EGU General Assembly 2024

19 Apr 2024

PDAF Parallel Data Assimilation Framework

SC5.12 Getting Started with Data Assimilation: Theory and Application

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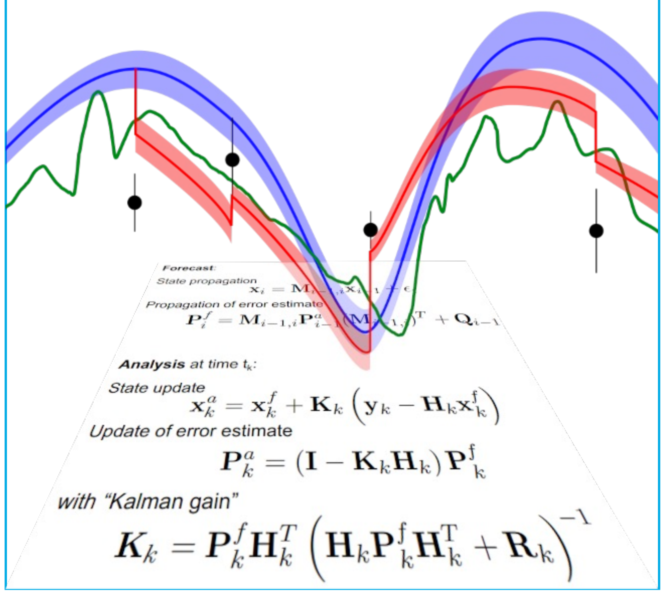
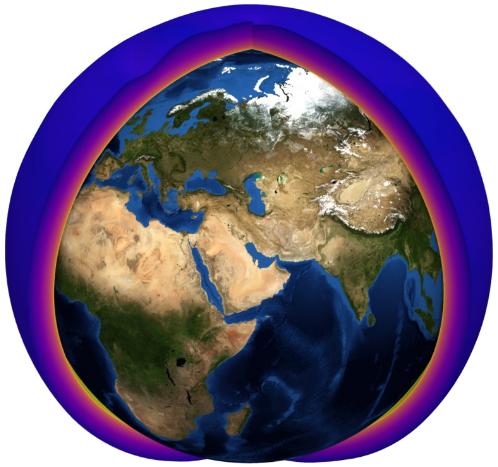
Schedule

PDAF Parallel
Data Assimilation
Framework

I Theory (25 min)



II Applications (20 min)



III Hands-on (45 min)

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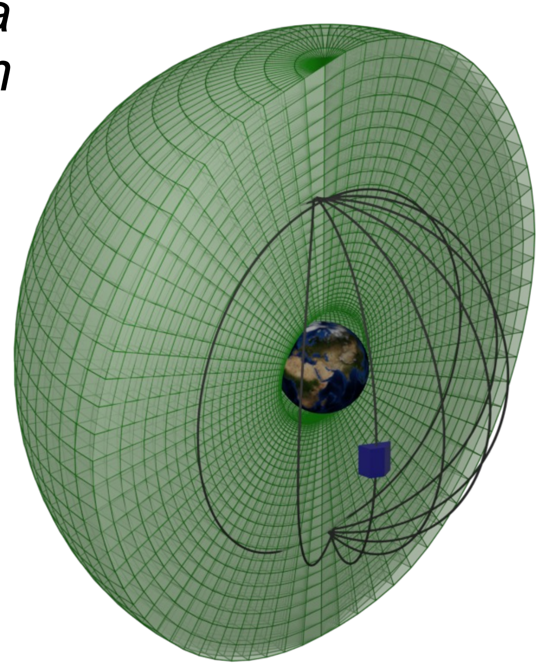
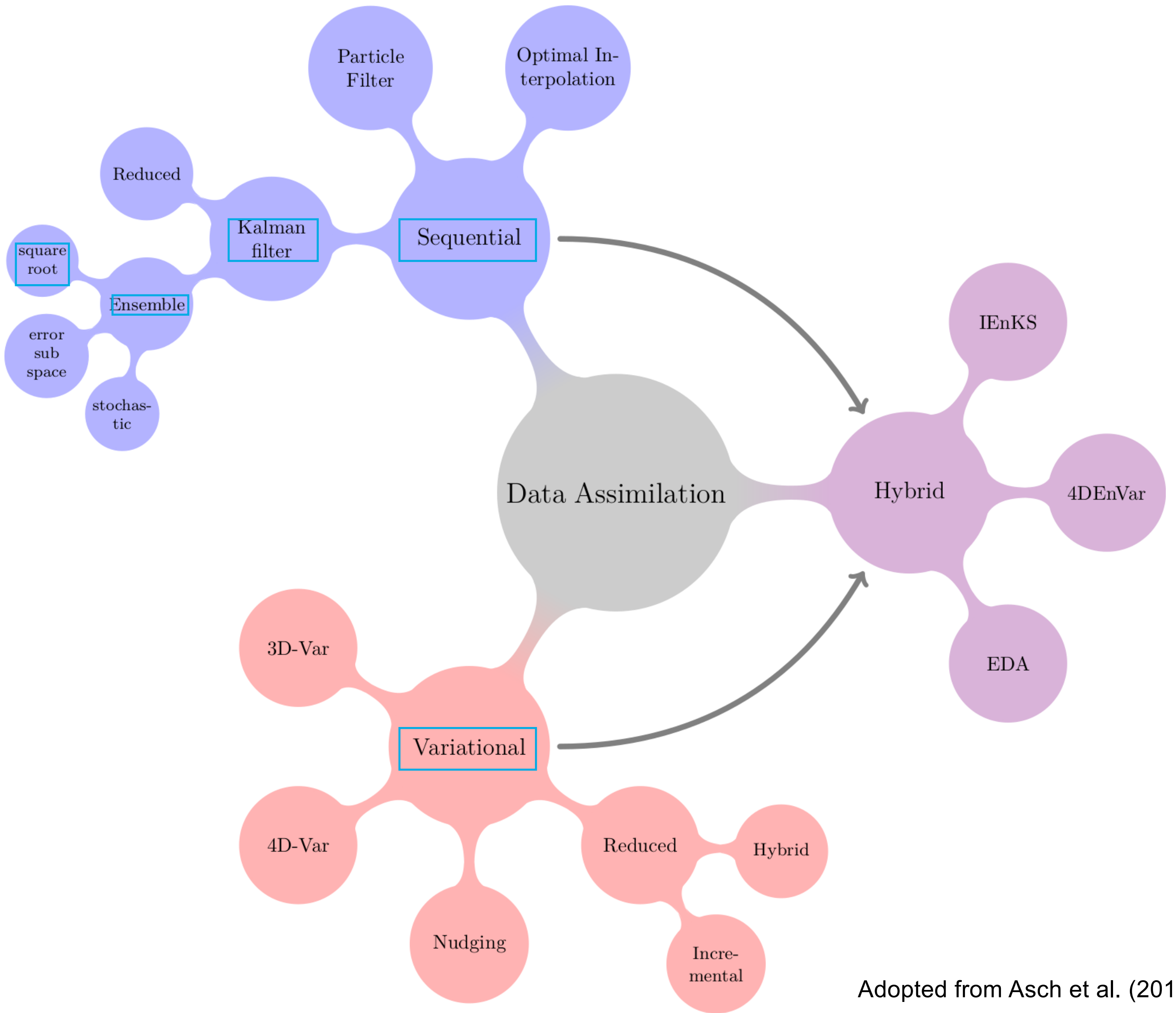
I Theory

Data Assimilation (DA)

Data assimilation (DA) is the science of ***combining observations*** *of a system,* ***including their uncertainty****, with estimates of that system from a dynamical* ***model****, including its* ***uncertainty****, to obtain a new and more accurate description of the system including an uncertainty estimate of that description.*

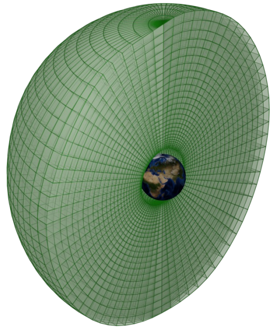
Vetra-Carvalho et al. (2018)





Adopted from Asch et al. (2016)

Requirements for DA



1. Model
   - With some skill

2. Observations
   - With finite errors
   - Related to model fields

3. Data assimilation method

PDAF Parallel Data Assimilation Framework

Observation Operator

PDAF Parallel Data Assimilation Framework

observations — state — observation errors

$$y(t) = \mathcal{H}\left(x(t)\right) + \varepsilon(t)$$

observation operator: maps state to observation

Linearized Operator: $$H = \left.\frac{\partial \mathcal{H}(x)}{\partial x}\right|_{x=x(t)}$$

Model Operator

state

model errors

$$x(t) = \mathcal{M}_{s,t}(x(s)) + \eta(t)$$

model/forward operator: propagates state from time s to t

Linearized Operator: $$M_{s,t} = \left.\frac{\partial \mathcal{M}_{s,t}(x)}{\partial x}\right|_{x=x(s)}$$

Sequential and Variational DA

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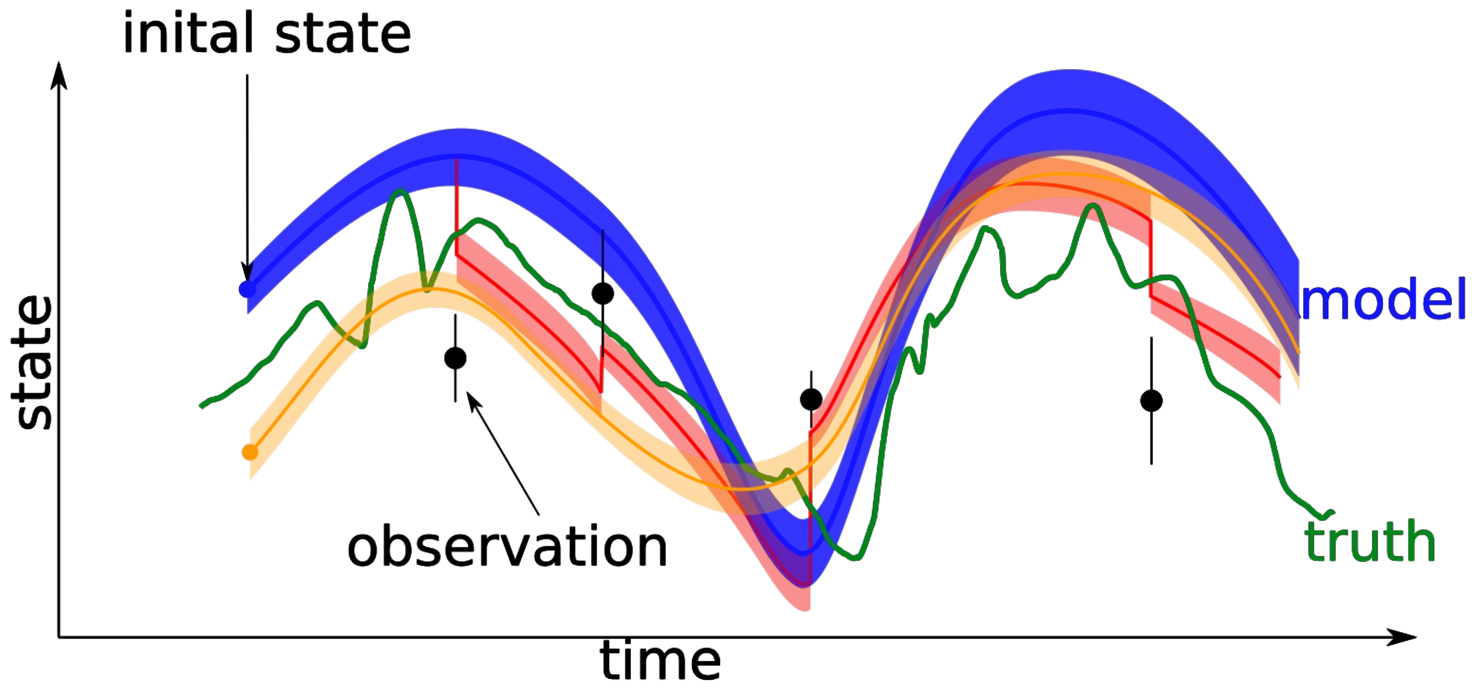

Optimization

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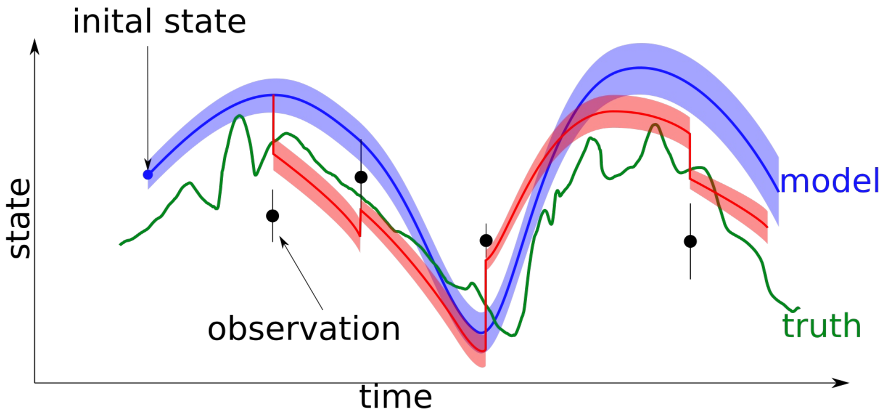
Sequential



forecast

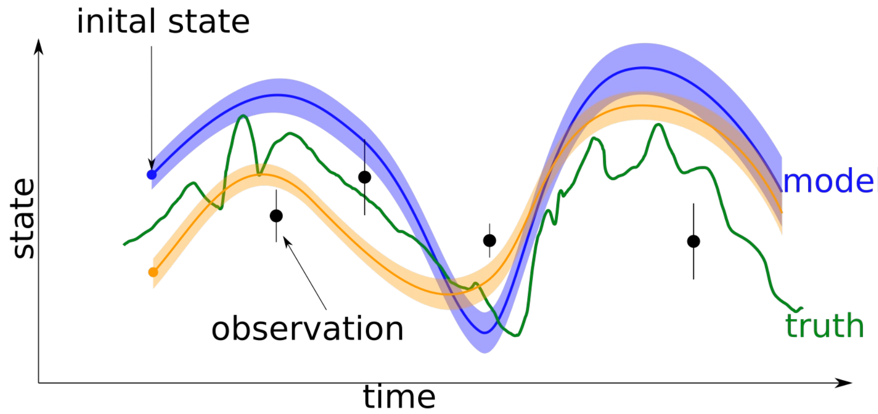
observations

$$J(x) = \left|x - x_i^f\right|^2_{\left(P_i^f\right)^{-1}} + \left|\mathcal{H}(x) - y_i^o\right|^2_{(R_i)^{-1}}$$

state

observation operator

Variational (4D Var)



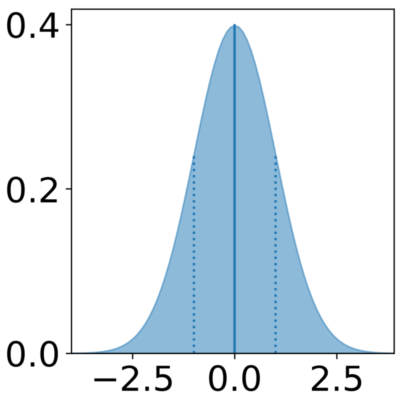
$$J(x_0) = \left|x_0 - x_0^b\right|^2_{(P_0)^{-1}} + \sum_{i=0}^{n} \left|\mathcal{H}(x_i) - y_i^o\right|^2_{(R_i)^{-1}}$$

Kalman filter is optimal

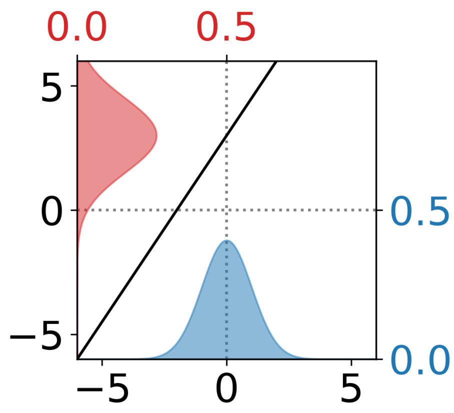
Optimal: state is **unbiased** and has **minimal variance**

Assumptions:

1. everything is Gaussian



2. model and observation operator are linear



3. model errors are not correlated with state or observation errors

$$\begin{bmatrix} R & 0 \\ 0 & P \end{bmatrix}$$

Kalman Filter

PDAF Parallel Data Assimilation Framework

1. Forecast/Prediction

State propagation

$$x_i = M_{i-1,i} x_{i-1} + \varepsilon_i$$

Propagation of error estimate

$$P_i^f = \boxed{M_{i-1,i} P_{i-1}^a M_{i-1,i}^T} + Q_{i-1}$$

1. M explicitly required
2. Scales poorly with the size of the problem

2. Analysis/Update at time t_k

State update

$$x_k^a = x_k^f + K_k (y_k^o - H_k x_k^f)$$

Propagation of error estimate

$$P_k^a = (I - K_k H_k) P_k^f$$

with Kalman gain

$$K_k = P_k^f H_k^T \left(H_k P_k^f H_k^T + R_k \right)^{-1}$$

Large Scale Models

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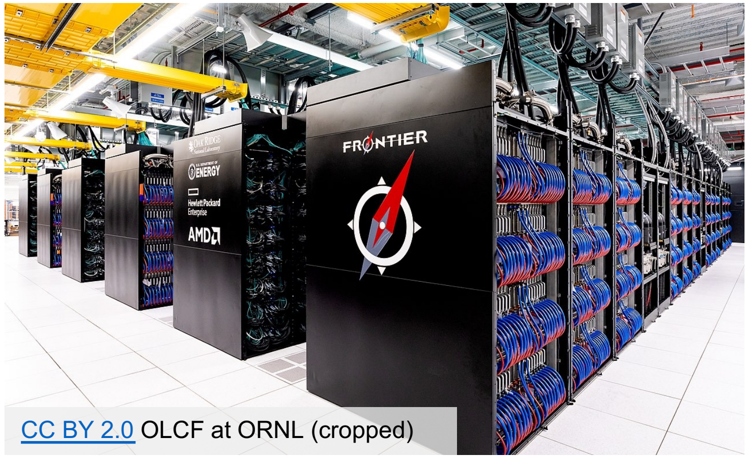
Dimension of state vector	Required memory (double)	
	x	P
1 000 000	8 MB	8 TB
10 000 000	80 MB	800 TB
100 000 000	800 MB	80 000 TB

Combined memory of best super computer[1] accumulates to **9 200 TB**

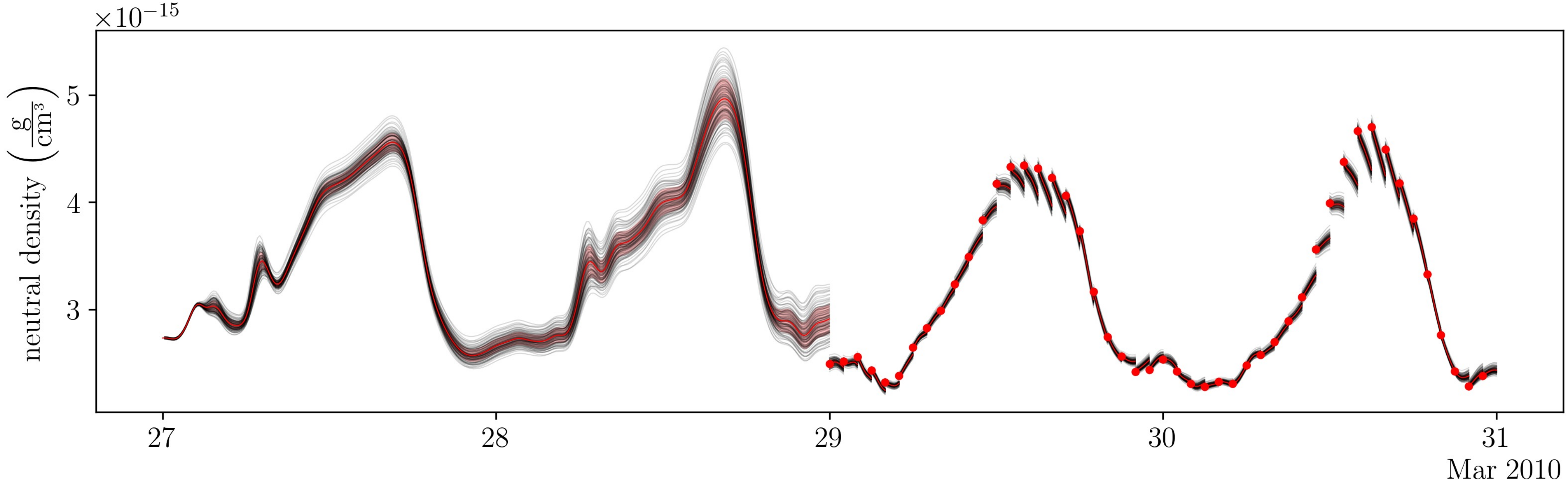


Storing and multiplication of the covariance matrix of the state becomes too expensive

[1]According to TOP500 List of Nov 2023

Ensemble Kalman Filters

PDAF Parallel Data Assimilation Framework



ensemble matrix

$$X = [x_1\, x_2\, \cdots\, x_n]$$

ensemble mean

$$\bar{x} = \frac{1}{n} X I$$

ensemble variance

$$P^f \approx \frac{1}{n-1}(X - \overline{X})(X - \overline{X})^T$$

Filters

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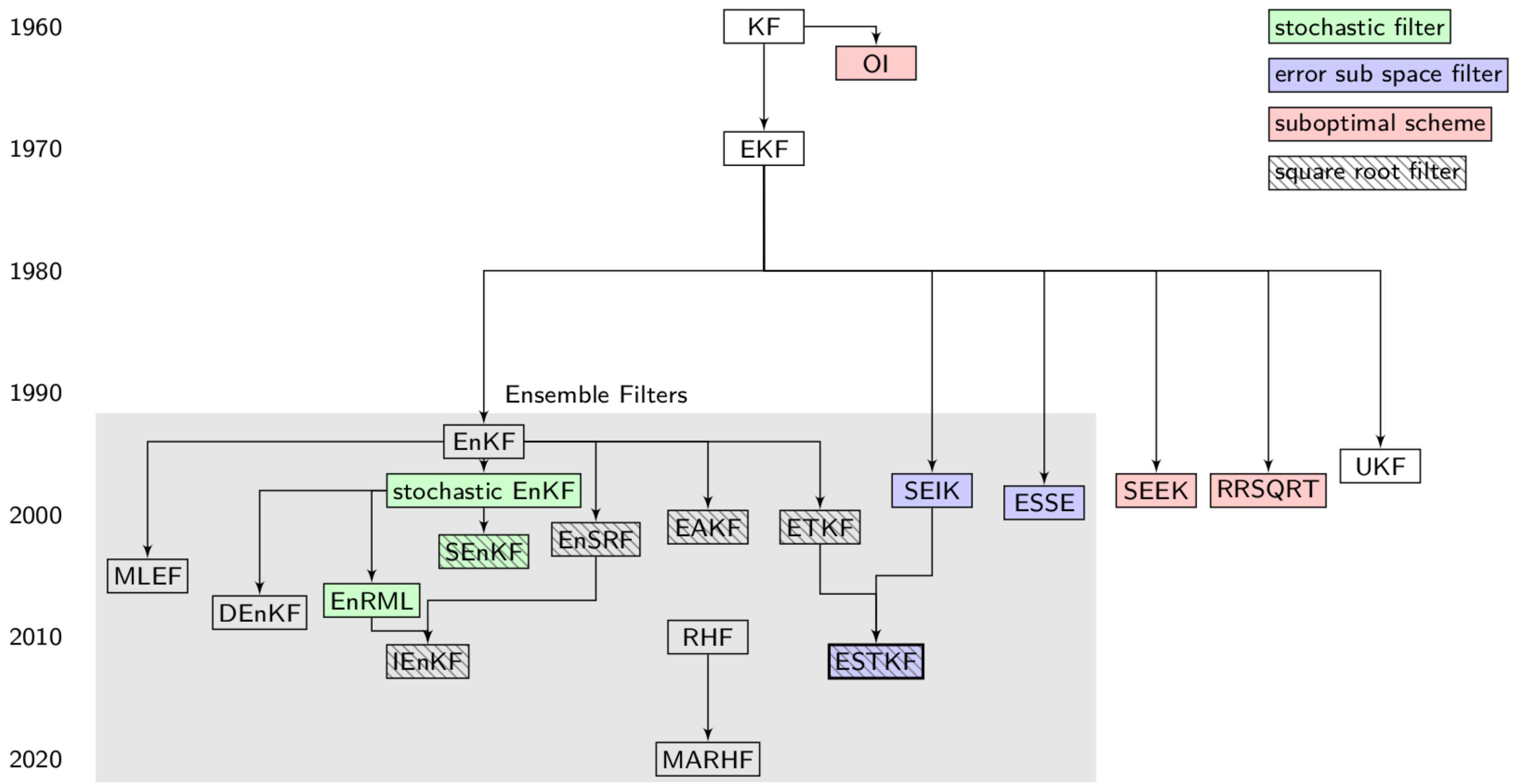
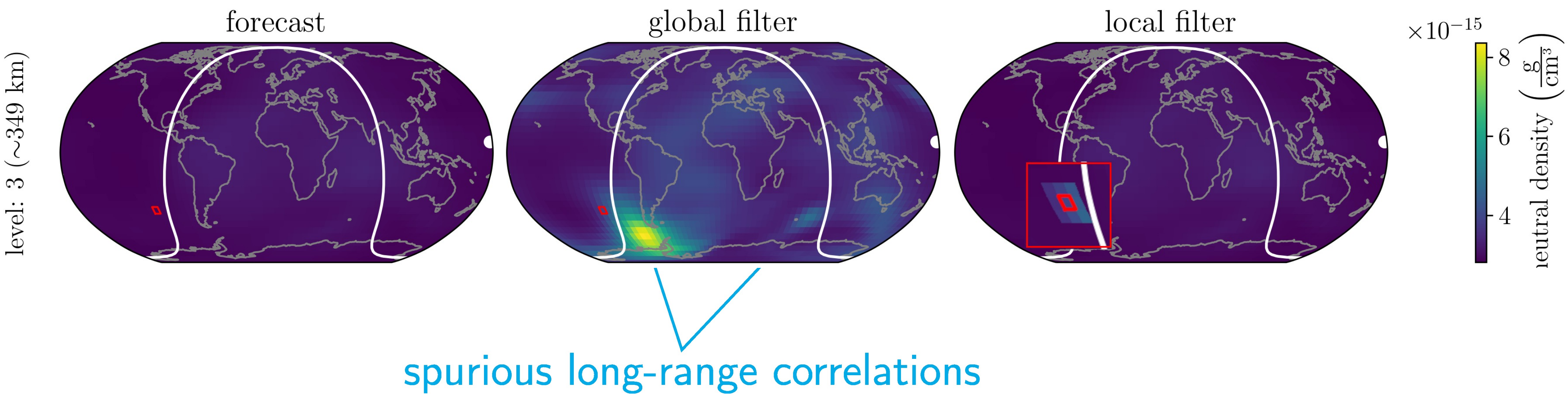
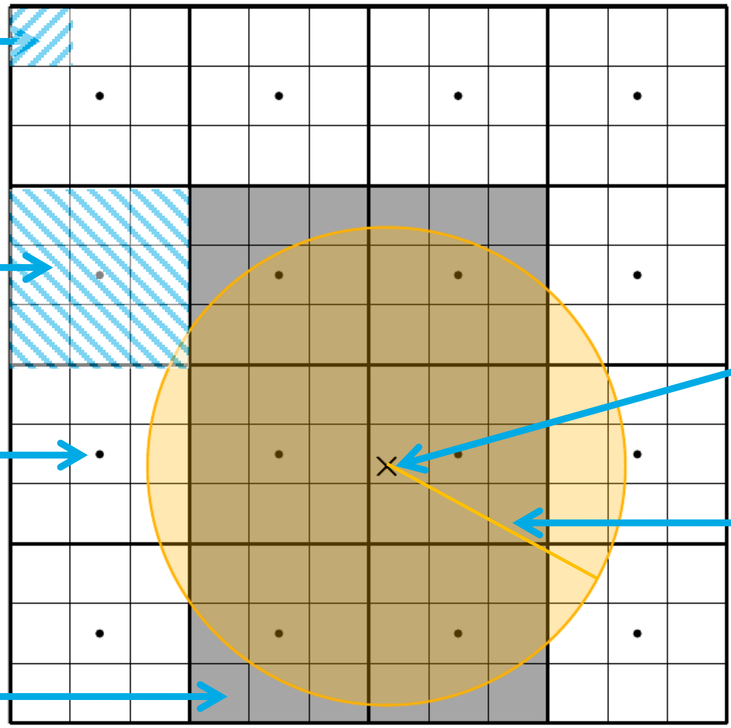


Localization



Domain Localization

- subdivide model into disjoint sub-domains
- update each sub-domain individually taking only observations within specific distance into account



Covariance Localization

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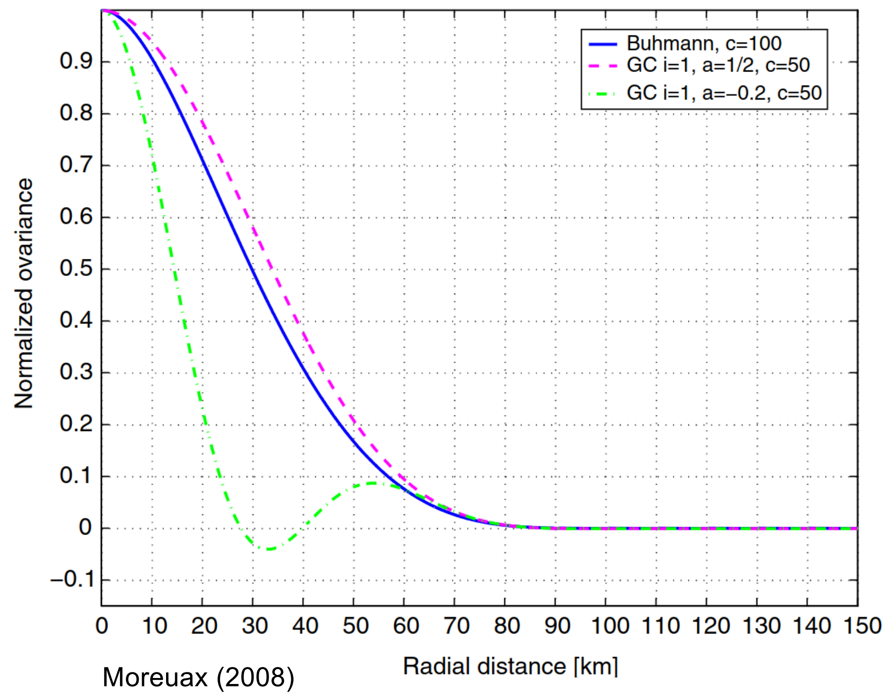
- Multiply covariance matrix of forecasted state with finite covariance function

properties of auto covariance functions
- positive semi-definite
- $f(0) \geq 0$
- $|f(x)| \leq f(0)$
- $f(-x) = f(x)$



Moreuax (2008)

Inflation

PDAF Parallel Data Assimilation Framework

- True variance is always underestimated
  - small ensemble size
  - sampling errors (unknown structure of P)
  - model errors

→ can lead to filter divergence

- Simple remedy

→ Increase error estimate before analysis

- Inflation
  - Increase ensemble spread by constant factor
  - Some filters allow multiplication of a small matrix
  - Needs to be experimentally tuned

Co-Estimation of Model Dynamics (Model Calibration)

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augment state vector with model parameters

state

$$z = \begin{bmatrix} x \\ c \end{bmatrix}$$

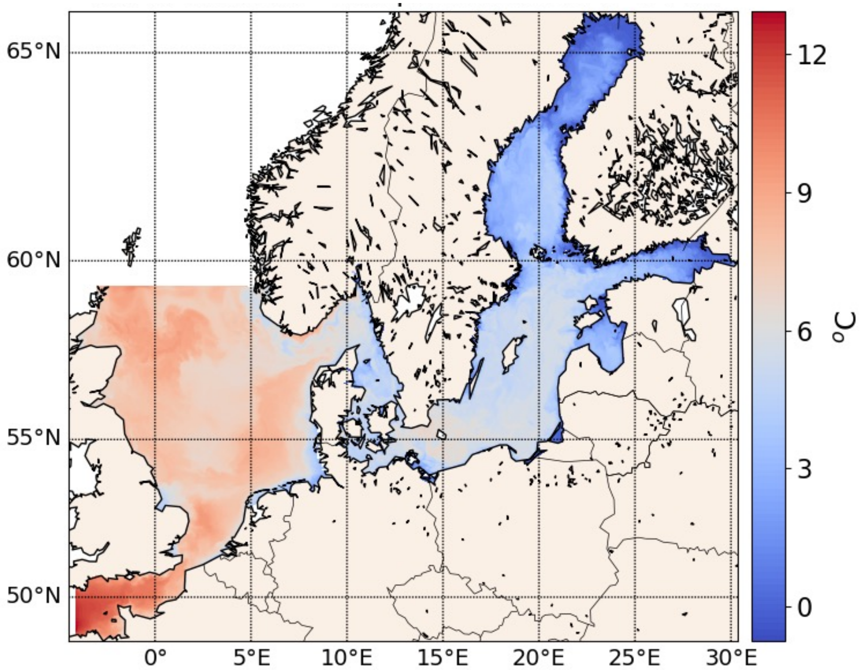
model parameters

II Applications

Coastal Ocean DA

Improving forecasts of **ocean physics** and **biogeochemistry**

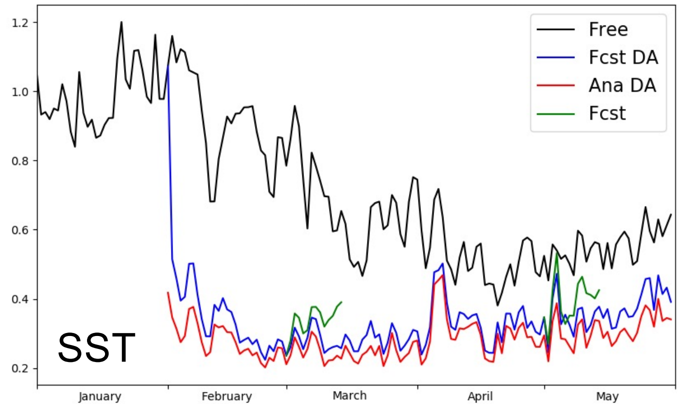
Model domain: North Sea and Baltic Sea
1.8km resolution, 56 layers

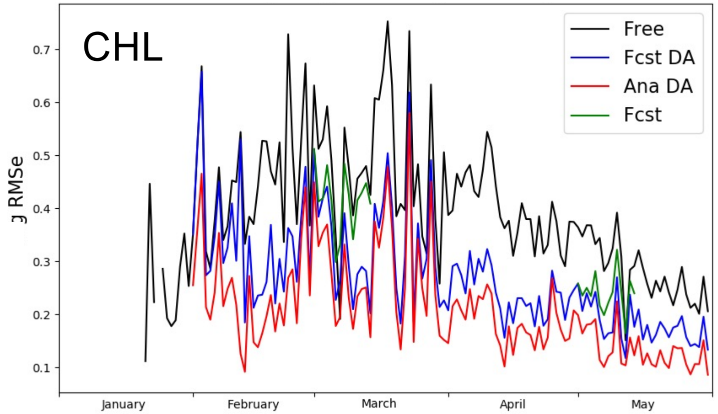


Surface temperature:
RMSe in Baltic Sea

Black: no DA
Blue: 1-day forecasts
Red: analysis
Green: 14-day forecasts

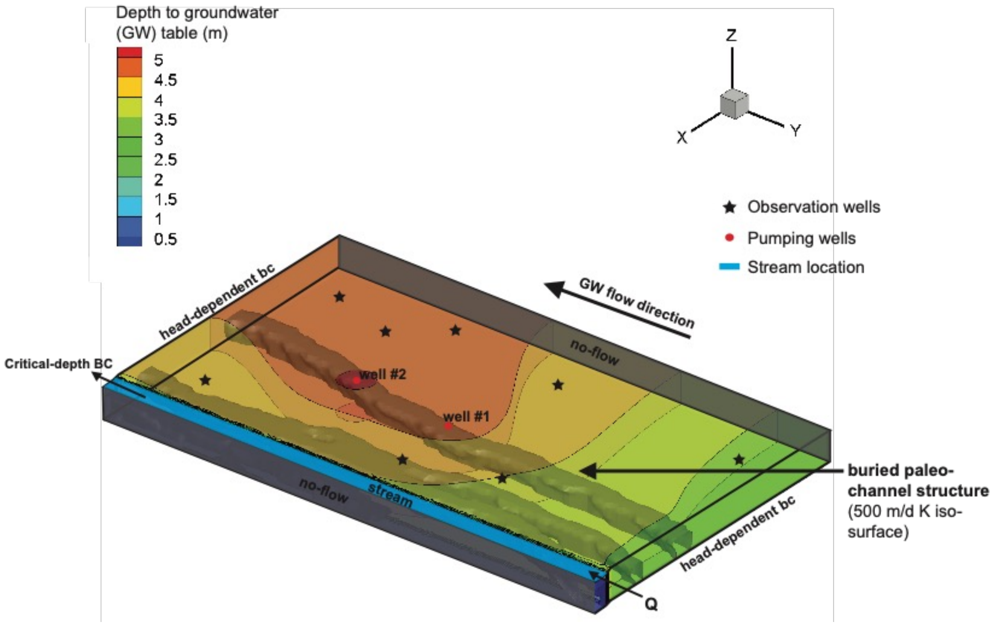
Chlorophyll:
Log10-RMSe
in Baltic Sea

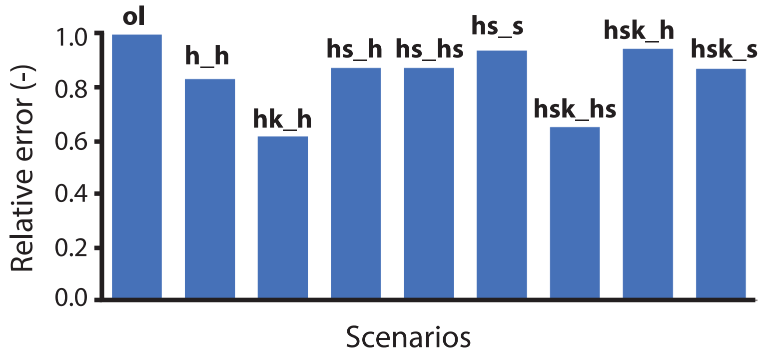


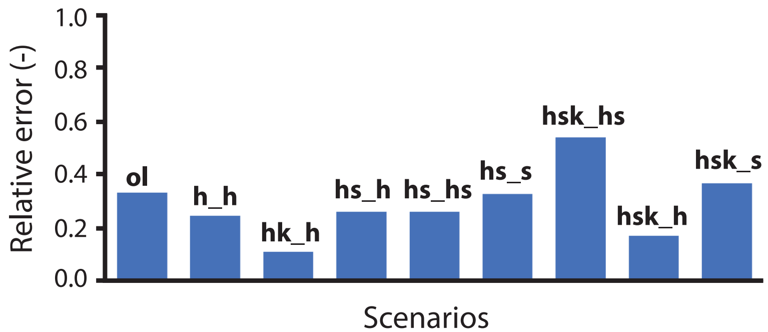


HGS-PDAF

A modular data assimilation framework for an integrated surface and subsurface **hydrological** model





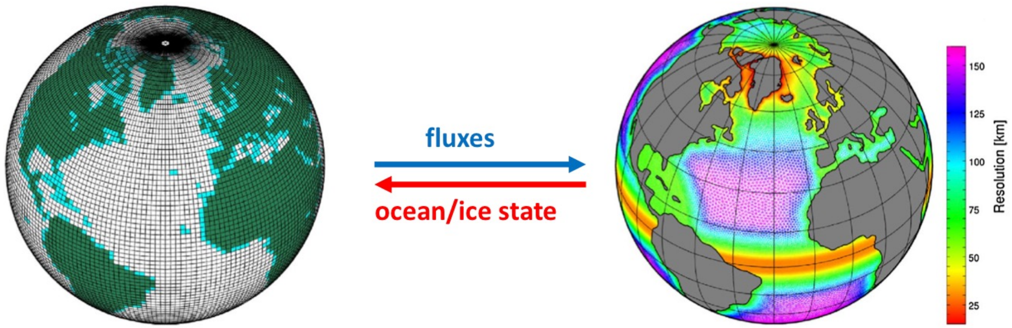


Tang et al. (2023): HGS-PDAF (version 1.0): A modular data assimilation framework for an integrated surface and subsurface hydrological model, Geosci. Model Dev. Discuss.

PDAF Parallel Data Assimilation Framework

AWI-CM-PDAF

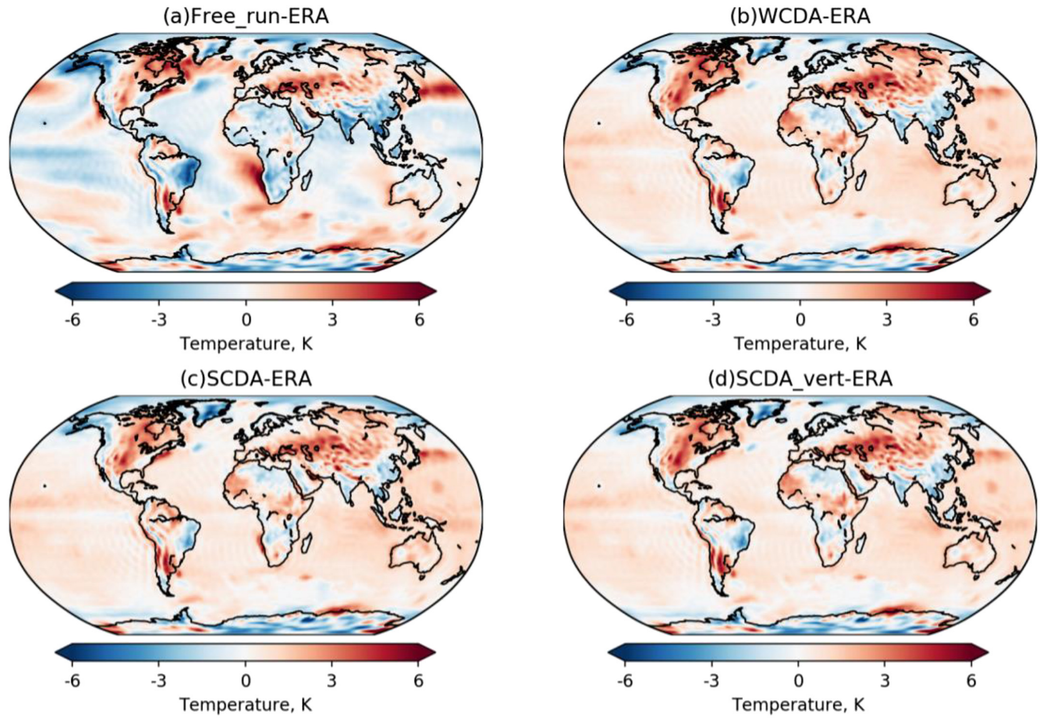
A data assimilation framework for coupled **ocean-atmosphere** models



Atmosphere
ECHAM6
JSBACH land

Coupler library
OASIS3-MCT

Ocean
FESOM
includes sea ice

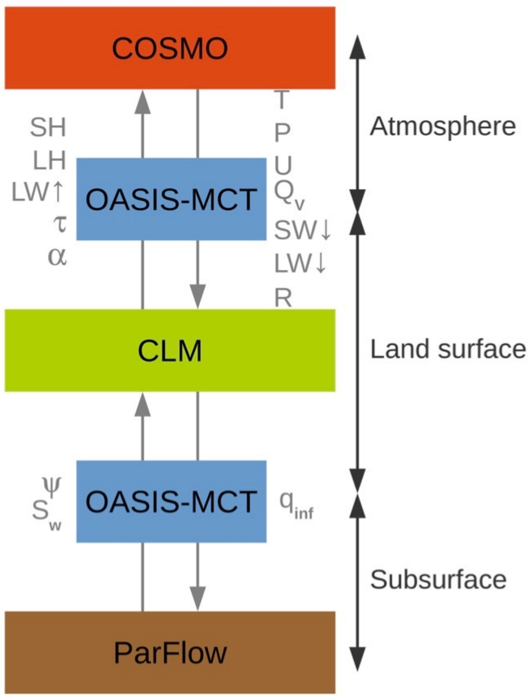


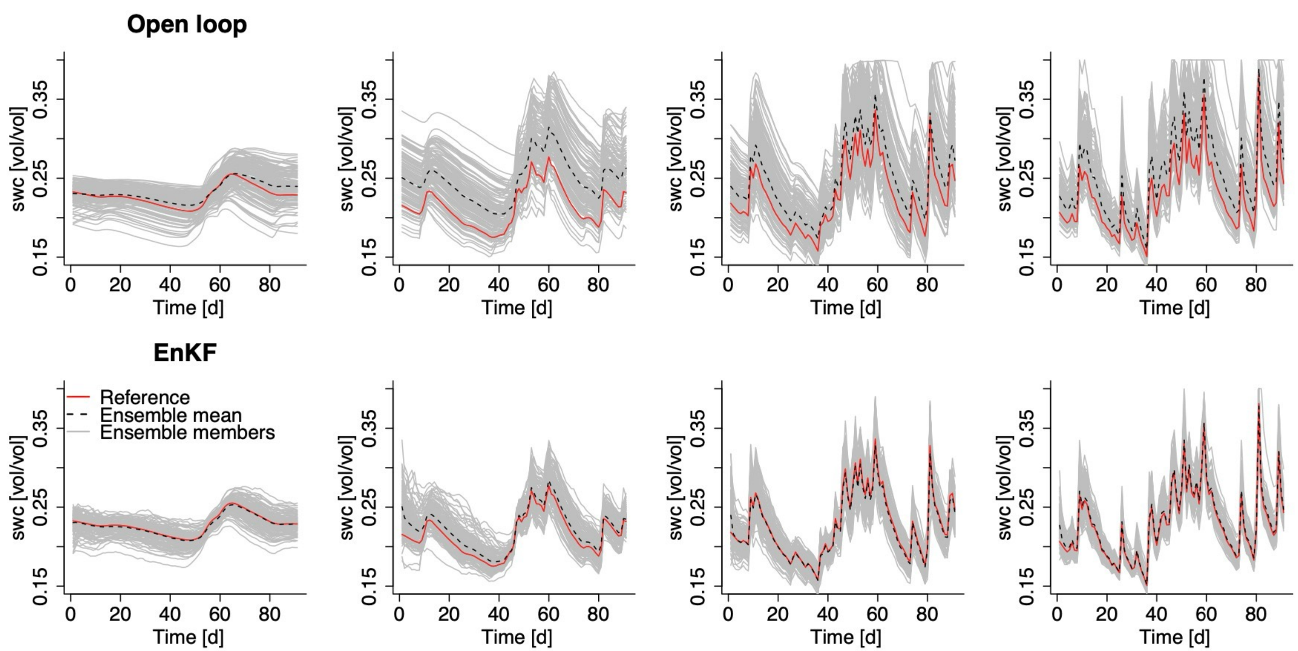
Nerger et al. (2020): Efficient ensemble data assimilation for coupled models with the Parallel Data Assimilation Framework: example of AWI-CM (AWI-CM-PDAF 1.0), Geosci. Model Dev.
Tang et al. (2021): Strongly coupled data assimilation of ocean observations into an ocean-atmosphere model. Geophysical Research Letters

TerrSysMP–PDAF

PDAF Parallel Data Assimilation Framework

a modular high-performance data assimilation framework for an integrated **land surface–subsurface** model

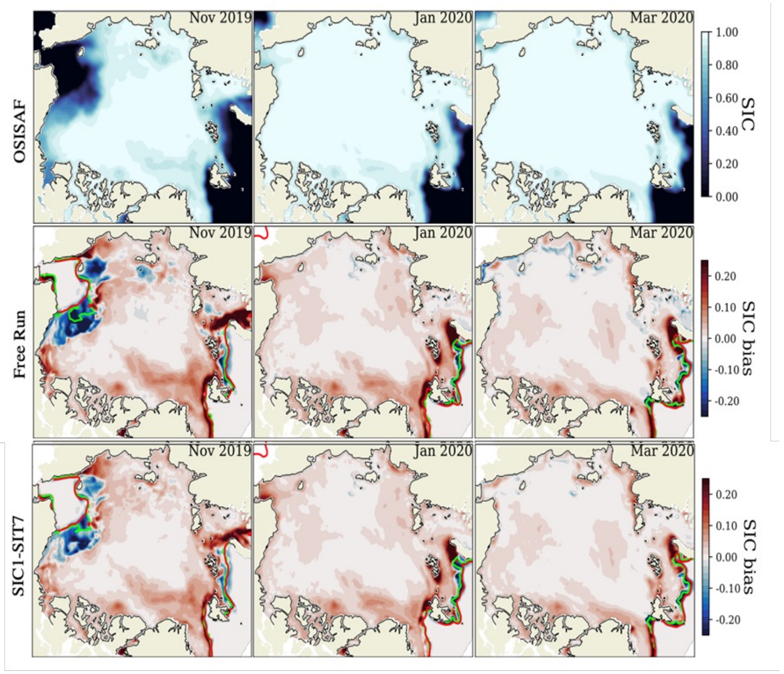




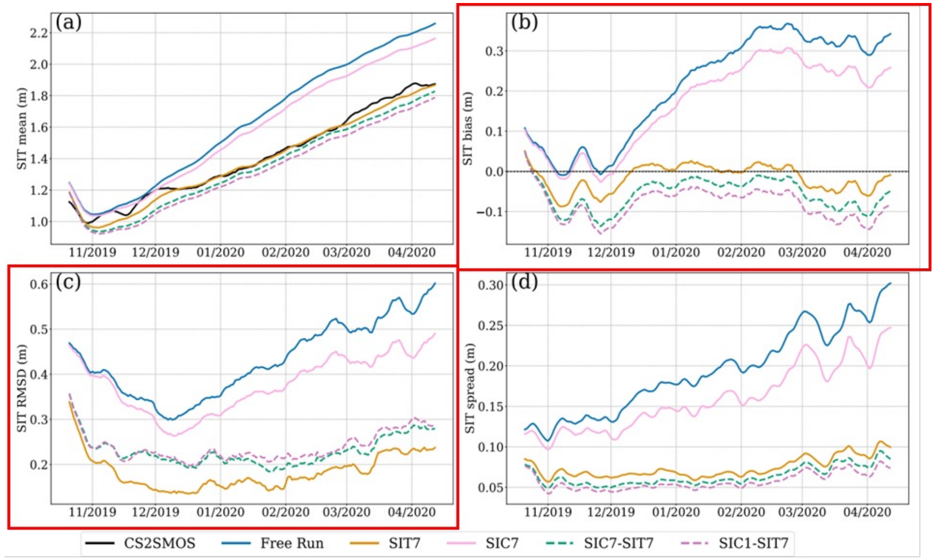
Kurtz et al. (2016): TerrSysMP–PDAF (version 1.0): a modular high-performance data assimilation framework for an integrated land surface–subsurface model, Geosci. Model Dev.

DEnKF on a Lagrangian **sea ice** model

PDAF Parallel Data Assimilation Framework



Reduction in sea ice extent bias (green: obs., red:forecast)



Improved sea ice thickness estimates

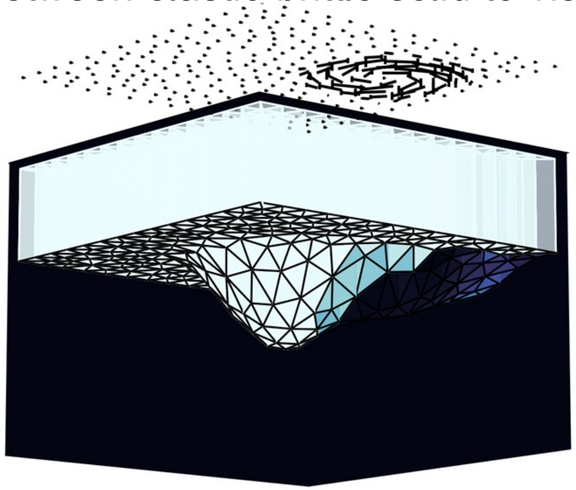
Cheng, S., Chen, Y., Aydoğdu, A., Bertino, L., Carrassi, A., Rampal, P., and Jones, C. K. R. T.: Arctic sea ice data assimilation combining an ensemble Kalman filter with a novel Lagrangiansea ice model for the winter 2019–2020, The Cryosphere, 17, 1735–1754, https://doi.org/10.5194/tc-17-1735-2023, 2023.

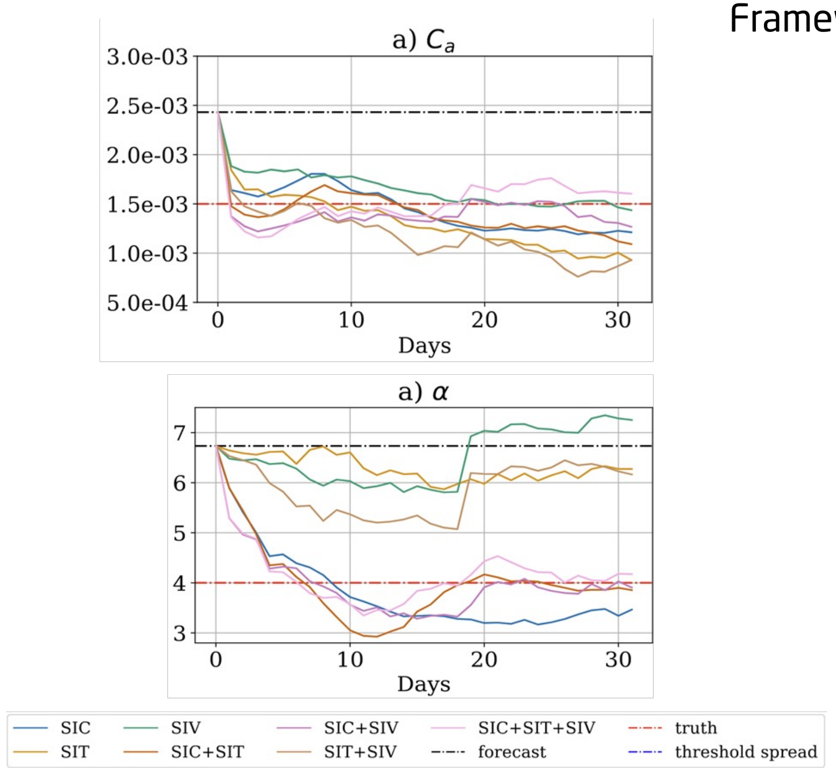
University of Reading SCHMIDT FUTURES National Centre for Earth Observation NATURAL ENVIRONMENT RESEARCH COUNCIL

Joint state and parameter estimation for sea ice model

- Idealised experiment on parameter estimation for a dynamics-only Arctic sea ice model

- Two parameters are estimated:
  - Air drag coefficient () - determines the influence of wind on the sea ice motion
  - Damage parameter (α) – determines the transition between elastic-brittle solid to viscous fluid behaviour





- **Estimation can get close to the truth**
- **Some issues exist**

Chen, Y., Smith, P., Carrassi, A., Pasmans, I., Bertino, L., Bocquet, M., Finn, T. S., Rampal, P., and Dansereau, V.: Multivariate state and parameter estimation with data assimilation on sea-ice models using a Maxwell-Elasto-Brittle rheology, EGUsphere [preprint], https://doi.org/10.5194/egusphere-2023-1809, 2023.

NCAR TIE-GCM PDAF

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Improving neutral mass density estimation in **upper atmosphere**

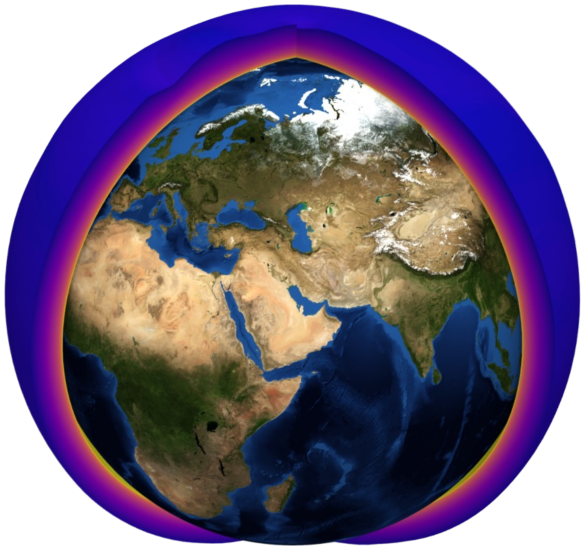
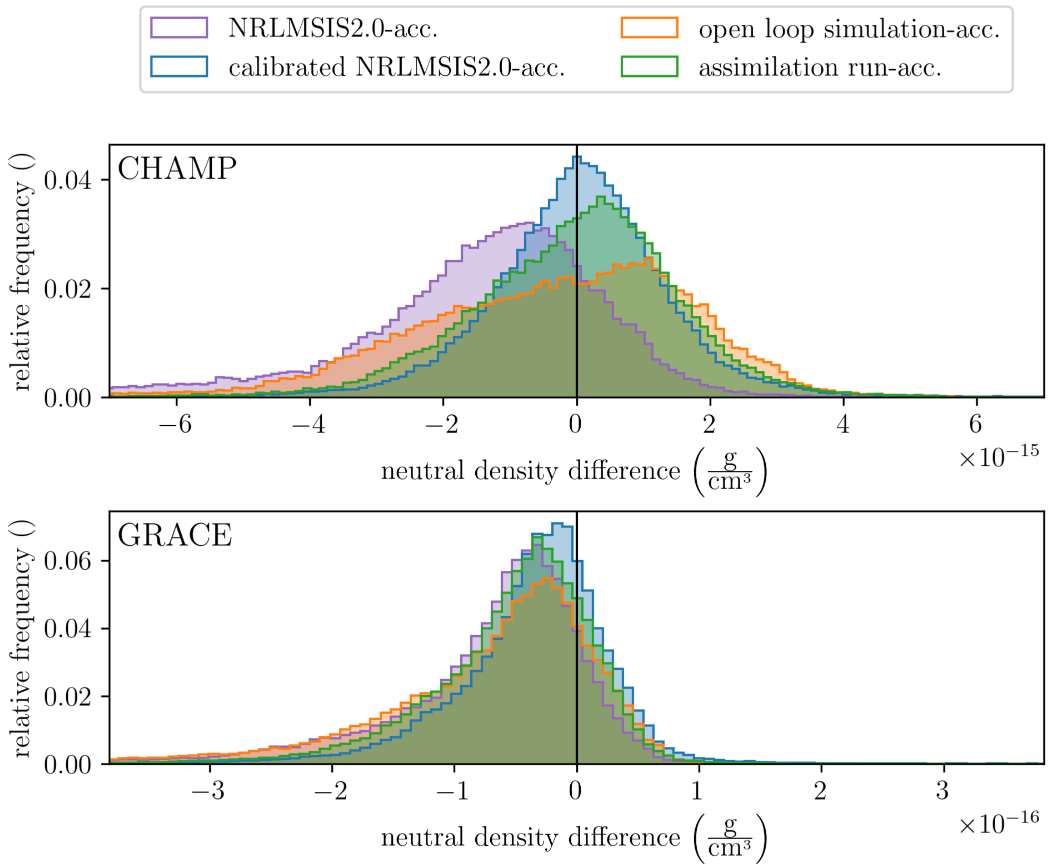


Image of Earth: Reto Stöckli, NASA Earth Observatory



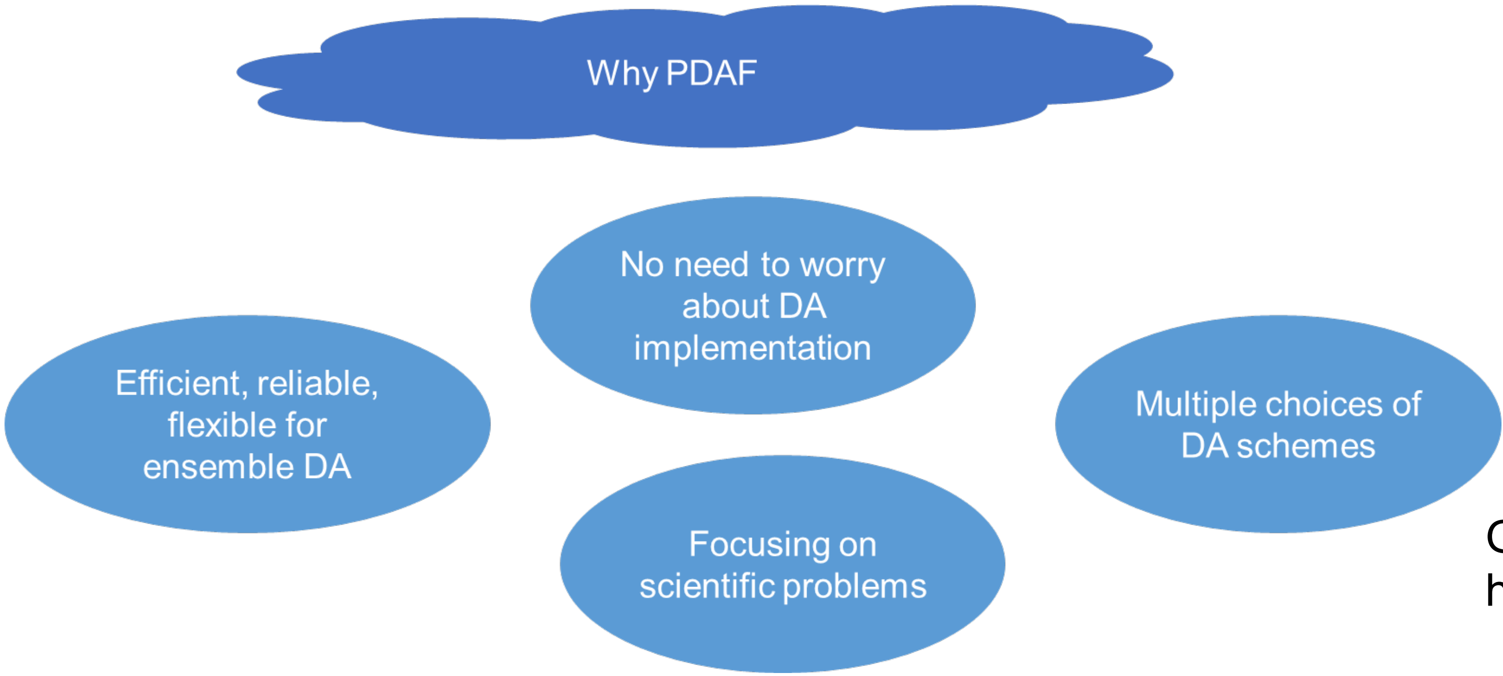
Corbin, A. & Kusche, J. Improving the estimation of thermospheric neutral density via two-step assimilation of in situ neutral density into a numerical model. Earth, Planets and Space 74, 183 (2022).

III Hands On

Building a DA system

PDAF Parallel **Data Assimilation** Framework

- We will use PDAF to build a simple data assimilation system



Website: https://pdaf.awi.de/trac/wiki

Github repo: https://github.com/PDAF/PDAF

pyPDAF – A Python interface to PDAF

PDAF Parallel Data Assimilation Framework

Efficient

Fortran models/
Offline DA

git repository:
https://github.com/yumengch/pypdaf

Python models

PDAF
(Fortran)

pyPDAF
(Python)

Intensive code
development

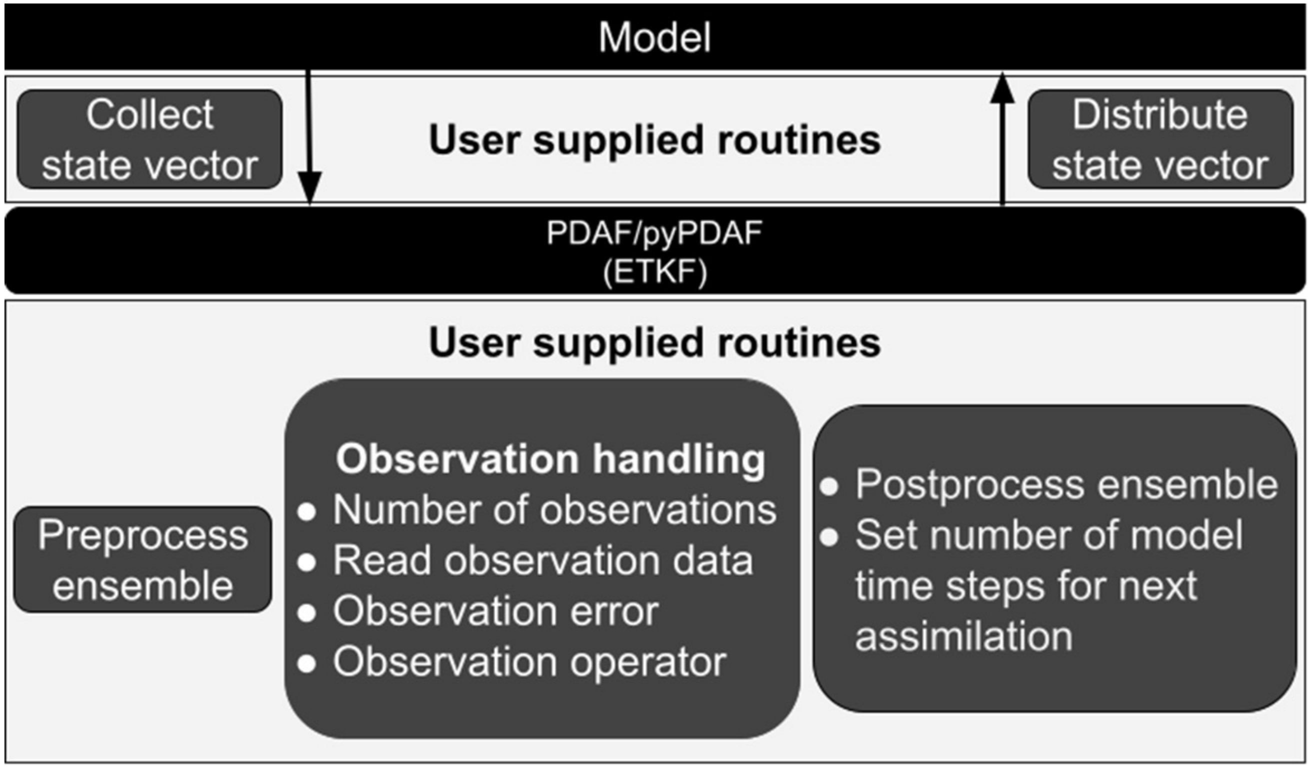
High-dimensional
systems

Less
efficient

Easier code
development

Overview of DA system

PDAF Parallel Data Assimilation Framework



Forecasts and their uncertainties

$$x_k^a = x_k^f + K_k\left(\boxed{y_k^o} - \boxed{H_k} x_k^f\right)$$

$$K_k = P_k^f \boxed{H_k^T}\left(\boxed{H_k} P_k^f \boxed{H_k^T} + \boxed{R_k}\right)^{-1}$$

Observations and their uncertainties

Hands-on example

PDAF Parallel Data Assimilation Framework

https://tinyurl.com/2p938fne

- The jupyter notebook can be run directly in Google colab

- If you download the jupyter notebook on your local computer, you can also install pyPDAF and jupyter notebook with conda using

```
conda install -c yumengch -c conda-forge pypdaf jupyter
```

and running jupyter notebook from the terminal with

```
jupyter notebook
```

References

Asch, M, M. Bocquet, M. Nodet, *Data Assimilation: Methods, Algorithms, and Applications*, SIAM, 2017

Moreaux, G., *Compactly Supported Radial Covariance Functions*, Journal of Geodesy 82.7, 2008

Vetra-Carvalho, S., Van Leeuwen, P.J., Nerger, L., Barth, A., Altaf, M.U., Brasseur, P., Kirchgessner, P. and Beckers, J.-M., *State-of-the-art stochastic data assimilation methods for high-dimensional non-Gaussian problems,* Tellus A: Dynamic Meteorology and Oceanography, 70(1), 2018

Evensen, G., F. Vossepoel, P. J. van Leeuwen, *Data Assimilation Fundamentals*, Springer, 2022, doi:10.1007/978-3-030-96709-3 (open access)