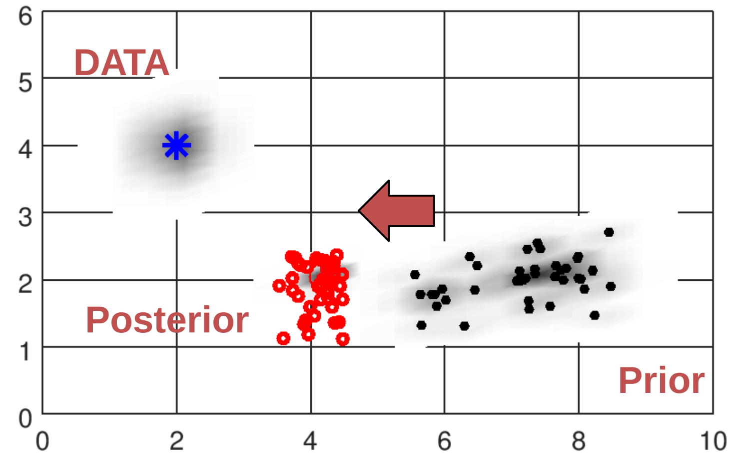
LMCPF = Local Markov Chain Particle Filter

- **Weights *W*** are calculated by drawing from the posterior

$$W = W + A_{shift} * W + B_{post} * R_{nd} * \sigma$$

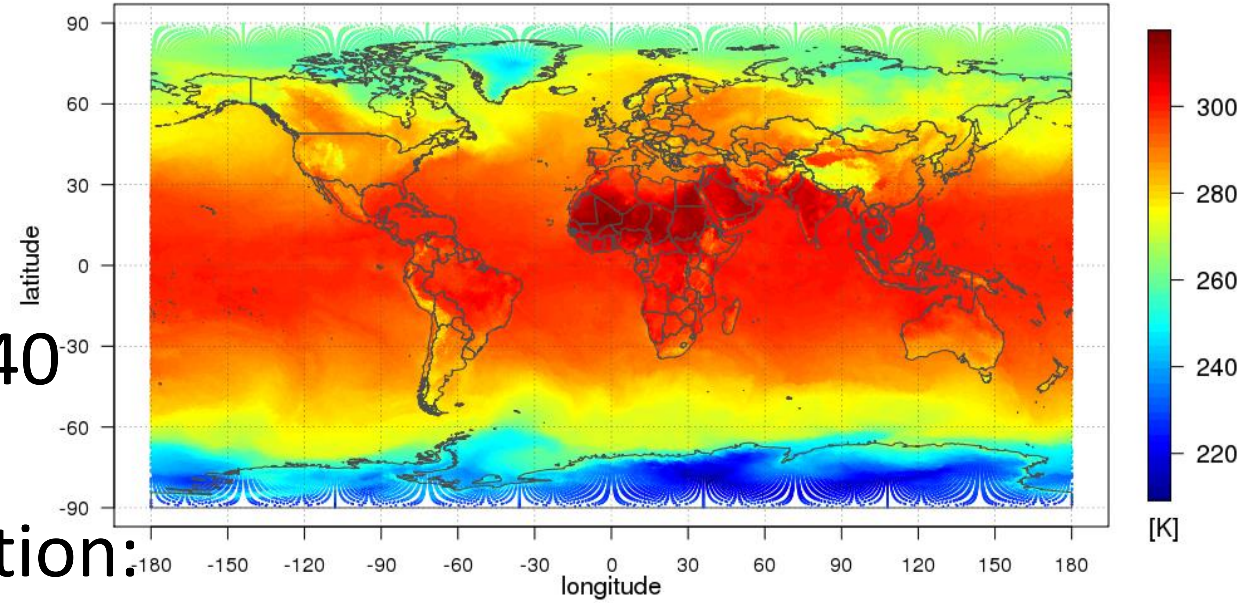
with R_{nd} normally distributed random numbers,
A_{shift} and B_{post} calculated with Gaussian radial basis function (rbf) Approximation for prior density and observation error



✓ It is an **explicit calculation** of the **Bayes posterior** based on **radial basis function approximation** of the prior, with subsequent draws from that distribution in the MCMC sense.

Large-Scale Experimental Set-up

Deutscher Wetterdienst
Wetter und Klima aus einer Hand



- Full ensemble: 40 members
- Reduced resolution:
  - 26km deterministic
  - 52km ensembles
- Period: 01.05.2016 – 31.05.2016

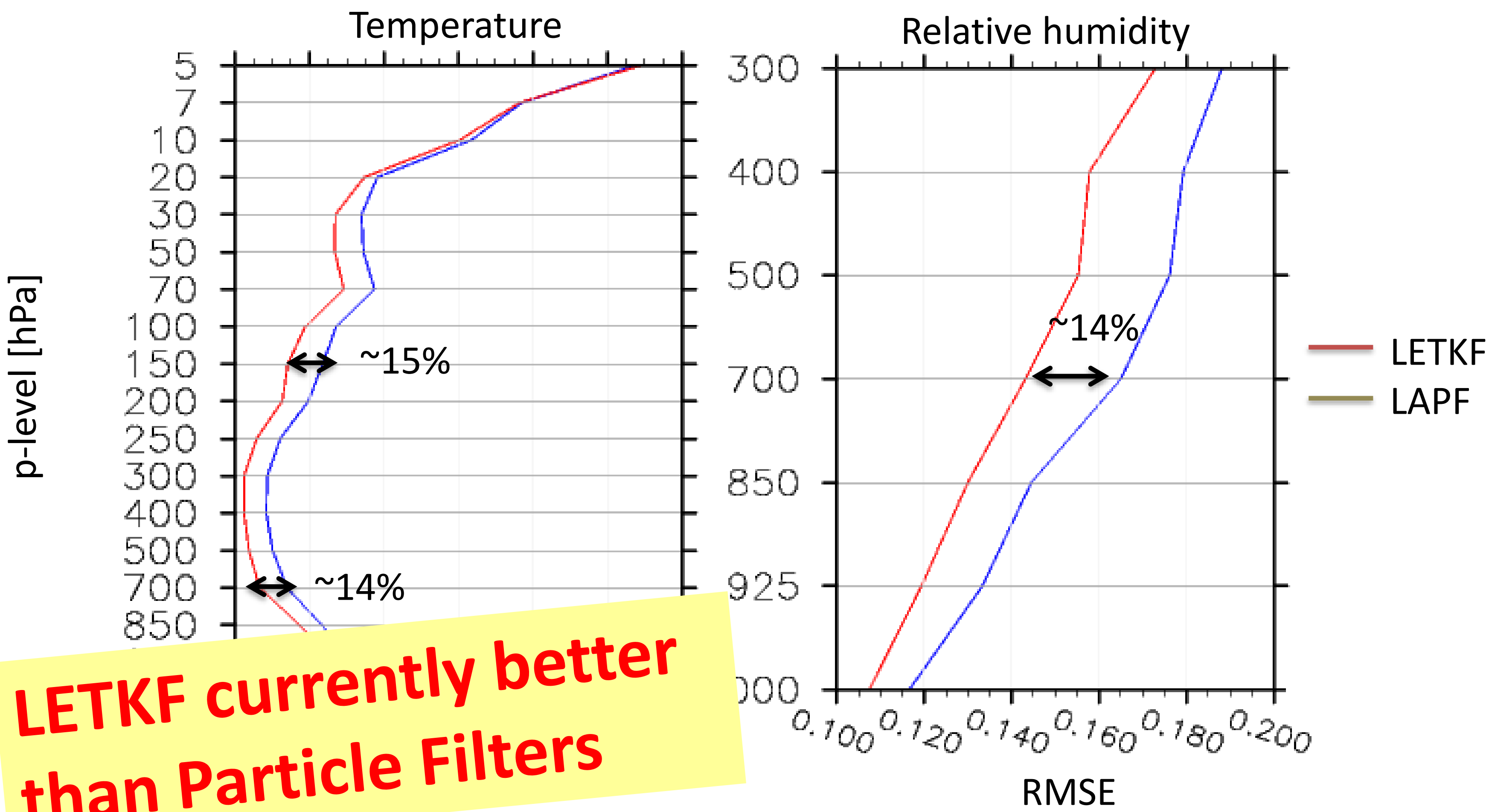
Experiments programmed and carried out **by Anne Walter, DWD& Uni Reading**, and Roland Potthast, DWD& Uni Reading

In Cooperation with Peter-Jan van Leeuwen , Uni Reading

LAPF Scores vs LETKF

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

Global **RMSE** for **obs-fg** statistics (Radiosondes vs. Model)
Period: 08.05.2016 – 31.05.2016

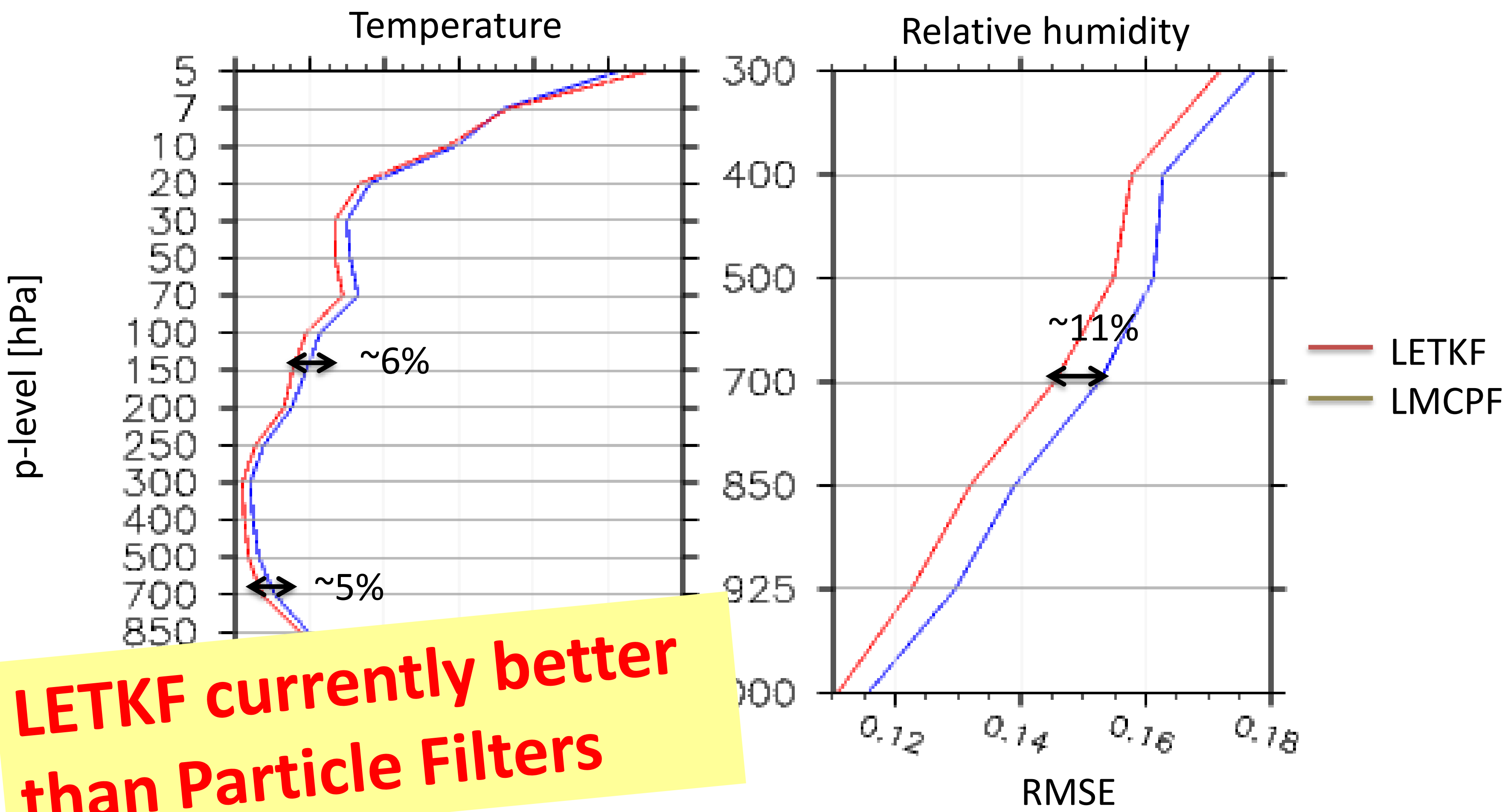


LETKF currently better than Particle Filters

Experiments programmed and carried out **by Anne Walter, DWD & Uni Reading**, and Roland Potthast, DWD & Uni Reading

LMCPF Scores vs LETKF

Global **RMSE** for **obs-fg** statistics (Radiosondes vs. Model)
Period: 08.05.2016 – 22.05.2016



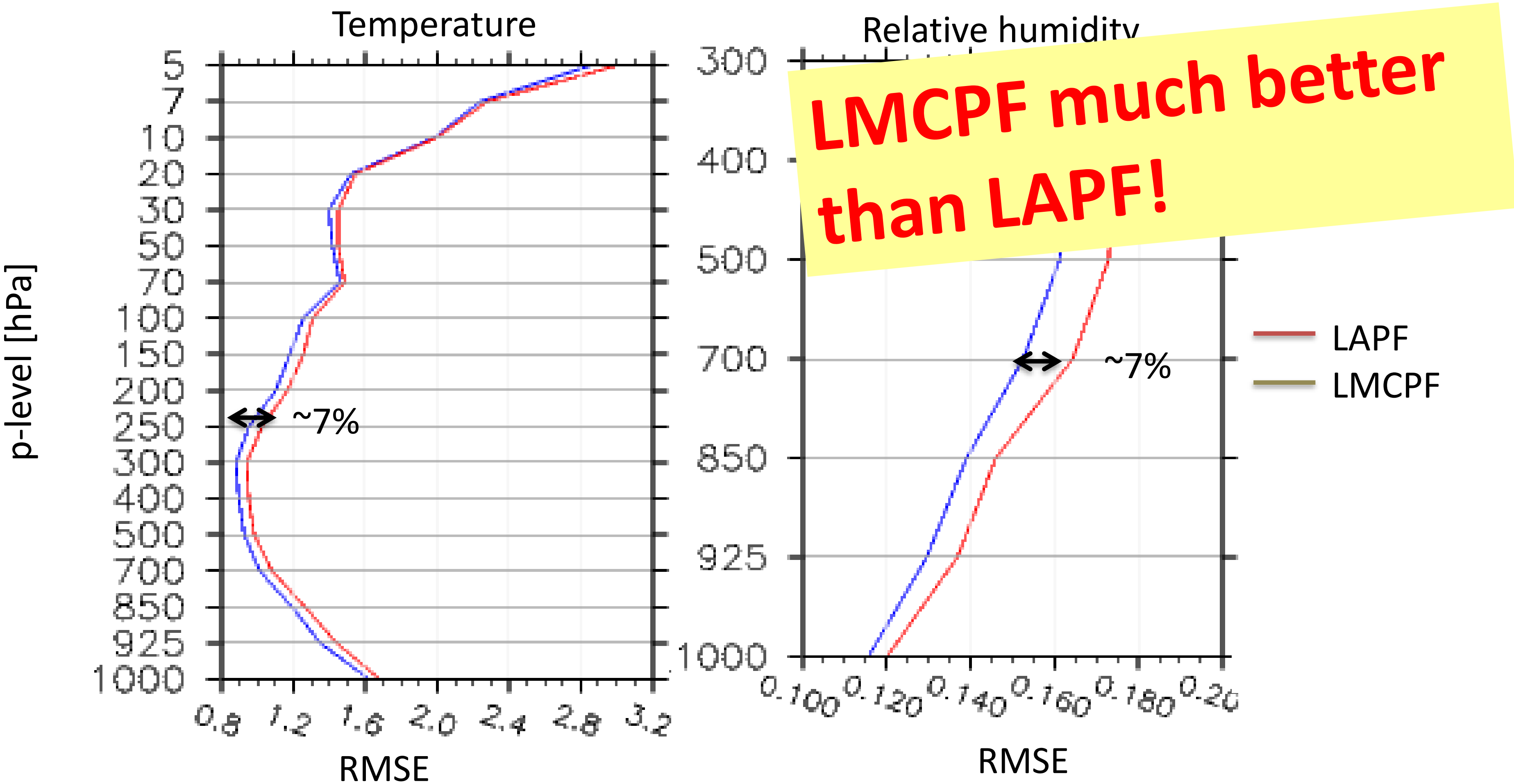
LETKF currently better than Particle Filters

Experiments programmed and carried out by Anne Walter, DWD & Uni Reading, and Roland Potthast, DWD & Uni Reading

LMCPF Scores vs LAPF

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

Global **RMSE** for **obs-fg** statistics (Radiosondes vs. Model)
Period: 08.05.2016 – 22.05.2016

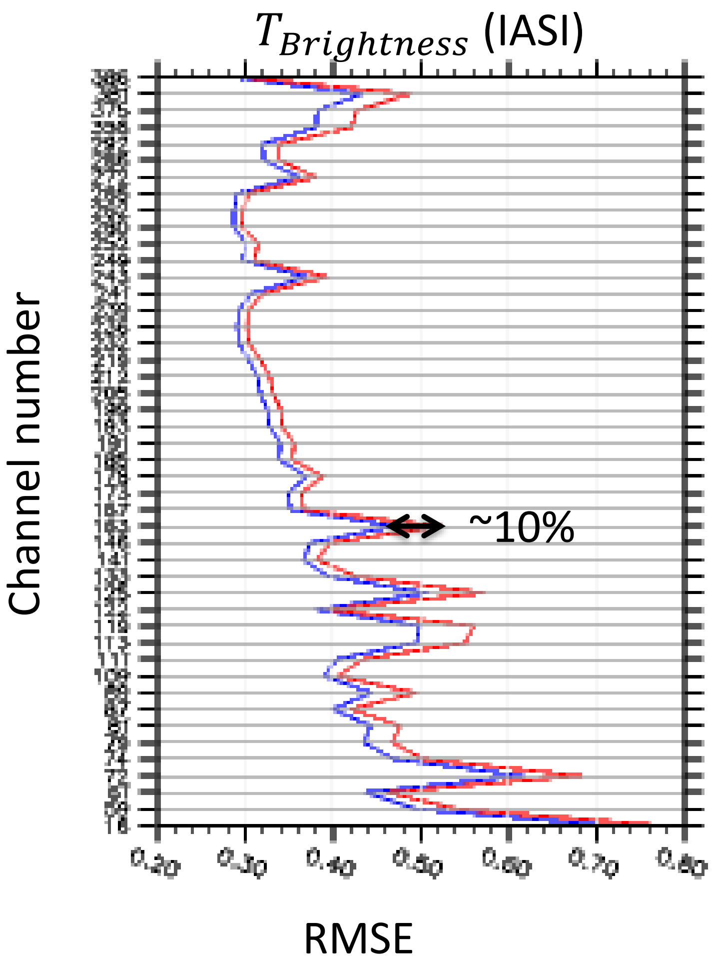


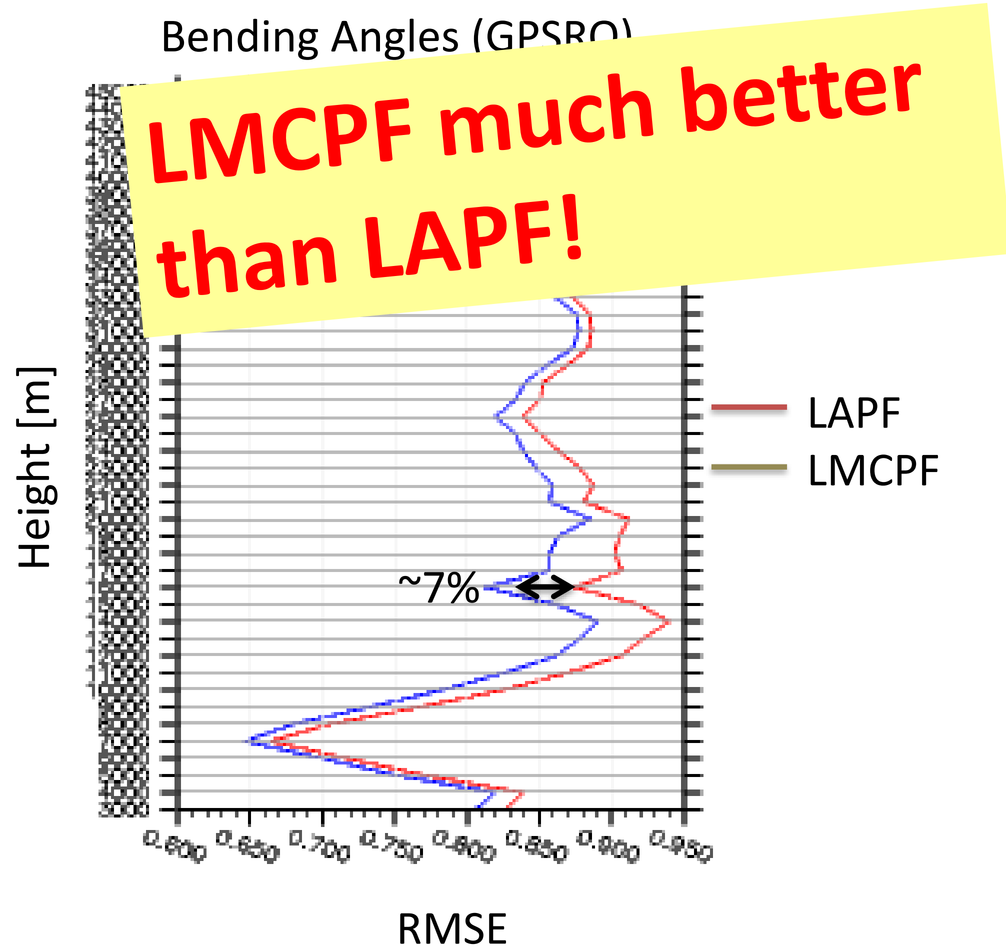
Experiments programmed and carried out **by Anne Walter, DWD & Uni Reading**, and Roland Potthast, DWD & Uni Reading

LMCPF Scores vs LAPF

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

Global **RMSE** for **obs-fg** statistics
Period: 08.05.2016 – 22.05.2016

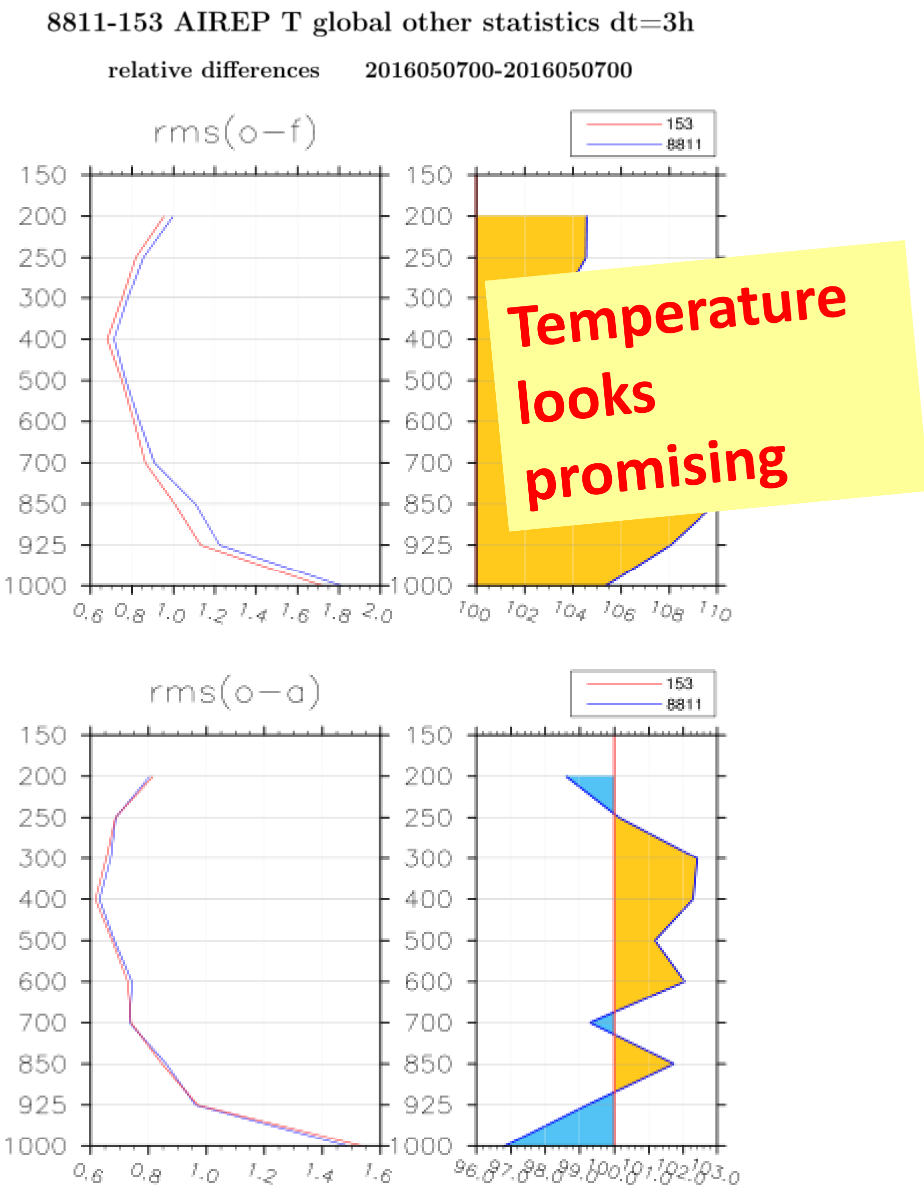


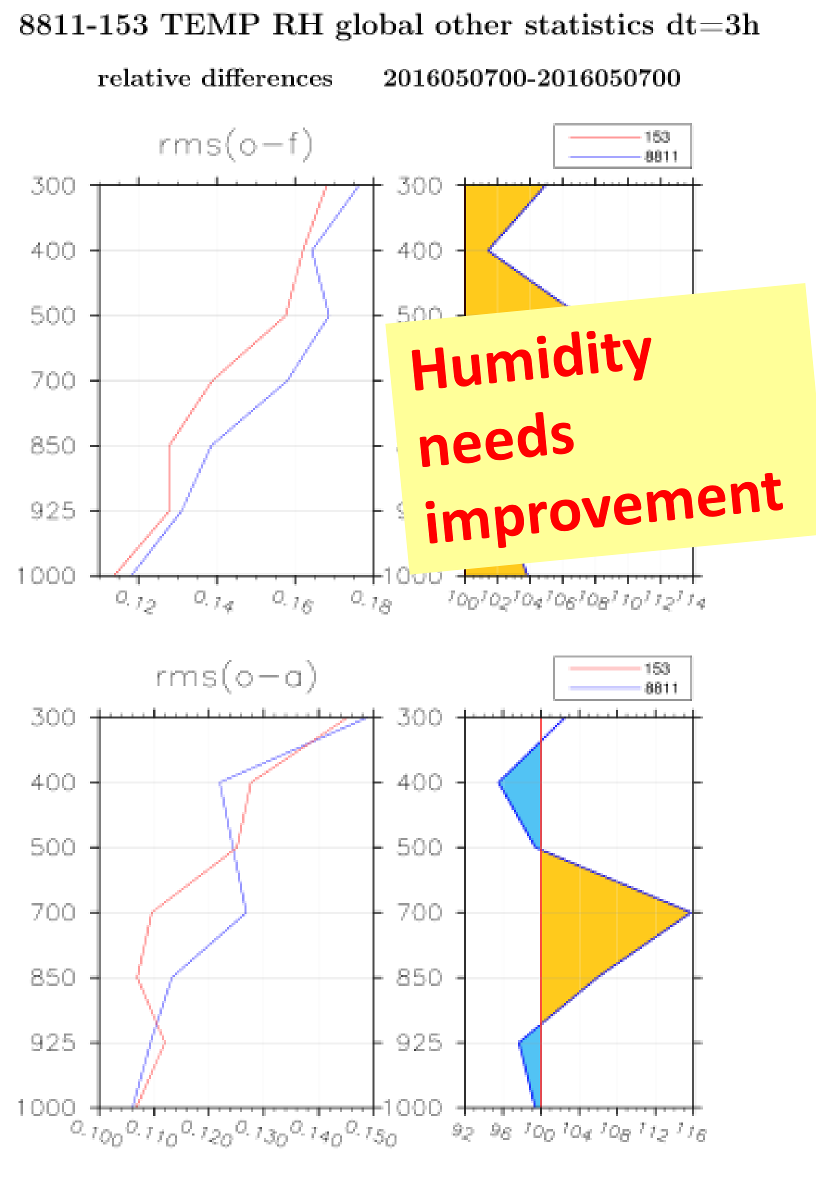


Experiments programmed and carried out **by Anne Walter, DWD & Uni Reading**, and Roland Potthast, DWD & Uni Reading

New LAMCPF Scores vs LETKF

Deutscher Wetterdienst
Wetter und Klima aus einer Hand





LAPF Spread vs LMCPF & LETKF

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

Global **spread** of T [K] ~ 500 hPa

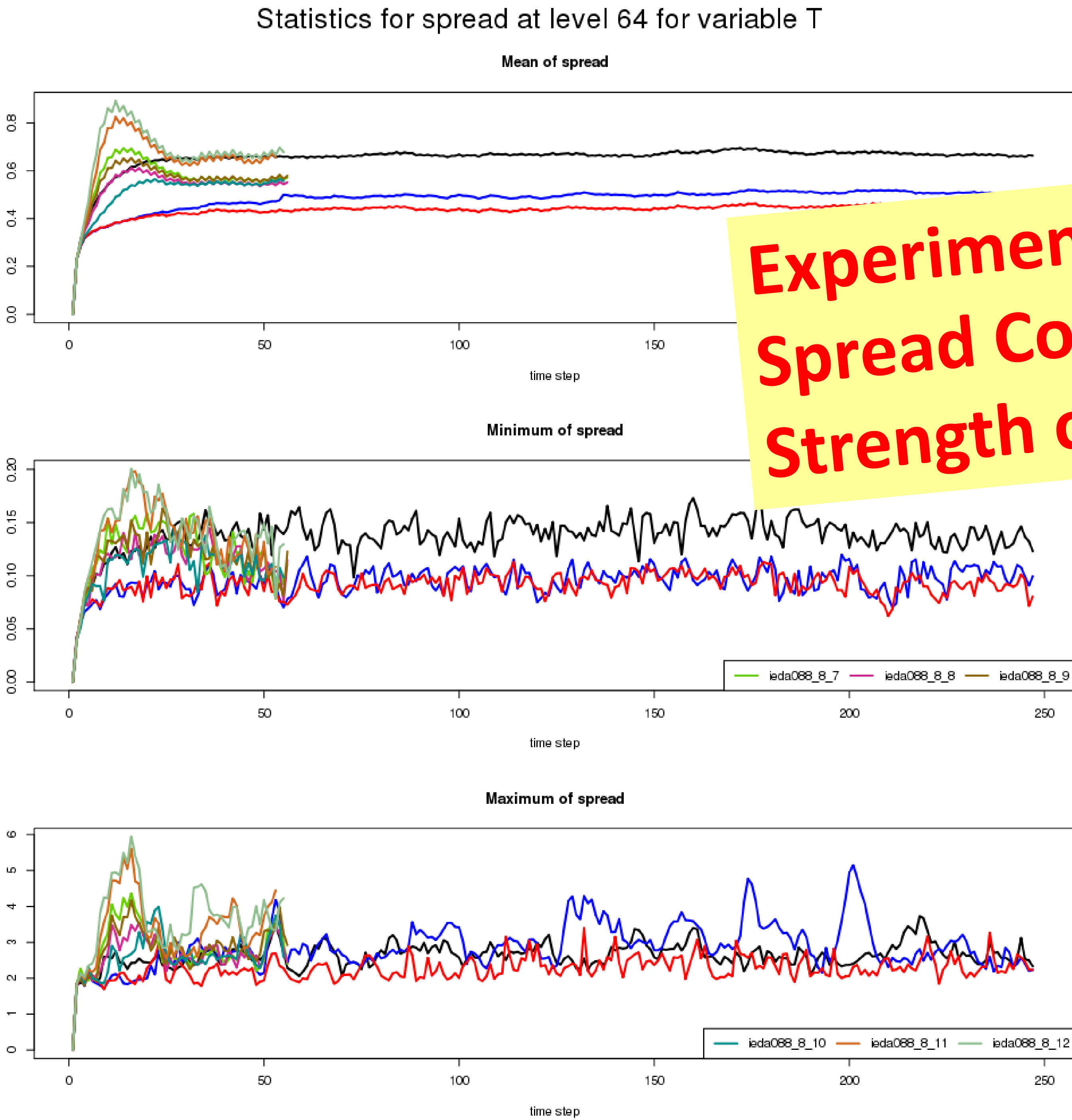
Experiments programmed and carried out **by Anne Walter, DWD & Uni Reading**, and Roland Potthast, DWD & Uni Reading

DWD

utscher Wetterdienst

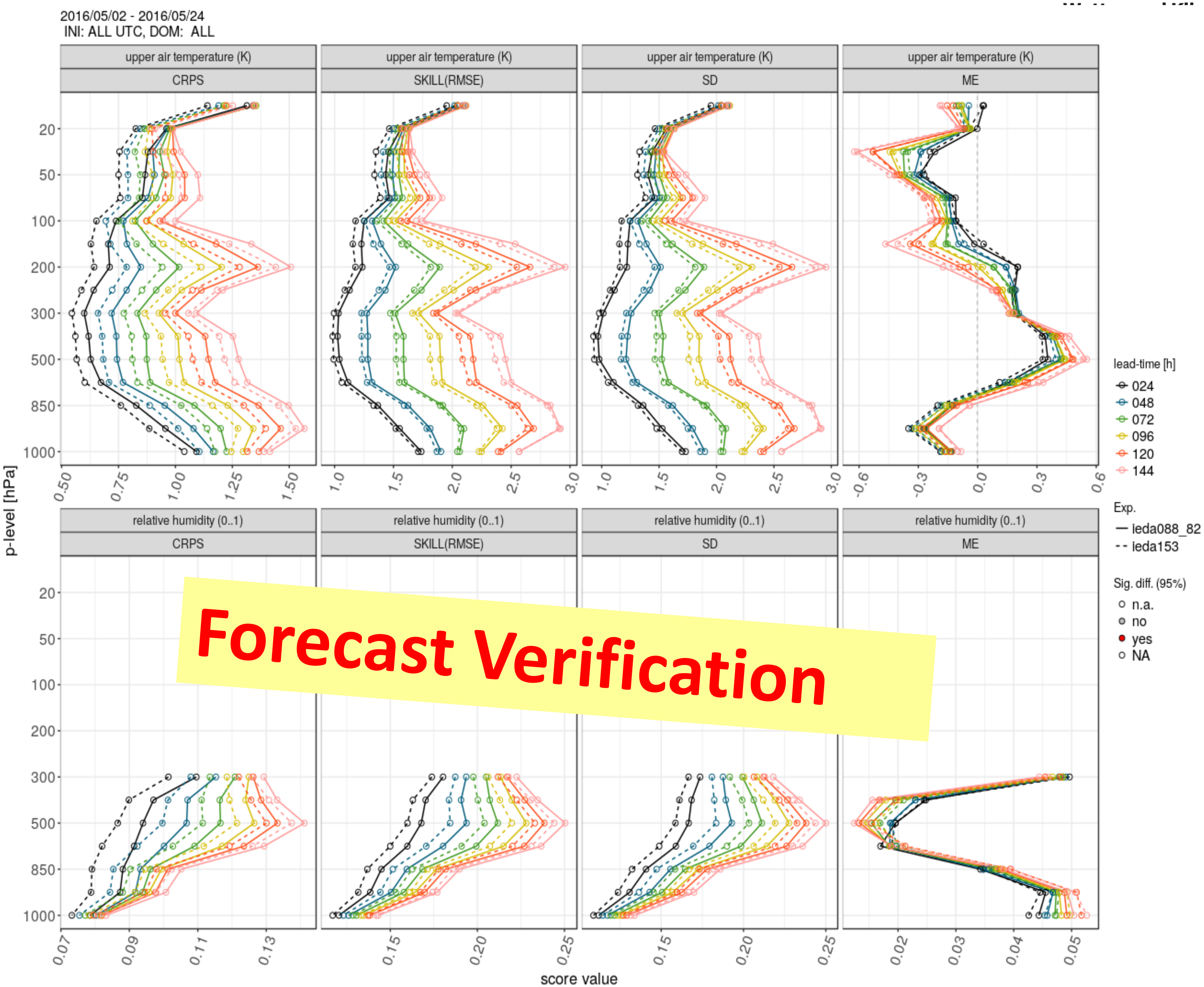
tter und Klima aus einer Hand

Experiments with Spread Control and Strength of Shifts



LMCPF Scores vs LETKF

Deutscher Wetterdienst
a aus einer Hand

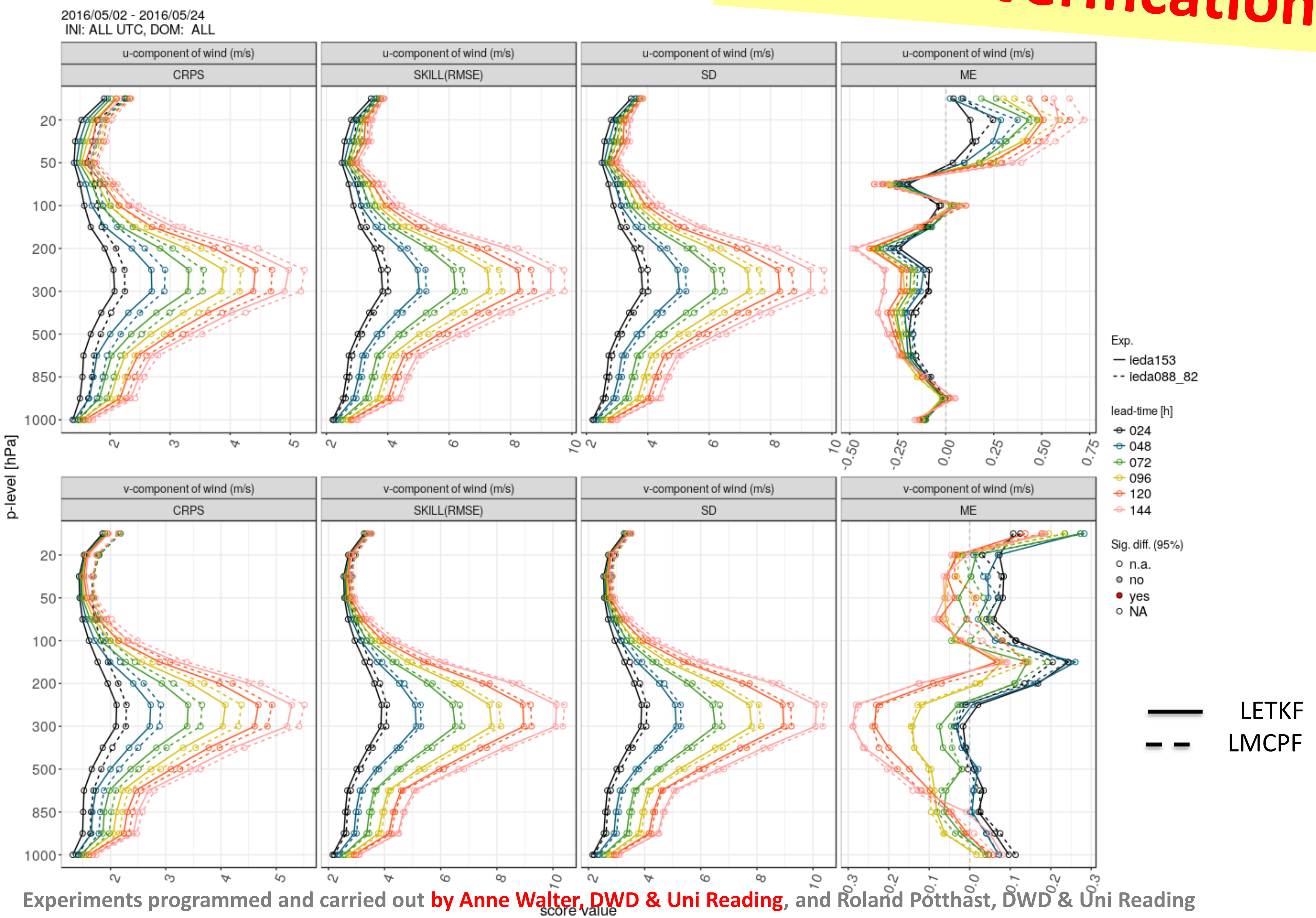


LETKF
LMCPF

Experiments programmed and carried out by Anne Walter, DWD & Uni Reading, and Roland Potthast, DWD & Uni Reading

LMCPF Scores vs LETKF

Forecast Verification



Experiments programmed and carried out by Anne Walter, DWD & Uni Reading, and Roland Potthast, DWD & Uni Reading

Summary LAPF and LMCPF

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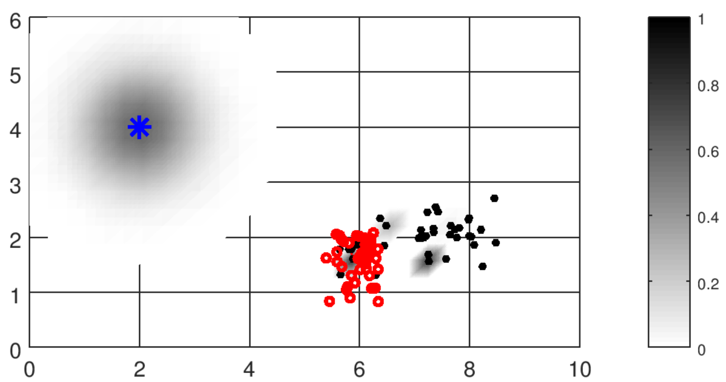
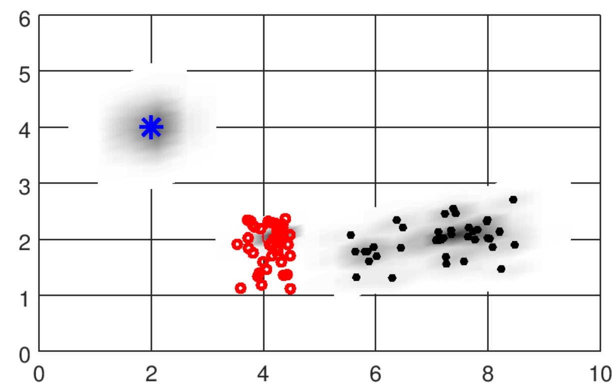
Wetter und Klima aus einer Hand

LAPF



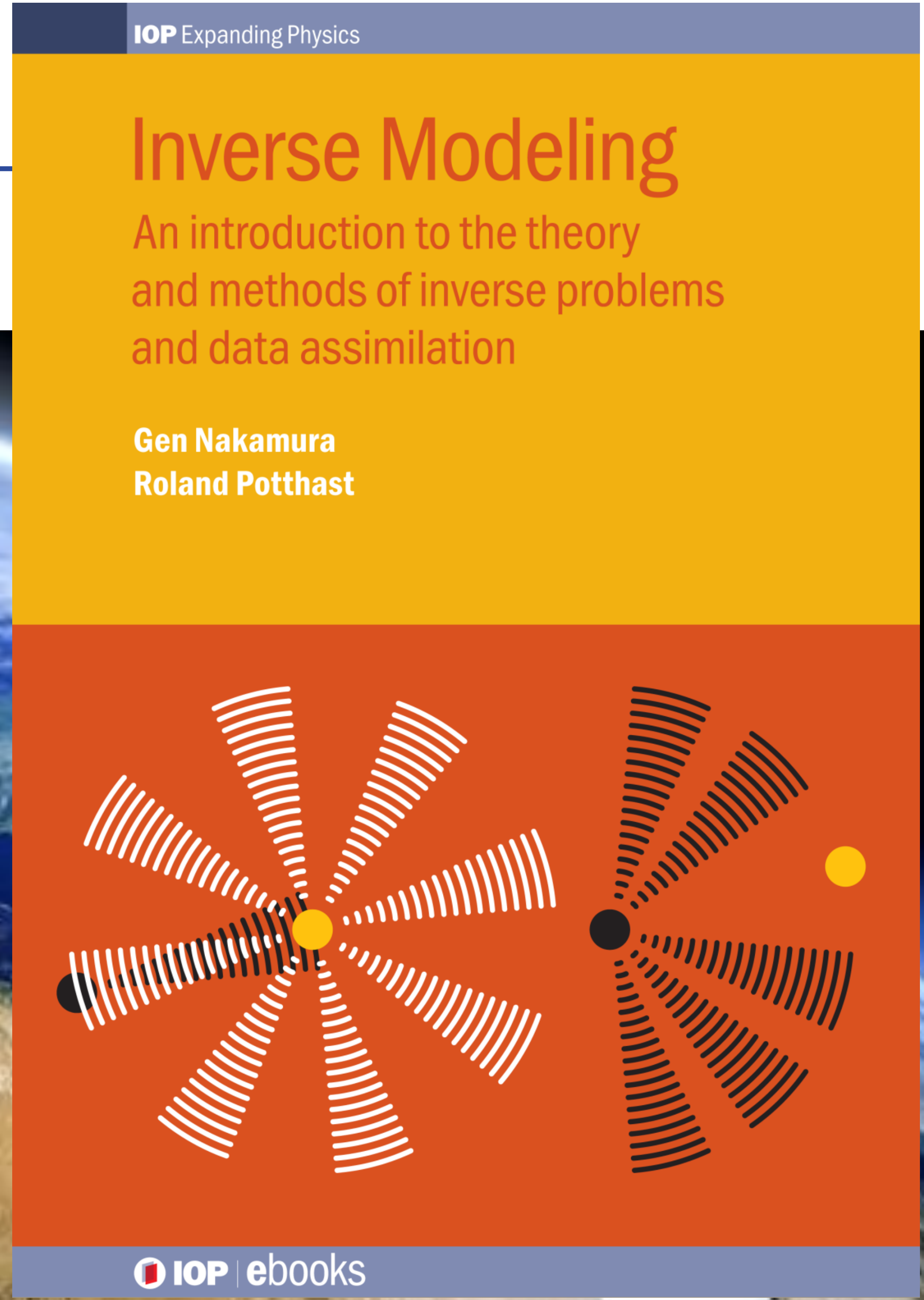
LMCPF



- LAPF and LMCPF are implemented in an **operational NWP system:** **Globally + mesoscale, convective scale**
- Both Particle Filters are able to provide **reasonable atmospheric analysis** in a large-scale (high-dimensional) environment and are running stably over a period of one month
- The LMCPF outperforms the LAPF but not yet the LETKF, but both Particle Filters are not far behind the operational LETKF

Both Particle Filters are showing promising results; further tuning and development is in progress.

Many Thanks!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