

On Ensemble and Particle Filters for Large-Scale Data Assimilation

Roland Potthast

Hendrik Reich, Christoph Schraff

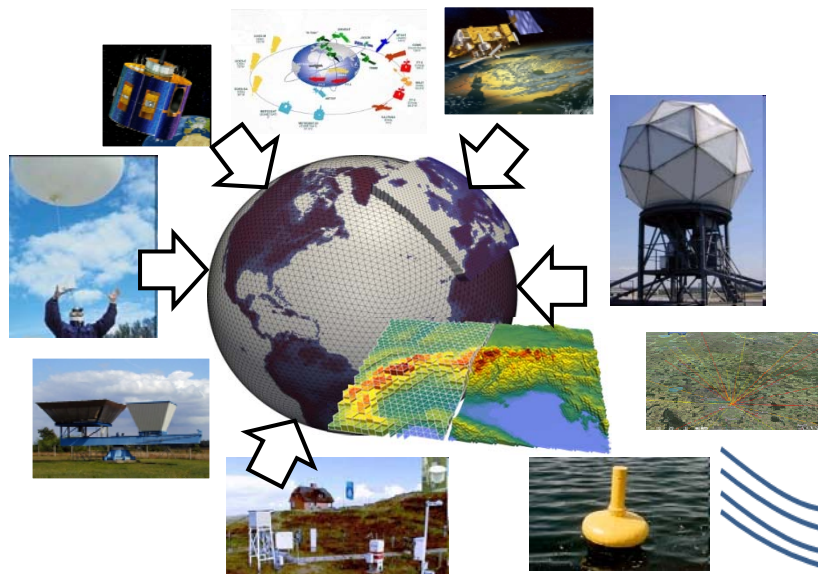
Andreas Rhodin, Ana Fernandez

Alexander Cress, Dora Foring

Annika Schomburg, Africa Perianez

Jason Otkin, Robin Faulwetter

Daniel Leuenberger, Hans Rdi Knsch

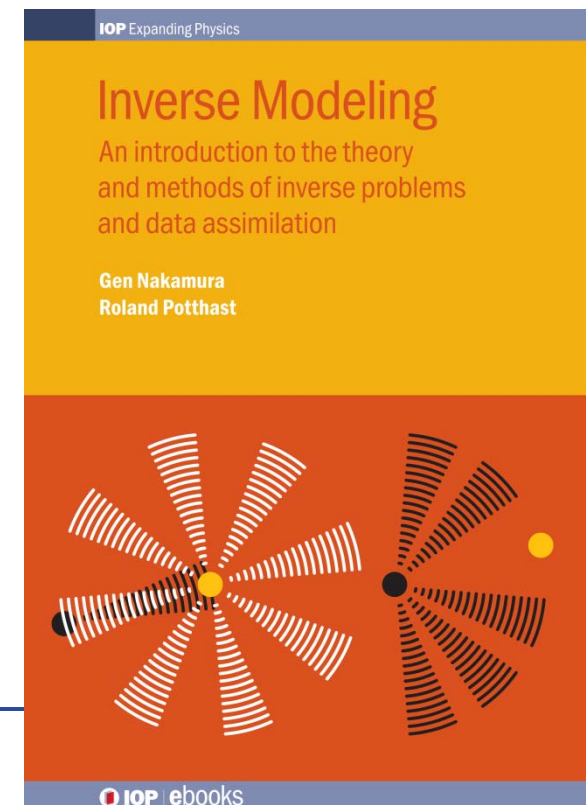


**DWD, Germany &
University of Reading, UK**

- ❖ **Ensemble Systems at Deutscher Wetterdienst (DWD)**
 - I DWD Research Environment
 - II VarEnKF and III KENDA (Kilometer Scale EDA)

- ❖ **Research Projects based on Ensemble Data Assimilation**

- ❖ **IV Particle Filters for NWP**
 - Local Markov Chain Particle Filter
 - Gaussian-Particle Filter



Part I: Research Environment

- **Deutscher Wetterdienst (DWD) is the national weather service of Germany**
- **We are a part of the Ministry of Transport and Digital Infrastructure**
- **National and European Measurement Networks (e.g. Satellites) are controled and developed**
- **We develop our systems within a network of partnerships with other states, with research institutes and universities**



Weather Prediction and Warnings for Central Europe.





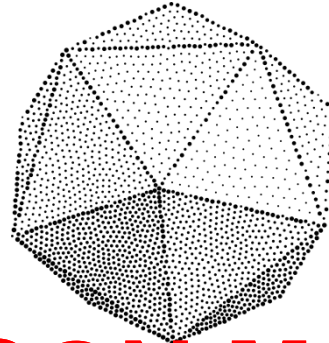
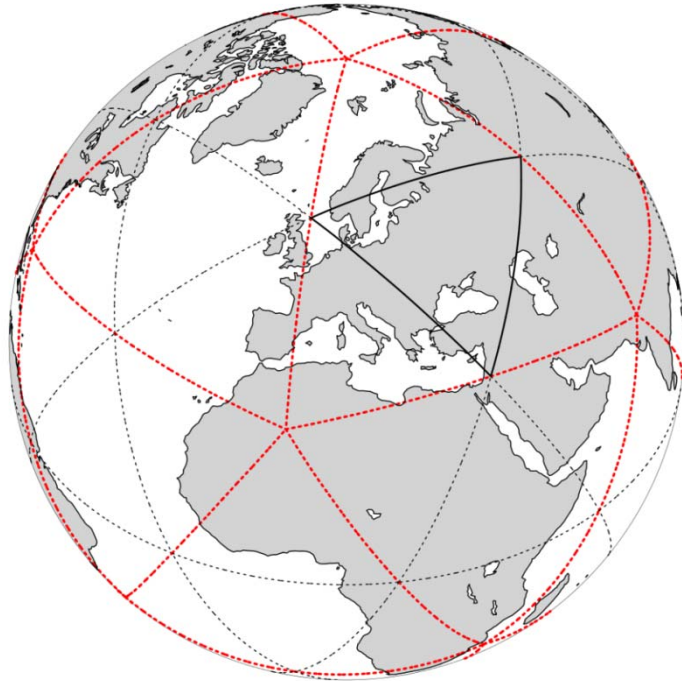
DWD operates two
CRAY
Supercomputers

Cray XC40, Intel Xeon E5-2670v2 10C 2.5GHz/E5-2680v3 12C 2.5Ghz, Aries interconnect,

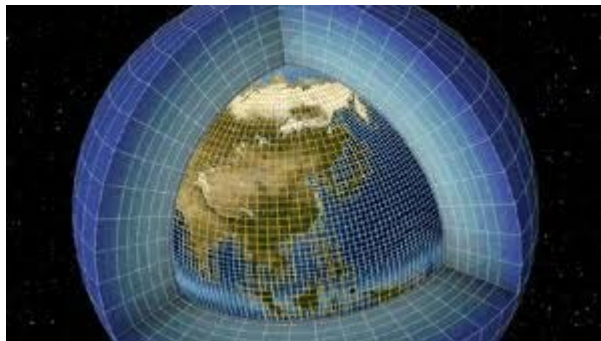
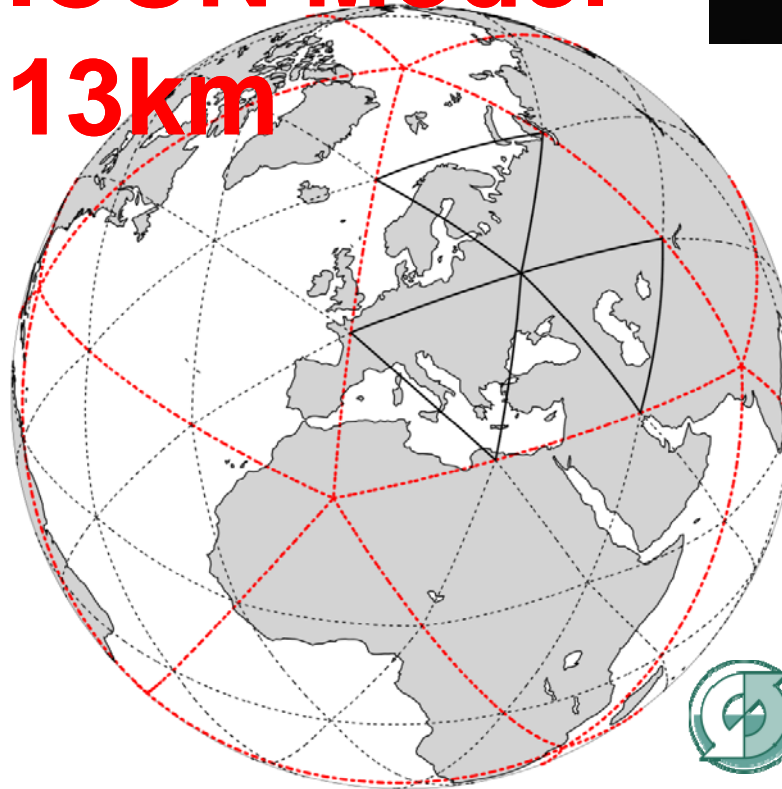
Rank 128 on the TOP 500 supercomputer list in 2014/11.



Part I: Model Chain



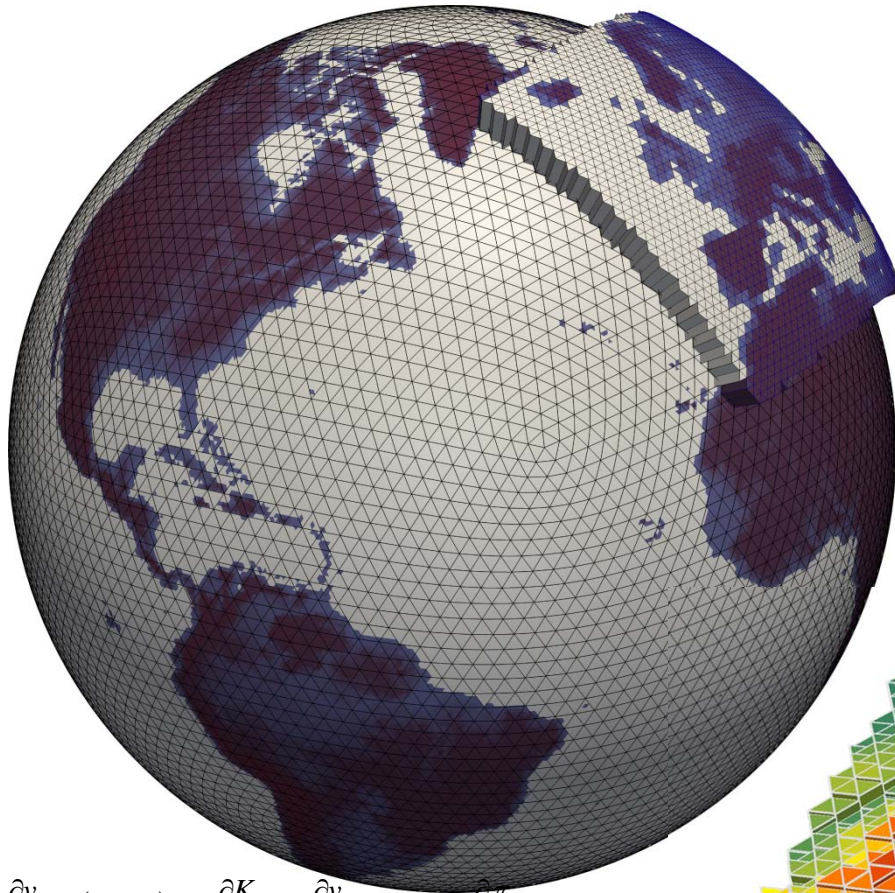
**ICON Model
13km**



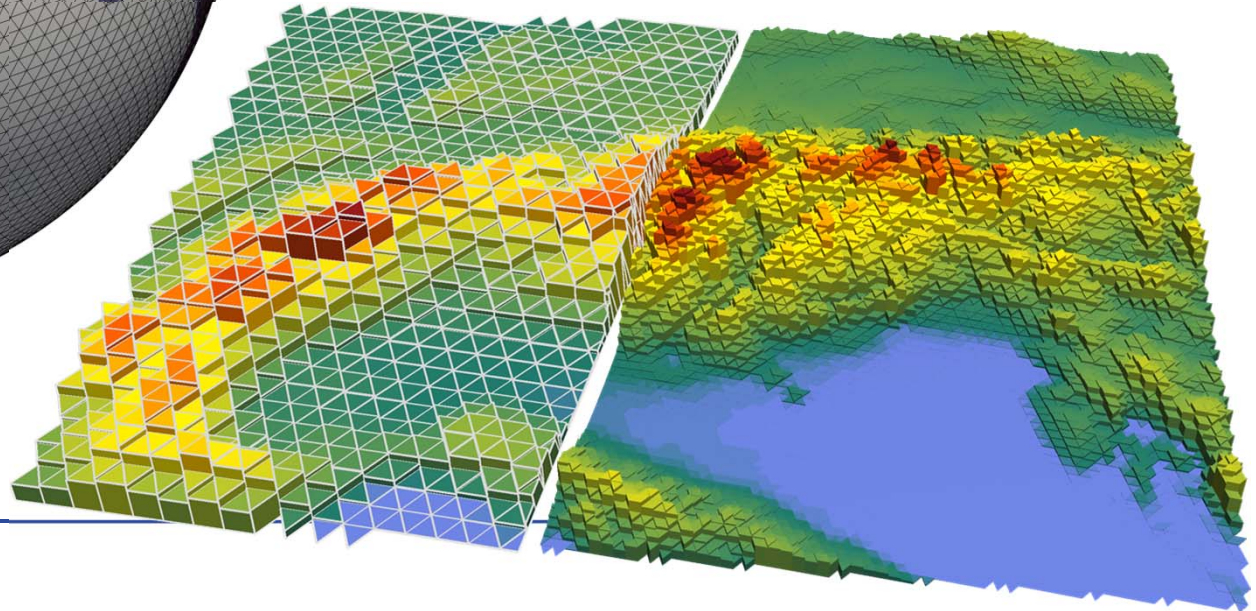
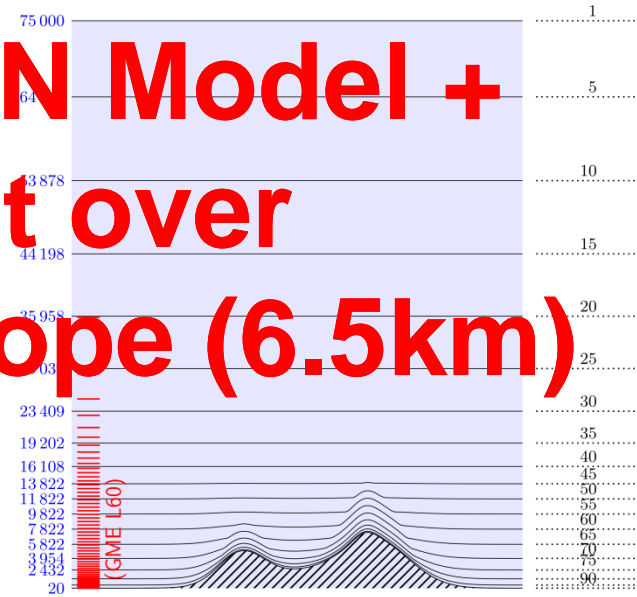
0-7 Days

Global Modelling

Deutscher Wetterdienst
Wetter und Klima aus einer Hand



ICON Model + Nest over Europe (6.5km)



$$\frac{\partial v_n}{\partial t} + (\zeta + f)v_i + \frac{\partial K}{\partial n} + w \frac{\partial v_n}{\partial z} = -c_{pd} \theta_v \frac{\partial \pi}{\partial n}$$

$$\frac{\partial w}{\partial t} + \bar{v}_h \cdot \nabla w + w \frac{\partial w}{\partial z} = -c_{pd} \theta_v \frac{\partial \pi}{\partial z} - g$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\bar{v} \rho) = 0$$

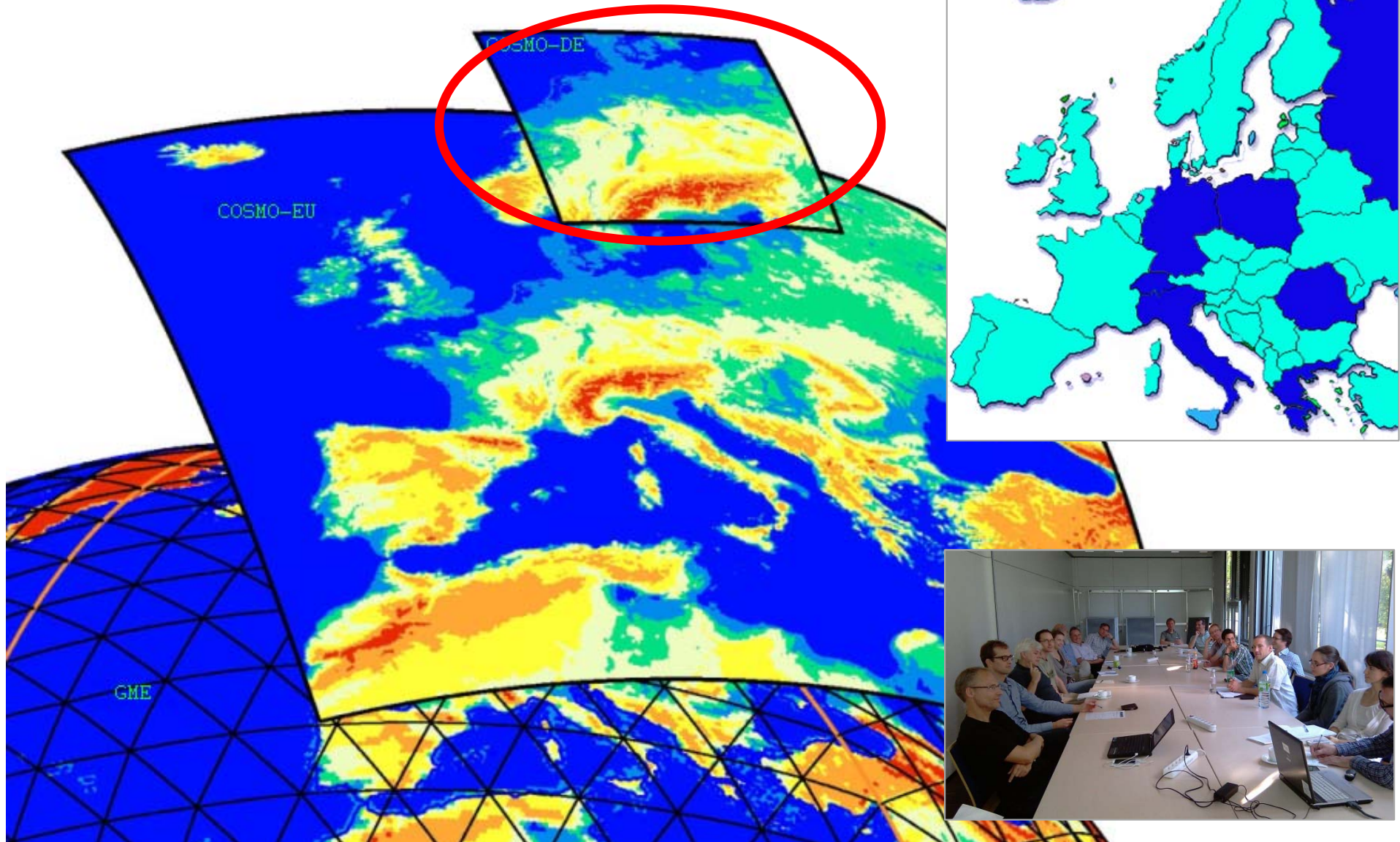
$$\frac{\partial \rho \theta_v}{\partial t} + \nabla \cdot (\bar{v} \rho \theta_v) = 0$$



02-24 Hours

High Resolution Modelling

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

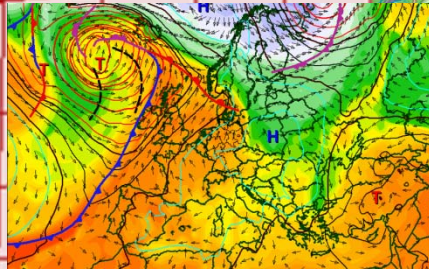
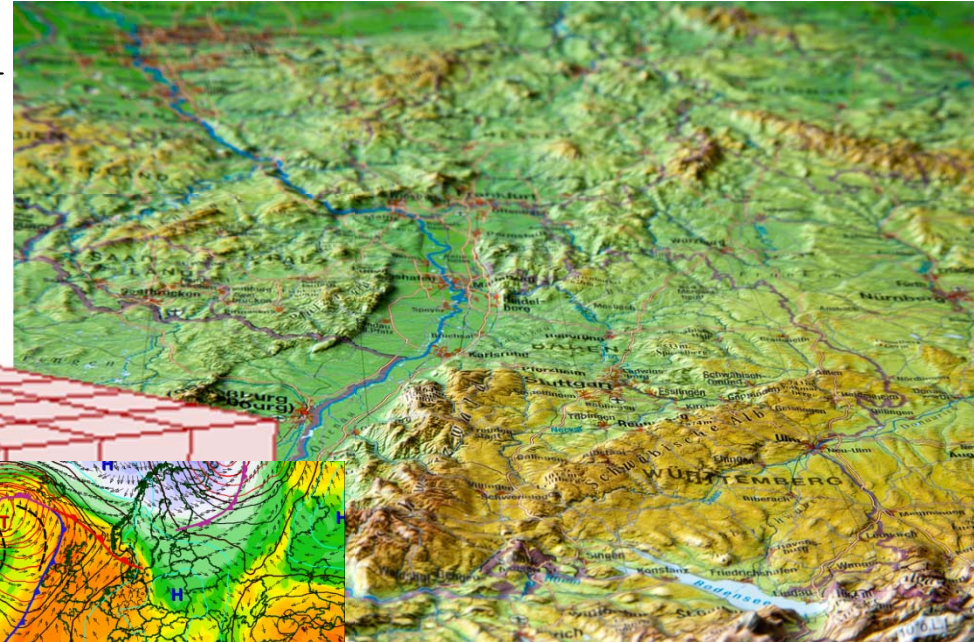


$$\frac{\partial v_n}{\partial t} + (\zeta + f)v_t + \frac{\partial K}{\partial n} + w \frac{\partial v_n}{\partial z} = -c_{pd} \theta_v \frac{\partial \pi}{\partial n}$$

$$\frac{\partial w}{\partial t} + \vec{v}_h \cdot \nabla w + w \frac{\partial w}{\partial z} = -c_{pd} \theta_v \frac{\partial \pi}{\partial z} - g$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\vec{v} \rho) = 0$$

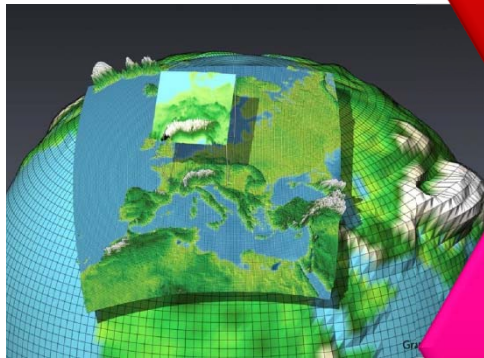
$$\frac{\partial \rho \theta_v}{\partial t} + \nabla \cdot (\vec{v} \rho \theta_v) = 0$$



2.8 (2.2 or 1)km
65 vertical layers
24km height



Part I: Research Network



COSMO
International consortium

HErZ
Hans Ertel Center

BMVI
Ministry Projects

DWD

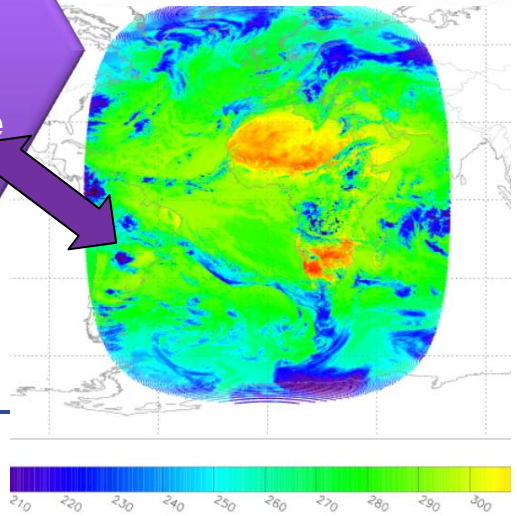
EMF
University research

Further Partners

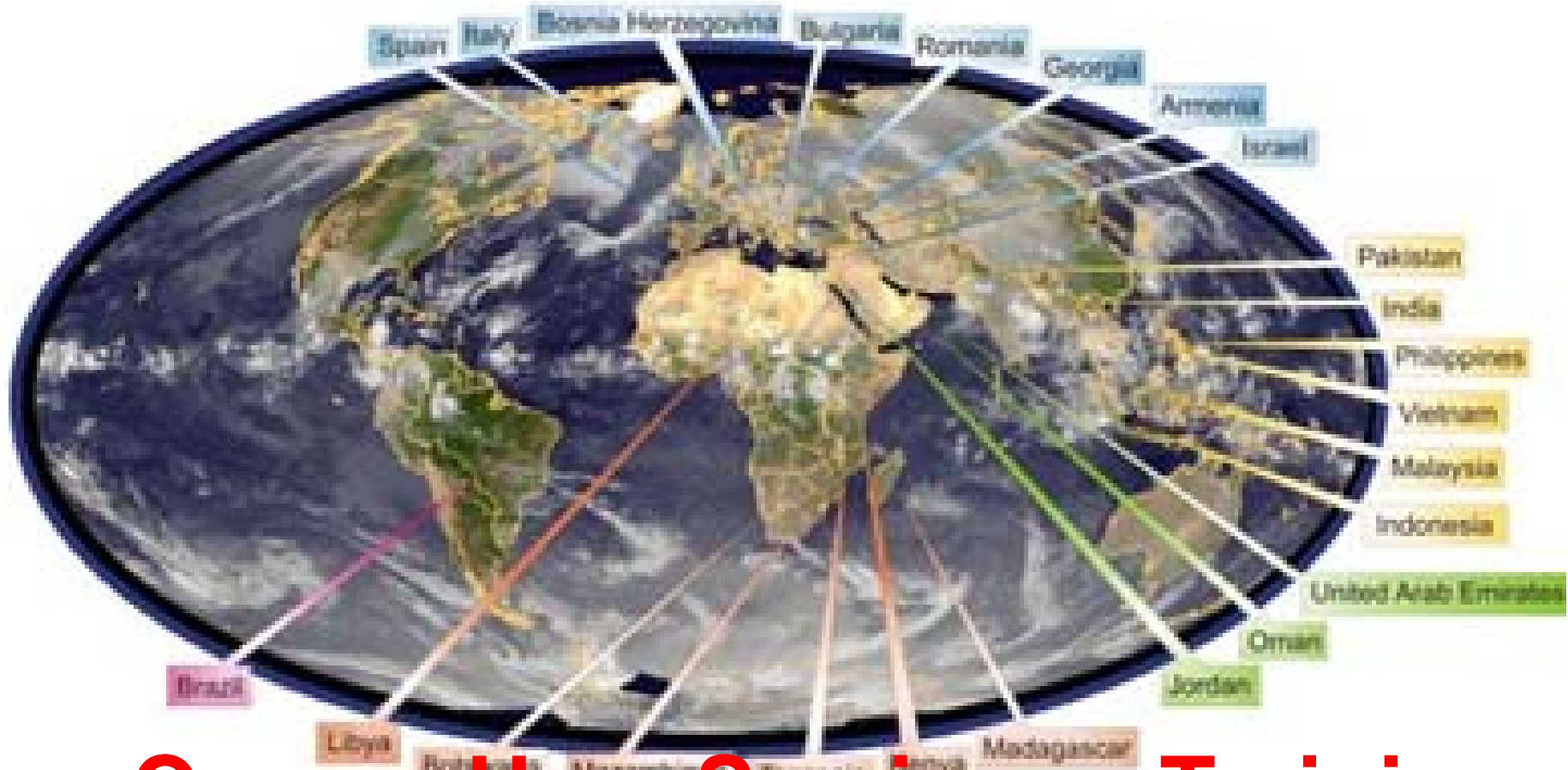
IAFE
Innovation programme



Bundesministerium für Verkehr und digitale Infrastruktur



40 Countries



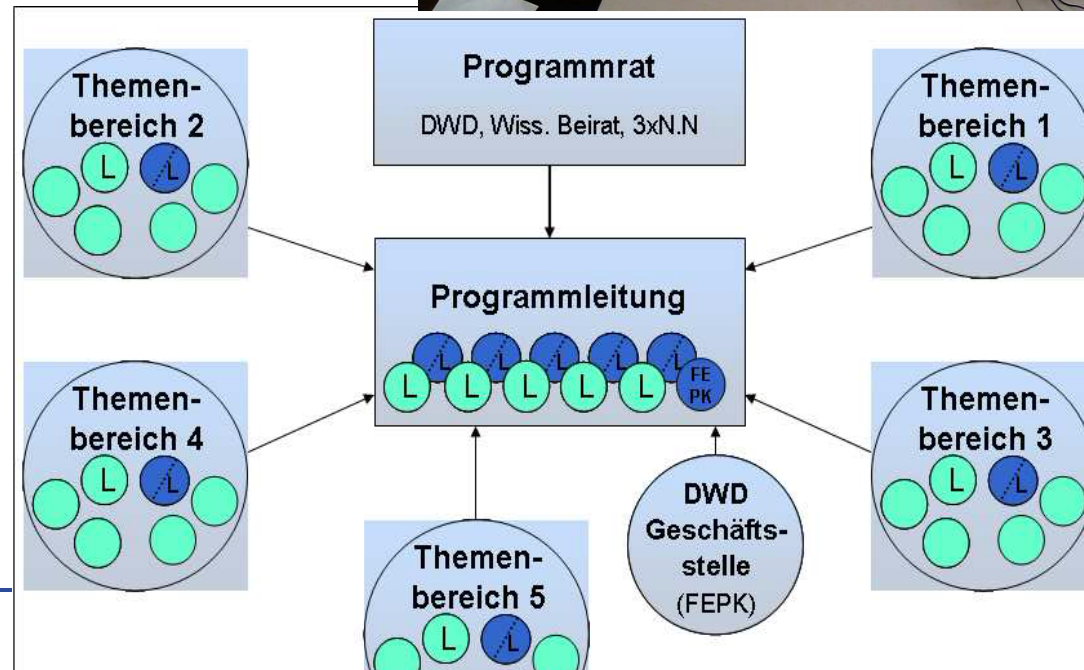
**Cosmo User Seminar + Training
Course + Symposium**



Research Network 2

Hans Ertel Center for Weather Research (HErZ)

- ➔ MPI Hamburg
- ➔ LMU Munich
- ➔ Uni Bonn
- ➔ Uni Frankfurt
- ➔ Uni Berlin



**SEE Talk of
Hendrik Reich**



Research in HErZ-DA and associated projects

Subproject A: Assimilation of potential high-impact observations

HErZ funded

HErZ funded

HErZ associated

HErZ associated

Black: Proposed
Green: Externally funded complementary projects

- Feature-based scores
- Different assimilation settings
- Operator refinement
- Model error repr. from B

Subproject B: Accounting for model error in DA

HErZ finanziert

Post-Doc Conservation in DA

HErZ associated

Work on stochastic perturbation schemes (LMU and w2W)

Subproject C: Predictability and ensemble generation

HErZ funded

PhD

Repr. of model error, predictability

PhD

Observation impact

HErZ associated

visualization of uncertainty in 5D data

w related model errors

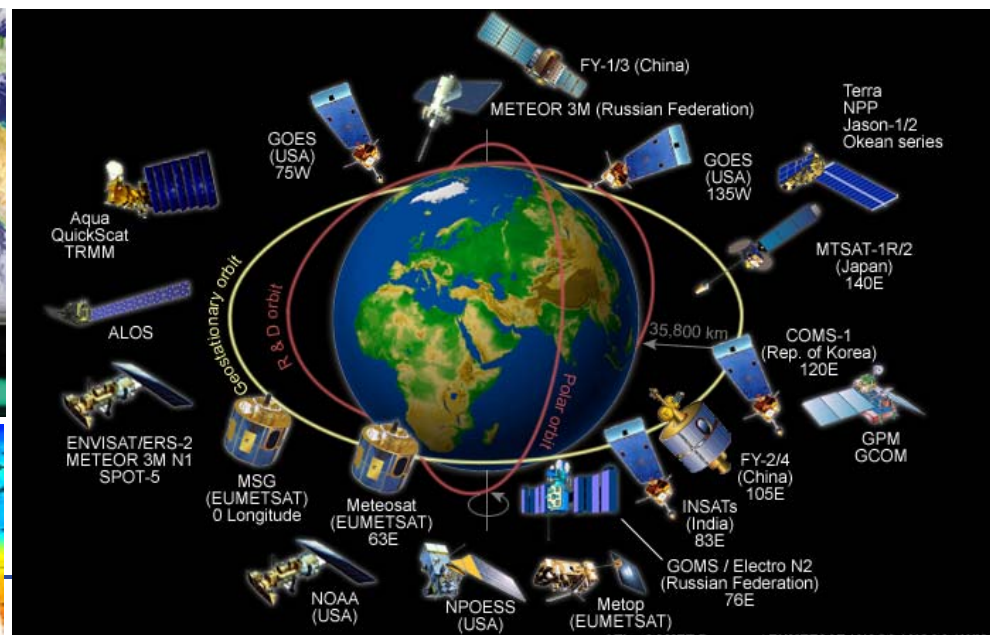
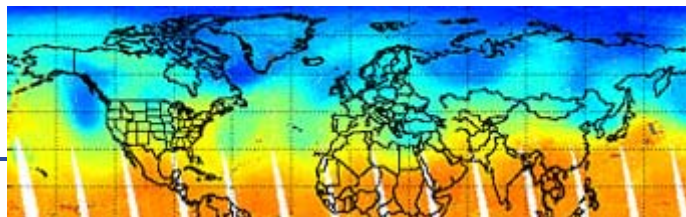
Subproject D: AMV height assignment

HErZ funded (2015)

Research Network 4:

IAFE Innovation in Applied Research and Development

Research and Development in Data Assimilation of Satellite Data



Innovation Programme (IAFE) +Eumetsat Positions Survey

Now filled ..

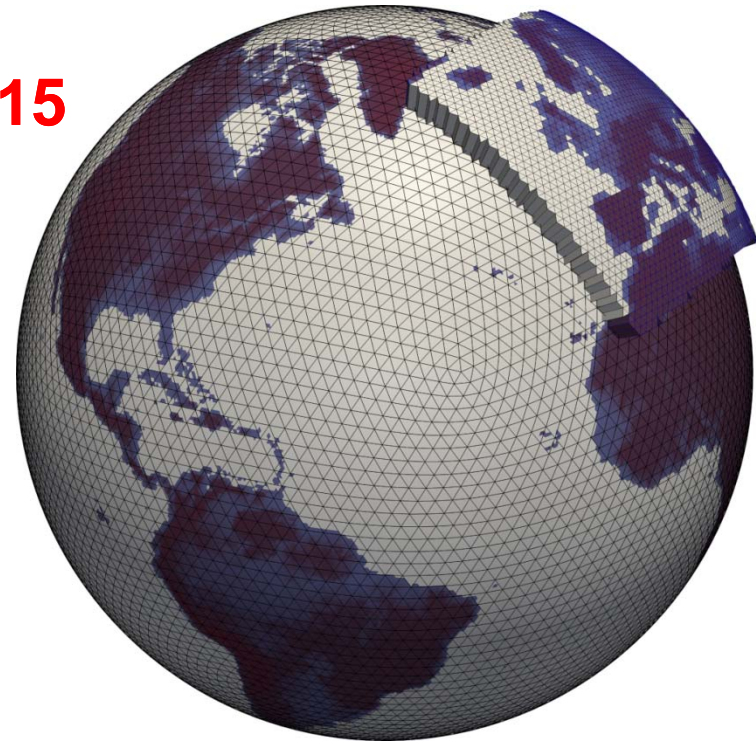
Nr	Position	Length in Years
1	SAT-GNSS-HUM	4
2	SAT-IR-ICON 1	4
3	SAT-IR-ICON 2	2 (+2 tbc)
4	SAT-IR-KENDA	4
5	SAT-MW-ICON 1	2 (+2 tbc)
6	SAT-MW-ICON 2	1+3
7	EUMETSAT Fellowship	1+2



Part II: New Global Model **ICON**

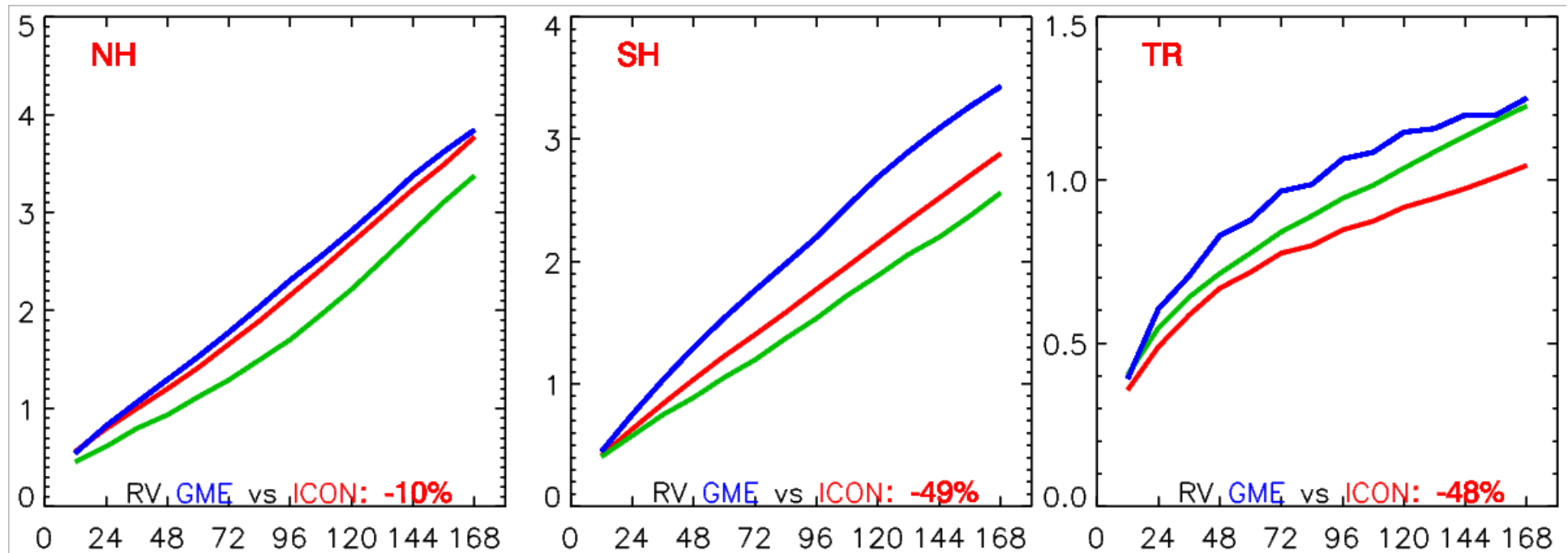
- **Operational since Jan 20, 2015**
- **Non-Hydrostatic**
- **13km resolution globally**
- **75km height**
- **90 vertical levels**

- **Still a lot in the pipeline!!**



Temperature at 700 hPa, RMSE in K

Blau: GME, rot: ICON, grün: IFS



Operational!

Part II: Global Ensemble Data Assimilation (EDA)

- **EnVar**
- **40 Members**
- **1 Deterministic**



Global EDA (EnVar) Development

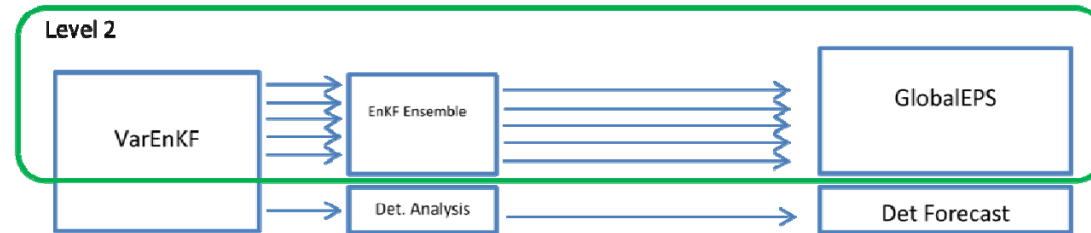
Current State



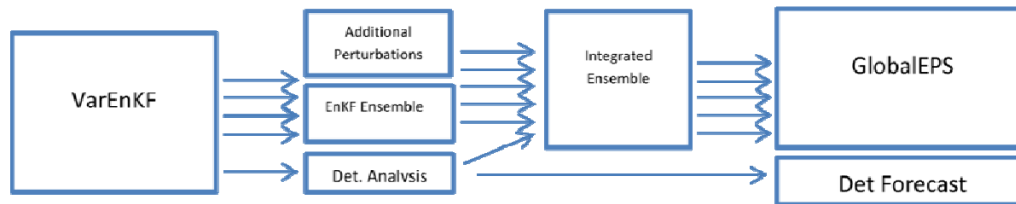
Level 1



Level 2

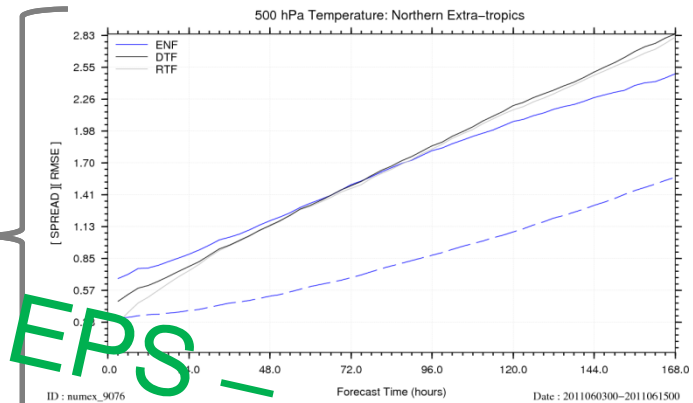


Level 3



Migration Done
Deterministic Forecast

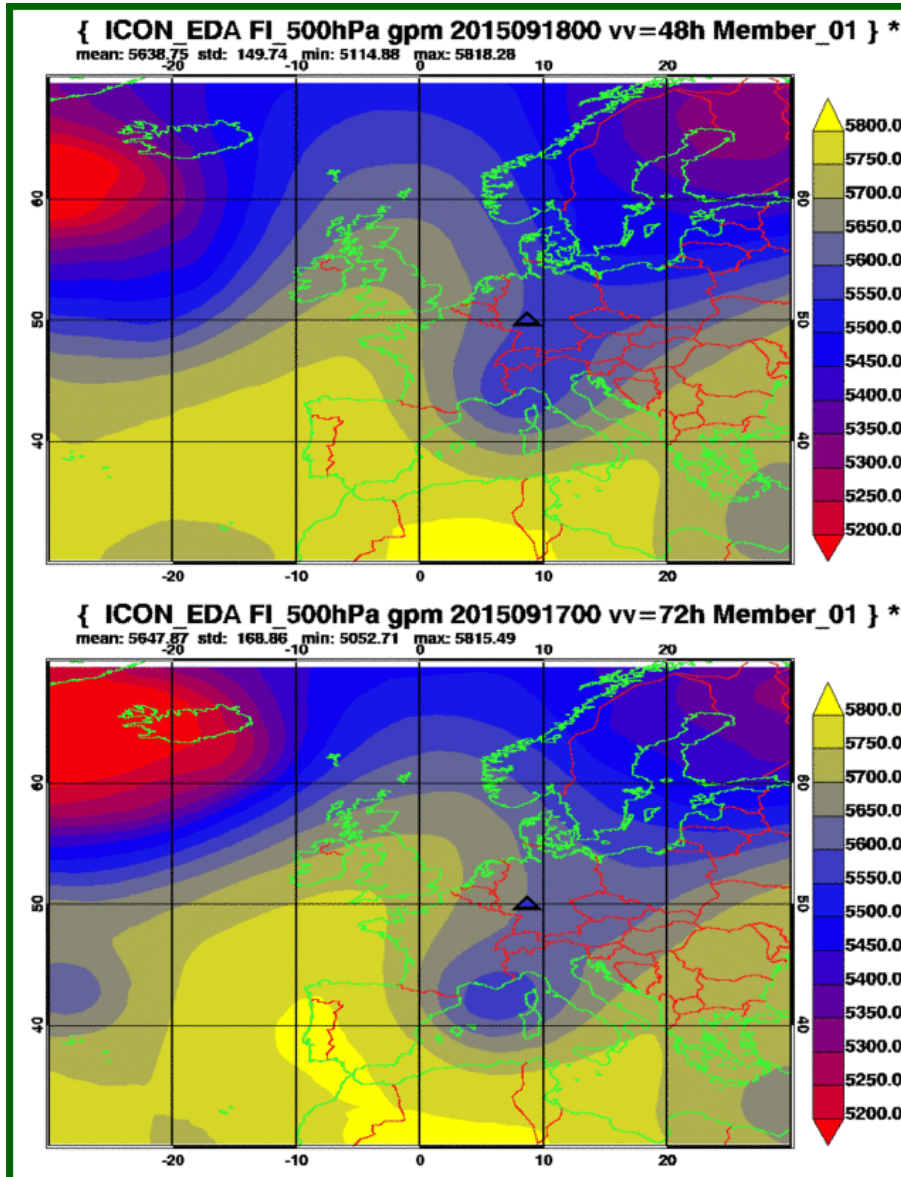
EPS - Ensemble Prediction



4. ICON Ensemble Datenassimilation

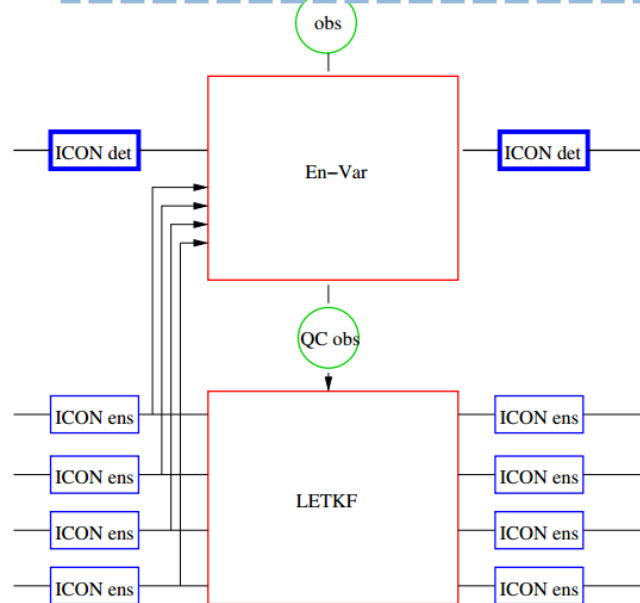
Pre-Operational since Sept 2015 : Rhodin, Fernandez, Cress, Anlauf, etc.

Ensemble Film by Bodo Ritter, FE14



We are running **ICON EDA** in our Parallel Routine since 10 Sept 2015

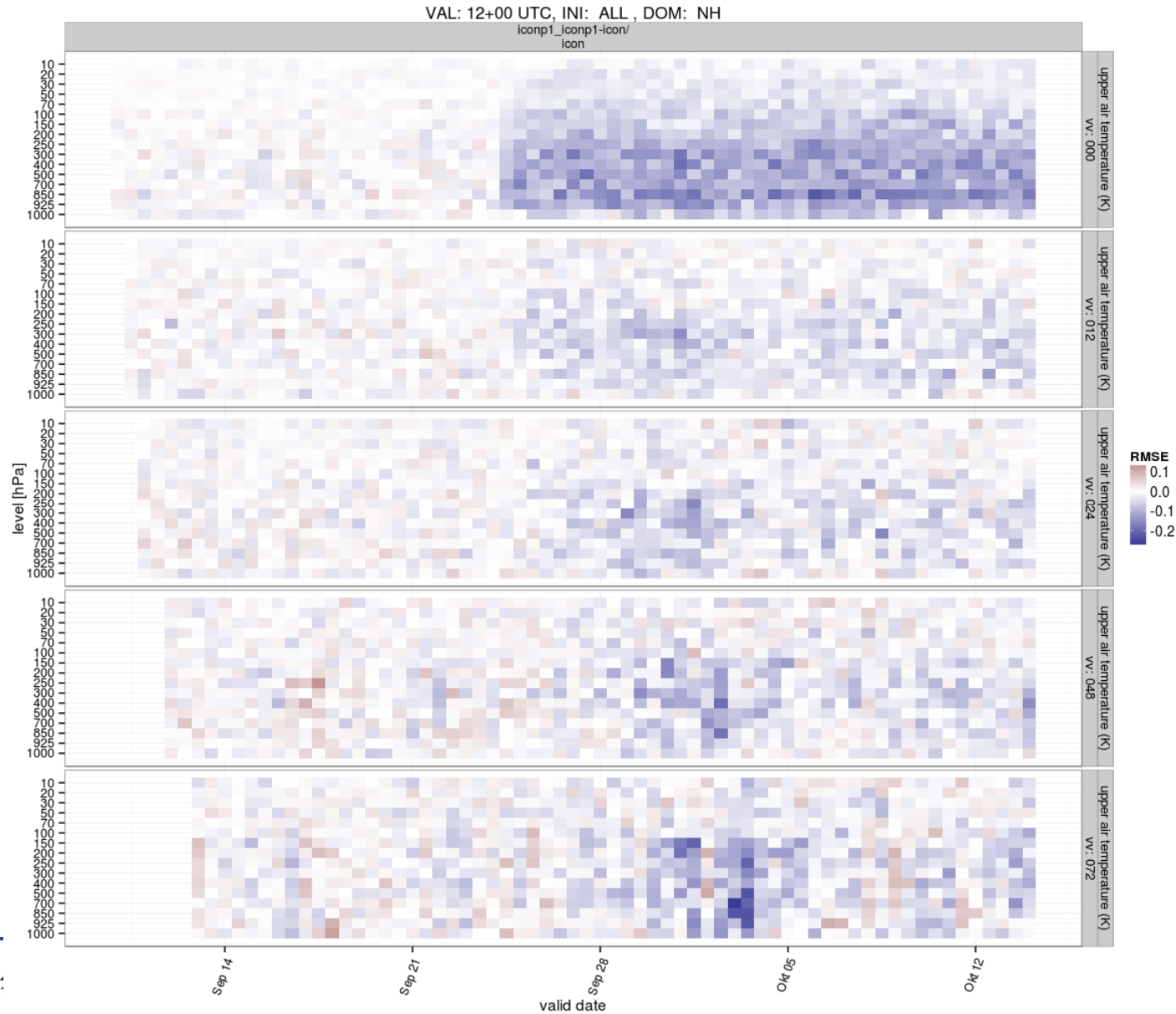
- 40 Members each with 40km global resolution and 20km NEST over Europe
- 1 deterministic 13km member
- **EPS forecasts** 40 Members 7 Days + 1 Deterministic
- Output for convective-scale EDA/EPS
- **Hybrid System** active since Sept 24, 2015



*Graphics and
ICON EDA Head
Andreas Rhodin,
FE12*

4. ICON Ensemble Datenassimilation

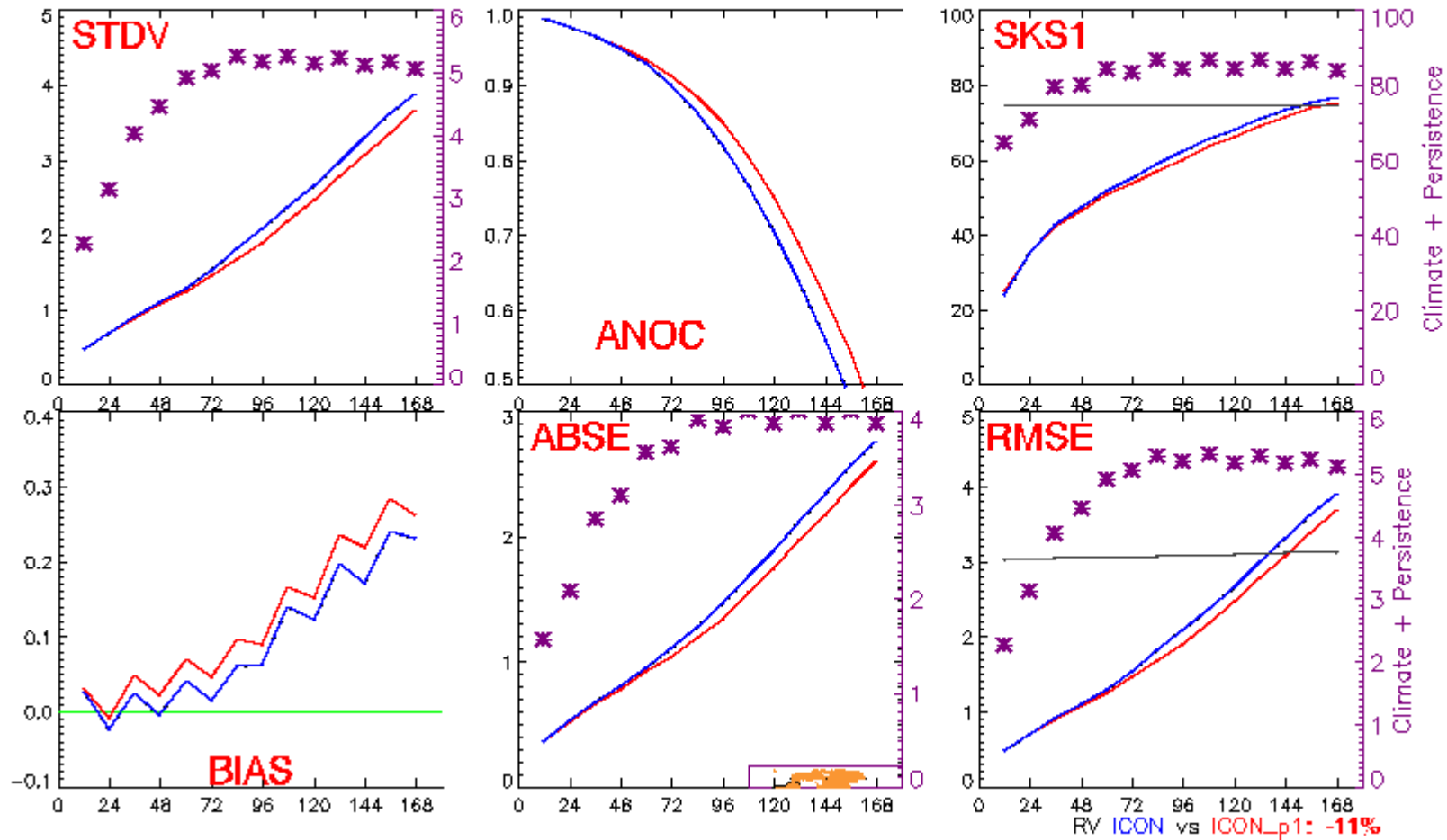
Verifikation: Felix Fundel, FE15, Michael Denhard, FE15 und A. Rhodin, FE12



4. ICON Ensemble Datenassimilation

Verifikation: Michael Denhard und Uli Damrath, FE15

Verification of forecasts from 24.09.2015 12UTC till 06.10.2015 12UTC (area mean) **ICON __**, **ICON_p1 __**, **Persistence**, Lines: climate(r
Parameter: **Temperatur**, region: **NH** , pressure level **0850 hPa**



Difference Routine/Parallelroutine: ICON with ENVAR



4. ICON Ensemble Datenassimilation

Verifikation: Felix Fundel, FE15, Michael Denhard, FE15 und A. Rhodin, FE12

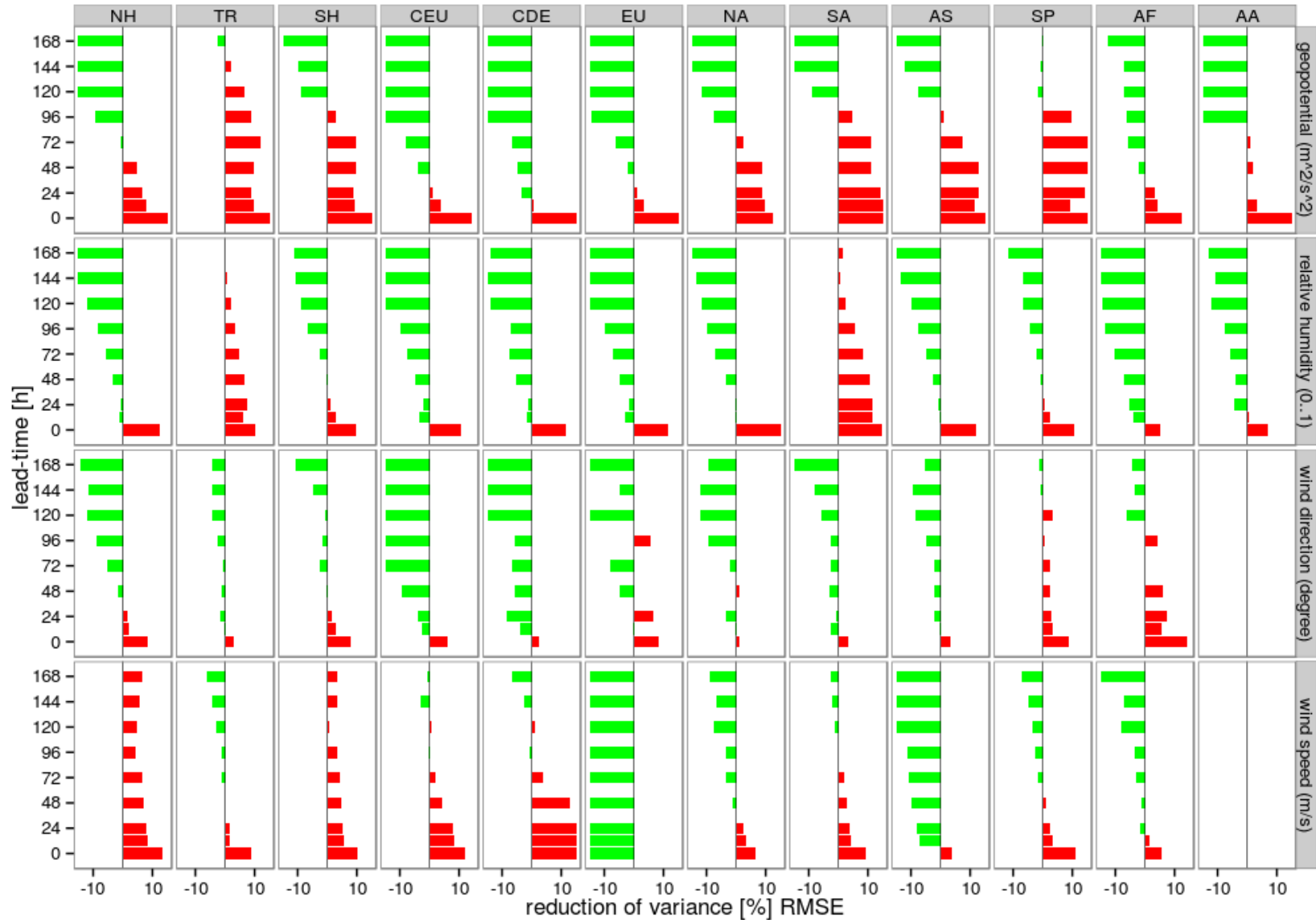
ICON EPS Ensemble Forecast 40/20km Verification Mean against TEMP



4. ICON Ensemble Datenassimilation

Verifikation: Felix Fundel, FE15, Michael Denhard, FE15 und A. Rhodin, FE12

ICON EPS Ensemble Forecast 40/20km Verification Mean Surface

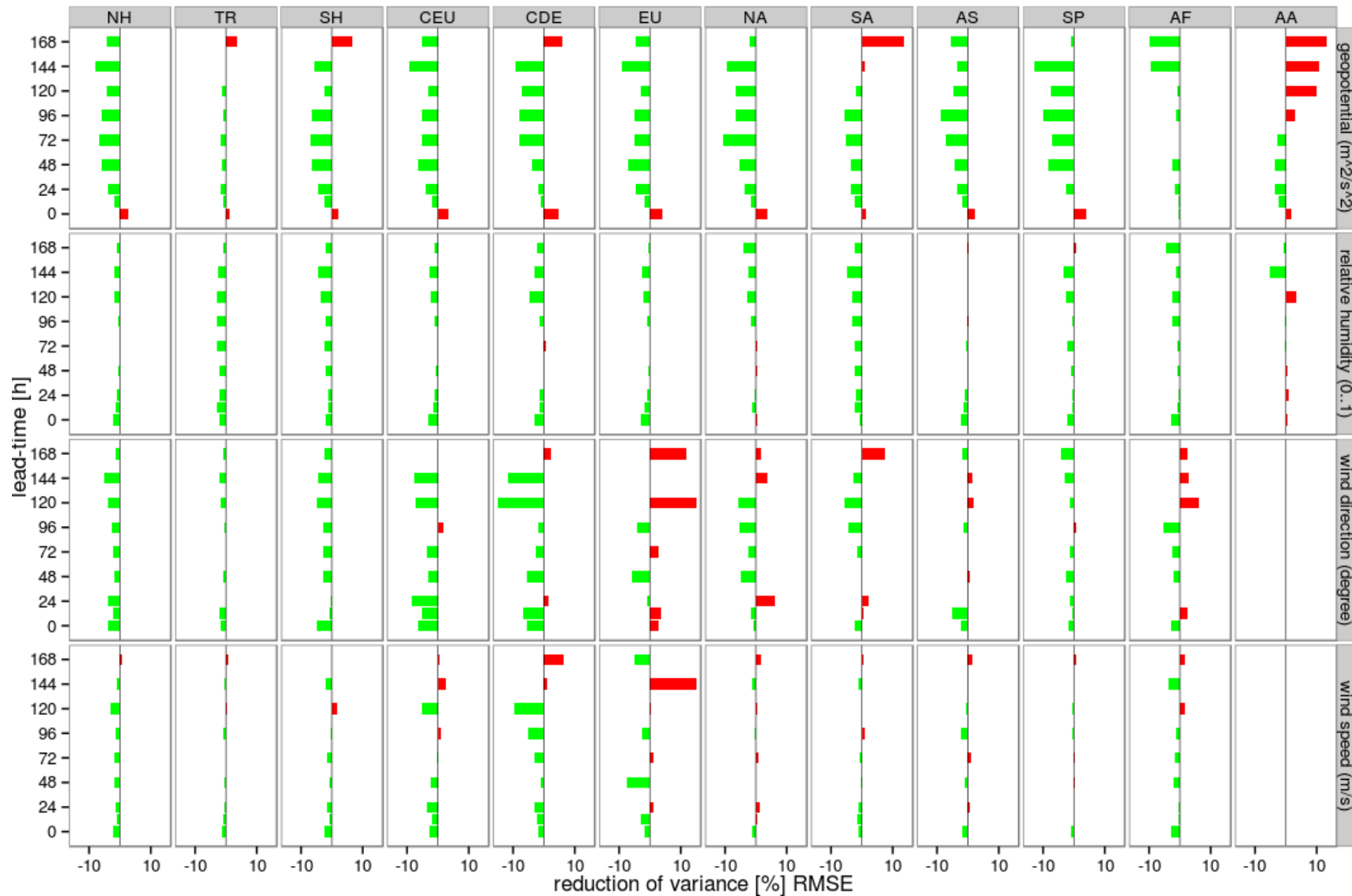


st

4. ICON Ensemble Datenassimilation

Verifikation: Felix Fundel, FE15, Michael Denhard, FE15 und A. Rhodin, FE12

ICON EnVar Forecast 13km Verification Surface vs. Routine

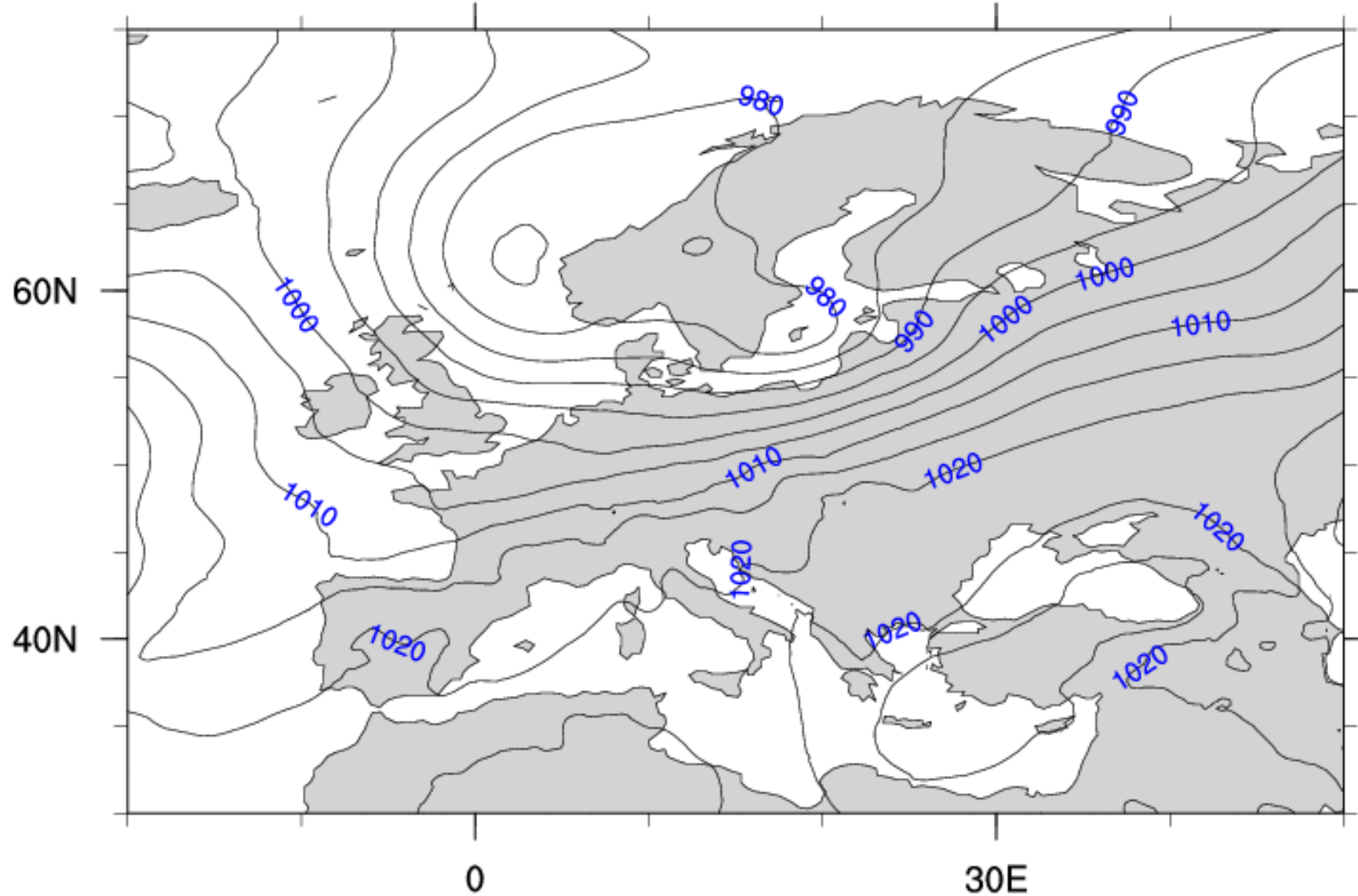


ICON Ensemble PMSL Mean Member 1

12/11/2014 (00:00)

42hr forecast

hPa



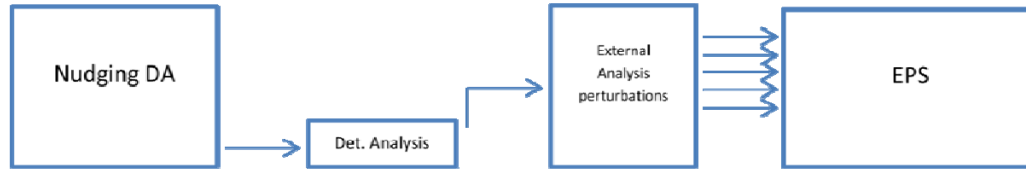
Part III: Kilometer Scale Ensemble Data Assimilation (KENDA)

- LETKF + DetAnalysis



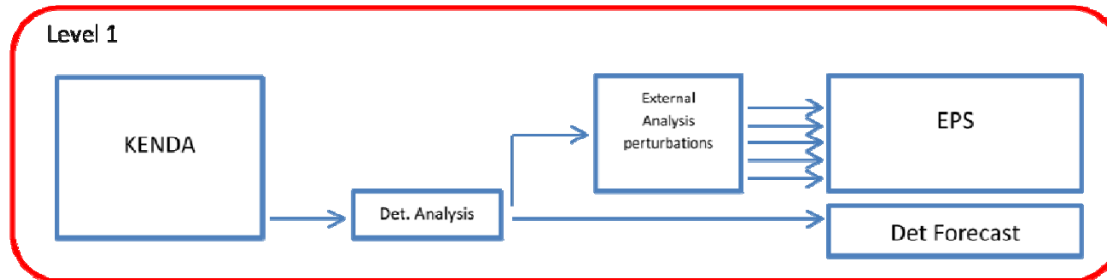
KENDA and EPS Development

Current State

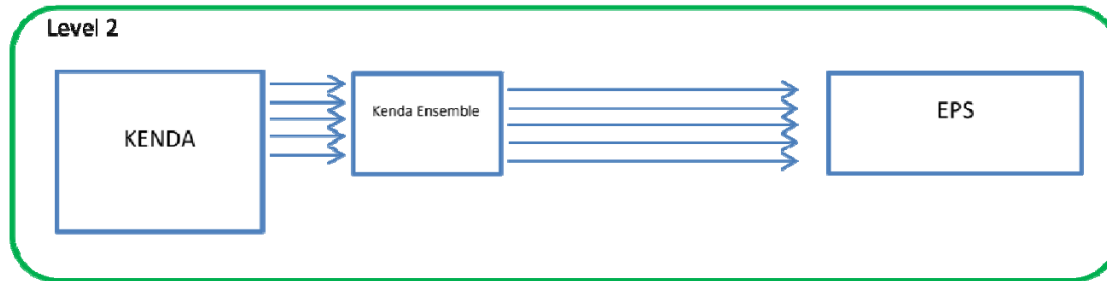


Migration ongoing
Deterministic Forecast

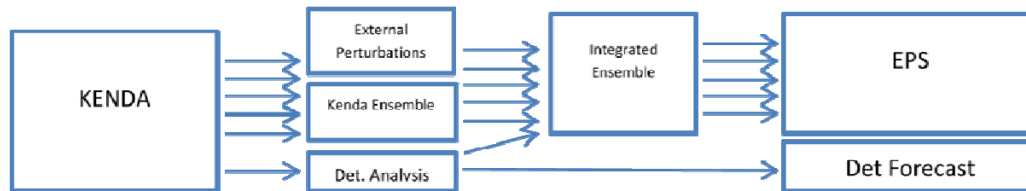
Level 1



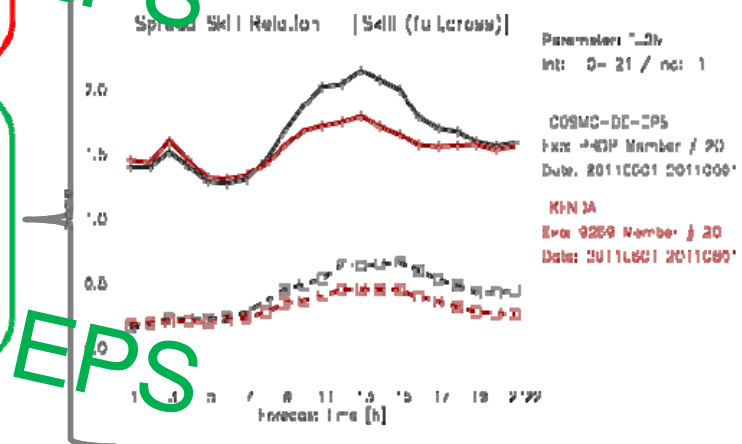
Level 2



Level 3

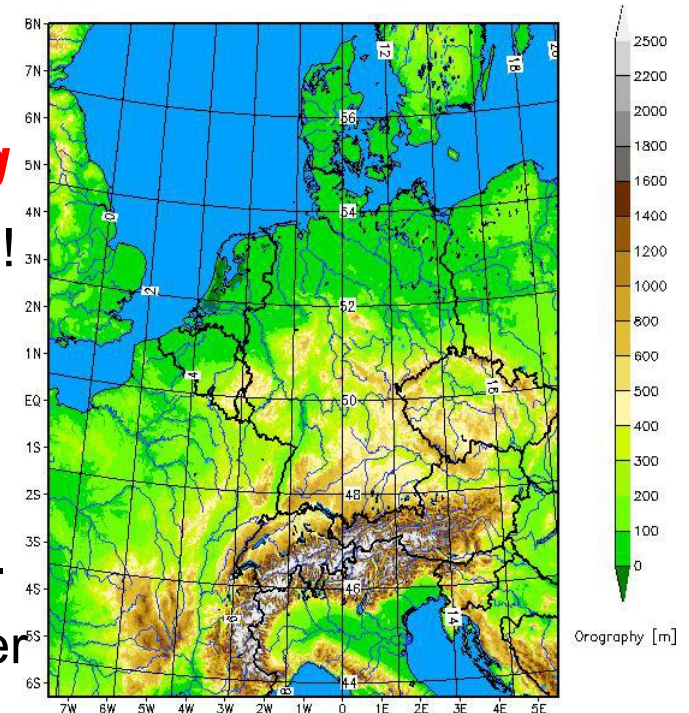


EPS
EPS



KENDA for COSMO

1. **Full System** with **conventional data** *running*
2. Work **Latent Heat Nudging**, done, works well!
3. Further **Observation Systems** under development
(e.g. **SEVIRI**, **GPS/GNSS**, Lidar, ...)
4. **Longer Periods/Winter Periods** to be tested.
5. **Technical work** on operational setup (member loss) done
6. **Archive/Storage** challenges remain severe
7. **Pattern Generator** and further **Refinements**
(Localiyation, Covariance Inflation, ...)

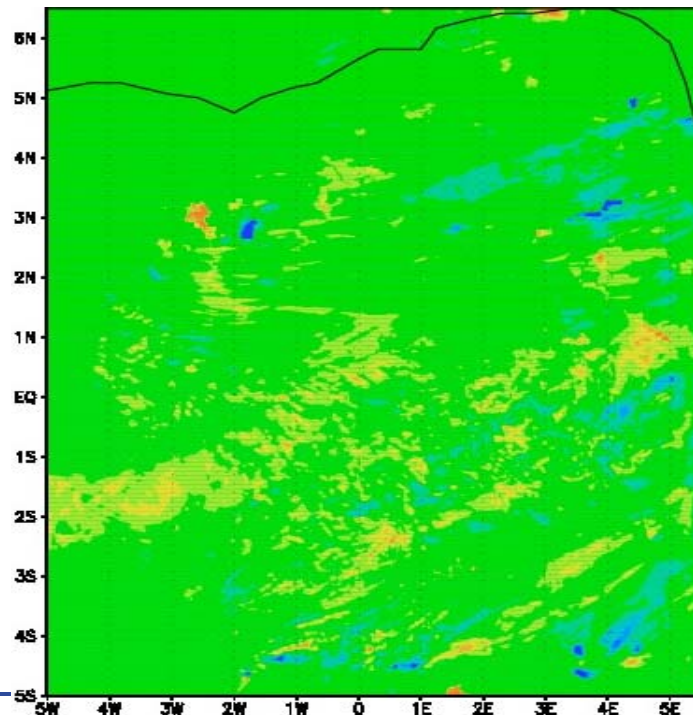


introduction of soil moisture (SM) perturbations (+ SST pert.)

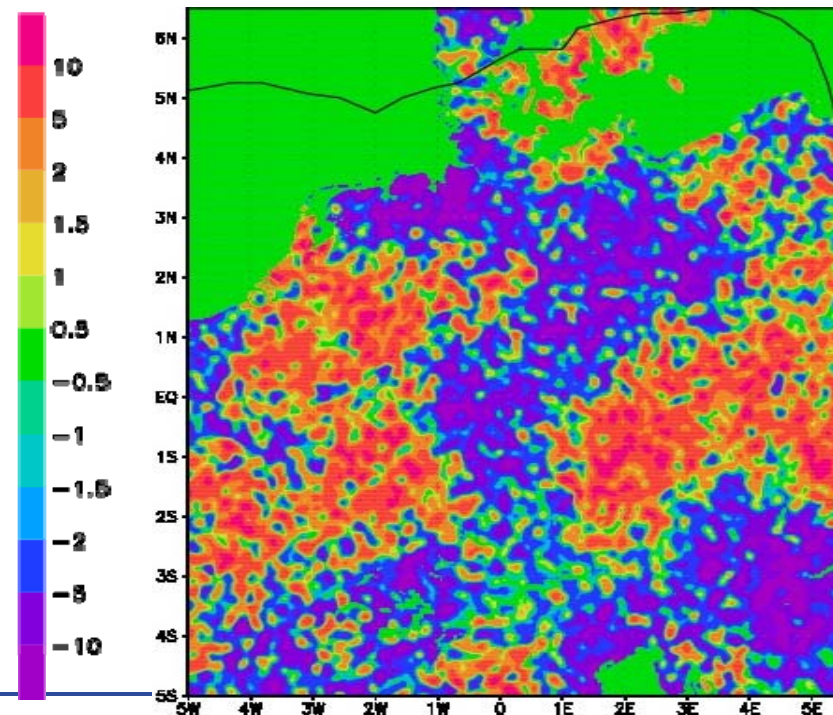
- ✓ simple superposition of Gaspari-Cohn (~ Gaussian) functions at each analysis g.p., with random amplitude and pre-specified horiz. / temporal correlation scale(s)
- ✓ scales : 100 km + 10 km ; 1 day ; std dev of amplitude: 0.1 soil moisture index

spread of soil moisture (WSO), layer 3 (3 – 9 cm), after 5 days

cycling without perturbations



cycling with SM perturbations



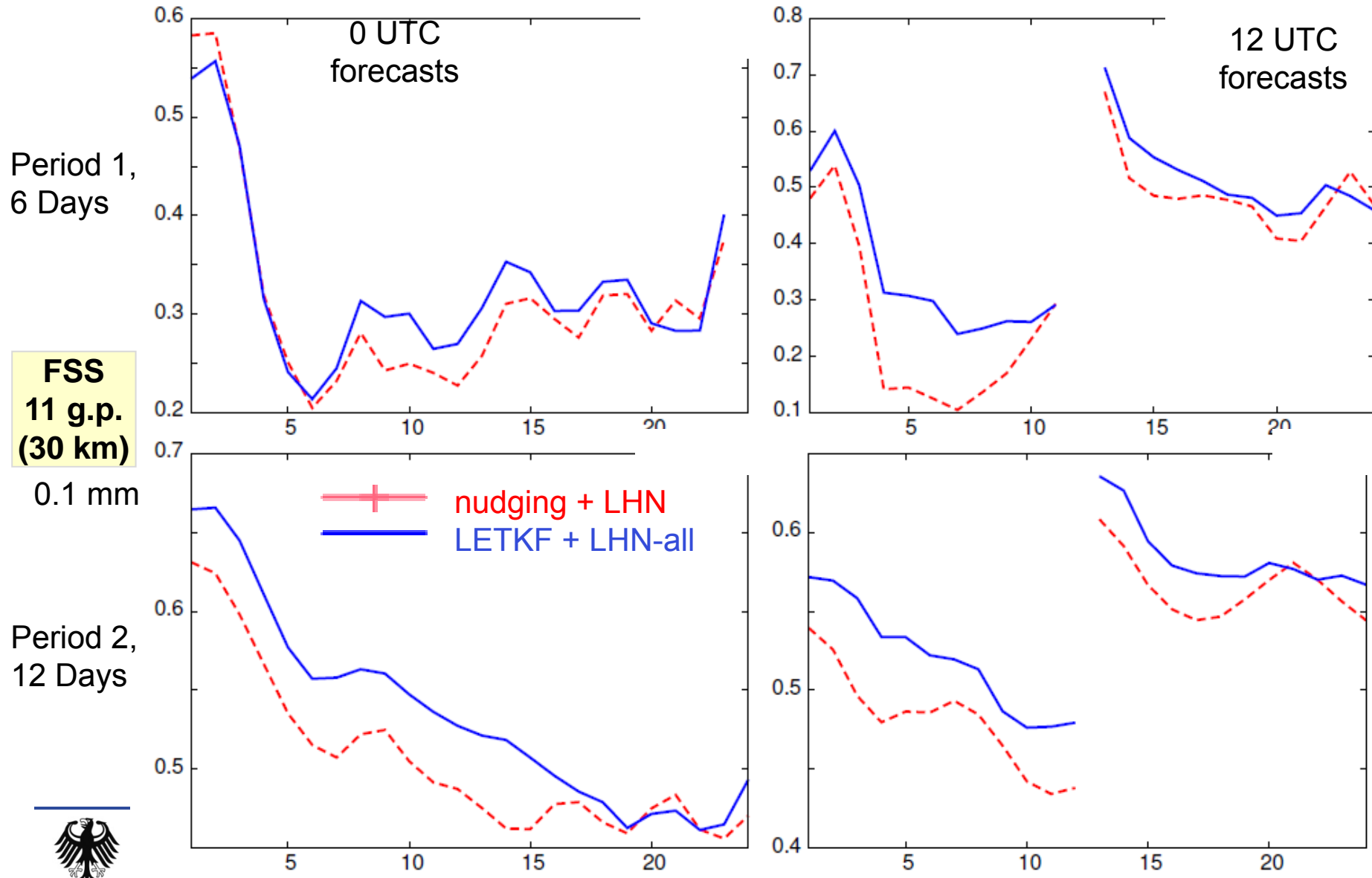
impact of including **LHN** in LETKF DA cycle (with ICON soil):
score chart

variable	LETKF LHN-det vs. no-LHN		LETKF LHN-all vs. LHN-det	
	RMSE ETS / FSS	Bias FBI	RMSE ETS / FSS	Bias FBI
upper-air	=	=	=	=
surface	=	=	=	=
precip 0 UTC , 0.1 mm	(+)	(+)	(+)	=
precip 0 UTC , 1 mm	=	=	(+)	=
precip 12 UTC, 0.1 mm	+	+	+	=
precip 12 UTC, 1 mm	+	=	+	=

- benefit from adding LHN small for 0-UTC runs, large for 12-UTC runs
- deterministic forecast improves if LHN also added to all ens members in LETKF



LETKF + LHN-all vs. Nudging + LHN : verification against radar precipitation



LETKF + LHN-all vs. Nudging + LHN :
KENDA score chart

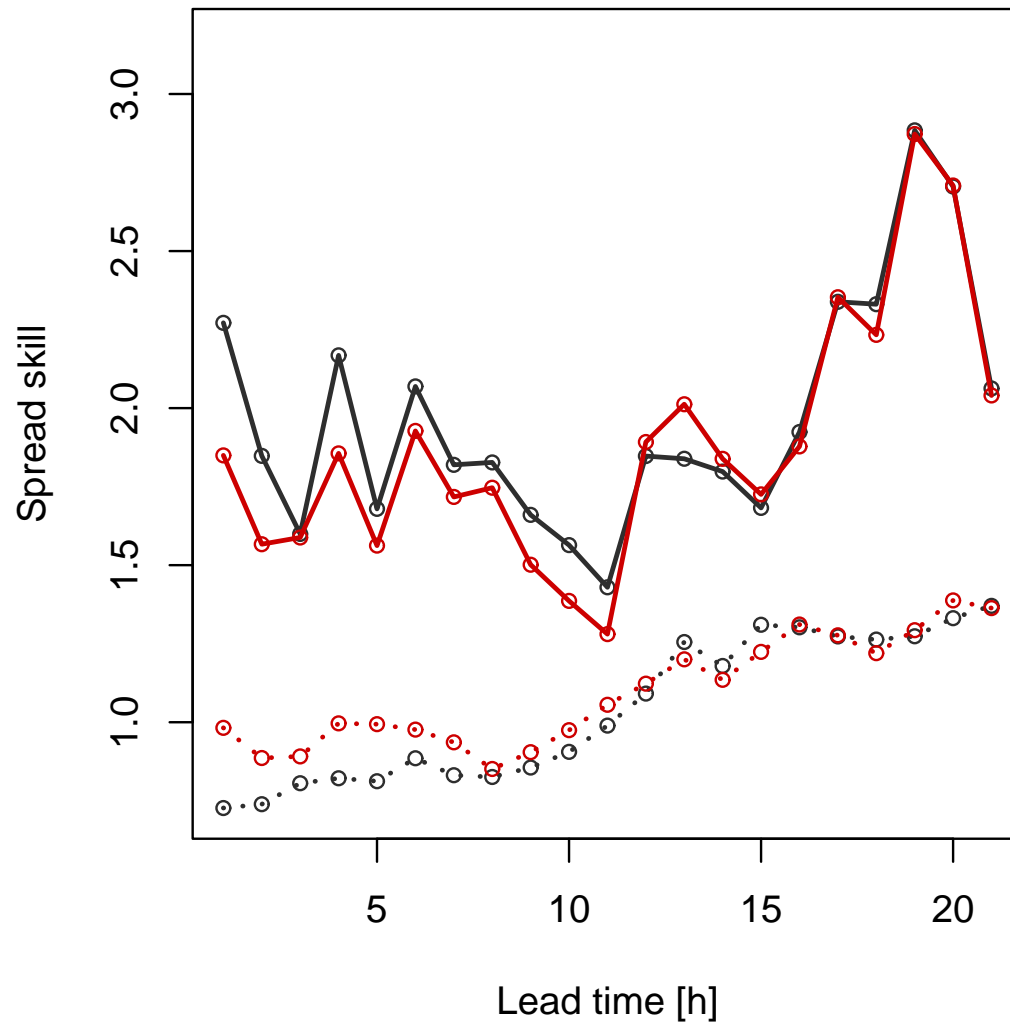
	variable	T2012		T2014	
		rmse	bias	rmse	bias
upper air	geopotential	=	=	=	=
	temperature	=	=	(+)	(+)
	relative humidity	=	=	=	-
	wind speed	+	=	+	=
	wind direction	+	=	(+)	=
surface	2-m temperature	=	=	+	=
	2-m dew point	=	=	+	+
	10-m wind	=	=	=	=
	surface pressure	-	=	+	=
	total cloud	=	=	=	=
	low cloud	+	+	-	=
	mid-level cloud	+	+	=	=
	high cloud	-	-	-	-
radar	precip 0 UTC runs	+ / (-)	+	++	++
	precip 12 UTC runs	++	++	++	++

LETKF:

- overall comparable / better results
- Mixed view for surface pressure
- Problem with high clouds

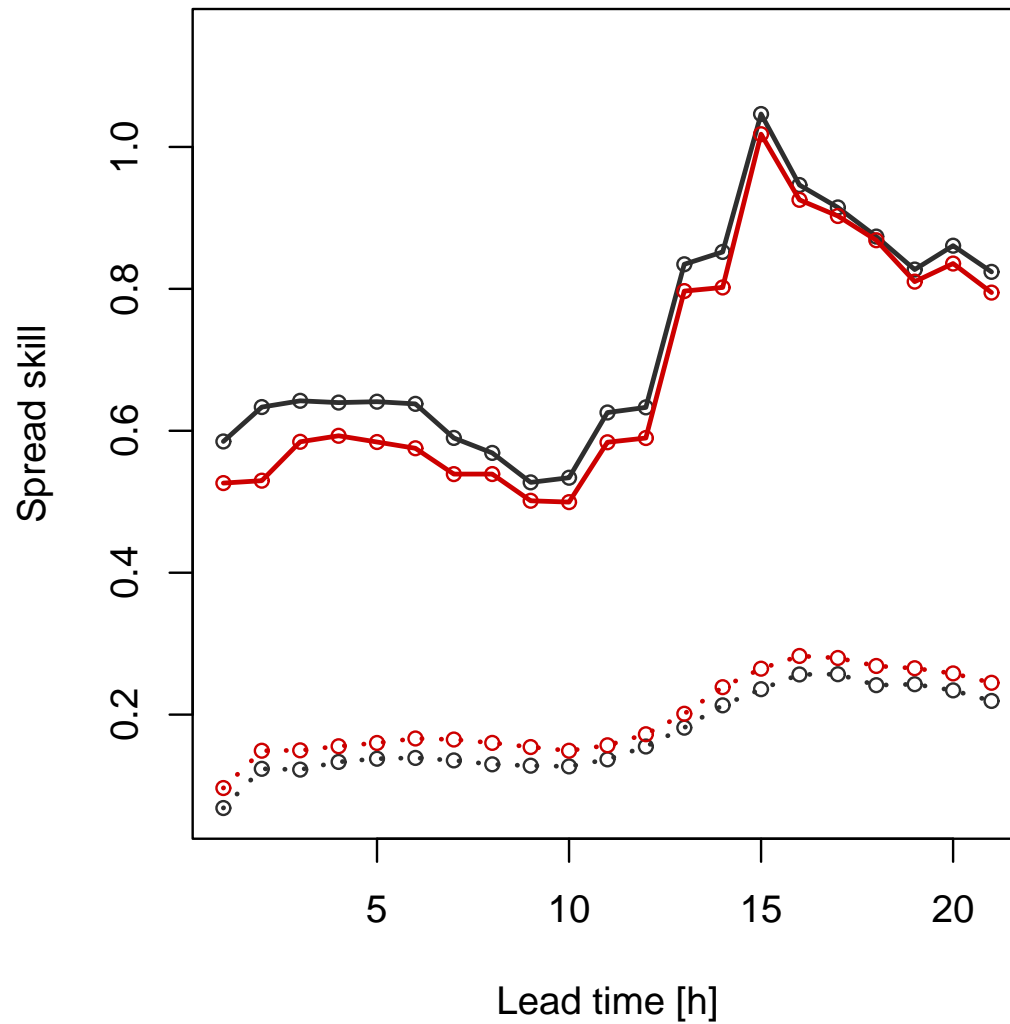
Stable Improvement

EPS 10-250 m Wind: RMSE + Spread



Nudging + BCEPS
KENDA

EPS Precipitation: RMSE + Spread



Nudging + BCEPS
KENDA

- Can a **Particle Filter** work for NWP?
- **Yes**, the EnKF is already working (as shown above)!
- The question is how to calculate the **posterior ensemble!**
- DWD is developing a **Local Markov Chain Particle Filter**
- MeteoSwiss + ETH Zurich + DWD are working on an **Ensemble Kalman Particle Filter**
- Uni Potsdam is developing a Particle Filter for our System



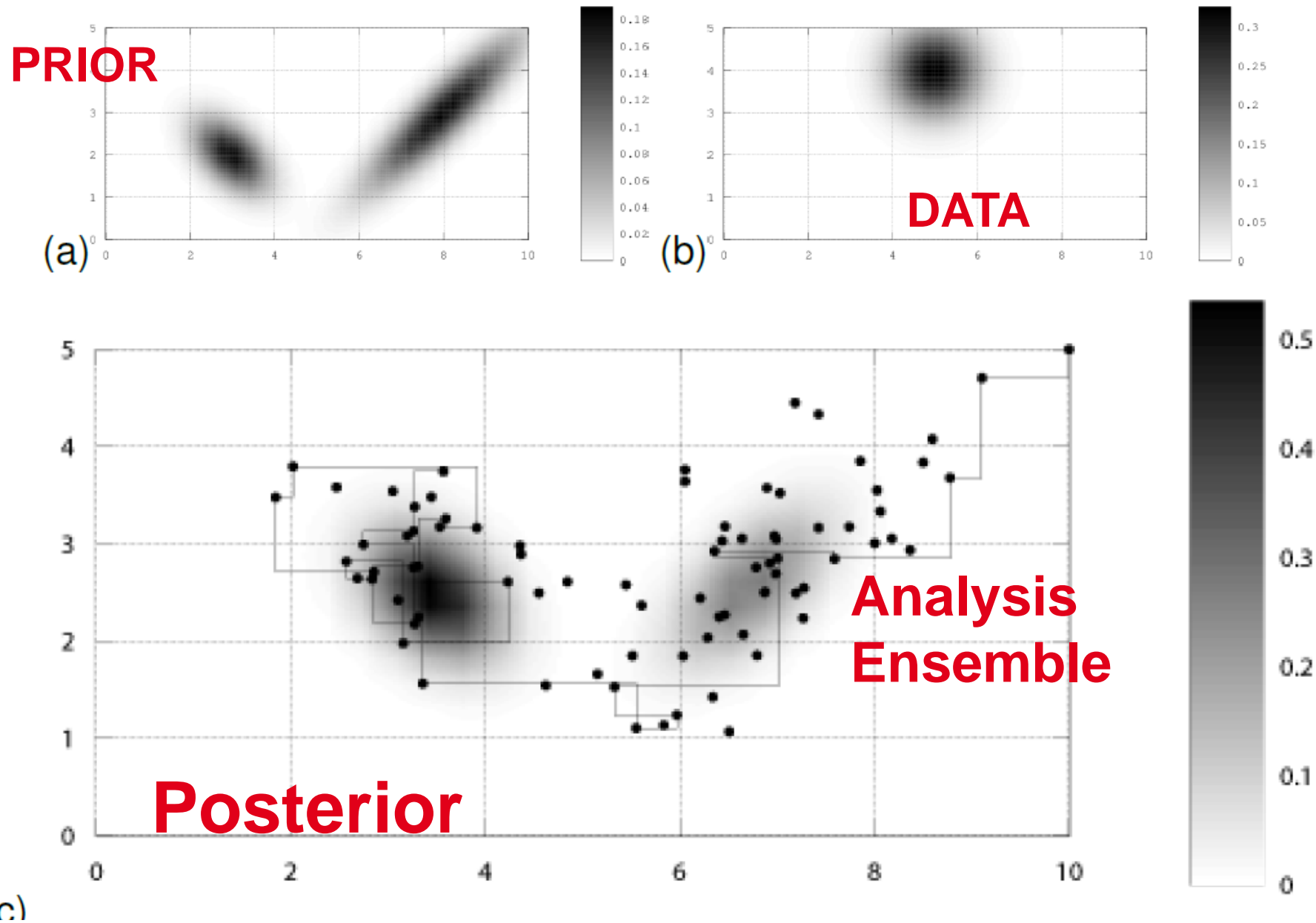
- You get a **prior distribution** $p(x)$ by some prior ensemble
- Measurements define a **data distribution** $p(y|x)$
- **Bayes theorem** defines a posterior distribution by
$$p(x|y) = c p(x) p(y|x)$$

The core game is

how to get an **analysis ensemble** from $p(x|y)$.



BAYES Data Assimilation



Let us start with some continuous transition probability $q(x', x)$ for the transition of x to x' , which we use as a **proposal density** to suggest draws as candidates for our transition probability density $k(x', x)$, $x, x' \in \Omega$. The goal is to construct a correction $\alpha(x', x)$ such that have

$$k(x', x) = \alpha(x', x)q(x', x), \quad x, x' \in \Omega, \quad (34)$$

is a transition kernel which satisfies the **detailed balance equation** (33). The choice

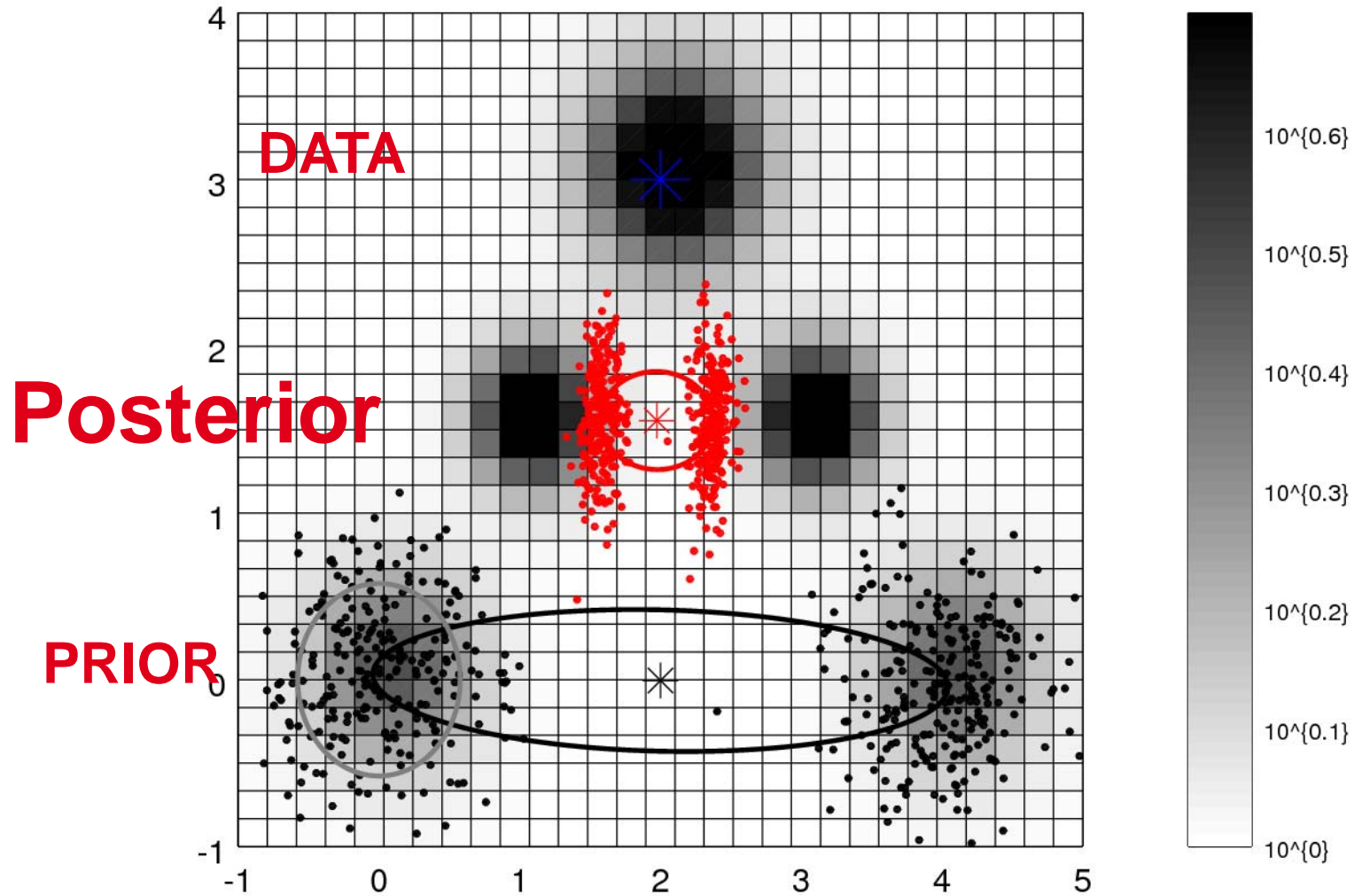
$$\alpha(x', x) := \min \left\{ 1, \frac{p(x')q(x, x')}{p(x)q(x', x)} \right\} \quad (35)$$

is known as **Metropolis-Hastings algorithm**.



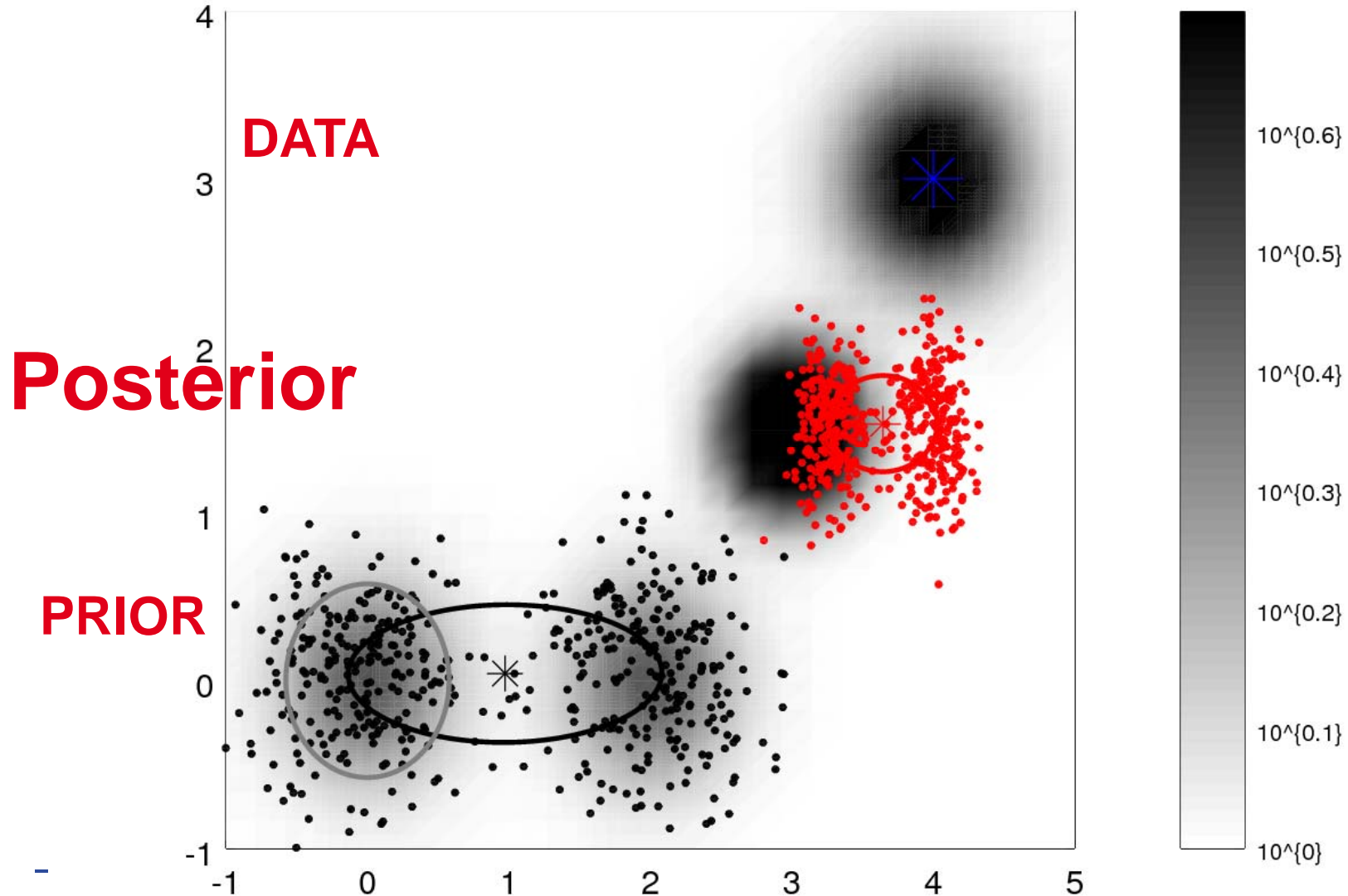
BAYES Data Assimilation

Bayes Theorem and the Ensemble Kalman Filter

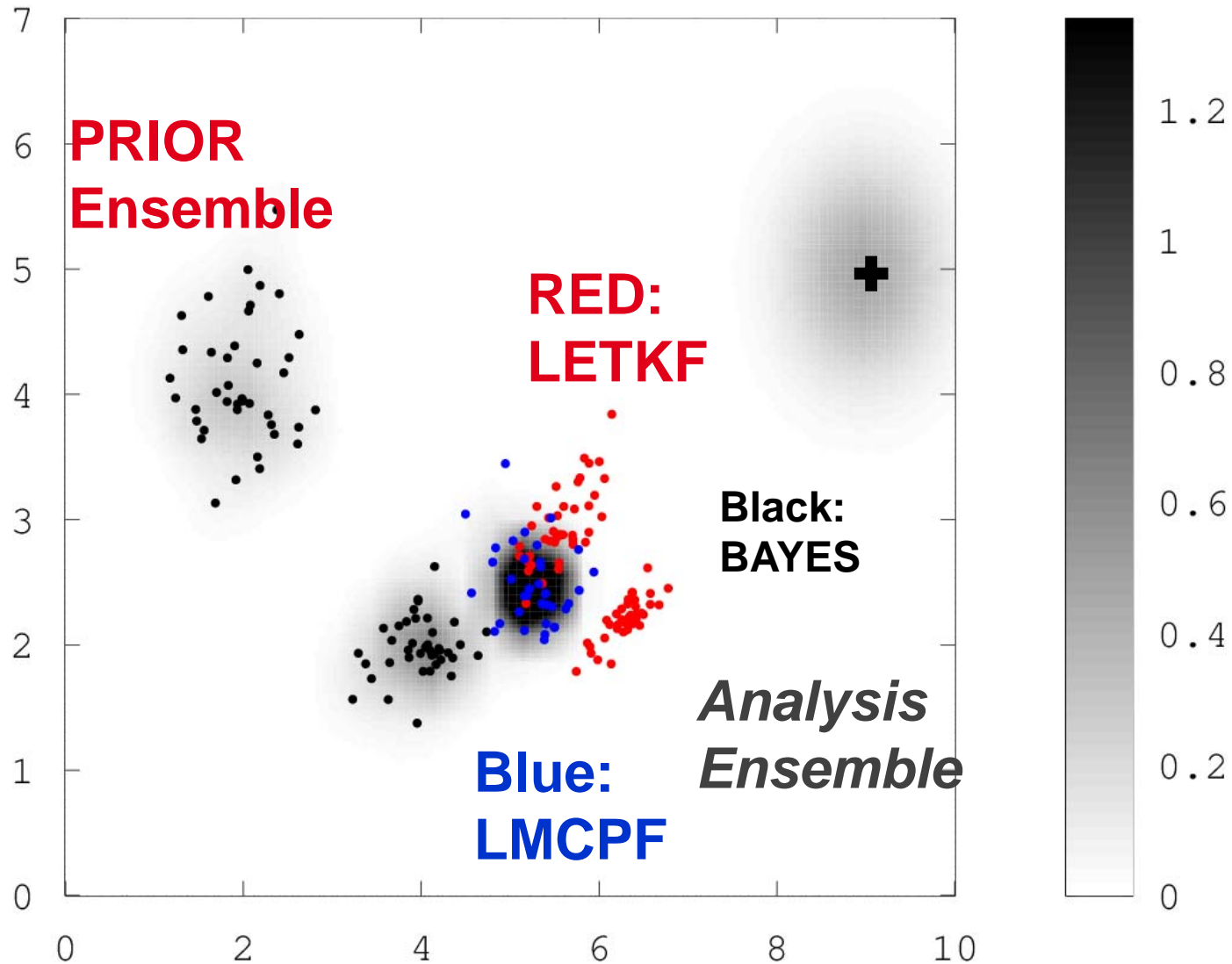


BAYES Data Assimilation

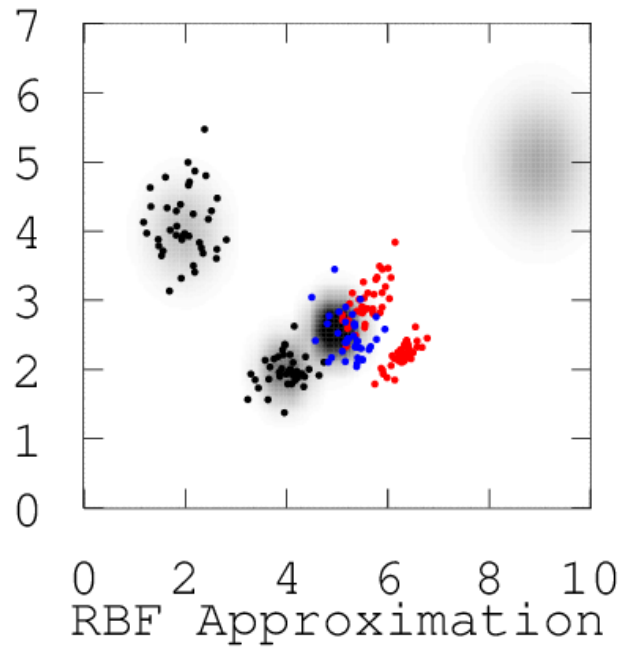
Bayes Theorem and the Ensemble Kalman Filter



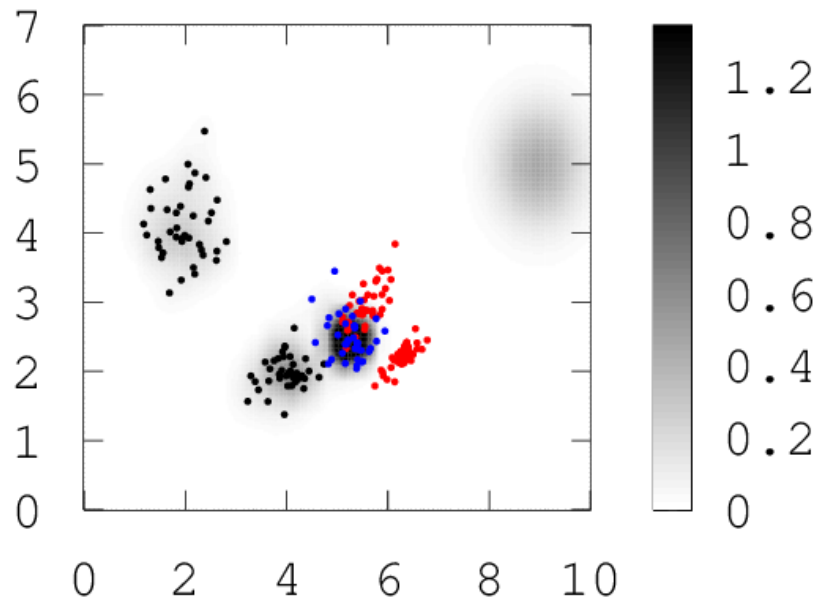
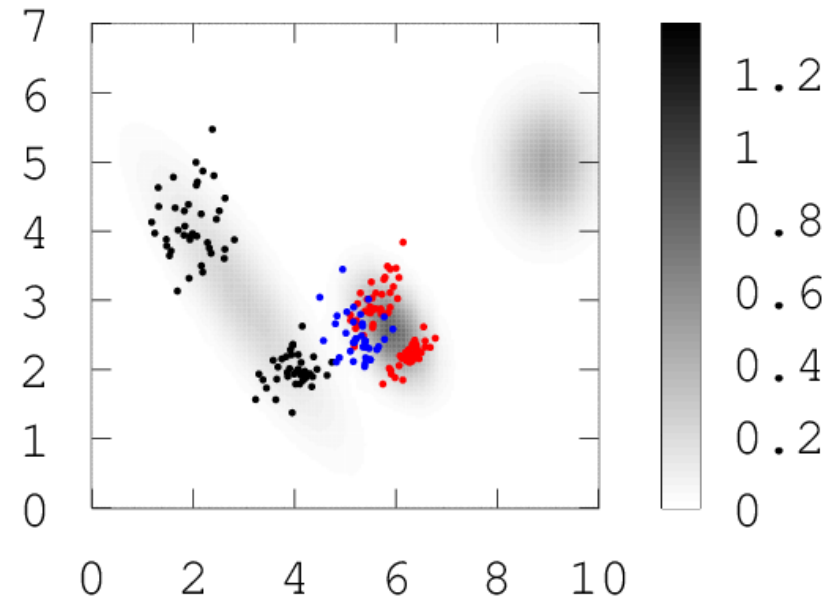
Particle Filter Example



Original



Gaussian Approximation



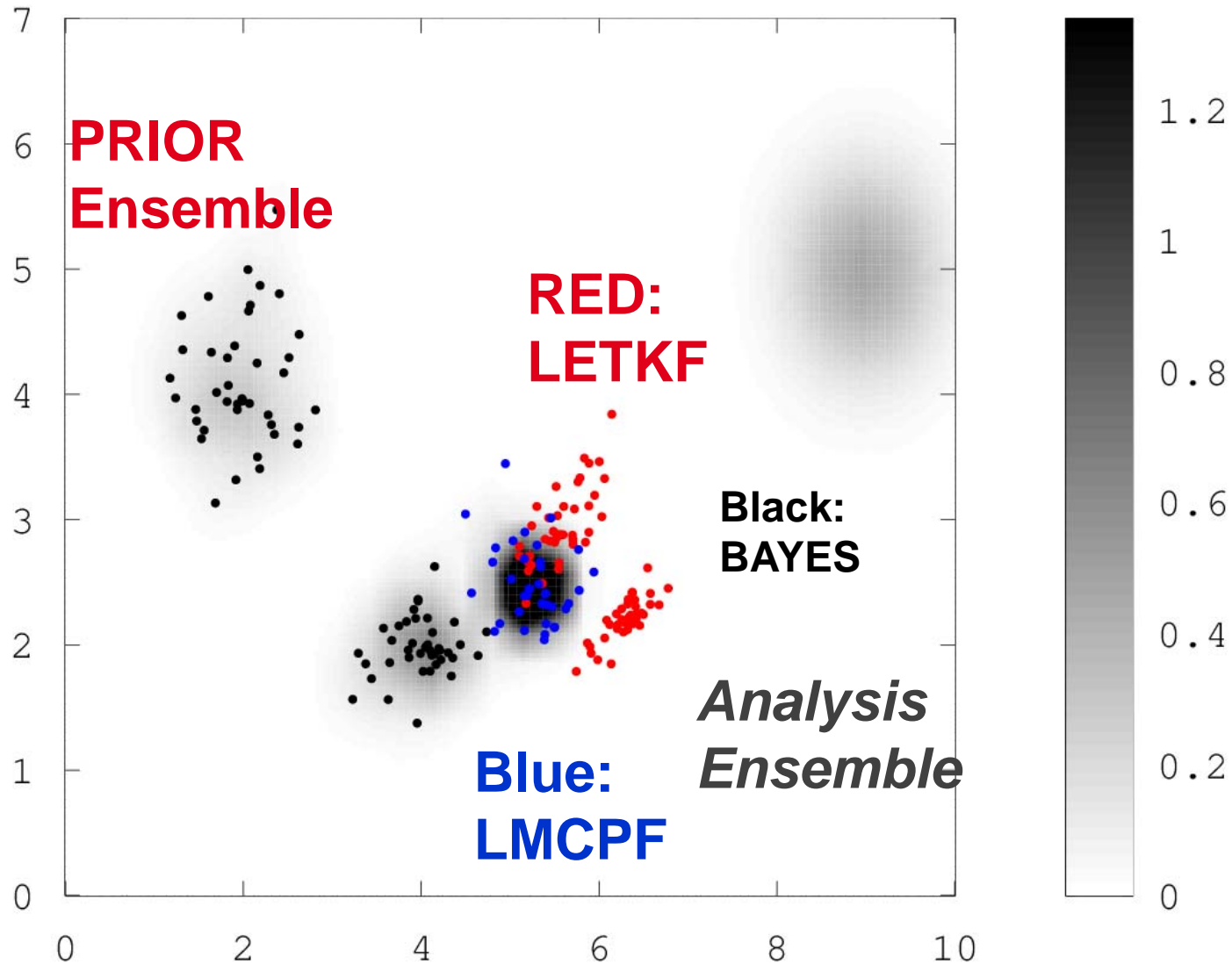
**LETKF
vs.
LMCPF**

The LMCPF Particle Filter

1. We carry out Bayes type data assimilation by creating an ensemble of states (the **particles** or **ensemble members**) $x^{(1)}, \dots, x^{(L)}$ in step t_k for $k = 0$ according to some initial probability distribution $p[t_0](x)$.
2. The ensemble is propagated from t_k to t_{k+1} . It samples the background or *prior* probability distribution $p[t_{k+1}](x)$ at time t_{k+1} .
3. Given measurement data $y \in Y$ we employ Bayes Theorem to calculate the **posterior distribution** $p(x) := p^{(a)}(x) = cp^{(b)}(x)p(y|x)$. This needs the ability to calculate $p(x)$ for some given state x as well as $p(y|x)$ given y for some state x .
4. We use MCMC with **Metropolis-Hastings kernel** to draw $x^{(1)}, \dots, x^{(L)}$ from $p(x)$. Then we proceed with Step 2.



Particle Filter Example



The LMCPF Particle Filter

- **Markov Chain Monte Carlo** Methods are a tool how to sample some given probability distribution $p(x)$.
- We need the ability to calculate $p(x)$ given some state x .
- Then we can employ MCMC, for example with Metropolis Hastings kernel.

- **Metropolis Hastings** is a particular way how to generate the posterior ensemble.
- The idea is to use a **proposal distribution $q(x)$** .
- For every proposal state a decision is made wether to take it or not.
- This depends on the Metropolis Hastings function α .



The LMCPF Particle Filter

- We can employ any **proposal distribution** q . In particular, we can use the result of the LETKF which brings us basically where we would like our particles to be - but with some wrong scaling in the directions of the LETKF-B-Matrix.
- Consequence: use a *relaxed* version of the LETKF to make sure we do not miss any states for our MCMC sampling! This is a form of **covariance inflation** for the LETKF which we have completely under our control.
- Our transition probability $q(x, x')$ can be independent of x , i.e. we can completely employ the **LETKF posterior probability distribution**! But we need the ability to calculate $p(x) = p^{(b, \text{LETKF})}(x)$. This is no problem when we have the estimate for $B^{(b, \text{LETKF})}$.



- We work in the **ensemble space**

$$U = \text{span}\{x^{(1)}, \dots, x^{(L)}\}, \quad x = \sum_{\ell=1}^L \alpha_{\ell} x^{(\ell)} \quad (37)$$

with the background ensemble propagated from the previous step.

- We might use a **localized** version of the space, i.e. we work around some point $p \in \mathbb{R}^3$.
- The term $p(y|x)$ can be calculated when we have observations in the same way as we do it for the LETKF.
- We need to calculate the **prior probability density** $p(x)$ for x given by (37) given the ensemble members $x^{(1)}, \dots, x^{(L)}$ many times in each analysis step of the LMCPF.



- To **approximate** $p(x)$ we can employ several methods. A very general approach is to attach a Gaussian to each ensemble member, i.e. to use

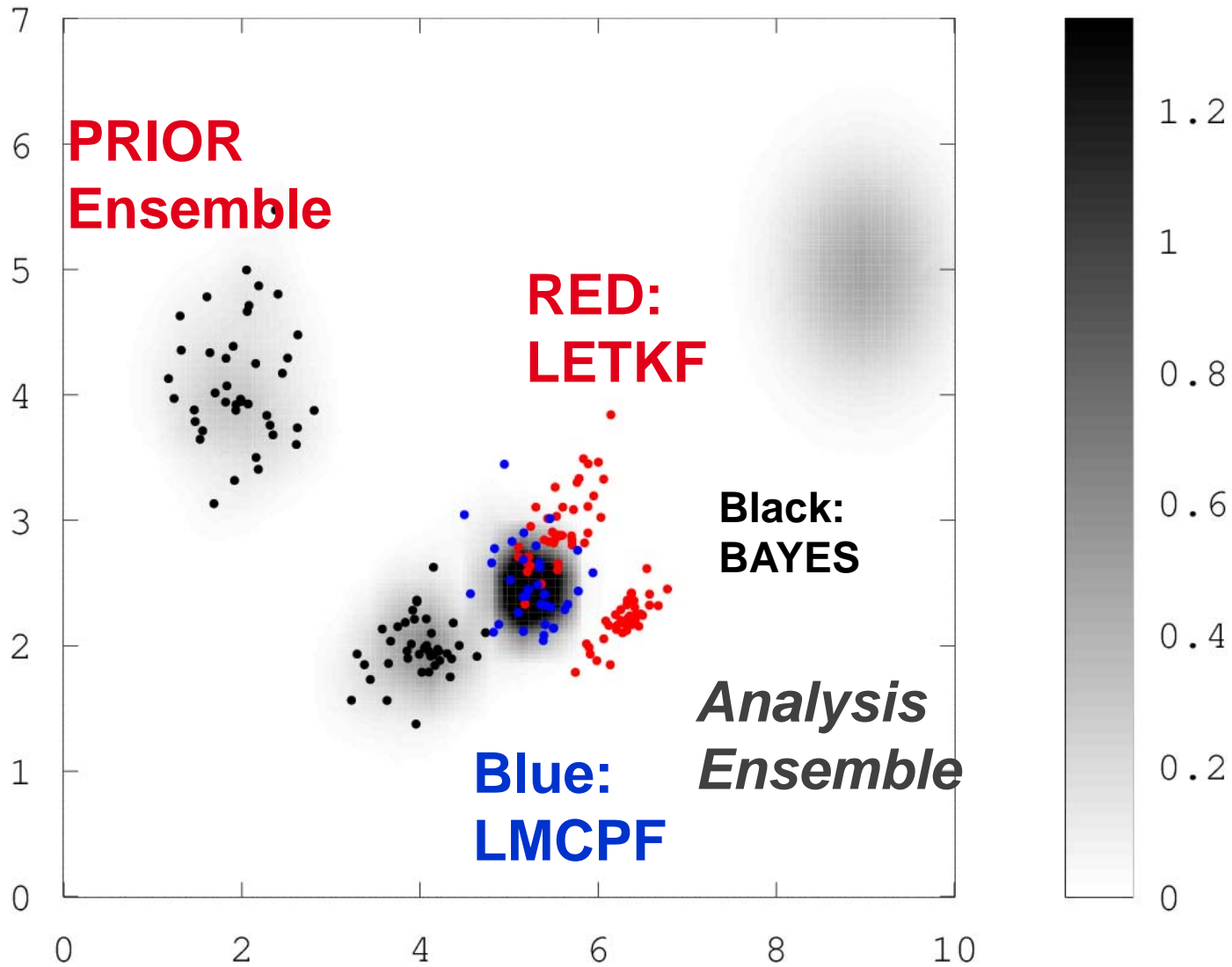
$$p(x) := \sum_{\ell=1}^L c_{\ell} e^{-\|x-x^{(\ell)}\|/b_{\ell}} \quad (38)$$

with constants b_{ℓ} and c_{ℓ} . Here, c_{ℓ} is chosen in dependence of b_{ℓ} such that the integral is equal to 1 for each of the Gaussian ensembles. The constants b_{ℓ} are **tuning constants** to get a best approximation of $p(x)$ based on $x^{(\ell)}$.

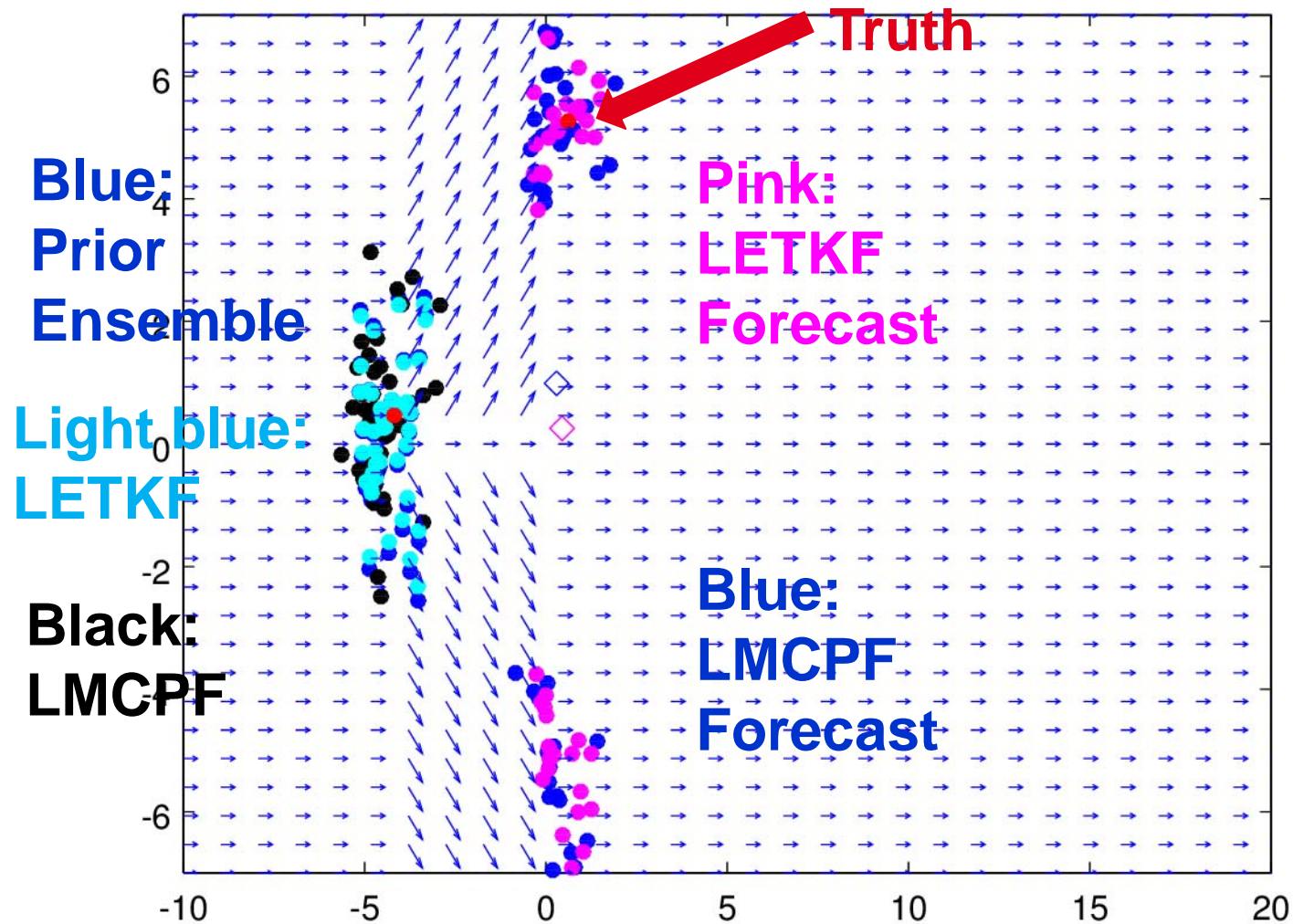
- *Some version of the **Ensemble Kalman Filter** can be obtained from the particular choice where we approximate $p(x)$ by a global Gaussian distribution!*



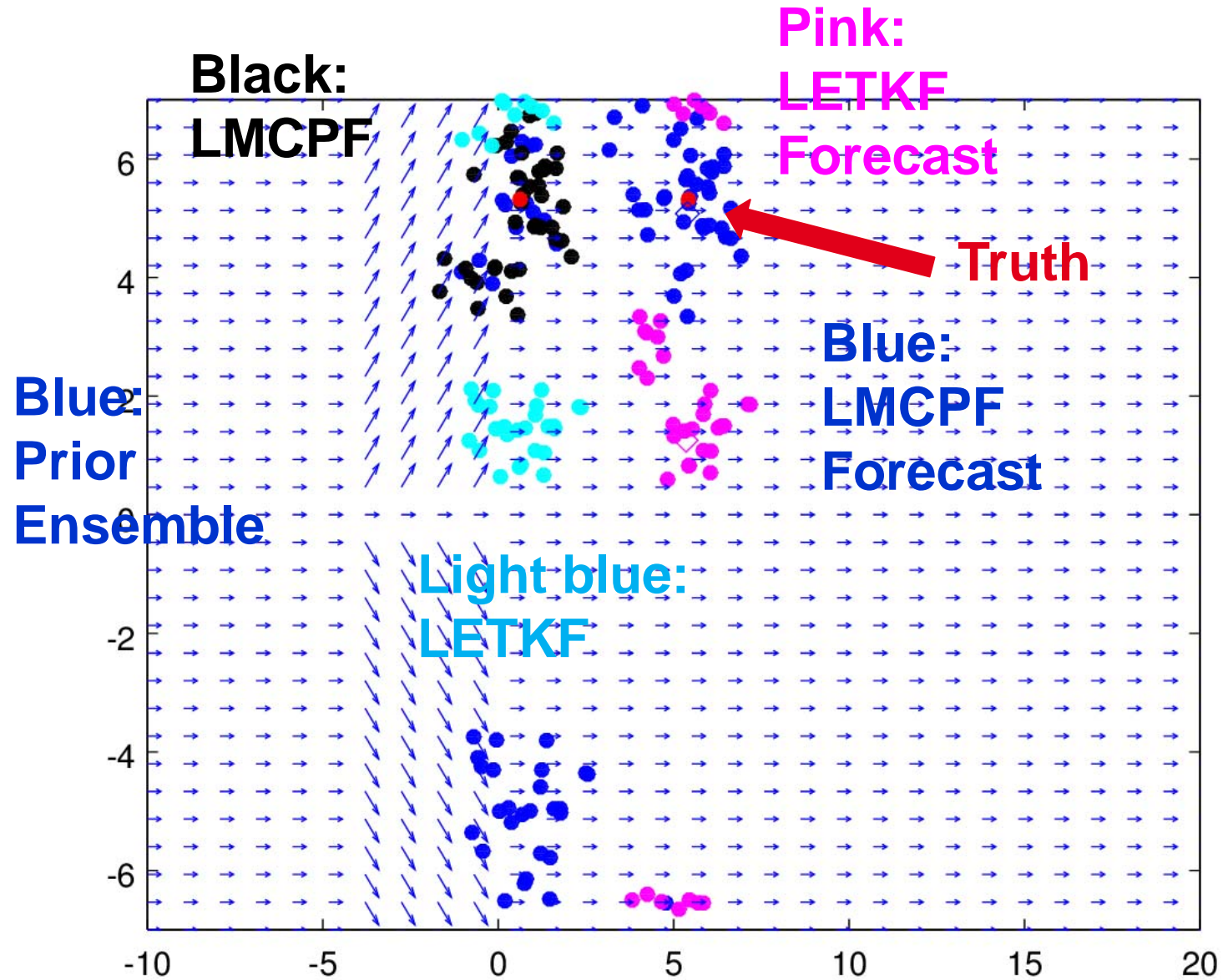
Particle Filter Example



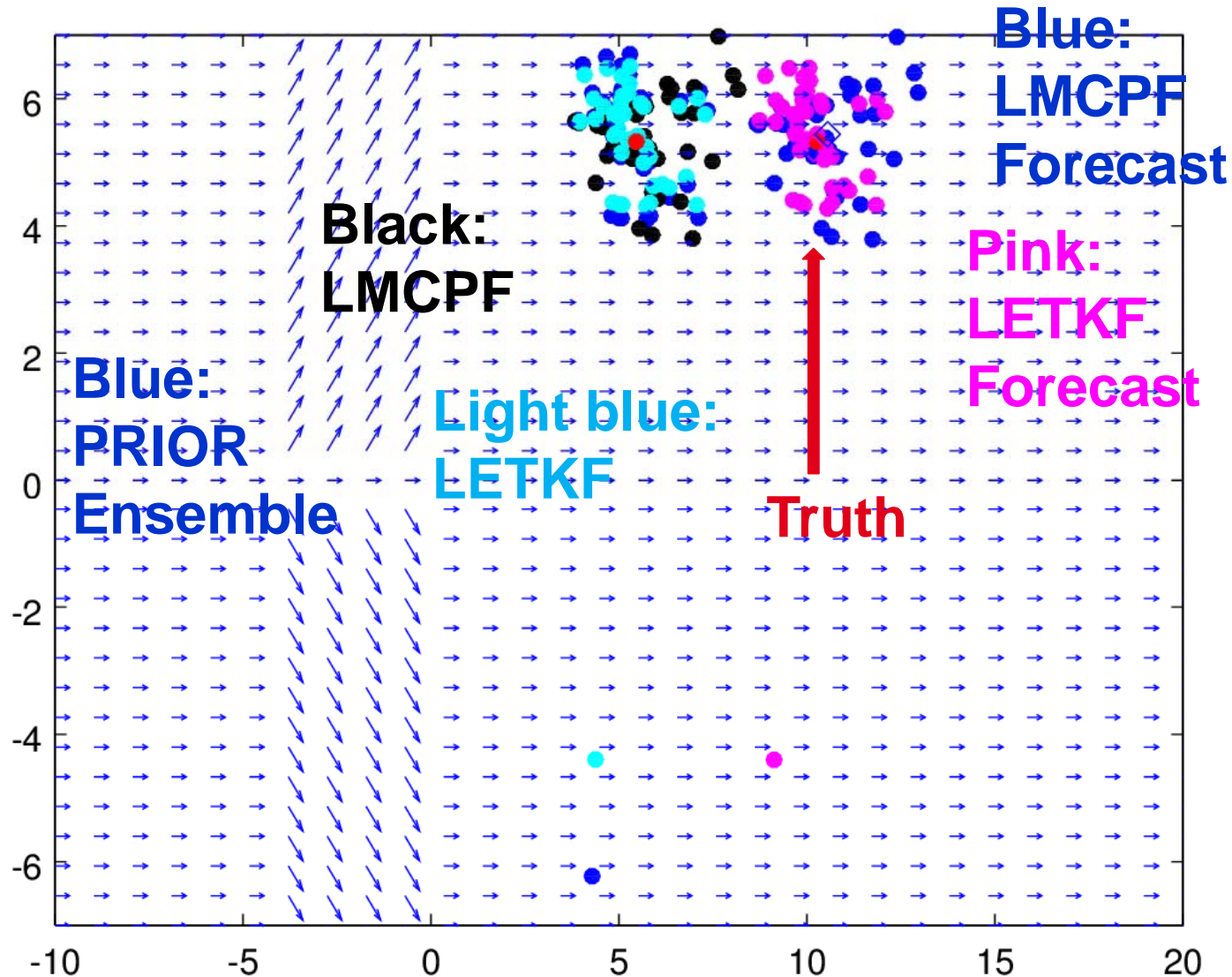
LMCPF Example: nonlinear gate



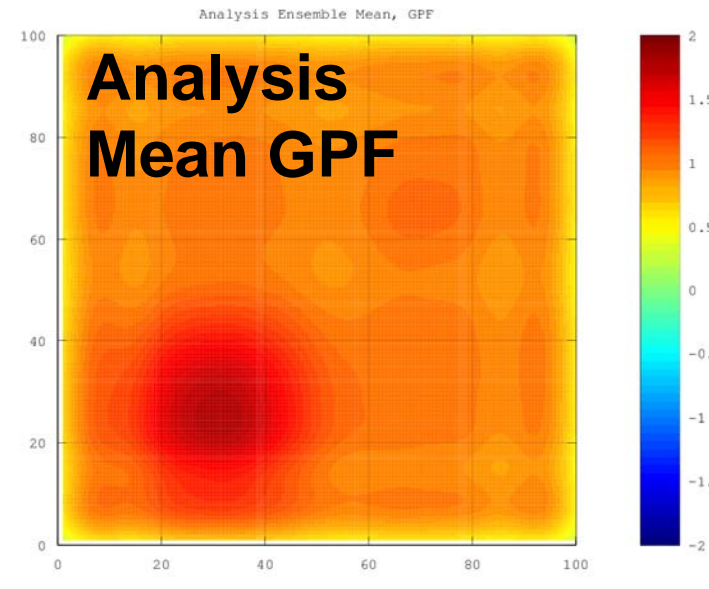
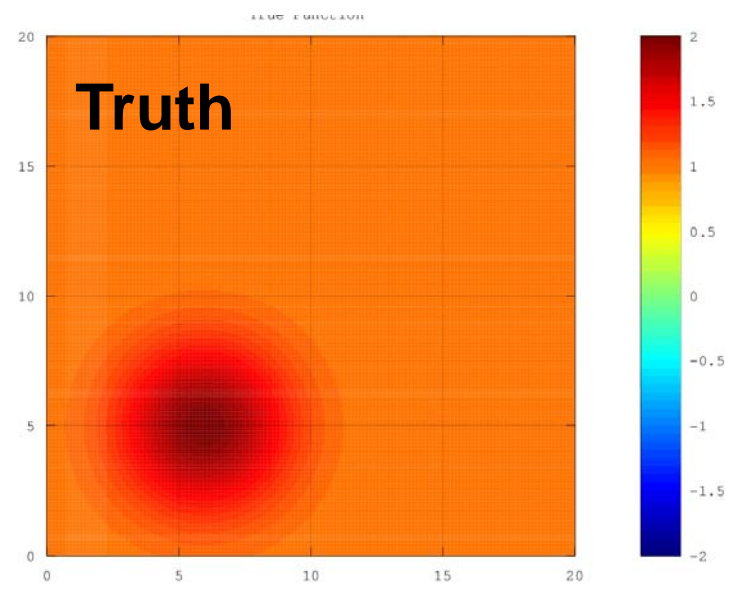
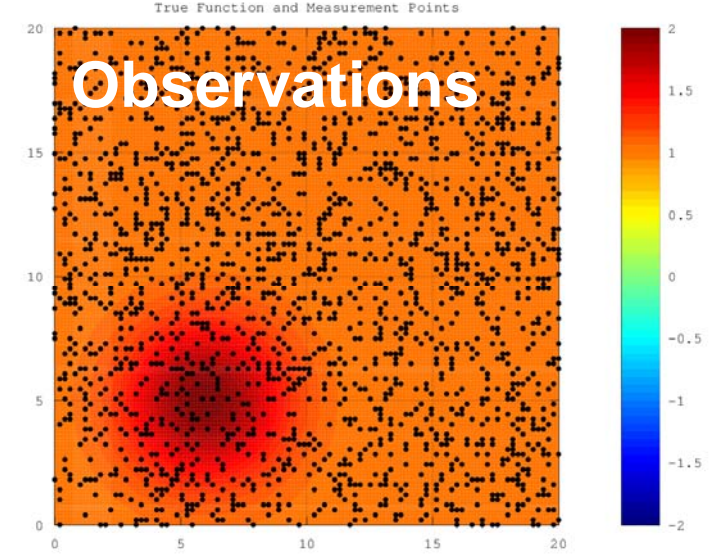
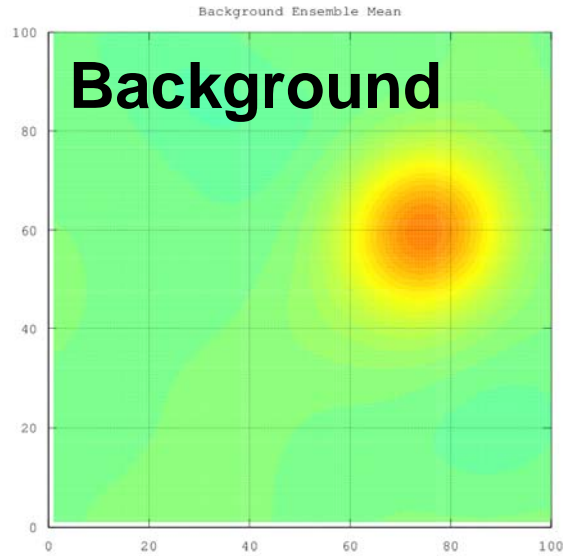
LMCPF Example: nonlinear gate



LMCPF Example: nonlinear gate

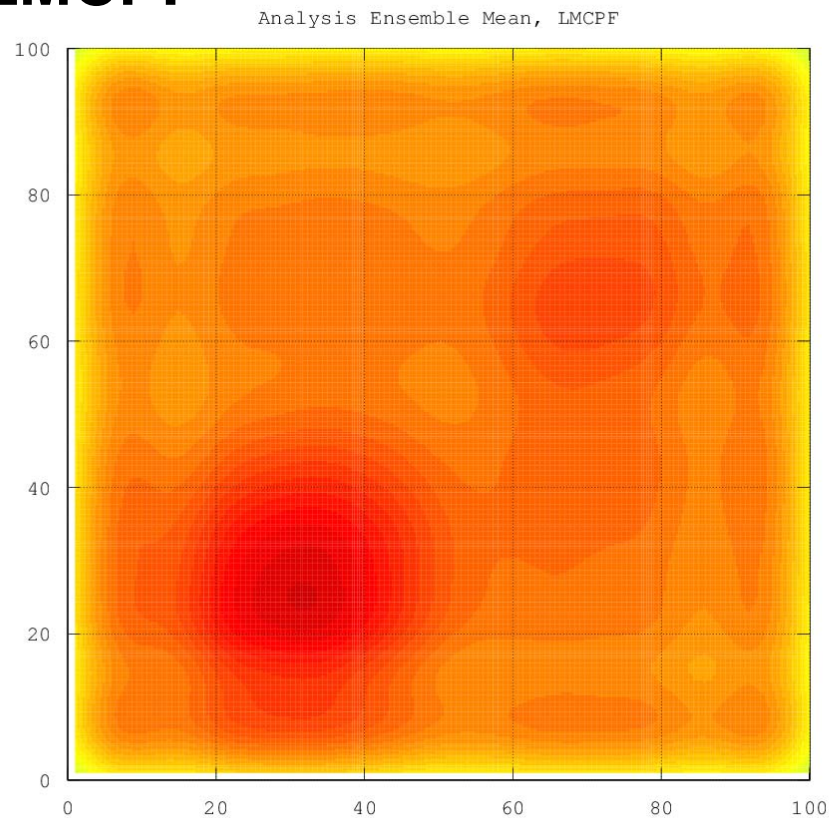


10.000 dimensional Example

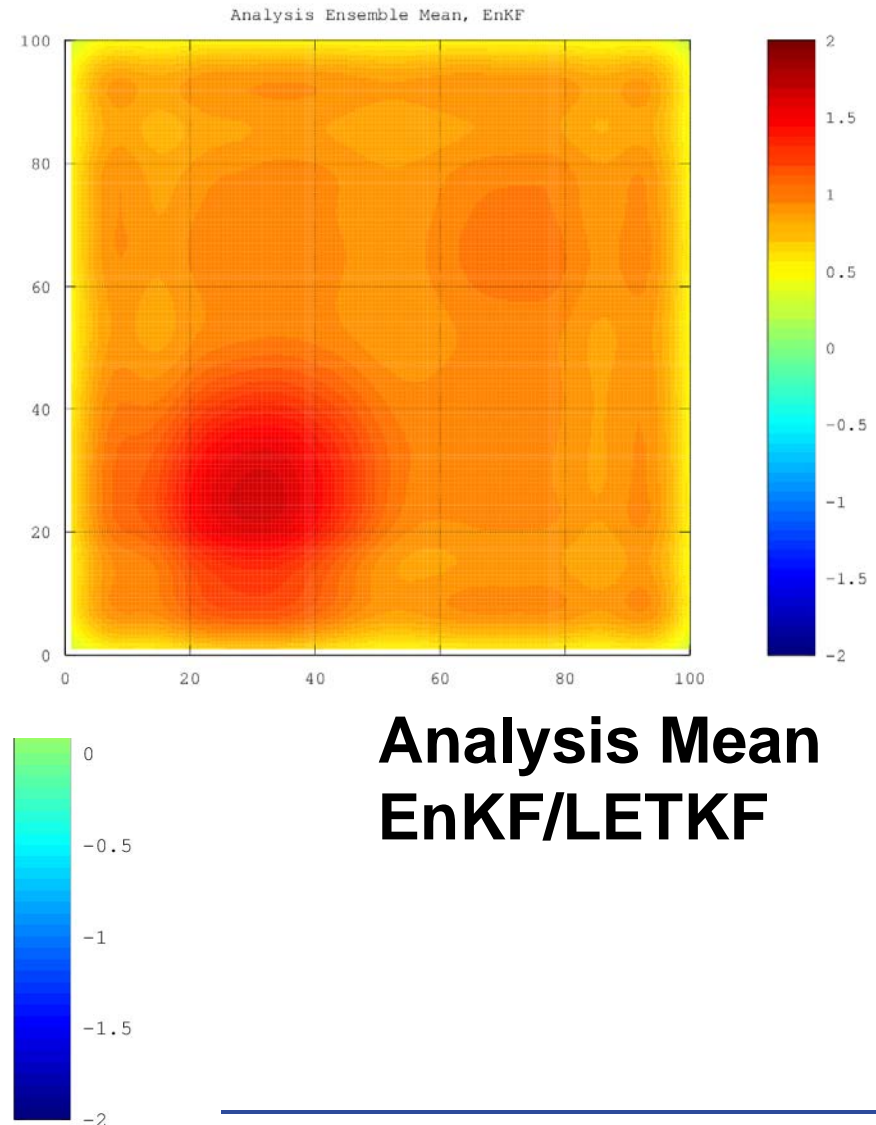


10.000 dimensional Example

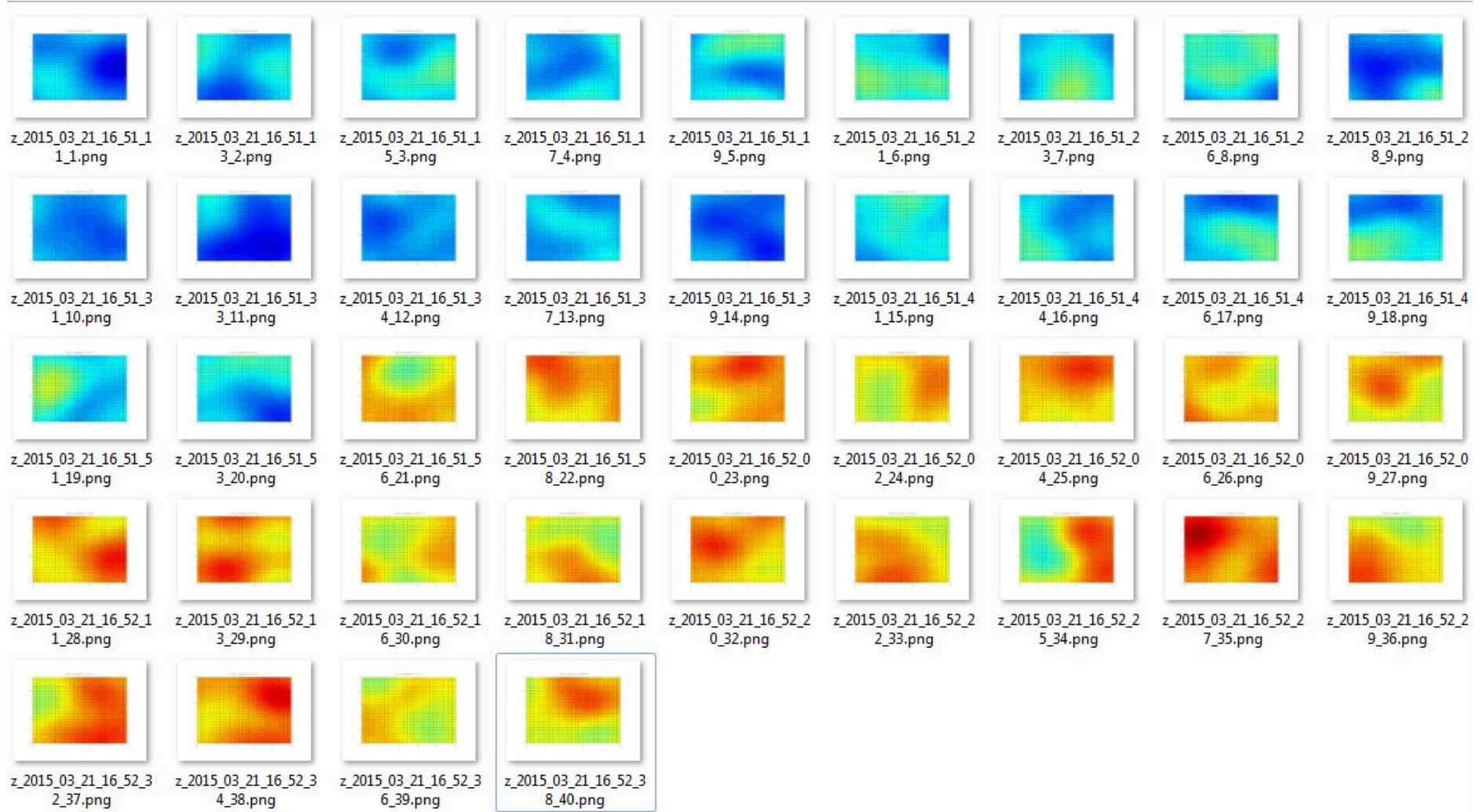
Analysis Mean LMCPF



Analysis Mean EnKF/LETKF



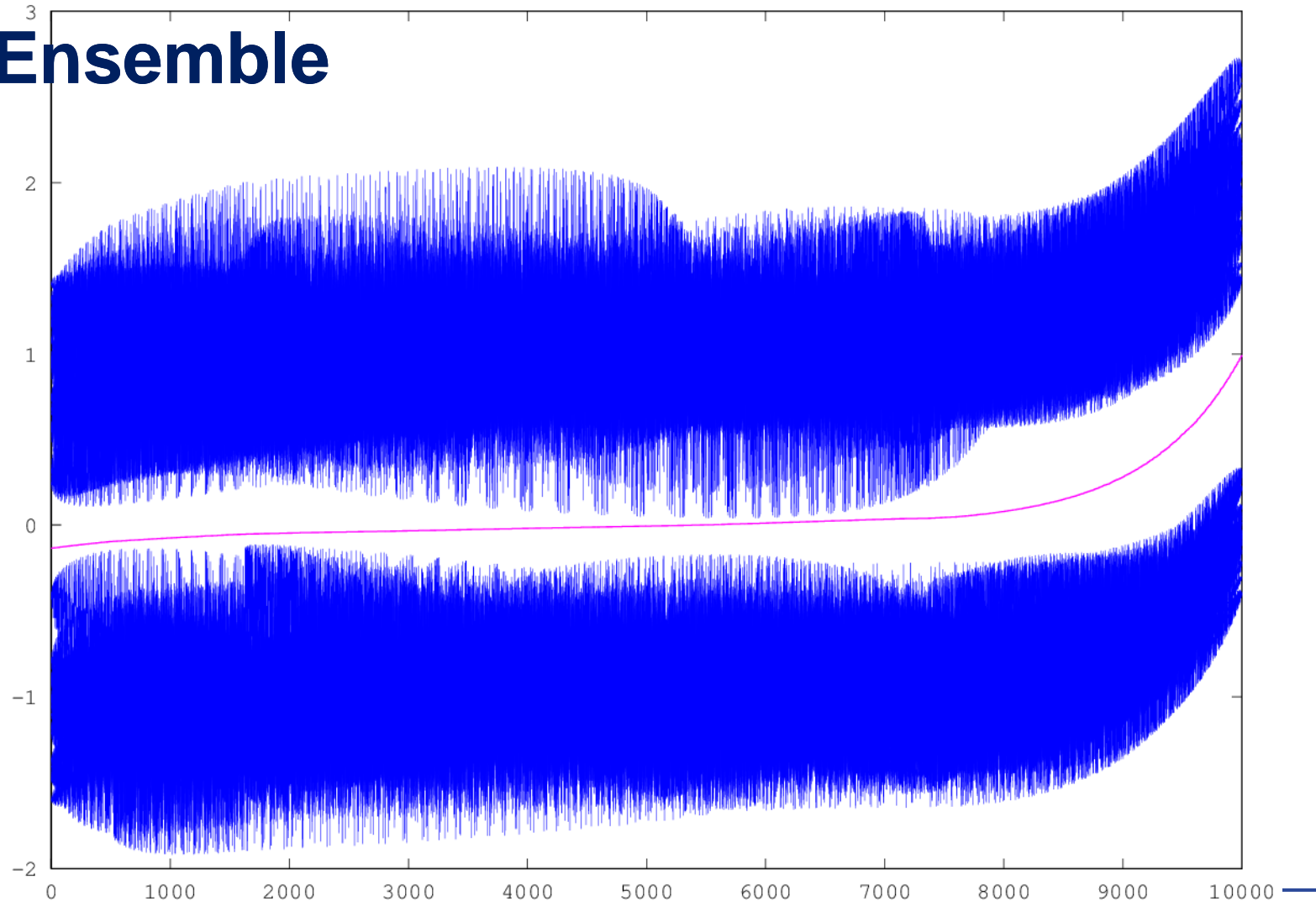
Prior Ensemble – Bi-Modal



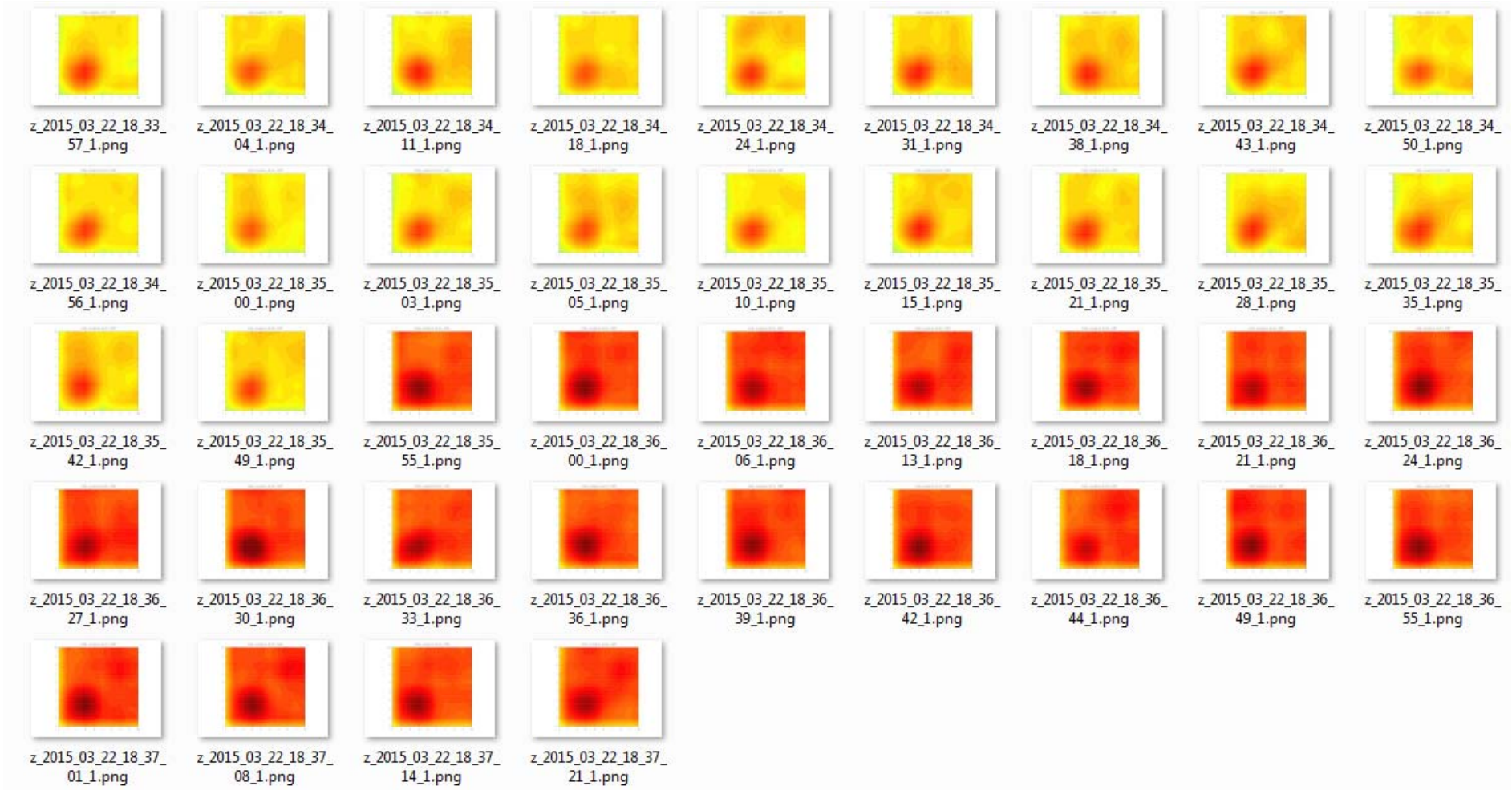
10.000 dimensional Example

Sequentially Sorted Diagram, Background Ensemble

Prior Ensemble



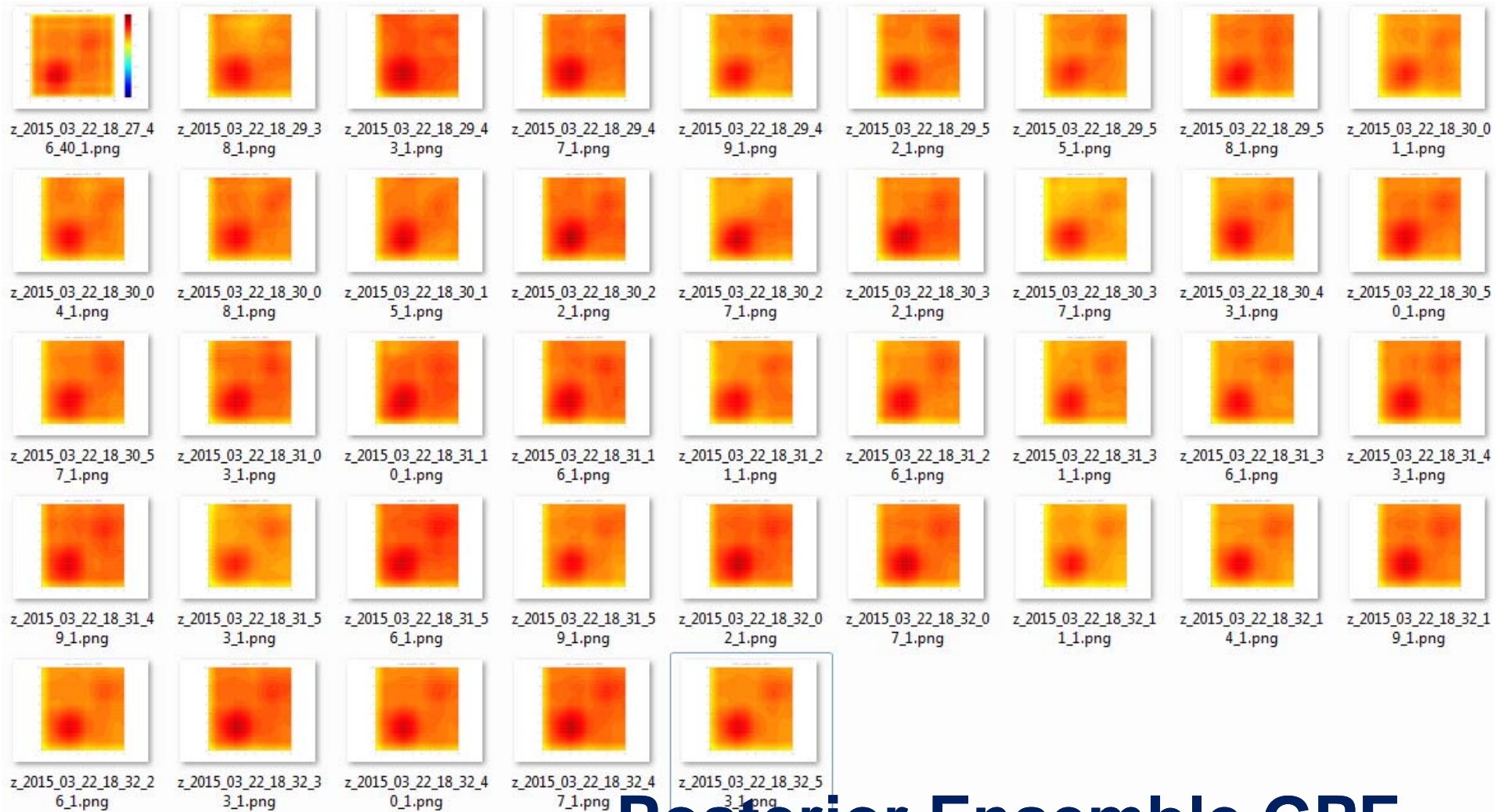
10.000 dimensional Example



Posterior Ensemble EnKF



10.000 dimensional Example

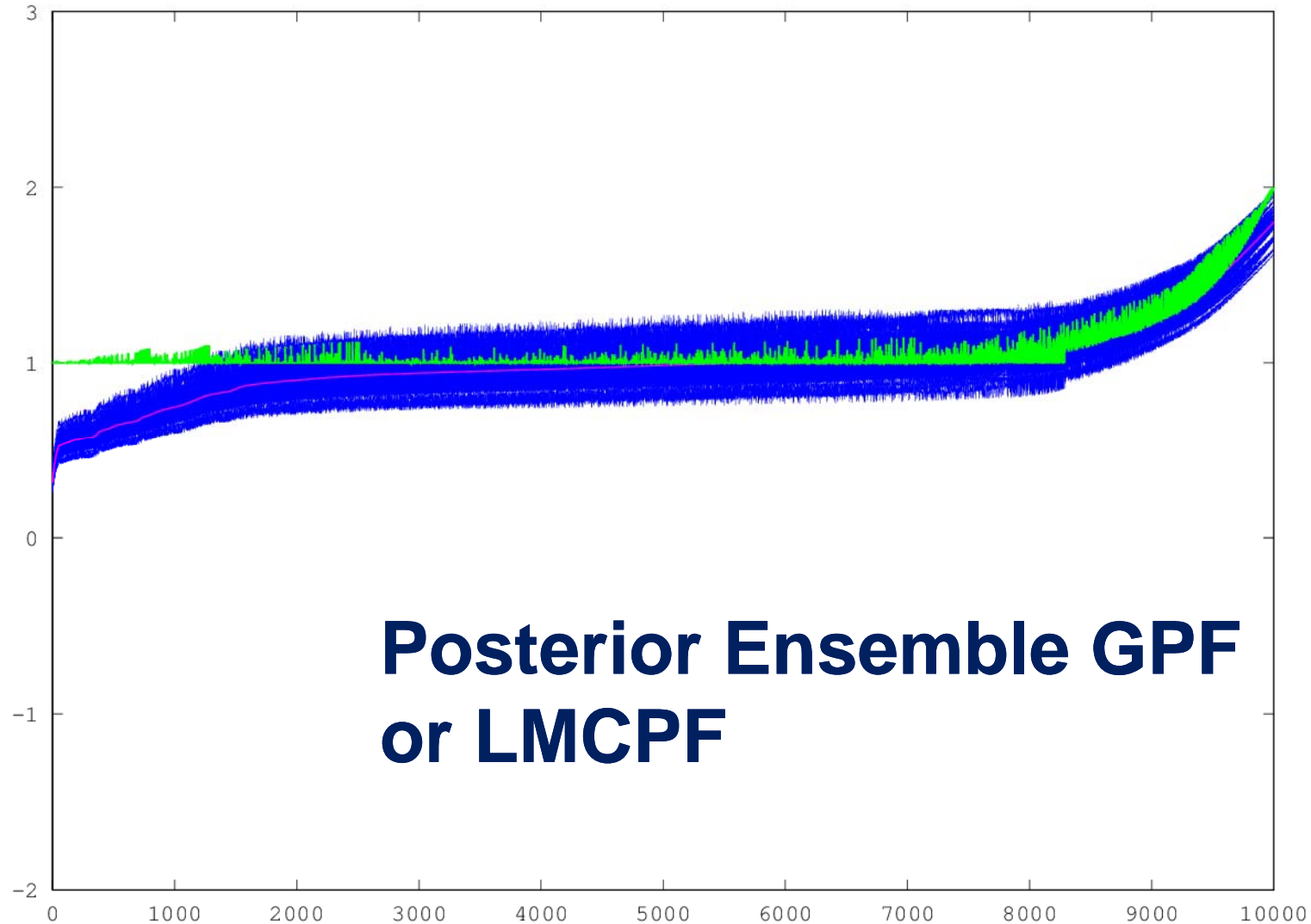


Posterior Ensemble GPF



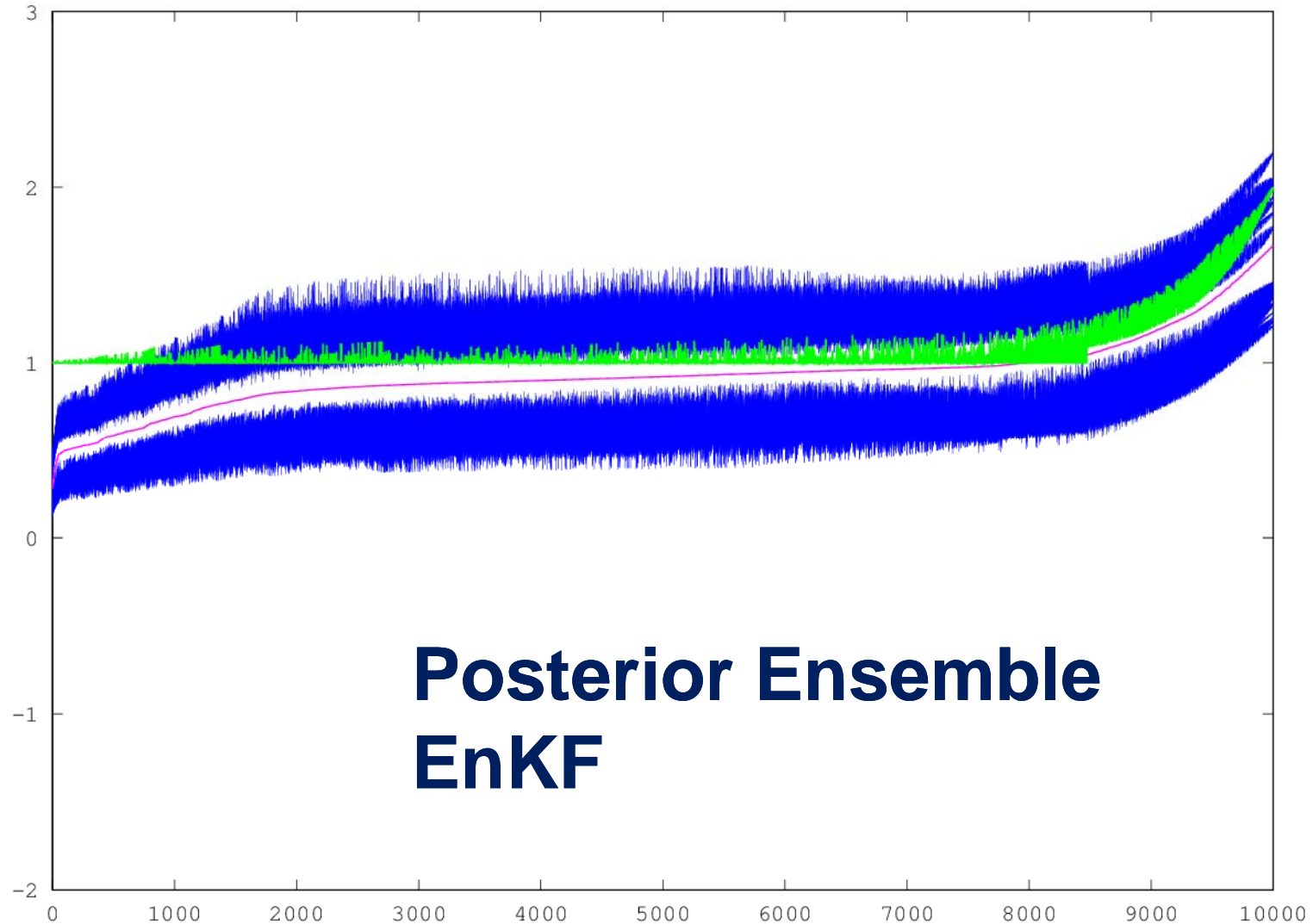
10.000 dimensional Example

Sequentially Sorted Diagram, Analysis Ensemble



10.000 dimensional Example

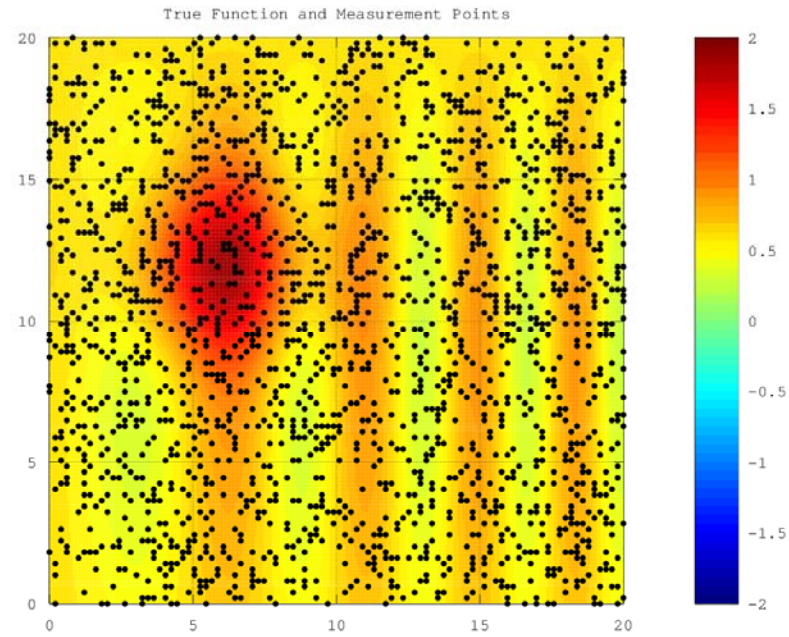
Sequentially Sorted Diagramm, Analysis Ensemble



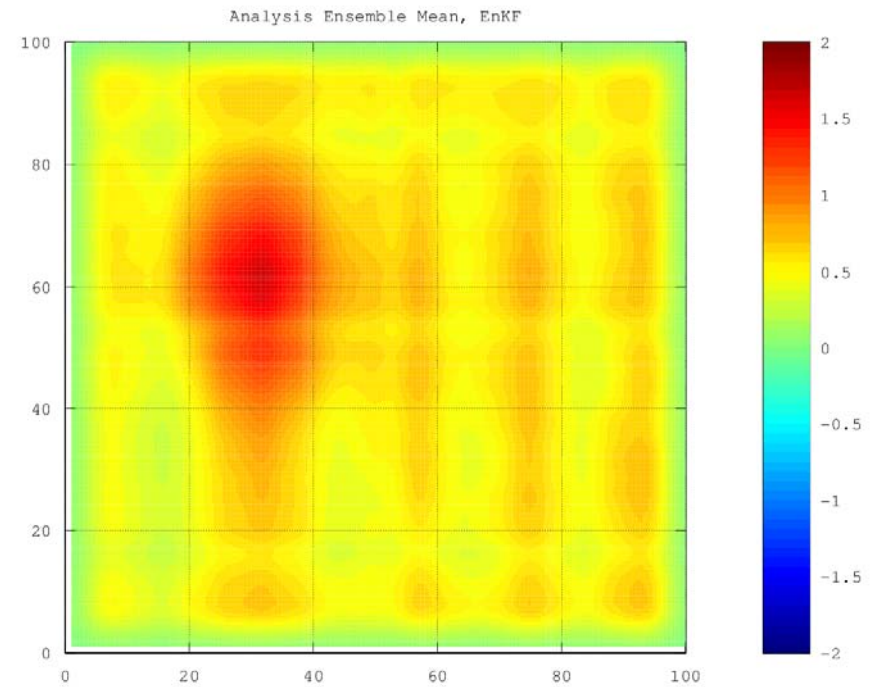
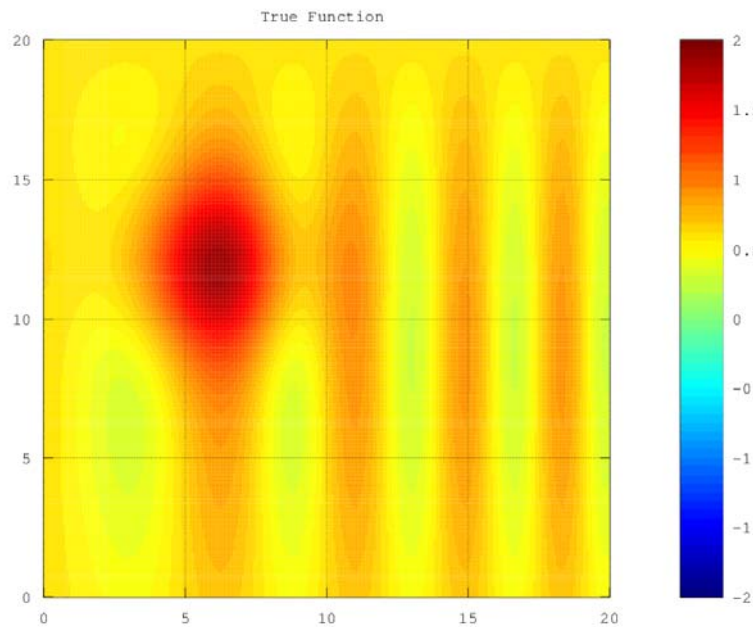
**Posterior Ensemble
EnKF**



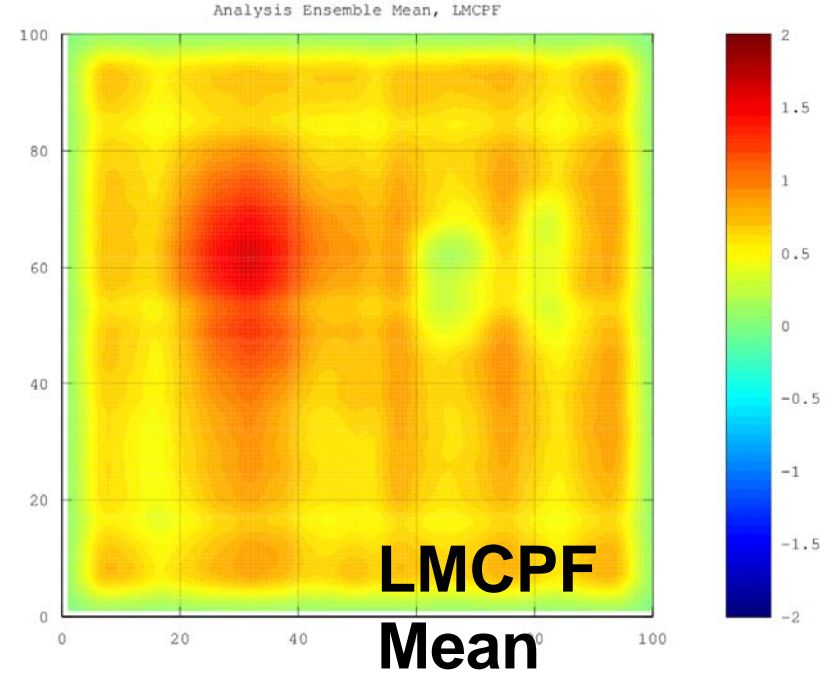
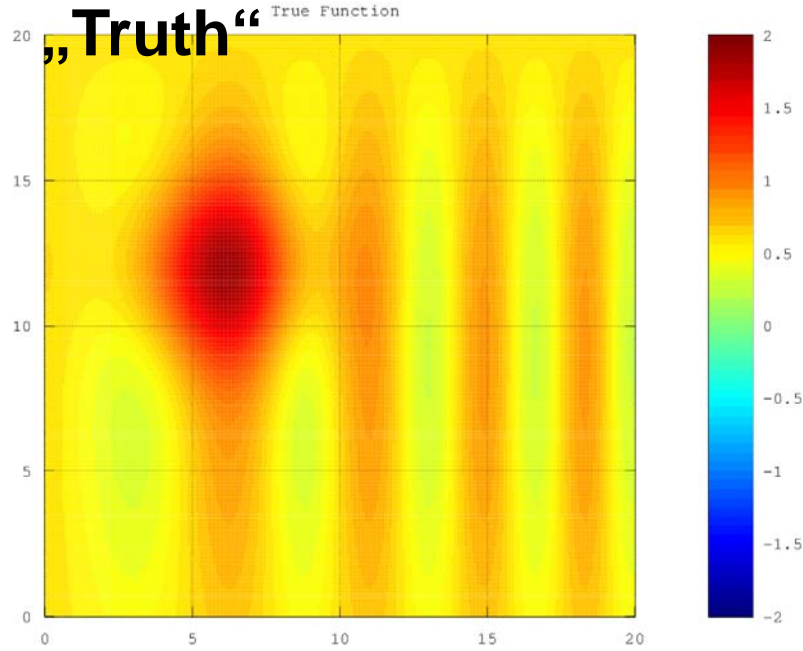
Higher Modes



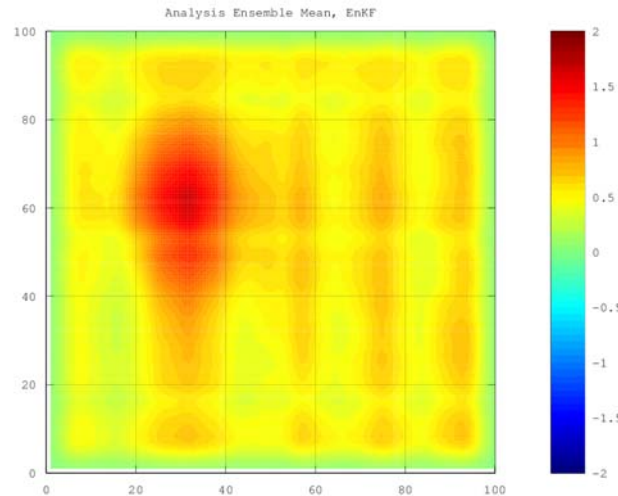
Deutscher Wetterdienst
Wetter und Klima aus einer Hand



Higher Modes LMCPF

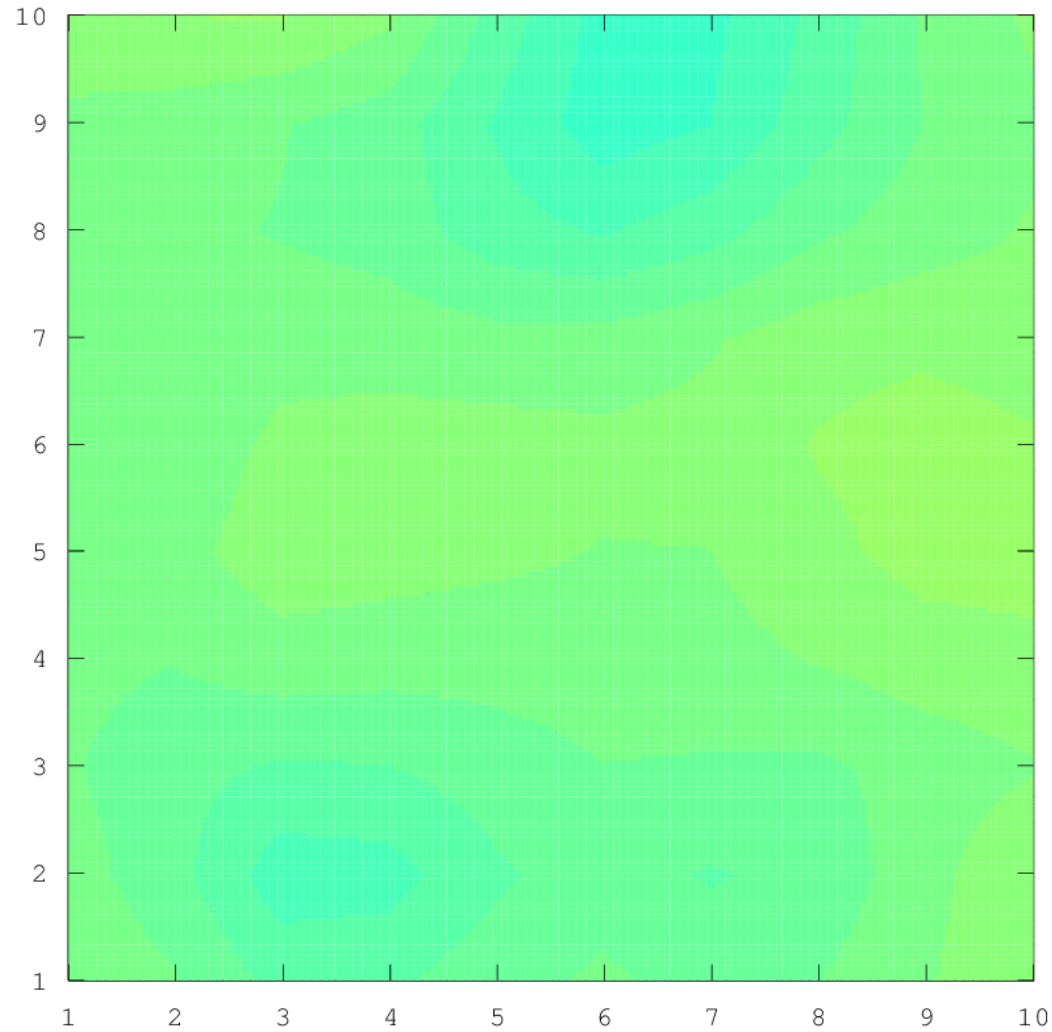


EnKF
Mean

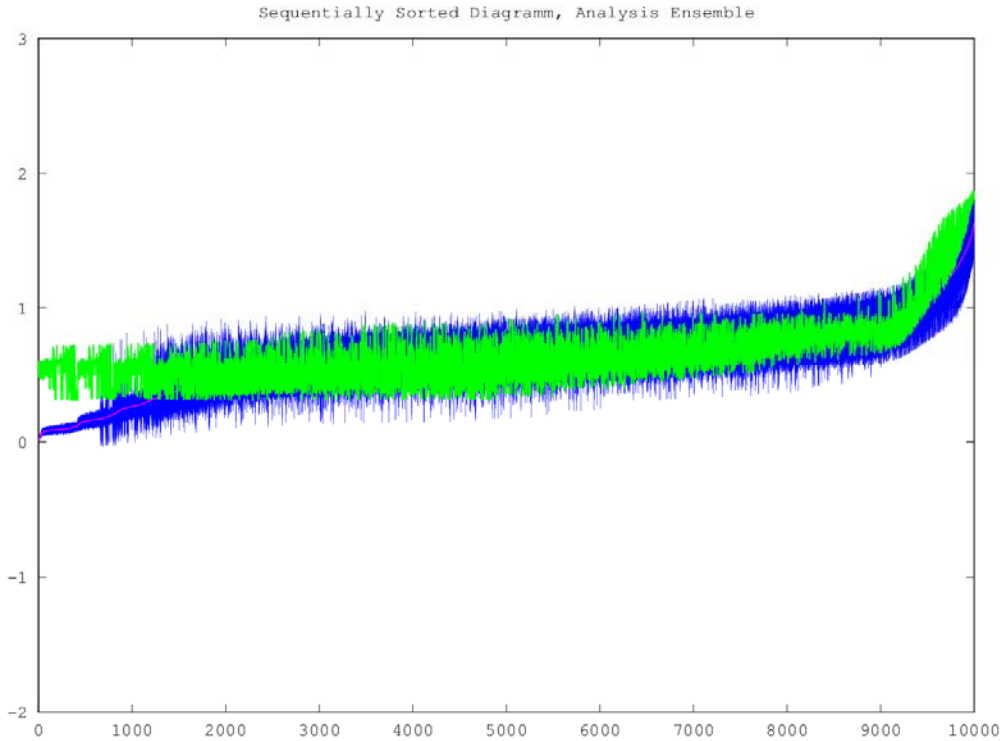


GPF Difference Ensemble

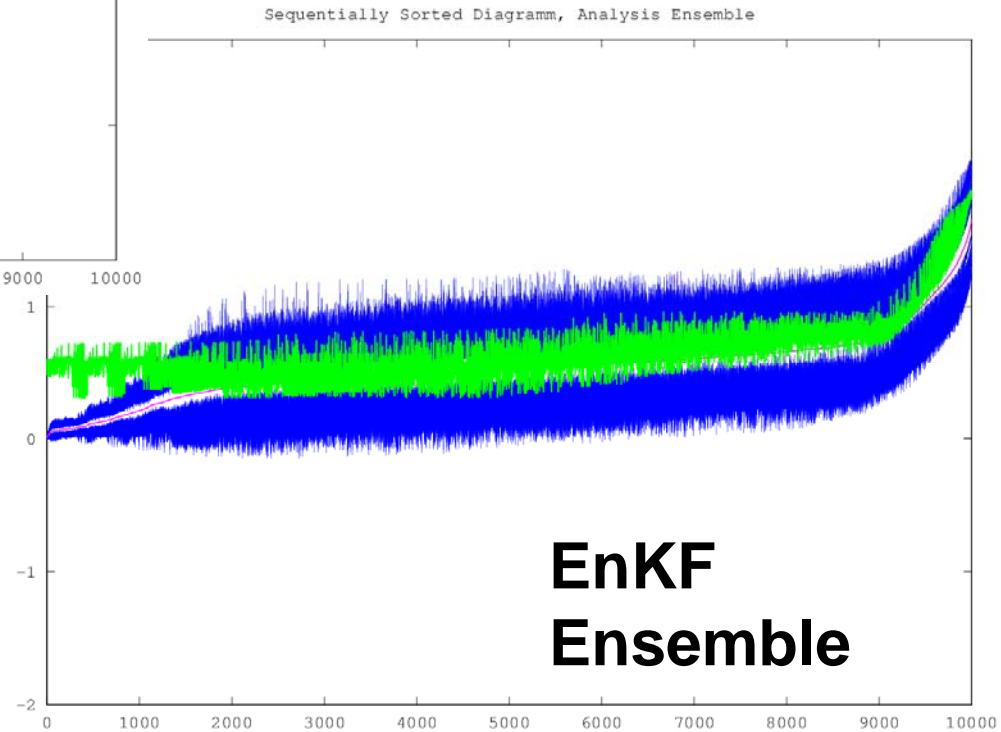
Combi ensemble No=1, GPF



LMCPF versus EnKF



**LMCPF
Ensemble**

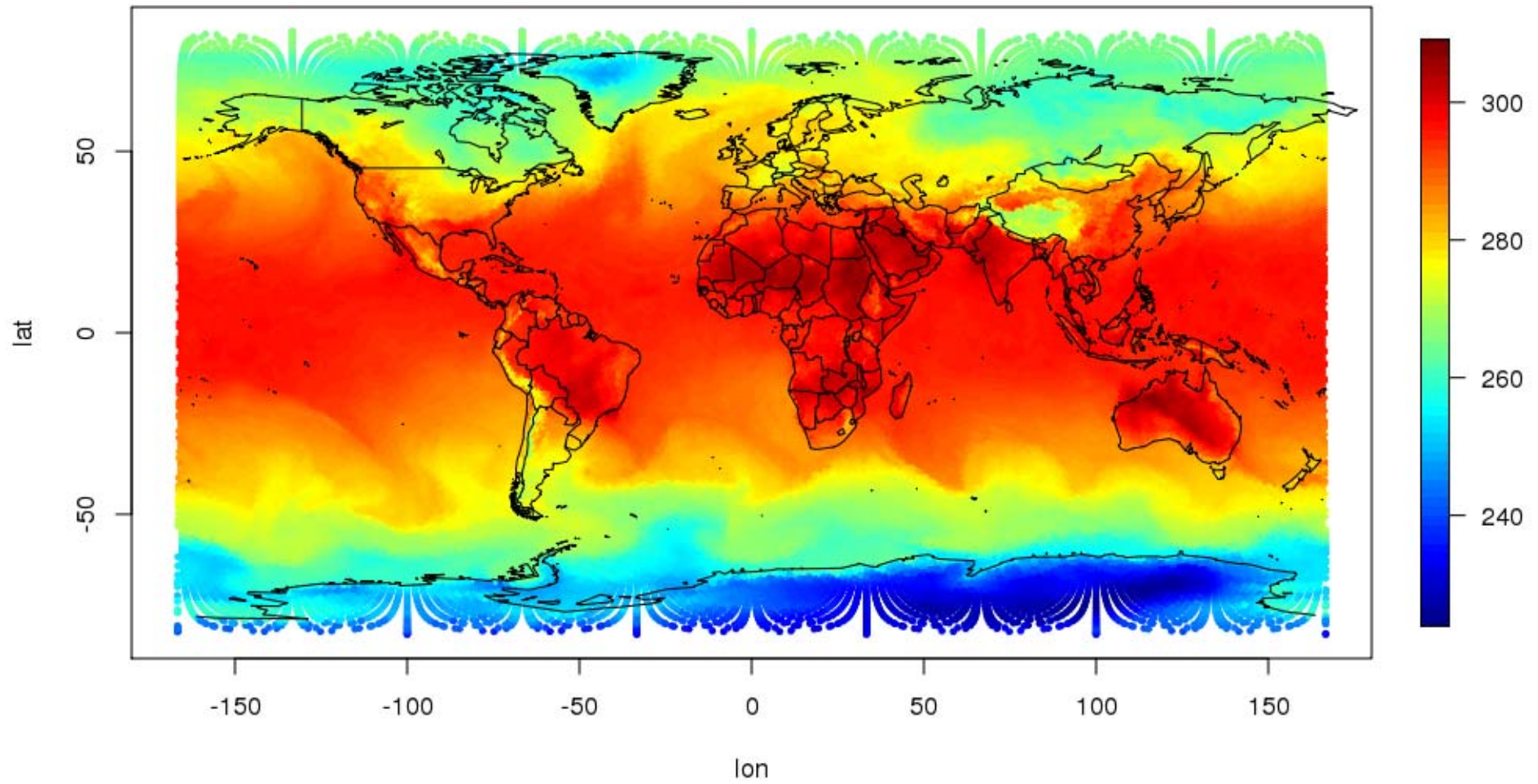


**EnKF
Ensemble**



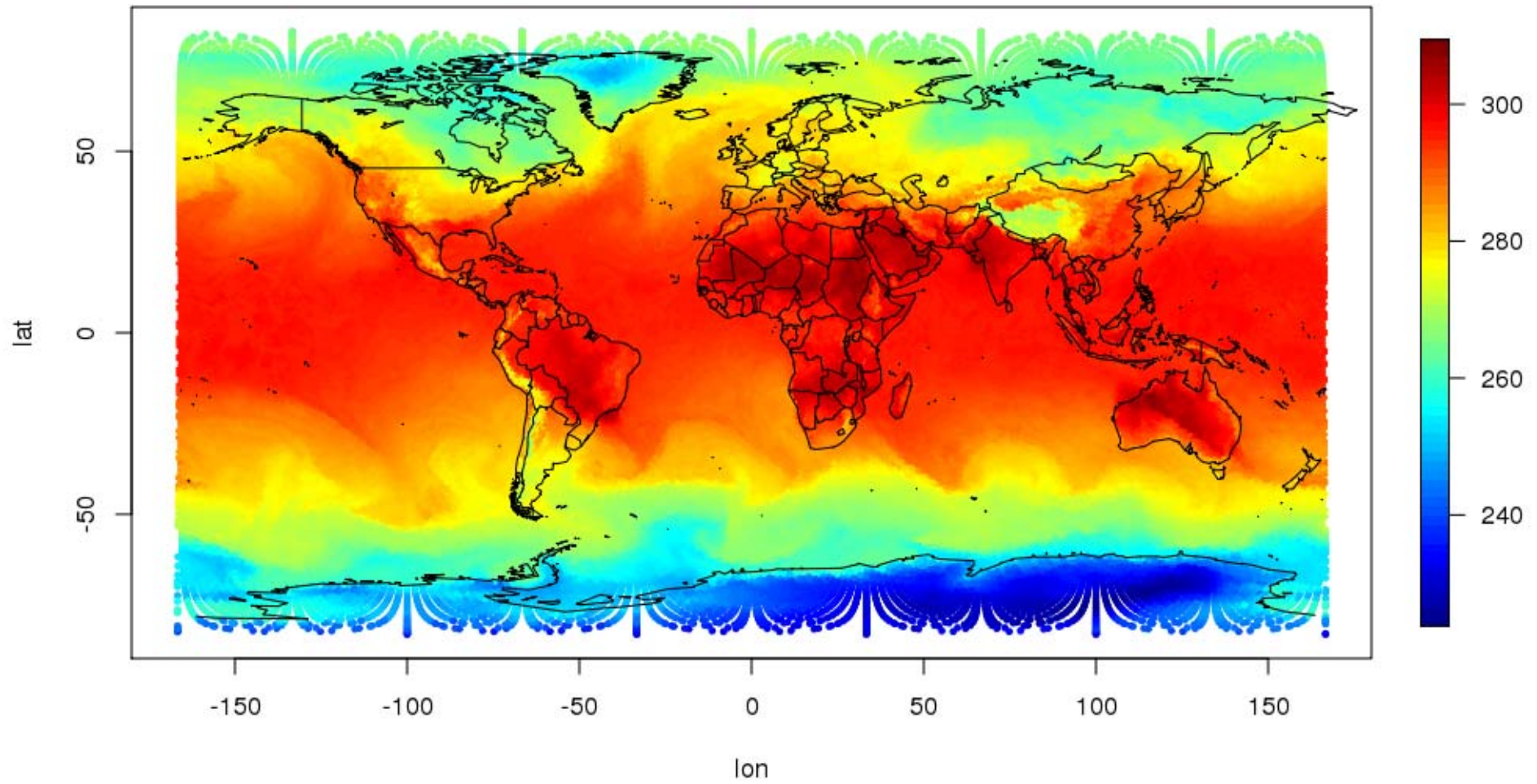
- ❖ Ongoing LMCPF and Ensemble Kalman Particle Filter **Implementations** for **Numerical Wether Prediction (270 Mio DoF)**
- ❖ Further **diagnostics** on nonlinear dynamics and the behaviour of particle filters (simple statistics are not sufficient)
- ❖ Test different **localization** schemes
- ❖ Extensive testing for **large-scale NWP systems.**





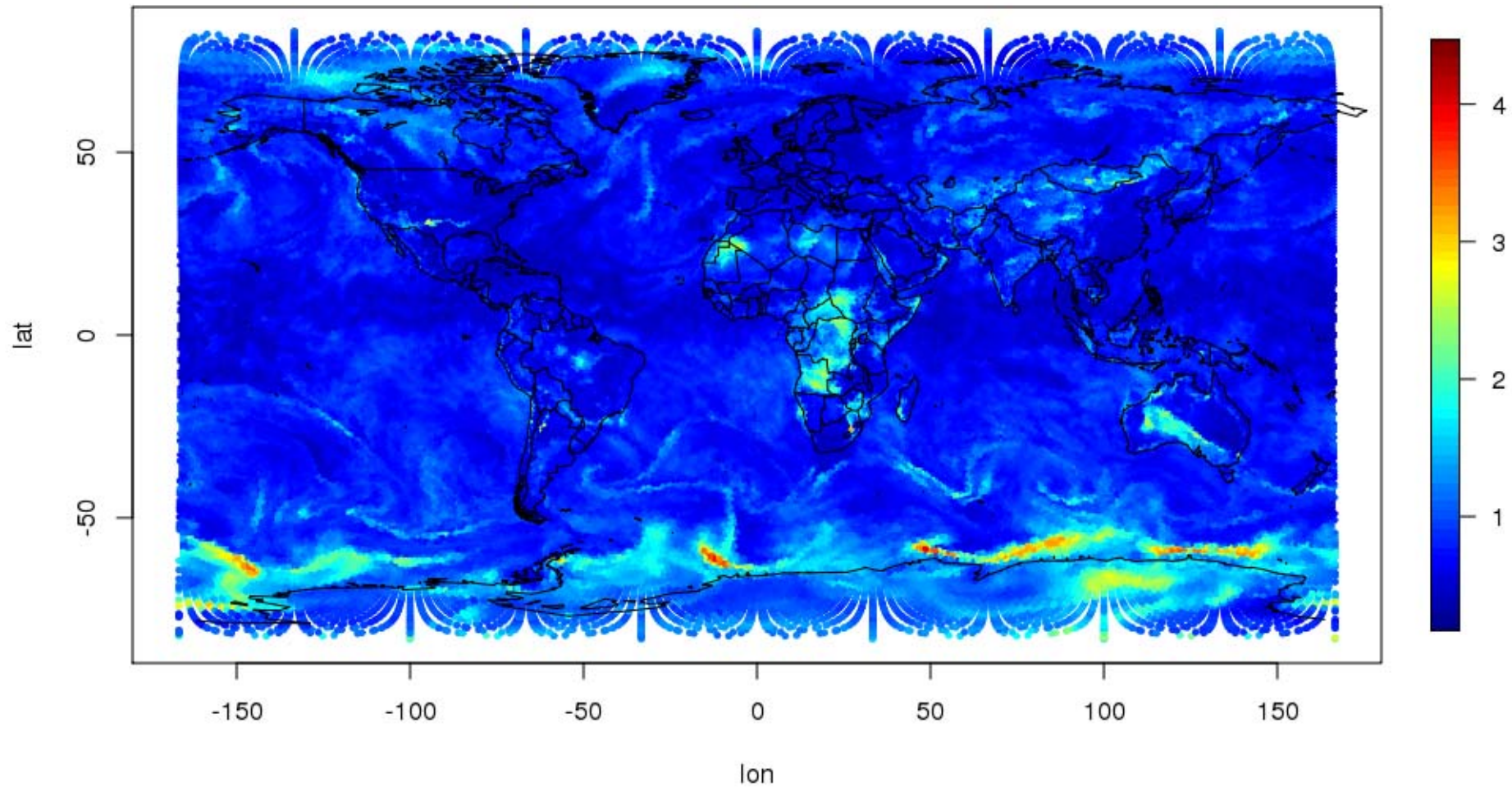
EnKF T on level 85





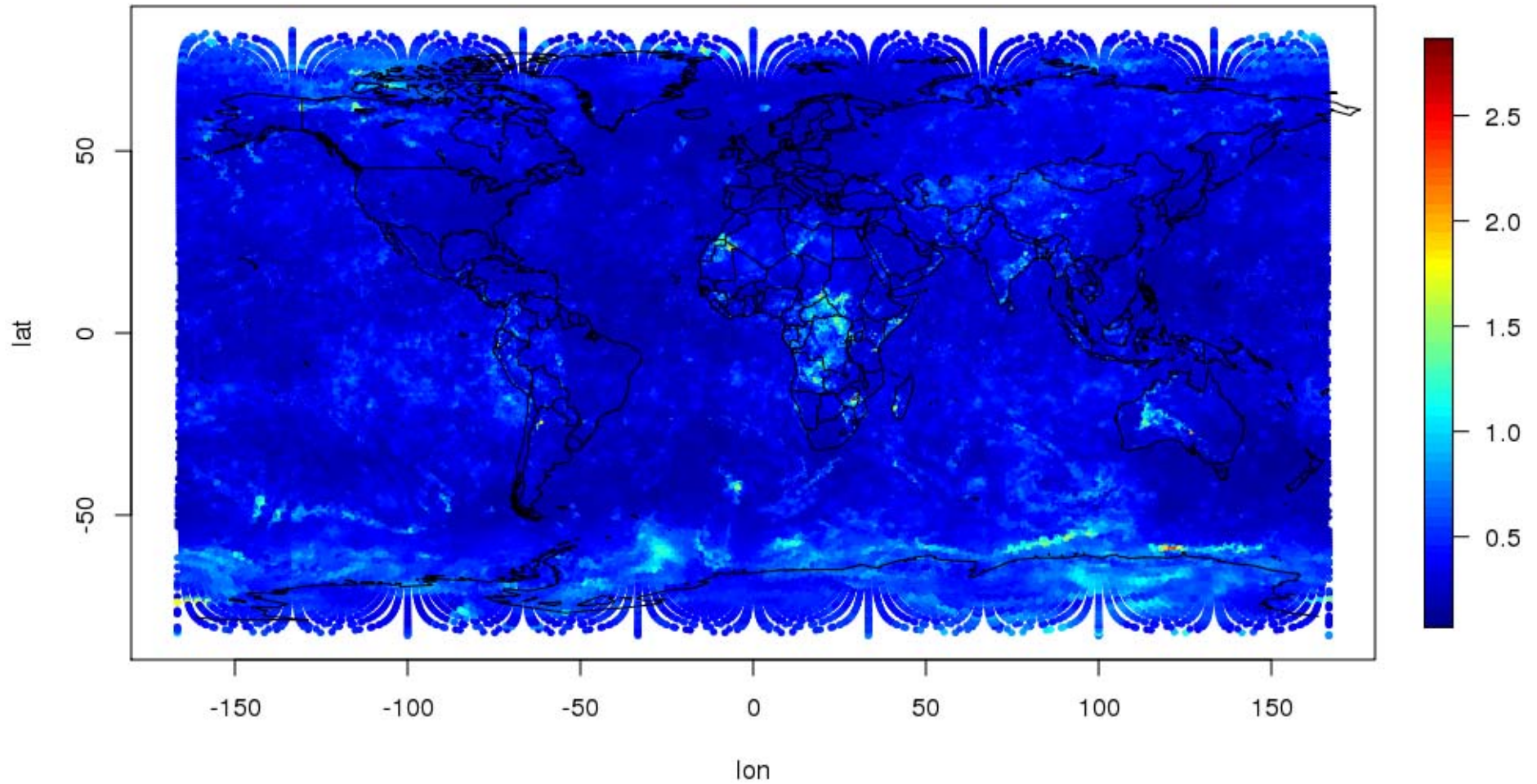
PF T on level 85





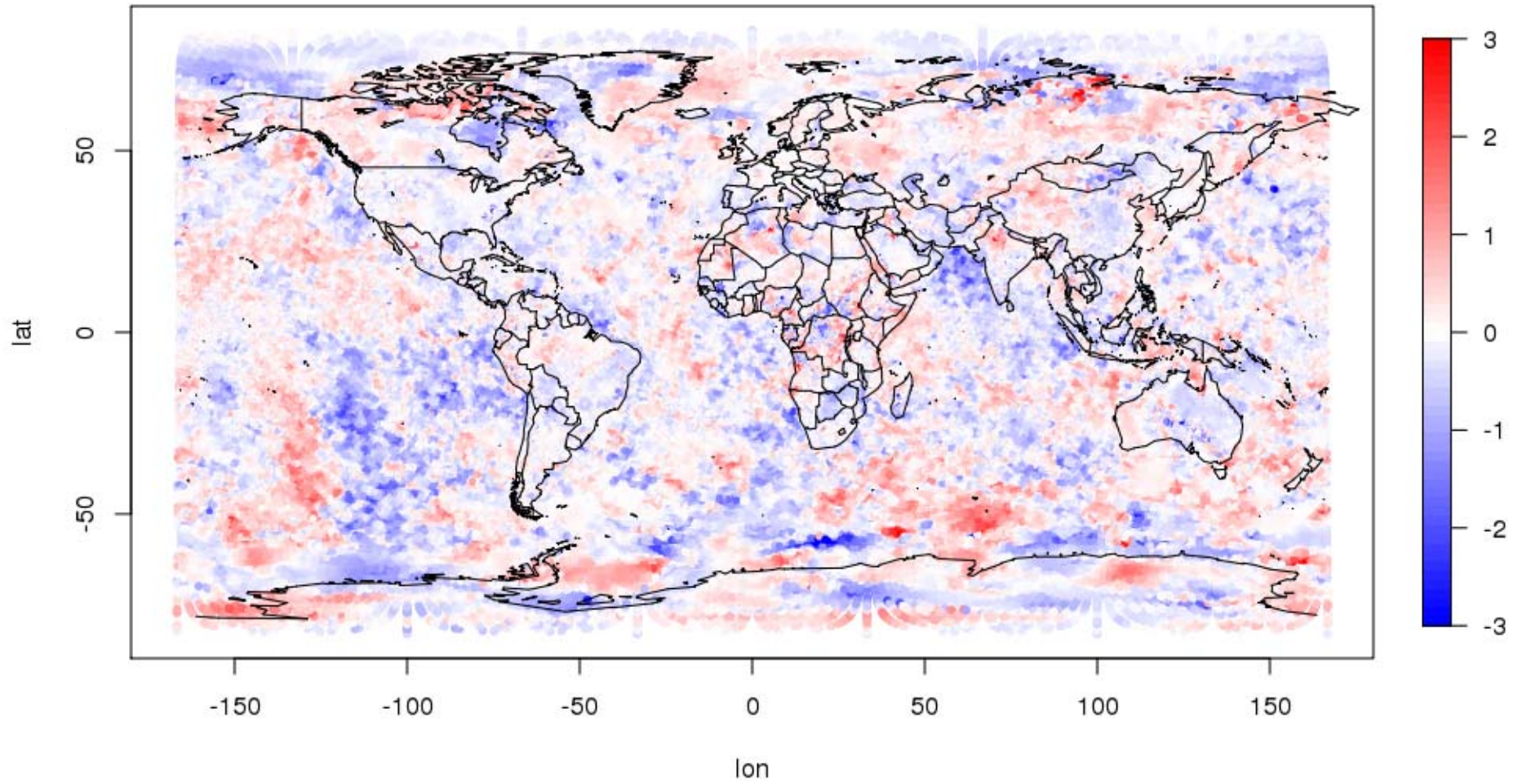
Spread EnKF T on level 85





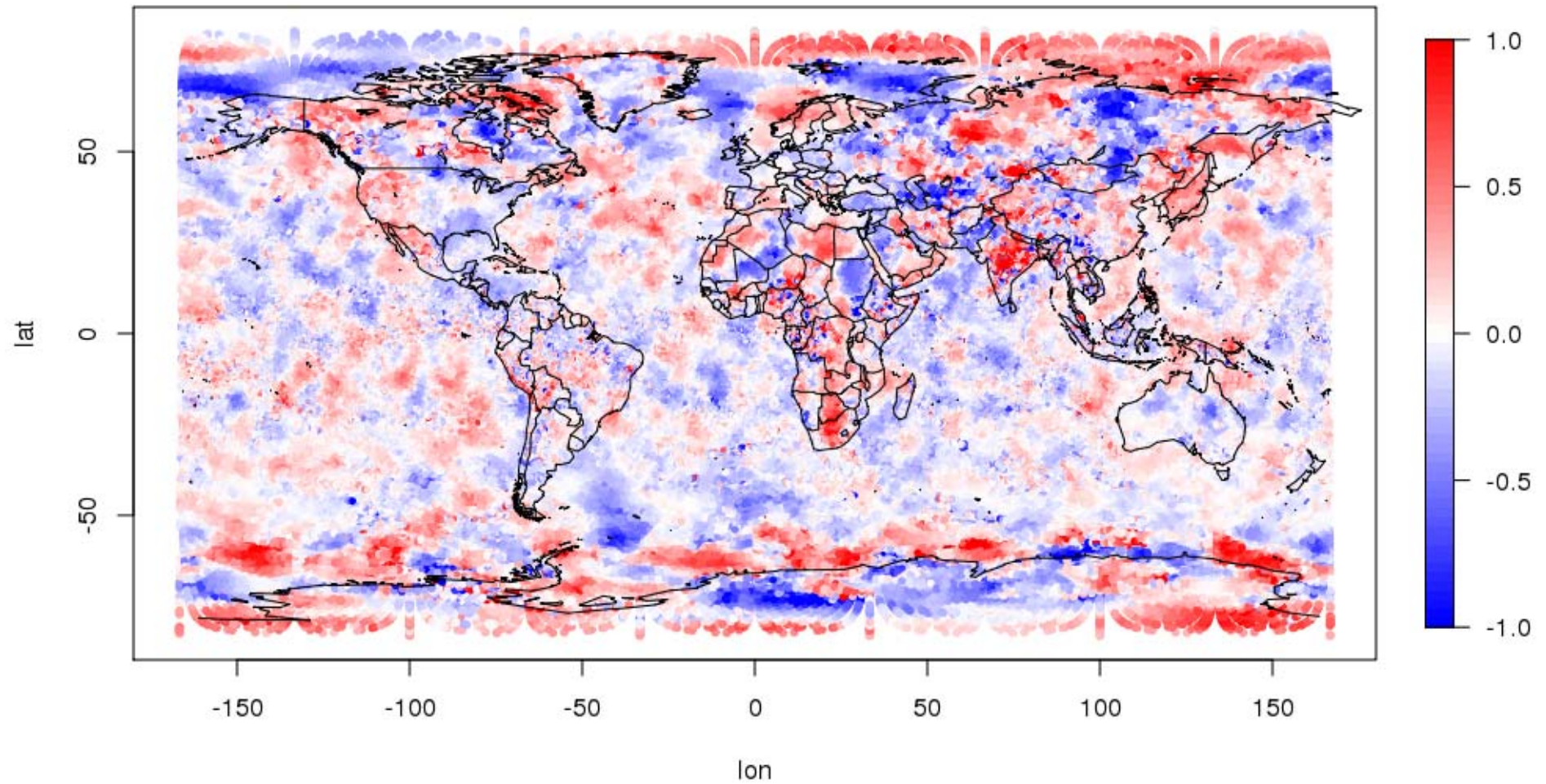
Spread PF T on level 85





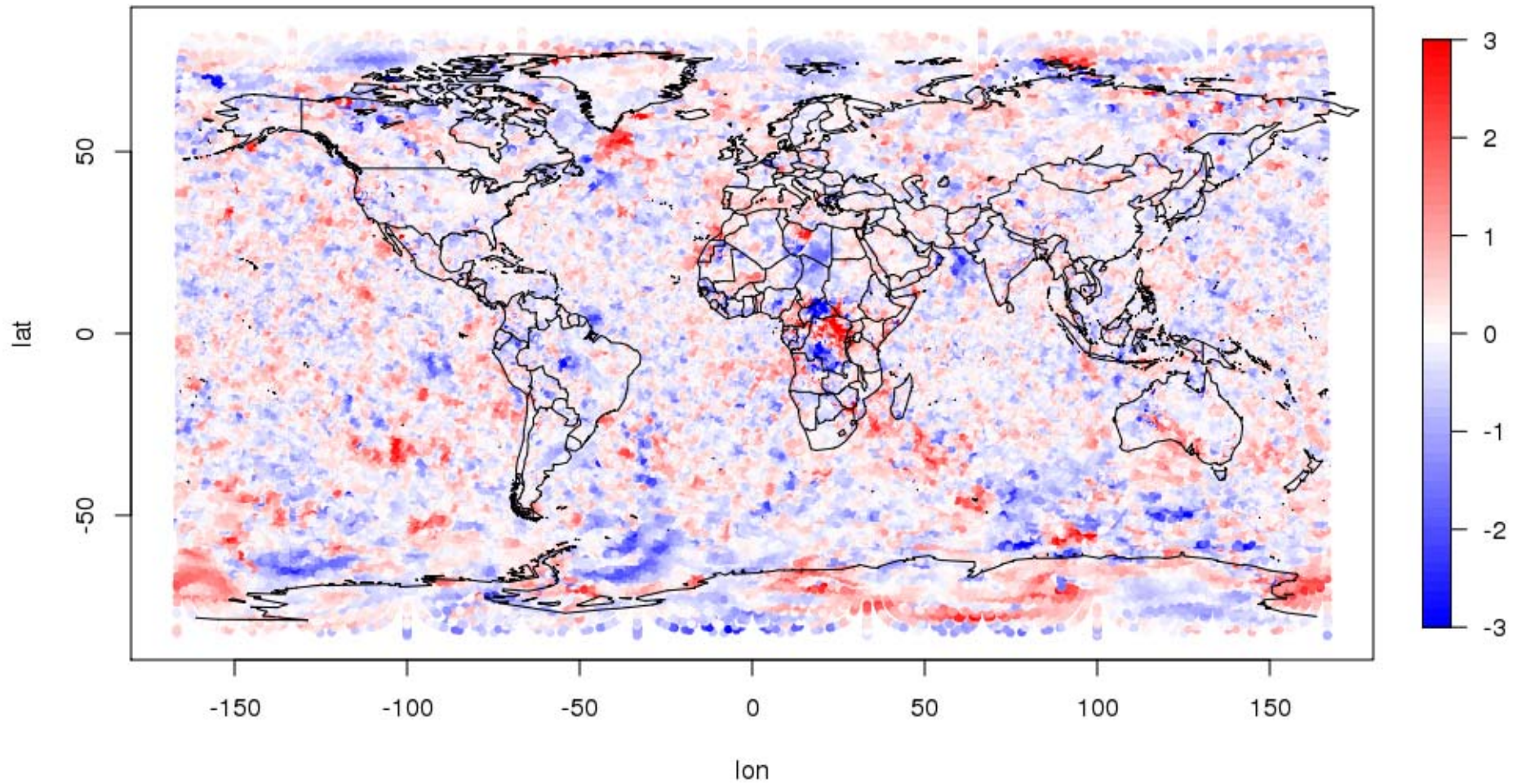
Ens 01-Mean, PF T 90





Ens 01-Mean, EKF T 90





Ens 01- Ens 01, PF1 vs PF2 T 90



Many Thanks!

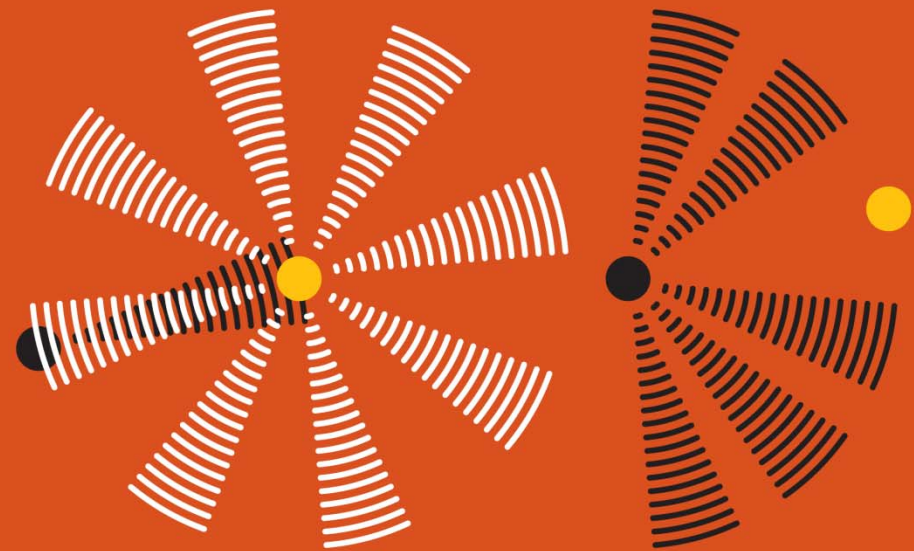


IOP Expanding Physics

Inverse Modeling

An introduction to the theory
and methods of inverse problems
and data assimilation

Gen Nakamura
Roland Potthast



IOP | ebooks