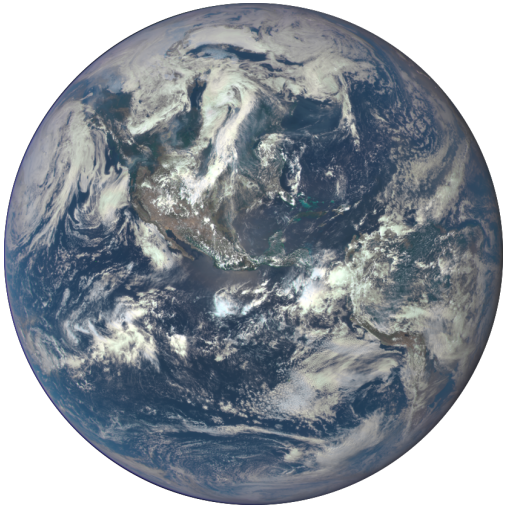
Data assimilation and conservation laws

Tijana Janjić[1], Yuefei Zeng[2], Yvonne Ruckstuhl[3]

[1] Mathematical Institute for Machine Learning and Data Science,
KU Eichstätt-Ingolstadt.
[2] Nanjing University of Information Science and Technology
[3] Ludwig-Maximilians-University of Munich

MIDS
Mathematical Institute for
Machine Learning and Data Science

Data assimilation



Data assimilation combines information in heterogeneous observations and a mathematical model to learn about and help predict phenomena of interest.

It employs a variety of mathematical methods from optimization, numerics, statistics.

Continuity:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$$

X – Momentum:

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho u v)}{\partial y} + \frac{\partial(\rho u w)}{\partial z} = -\frac{\partial p}{\partial x} + \frac{1}{Re_r}\left[\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z}\right]$$

Y – Momentum:

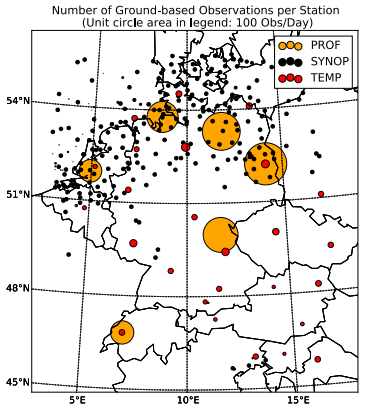
$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho u v)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} + \frac{\partial(\rho v w)}{\partial z} = -\frac{\partial p}{\partial y} + \frac{1}{Re_r}\left[\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z}\right]$$

Z – Momentum

$$\frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho u w)}{\partial x} + \frac{\partial(\rho v w)}{\partial y} + \frac{\partial(\rho w^2)}{\partial z} = -\frac{\partial p}{\partial z} + \frac{1}{Re_r}\left[\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z}\right]$$

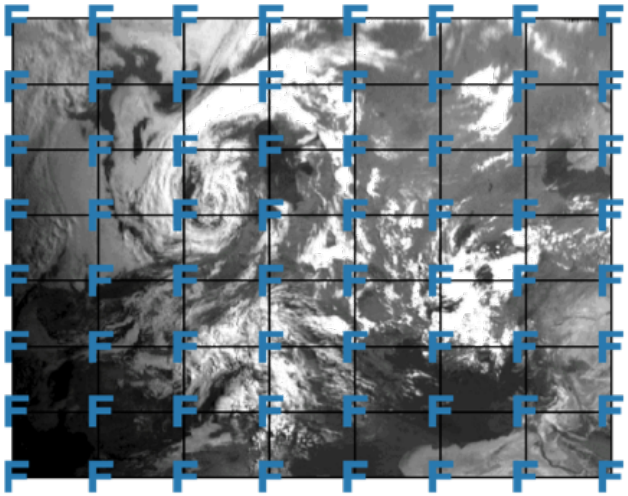
Energy:

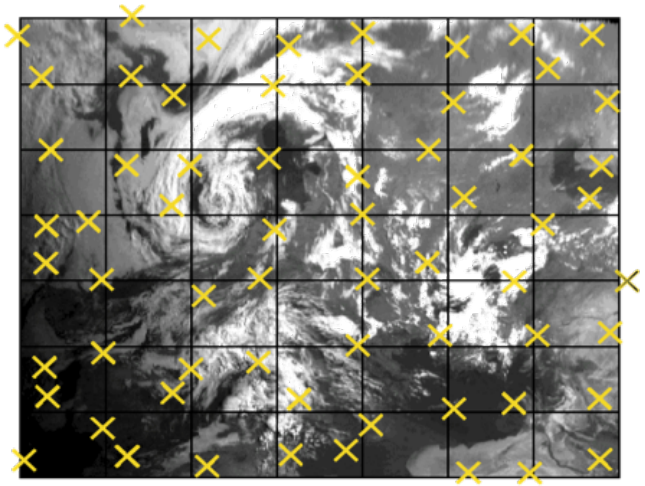
$$\frac{\partial(E_T)}{\partial t} + \frac{\partial(uE_T)}{\partial x} + \frac{\partial(vE_T)}{\partial y} + \frac{\partial(wE_T)}{\partial z} = -\frac{\partial(up)}{\partial x} - \frac{\partial(vp)}{\partial y} - \frac{\partial(wp)}{\partial z} - \frac{1}{Re_r Pr_r}\left[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right]$$
$$+ \frac{1}{Re_r}\left[\frac{\partial}{\partial x}(u\,\tau_{xx} + v\,\tau_{xy} + w\,\tau_{xz}) + \frac{\partial}{\partial y}(u\,\tau_{xy} + v\,\tau_{yy} + w\,\tau_{yz}) + \frac{\partial}{\partial z}(u\,\tau_{xz} + v\,\tau_{yz} + w\,\tau_{zz})\right]$$



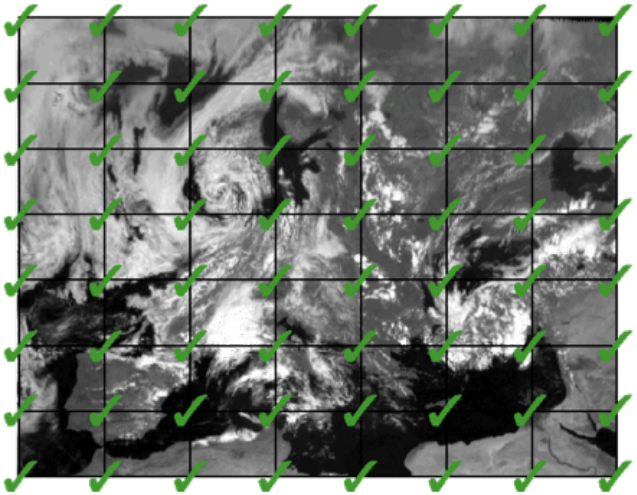
Data assimilation

$\mathbf{w}_k^b$





$\mathbf{w}_k^o$



$\mathbf{w}_k^a$

Analysis at time k

use, e.g., as initial conditions

Data assimilation algorithm

Data assimilation produces initial conditions for geophysical models by combining observations and a background (forecast) using estimates of their uncertainties.

Data assimilation algorithm

Data assimilation produces initial conditions for geophysical models by combining observations and a background (forecast) using estimates of their uncertainties.

$$\min_{\delta \mathbf{w}} J(\delta \mathbf{w}) = \min_{\delta \mathbf{w}} \delta \mathbf{w}^T \mathbf{P}^{b^{-1}} \delta \mathbf{w} + (\mathbf{d} - \mathbf{H}\delta \mathbf{w})^T \mathbf{R}^{-1} (\mathbf{d} - \mathbf{H}\delta \mathbf{w})$$

$$\text{with} \quad \delta \mathbf{w} = \mathbf{w} - \mathbf{w}_k^b \quad \text{and} \quad \mathbf{d} = \mathbf{w_k^o} - H(\mathbf{w_k^b})$$

Data assimilation algorithm

Data assimilation produces initial conditions for geophysical models by combining observations and a background (forecast) using estimates of their uncertainties.

$$\min_{\delta \mathbf{w}} J(\delta \mathbf{w}) = \min_{\delta \mathbf{w}} \delta \mathbf{w}^T \mathbf{P}^{b^{-1}} \delta \mathbf{w} + (\mathbf{d} - \mathbf{H}\delta \mathbf{w})^T \mathbf{R}^{-1} (\mathbf{d} - \mathbf{H}\delta \mathbf{w})$$

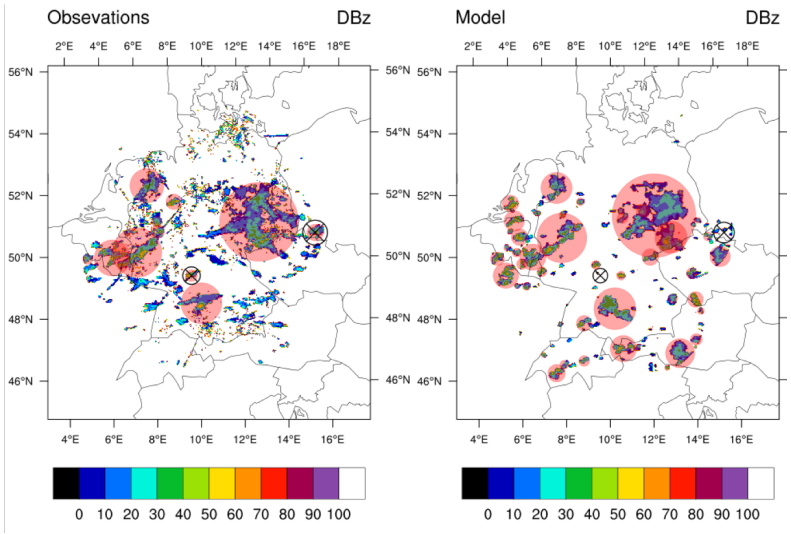
$$\text{with} \quad \delta \mathbf{w} = \mathbf{w} - \mathbf{w}_k^b \quad \text{and} \quad \mathbf{d} = \mathbf{w}_\mathbf{k}^\mathbf{o} - H(\mathbf{w}_\mathbf{k}^\mathbf{b})$$

$\mathbf{P}^b$ error covariance of the background (forecast)

$\mathbf{R}$ error covariance of the observations

Why is this hard?

- Geophysical models of atmosphere incorporate our knowledge of the dynamics and physics.

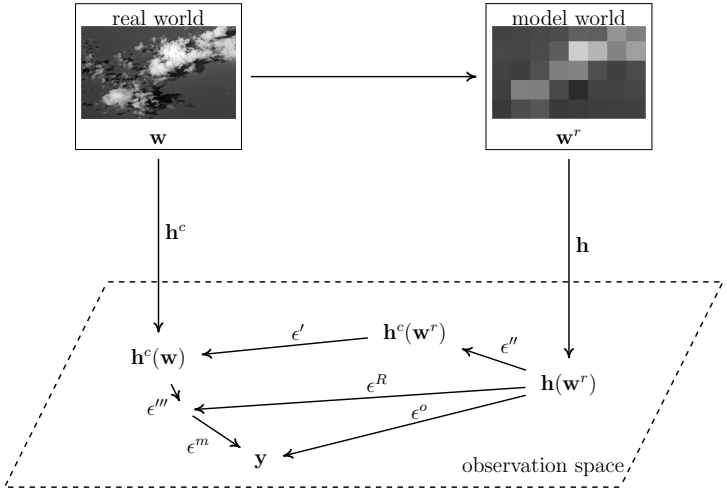


These models are not perfect.
We need to specify background uncertainty including model error uncertainty.

- The state vector $\mathbf{w}_k^b$ at time k consists of variables as temperature, wind components, humidity of the numerical model at all grid points
- For modern geophysical models this state vector is of size $10^6 - 10^8$.
We need fast algorithms applicable for large scale problems.

Why is this hard?

- Second source of the information about the state of the atmosphere is given through observations.
- Instruments have different spatial and temporal coverage as well as different accuracy.



The observations are not perfect.
We need to specify observation uncertainty including representation error uncertainty.

- The observation vector $\mathbf{w}_k^o$ at time k consists of all available data at that time. Observation vector is of size $10^5 - 10^6$.
At any given time data assimilation problem is underdetermined.

Kalman filter

Rudolf Emil Kalman

Trajectory estimation for the Apollo program in 1960s

Many different applications:

- Navigation
- Robotics
- Economic modeling
- Flood forecasting .....

Kalman filter

Propagation step. Propagate the mean and the covariance with the dynamics between observations. Prior to new observation we have $\mathbf{w}_k^b$ and its covariance $\mathbf{P}_k^b$.

$$\mathbf{w}_k^b = \mathcal{M}\mathbf{w}_{k-1}^a + \mathbf{q}_k$$
$$\mathbf{P}_k^b = \mathbf{M}\mathbf{P}_{k-1}^a\mathbf{M}^T + \mathbf{Q}$$

Kalman analysis.

$$\mathbf{w}_k^a = \mathbf{w}_k^b + \mathbf{K}_k(\mathbf{w}_k^o - \mathbf{H}_k\mathbf{w}_k^b),$$
$$\mathbf{K}_k = \mathbf{P}_k^b\mathbf{H}_k^T(\mathbf{H}_k\mathbf{P}_k^b\mathbf{H}_k^T + \mathbf{R}_k)^{-1}$$
$$\mathbf{P}_k^a = (\mathbf{I} - \mathbf{K}_k\mathbf{H}_k)^T\mathbf{P}_k^b$$

Derived using $q \sim \mathcal{N}(0, \mathbf{Q})$, $r \sim \mathcal{N}(0, \mathbf{R})$, $\mathbf{w}_0^b \sim \mathcal{N}(0, \mathbf{P_0^b})$ and all uncorrelated.

Ensemble Kalman filter

Idea: take Kalman filter equations and represent all the covariances using an ensemble of geophysical model simulations!

Ensemble Kalman filter

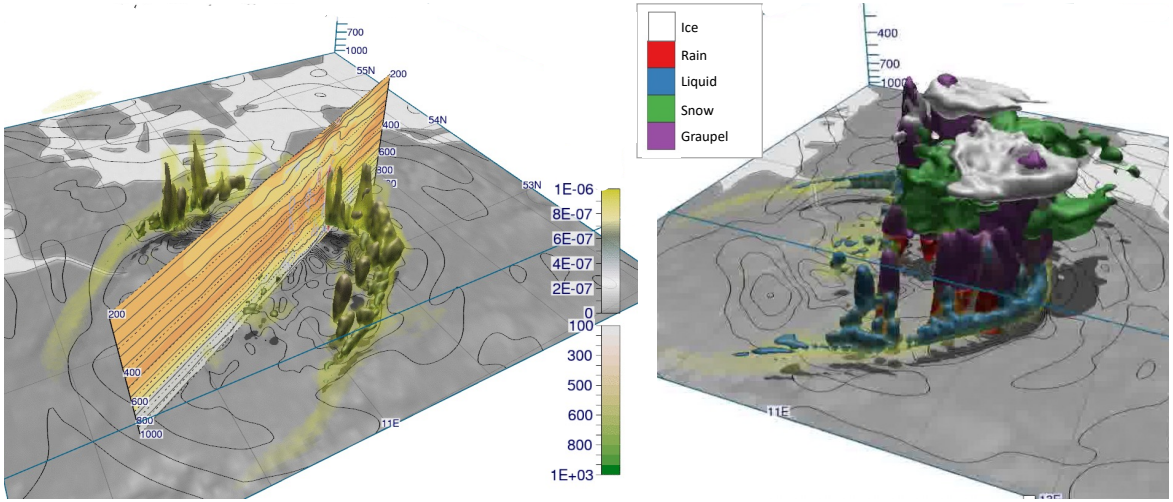
Idea: take Kalman filter equations and represent all the covariances using an ensemble of geophysical model simulations!

Covariances represented through

$$\mathbf{P}_k^b = \frac{1}{N-1} \sum_{i=1}^{N} [\mathbf{w}_k^{b,i} - \mathbf{w}_k^b][\mathbf{w}_k^{b,i} - \mathbf{w}_k^b]^T.$$

$\mathbf{P}_k^b$ is the ensemble derived background error covariance;
$\mathbf{w}_k^{b,i}$ are ensemble members $i = 1, \ldots, N$ of size $n \times 1$ at time t_k;
$\mathbf{w}_k^b$ is the average over ensemble, $\mathbf{w}_k^b = \frac{1}{N} \sum_{i=1}^{N} \mathbf{w}_k^{b,i}$.

Why ensemble Kalman filter



Met3D

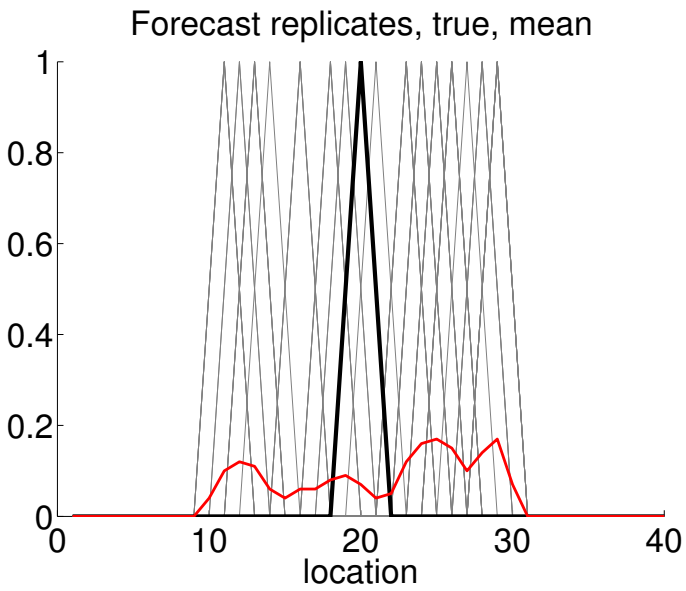
- Ensembles are propagated with full nonlinear numerical model. This can be done over long time period, and results in flow dependent covariances.
- Computationally efficient formulations using low dimensional ensemble space.

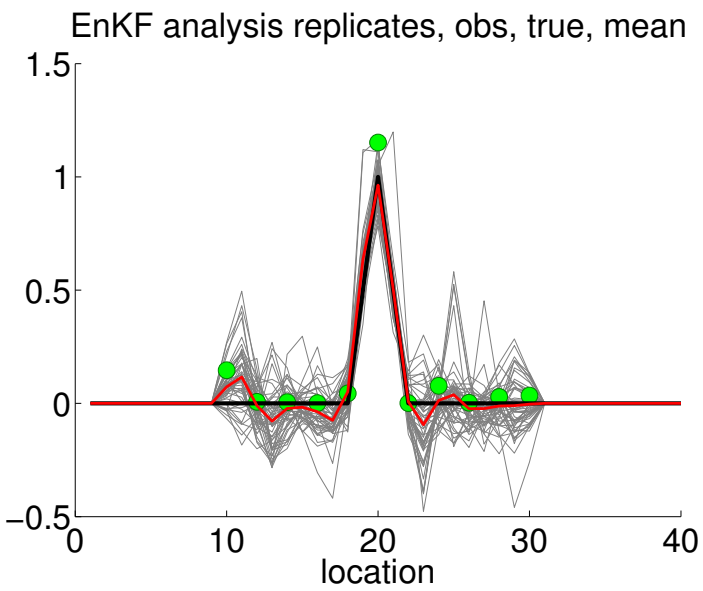
Issues with ensemble Kalman filter

- Small ensemble size requires localization.
- Still model and observation error need to be specified.
- Equations are not optimal for non-Gaussian problems.

— Fidelity to conservation laws —

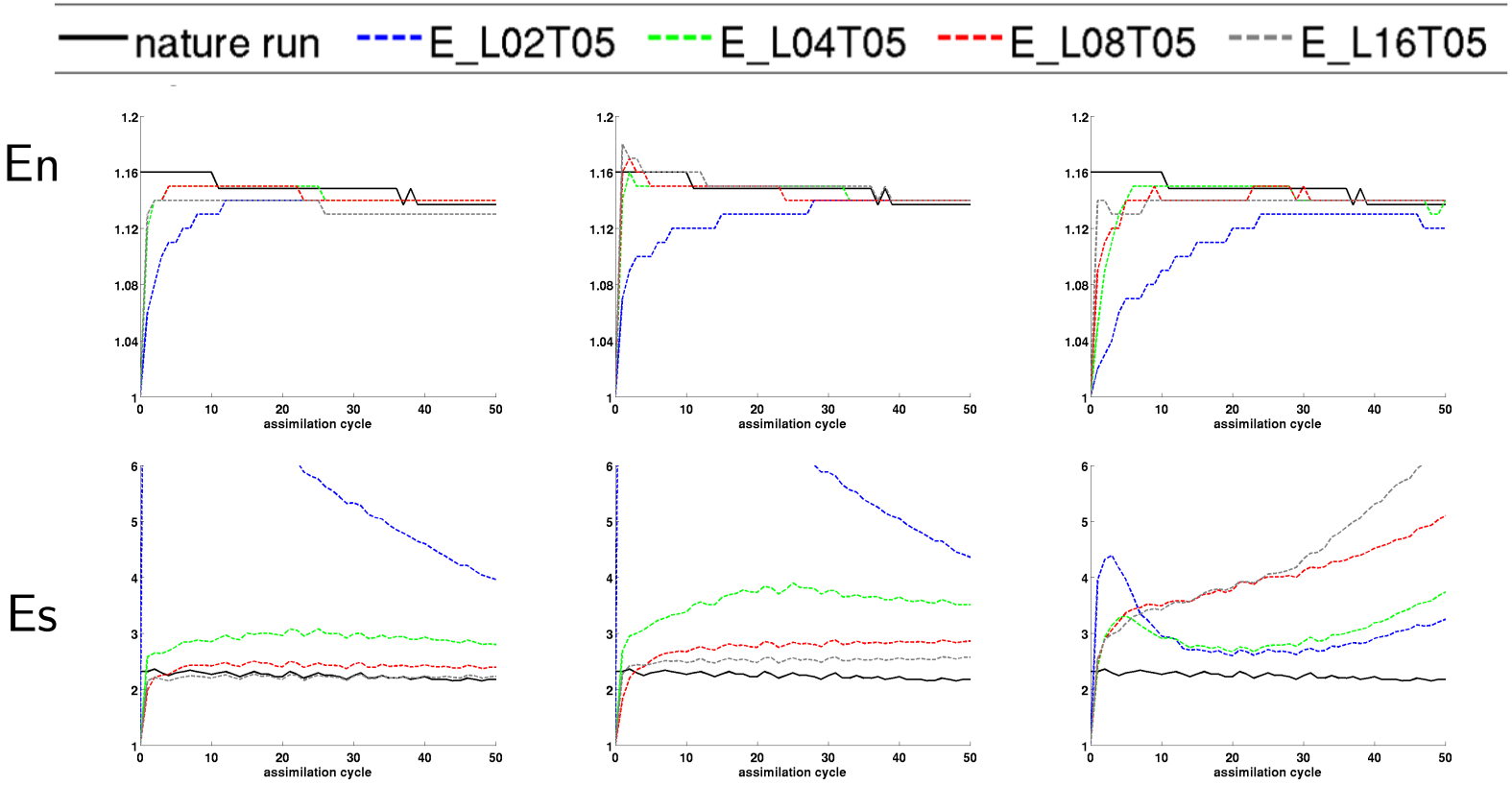
Physical properties lost in the analysis step





The mean (red line) with background ensemble (left) and analysis ensemble obtained with EnKF algorithm (right). Observations (green) are the true state plus log normal noise.

Energy and Enstrophy

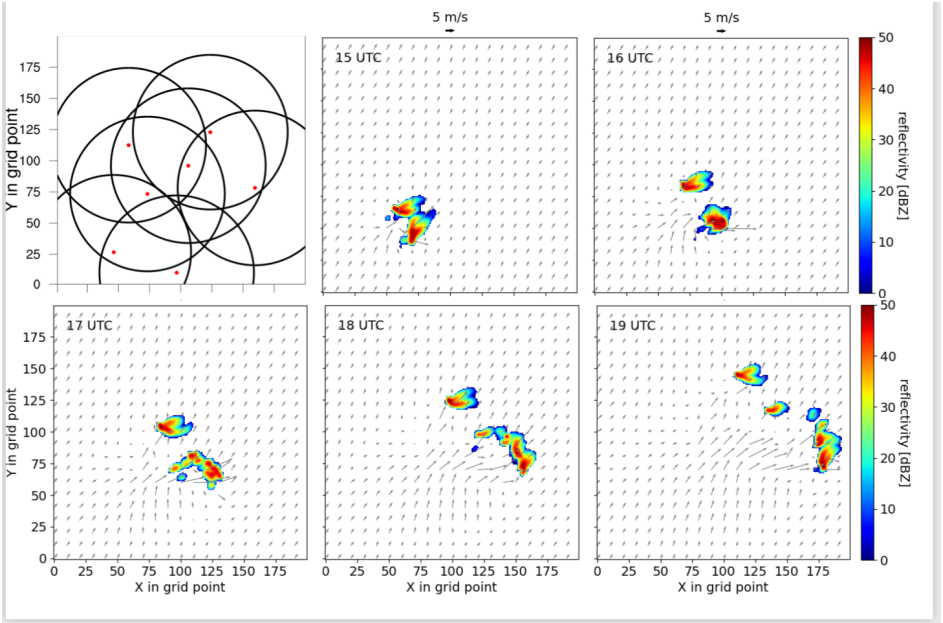


Obs u,v and h Obs u and v Obs h

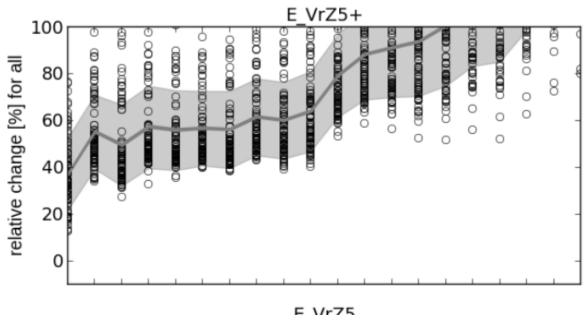
Y. Zeng and T. Janjic, 2016: Study of Conservation Laws with the Local Ensemble Transform Kalman Filter, Q. J. R. Meteorol. Soc.,142:699, 2359–2372.

Problem on convective scale

Idealized setup for radar DA



Zeng et al. 2021: Assimilating radar radial wind and reflectivity data in an idealized setup of the COSMO-KENDA system, Atmospheric Research, 249, 105282, https://doi.org/10.1016/j.atmosres.2020.105282.



Analysis mass of all hydrometeors compared to truth during DA.

QPEns

Propagation step. Propagate the mean and the covariance with the dynamics between observations. Prior to new observation we have $\mathbf{w}_k^b$ and its covariance $\mathbf{P}_k^b$.

$$\mathbf{w}_k^{b,i} = \mathcal{M}\mathbf{w}_{k-1}^{a,i} + \mathbf{q}_k^i \quad i = 1, \dots N$$

$$\mathbf{P}_k^b = \frac{1}{N-1}\sum_{i=1}^{N}[\mathbf{w}_k^{b,i} - \mathbf{w}_k^b][\mathbf{w}_k^{b,i} - \mathbf{w}_k^b]^T.$$

Kalman analysis.

$$\mathbf{w}_k^{a,i} = \mathbf{w}_k^{b,i} + \mathbf{K}_k(\mathbf{w}_k^o + r^i - \mathbf{H}_k\mathbf{w}_k^b),$$

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

$$\mathbf{P}_k^a = (\mathbf{I} - \mathbf{K}_k\mathbf{H}_k)^T\mathbf{P}_k^b$$

Derived using $q^i \sim \mathcal{N}(0, \mathbf{Q})$, $r^i \sim \mathcal{N}(0, \mathbf{R})$, $\mathbf{w}_0^b \sim \mathcal{N}(0, \mathbf{P_0^b})$ and all uncorrelated.

QPEns algorithm

- The idea is to extend the stochastic EnKF by imposing additional physical constraints on the atmospheric states when updating the ensemble members.
- This can yield more physically plausible states and also allows to consider nonlinear relationships and therefore non-Gaussian moments in the background PDF. If used without constraints, the QPEns equals the stochastic EnKF.
- The QPEns read:

$$\mathbf{w}_k^{a,i} = \arg\min_{\mathbf{w}} \mathcal{J}_k^i(\mathbf{w})$$

$$\text{subject to} \qquad c_l(\mathbf{w}) = 0,\ l \in \mathcal{E} \qquad \text{and/or} \qquad c_m(\mathbf{w}) \leq 0,\ m \in \mathcal{I},$$

$$\text{with} \qquad \mathcal{J}_k^i(\mathbf{w}) = \frac{1}{2}(\mathbf{w} - \mathbf{w}_k^{b,i})^T \mathbf{P}_k^{b\,-1}(\mathbf{w} - \mathbf{w}_k^{b,i}) + \frac{1}{2}(\mathbf{y}_k^i - \mathcal{H}(\mathbf{w}))^T \mathbf{R}_k^{-1}(\mathbf{y}_k^i - \mathcal{H}(\mathbf{w}))$$

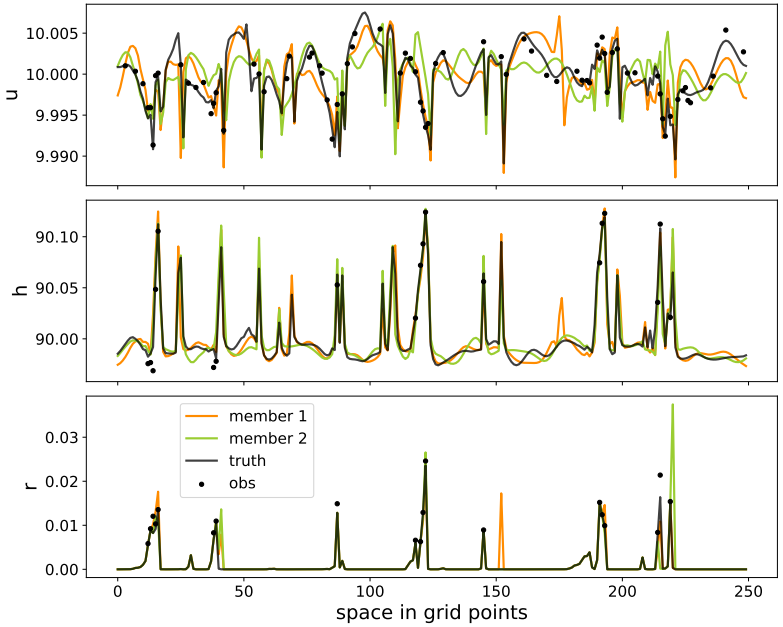
Janjic, T., D. McLaughlin, S. E. Cohn, M. Verlaan, 2014: Conservation of mass and preservation of positivity with ensemble-type Kalman filter algorithms, Mon. Wea. Rev., 142, No. 2, 755-773.

Modified shallow water model

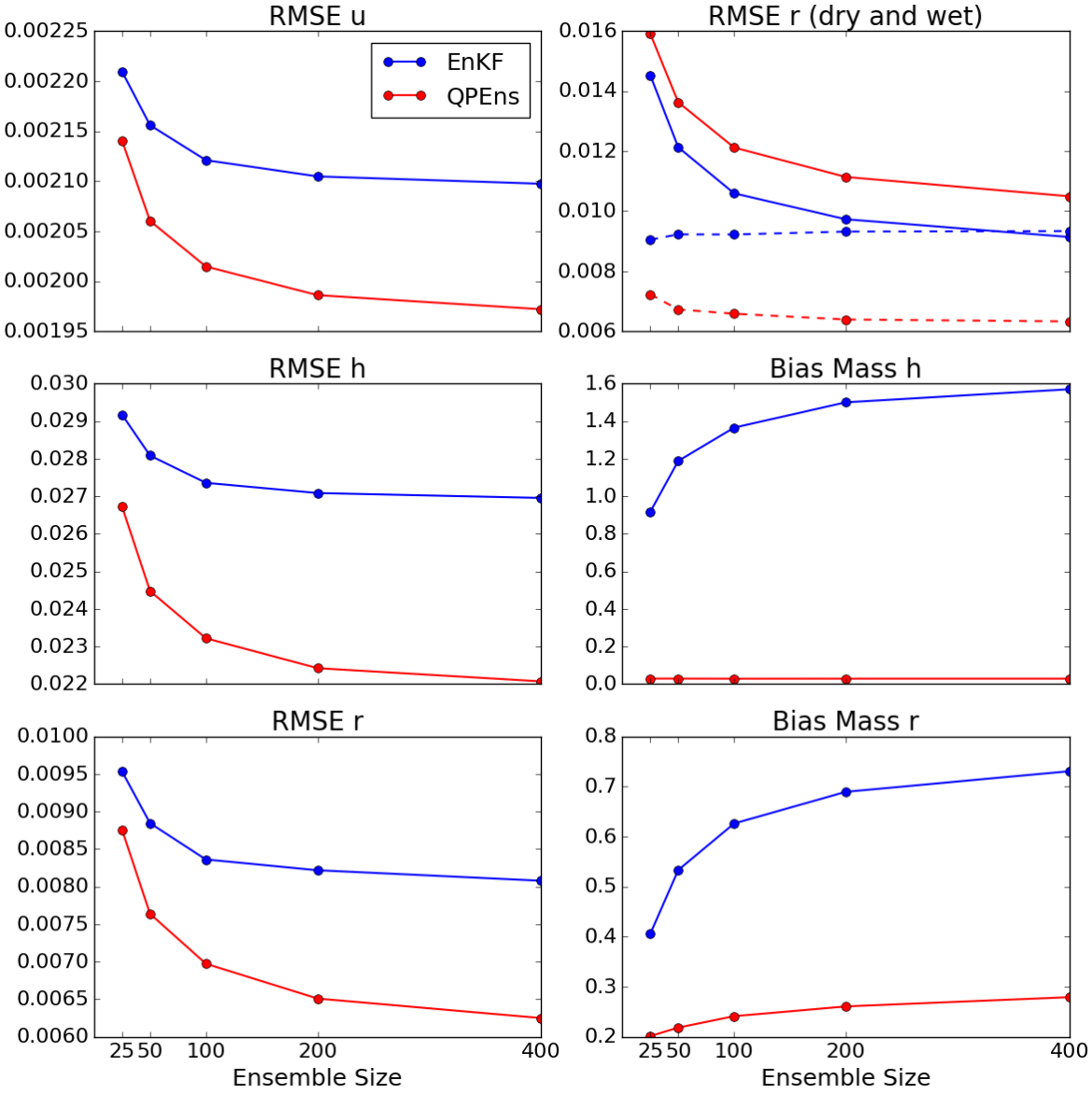
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \frac{\partial(\phi + \gamma^2 r)}{\partial x} = \beta_u + D_u \frac{\partial^2 u}{\partial x^2}, \phi = \begin{cases} \phi_c & \text{if } h > h_c \\ gh & \text{otherwise}, \end{cases}$$

$$\frac{\partial r}{\partial t} + u\frac{\partial r}{\partial x} = D_r \frac{\partial^2 r}{\partial x^2} - \alpha r - \begin{cases} \delta \frac{\partial u}{\partial x}, & \text{if } h > h_r \text{ and } \frac{\partial u}{\partial x} < 0 \\ 0 & \text{otherwise}, \end{cases}$$

$$\frac{\partial h}{\partial t} + \frac{\partial(uh)}{\partial x} = D_h \frac{\partial^2 h}{\partial x^2}.$$



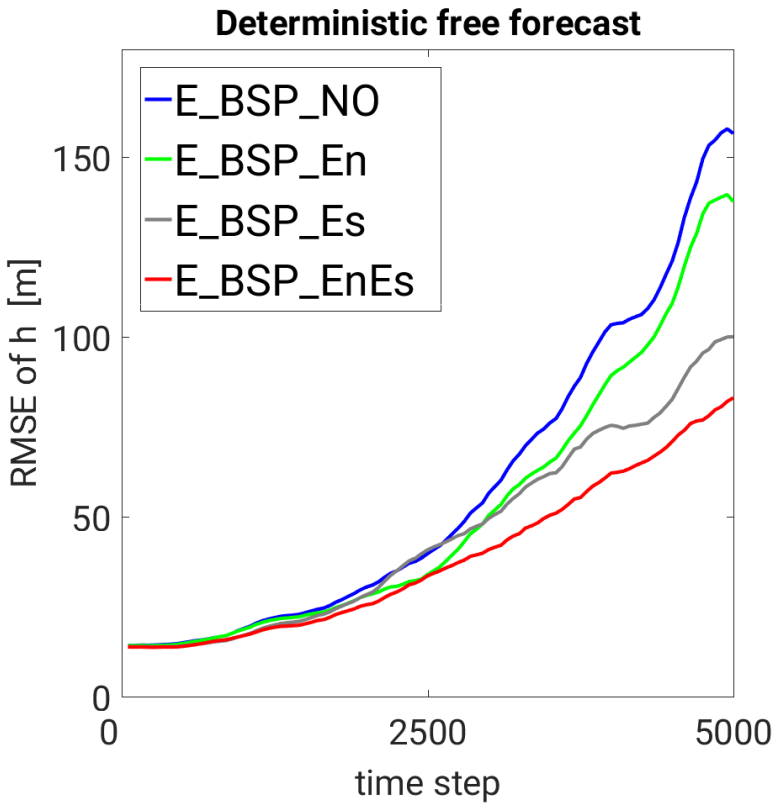
Wuersch and Craig 2014: A simple dynamical model of cumulus convection for data assimilation research., Meteorol. Z., 23, 483-490.



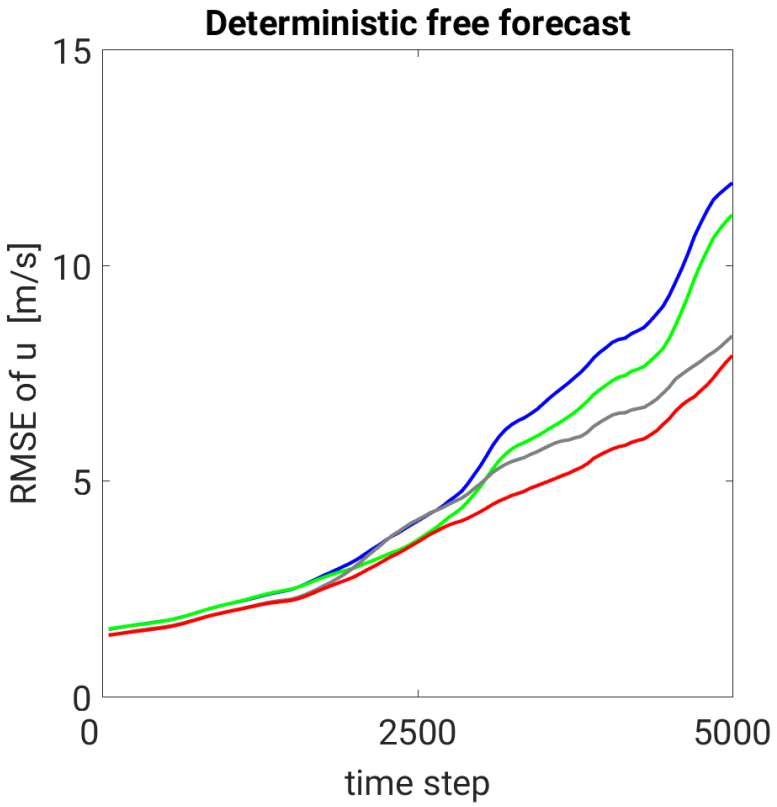
Ruckstuhl and Janjic 2018: Parameter and state estimation with ensemble Kalman filter based algorithms for convective scale applications. Q.J.R. Meteorol. Soc.. 144:712, 826–841, doi:10.1002/qj.3257.

2D shallow water model - Prediction

Northern Hemisphere, approximately 50 km horizontal resolution, midlatitudes



RMSE for h



RMSE for u

Zeng, Y., T. Janjić, Y. Ruckstuhl and M. Verlaan, 2017: Ensemble-type Kalman filter algorithm conserving mass, total energy and enstrophy, Q. J. R. Meteorol. Soc., 143:708, 2902–2914, doi:10.1002/qj.3142.

The MJO Skeleton Model

The Skeleton model is a dynamical model with intermediate complexity that simulates tropical intraseasonal variability, especially the MJO and its relevant tropical waves, at the planetary scale (Majda and Stechmann, 2011),

$$\frac{\partial u}{\partial t} - yv - \frac{\partial \theta}{\partial x} = 0 \tag{1a}$$

$$yu - \frac{\partial \theta}{\partial y} = 0 \tag{1b}$$

$$\frac{\partial \theta}{\partial t} - \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) = \overline{H}a - s^{\theta} \tag{1c}$$

$$\frac{\partial q}{\partial t} + \overline{Q}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) = -\overline{H}a + s^{q} \tag{1d}$$

$$\frac{\partial a}{\partial t} = \Gamma q a. \tag{1e}$$

Implementation

In this study, constraints to the following properties are taken into consideration:

- the total energy (TE),

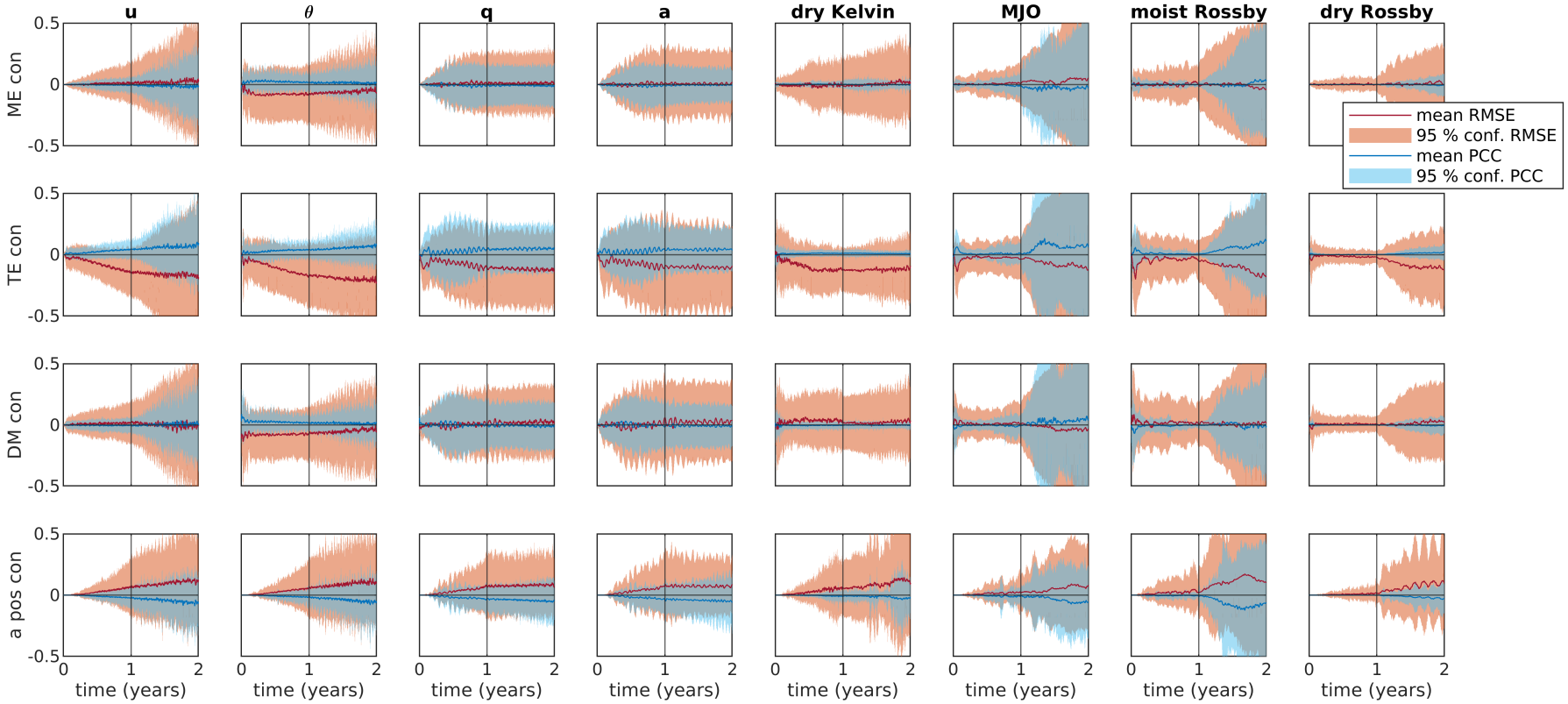
$$\int \left(\frac{u^2}{2} + \frac{\theta^2}{2} + \frac{1}{2} \frac{\overline{Q}}{1-\overline{Q}} \left(\theta + \frac{q}{\overline{Q}} \right)^2 + \frac{\overline{H}}{\Gamma \overline{Q}} a - \frac{s}{\Gamma \overline{Q}} \ln(a) \right) = \text{const.}$$

- the moist static energy (ME),
- the dry mass (DM), and
- the positivity of convective activity.

Gleiter, T., T. Janjić, N. Chen, 2022: Ensemble Kalman Filter based Data Assimilation for Tropical Waves in the MJO Skeleton Model, Q. J. R. Meteorol. Soc., 148, 1035–1056, https://doi.org/10.1002/qj.4245.

Results: Impact of the different constraints

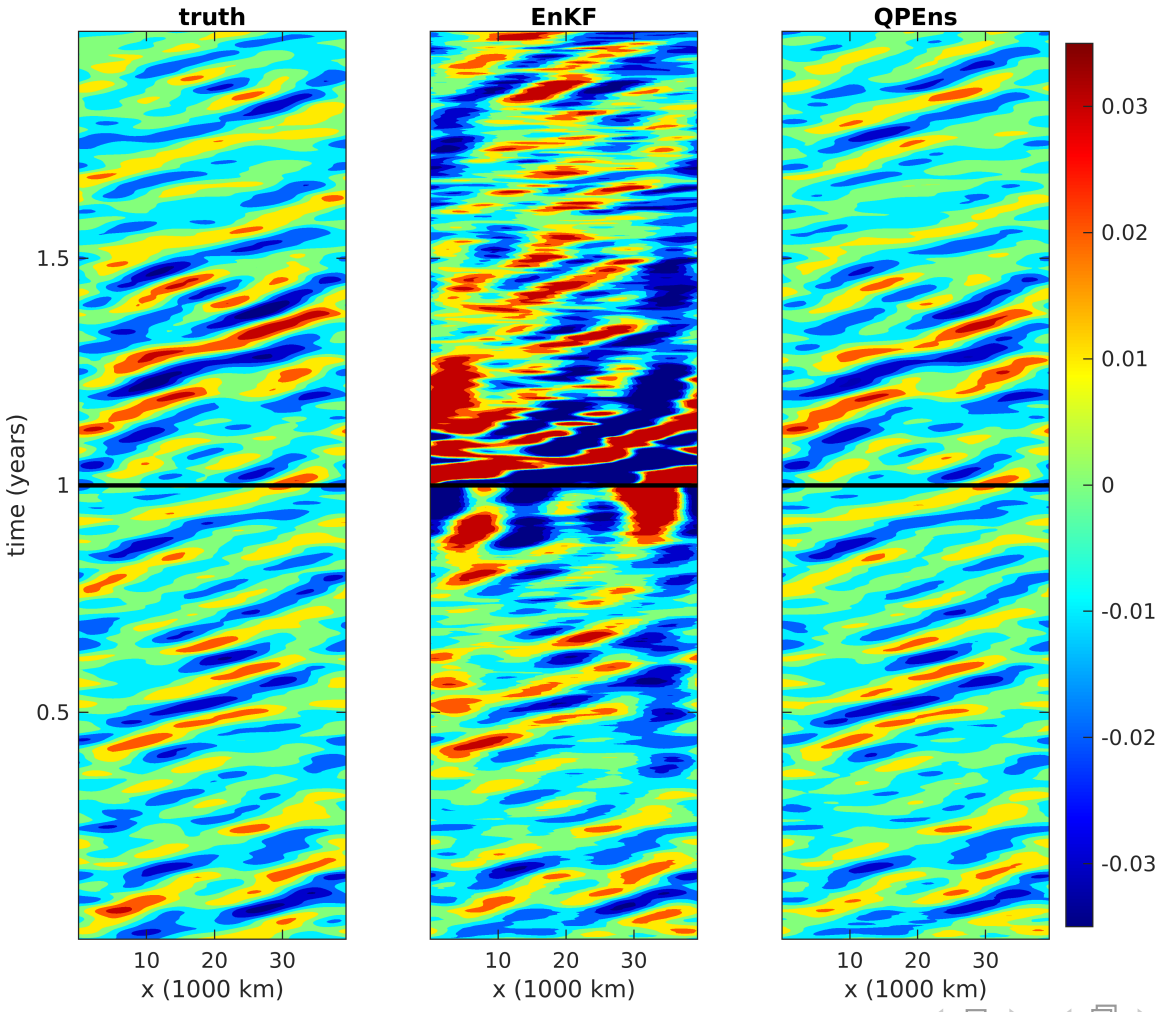
The differences in the RMSEs and pattern correlations for 1 year of DA followed by 1 year of free forecast. Calculated by subtracting the reference value of the stochastic EnKF from those of the QPEns. Only the zonal wind and the convective activity observed.



- Overall, during DA, the EnKF and QPEns produce more similar RMSEs. However, during the free forecast, initial small error differences amplify.
- There is a significant statistical benefit from the total energy (TE) constraint.

A stronger non-Gaussian test case for the QPEns with total energy constraint

Increasing the background warmpool parameter from 0.6 to 0.75 and assimilating zonal wind and the convective activity only.



Weakly Constrained LETKF

For positivity:

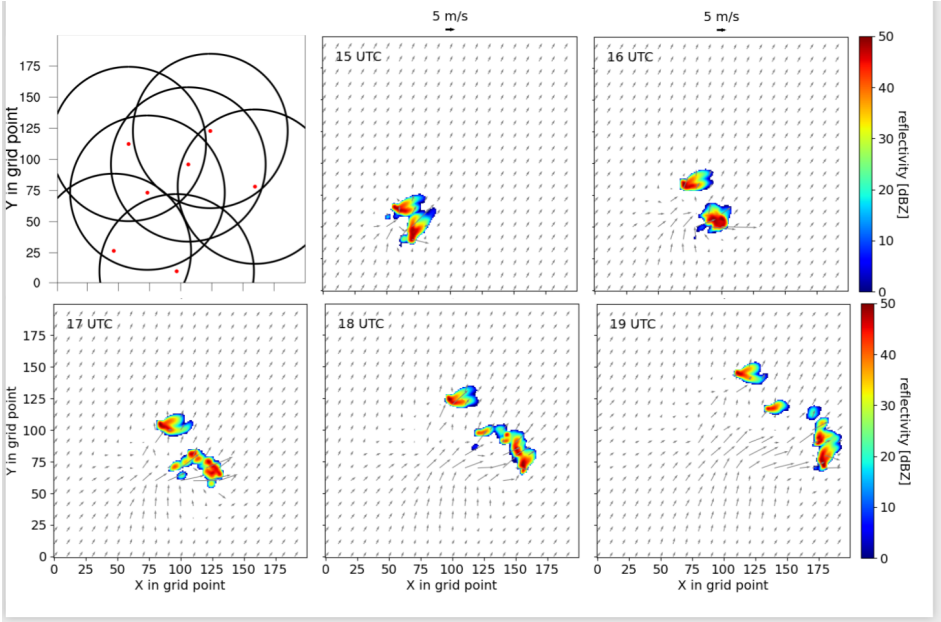
- To avoid spurious convection (Aksoy et al., 2009) clear-air reflectivity data are assimilated, i.e. non-negative threshold value is set for very small reflectivities.
- By assimilating additional clear-air reflectivity data, we are asking in the approximate weak sense that non-negativity is preserved in the analysis of hydrometeors

For mass: $\mathbf{S}$ is operator which calculates the domainwise (global) integral for each of the microphysical spieces. Constraint on mass is up to accuracy $\mathbf{M}_k$

$$\mathbf{M}_k = \frac{1}{N_{ens} - 1} \sum_{i=1}^{N_{ens}} \left[\mathbf{m}_k^* - \mathbf{S}\left(\mathbf{x}_k^{b(i)}\right) \right] \left[\mathbf{m}_k^* - \mathbf{S}\left(\mathbf{x}_k^{b(i)}\right) \right]^T$$

Experimental setup

Idealized setup for radar DA



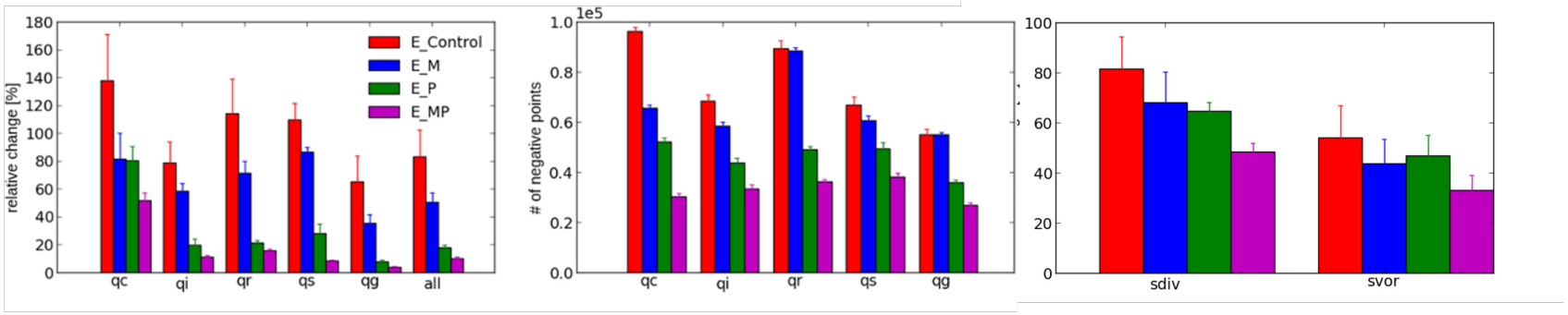
Zeng et al. 2021: Assimilating radar radial wind and reflectivity data in an idealized setup of the COSMO-KENDA system, Atmospheric Research, 249, 105282, https://doi.org/10.1016/j.atmosres.2020.105282.

- COSMO model with a 2-km horizontal resolution
- Efficient Modular VOlume scanning RADar Operator (EMVORADO, Zeng et al., 2014, 2016)
- Both radial wind and reflectivity data are assimilated
- Ensemble size is 80
- Assimilated observations are perturbation of nature run with Gaussian noise with a standard deviation of 5.0 dBZ and 1.0 m/s

Results: Impact of the different constraints

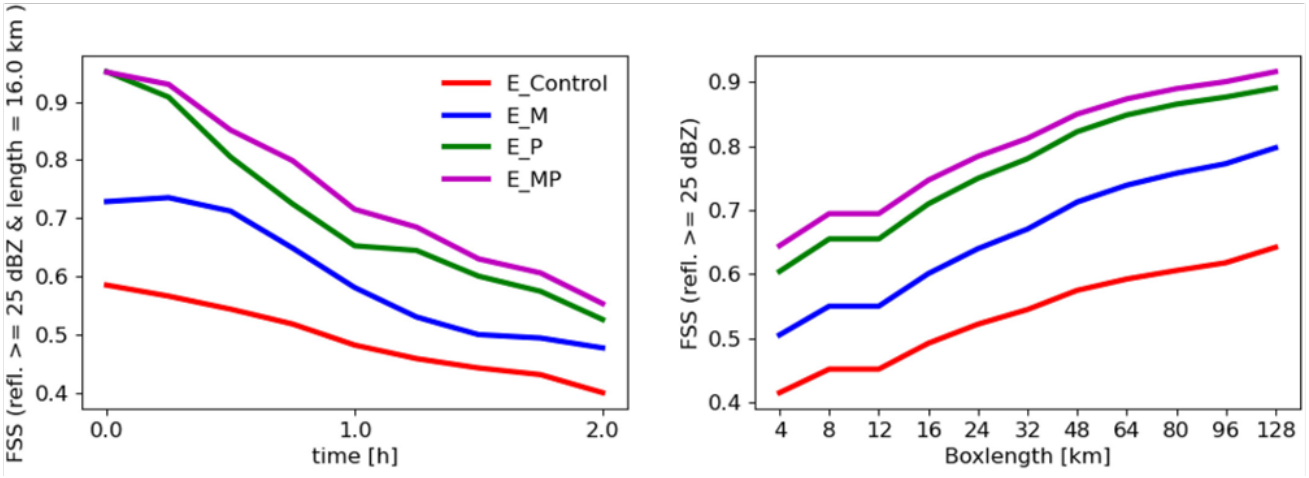
1. $E_{Control}$ Radar reflectivity and wind assimilated
2. E_M With mass constraint
3. E_P With positivity constraint (clear-air reflectivity data)
4. E_{MP} Both constraint

If clear-air reflectivity data are assimilated, a threshold value of 5 dBZ is set, that is, all reflectivity values smaller than 5 dBZ are set to 5 dBZ. If clear-air reflectivity data are not assimilated, all reflectivity values smaller than 5 dBZ are set to missing values.



Janjic, T. and Y. Zeng, 2021, Weakly constrained LETKF for estimation of hydrometeor variables in convective-scale data assimilation, Geophysical Research Letters, 48, e2021GL094962, https://doi.org/10.1029/2021GL094962.

Accuracy



FSS score. Accuracy of short term forecasts.

Conclusion

- The idea of representing the uncertainty through the ensemble of states allows inclusion of the time varying error structures in algorithm.

Conclusion

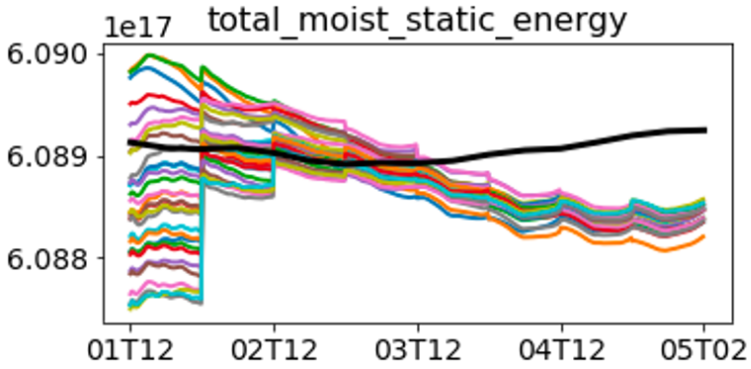
- The idea of representing the uncertainty through the ensemble of states allows inclusion of the time varying error structures in algorithm.
- We propose inclusion of conservation laws and physical constraints to tackle the difficult problem of small ensemble size and non-Gaussianity.
- Convective scale DA (higher dimensional problem with third of the variables that need to be nonnegative) requires new approaches.
- By including in addition physical properties, as mass and positivity for example we improve on prediction of convective events.

Conclusion

- The idea of representing the uncertainty through the ensemble of states allows inclusion of the time varying error structures in algorithm.
- We propose inclusion of conservation laws and physical constraints to tackle the difficult problem of small ensemble size and non-Gaussianity.
- Convective scale DA (higher dimensional problem with third of the variables that need to be nonnegative) requires new approaches.
- By including in addition physical properties, as mass and positivity for example we improve on prediction of convective events.
- Tests on models representing various dynamical properties show benefits of this approach.

Outlook

- The inclusion of model error and observation error are still required.
- Application of QPEns to high dimensional systems:
  1. Optimization research as in Janjic, T., Y. Ruckstuhl and P. L. Toint, 2021, QJRMS or
  2. through machine learning Ruckstuhl, Y., T. Janjic, S. Rasp 2021, Nonlinear Processes in Geophysics.



- Hierarchy of models for robustness across scales and in presence of sources and sinks, boundary conditions, etc.
- Predictability studies