High-Dimensional Applications of Ensemble-Based Data Assimilation in Geosciences

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Overview

Application-centric viewpoint of ensemble-based data assimilation

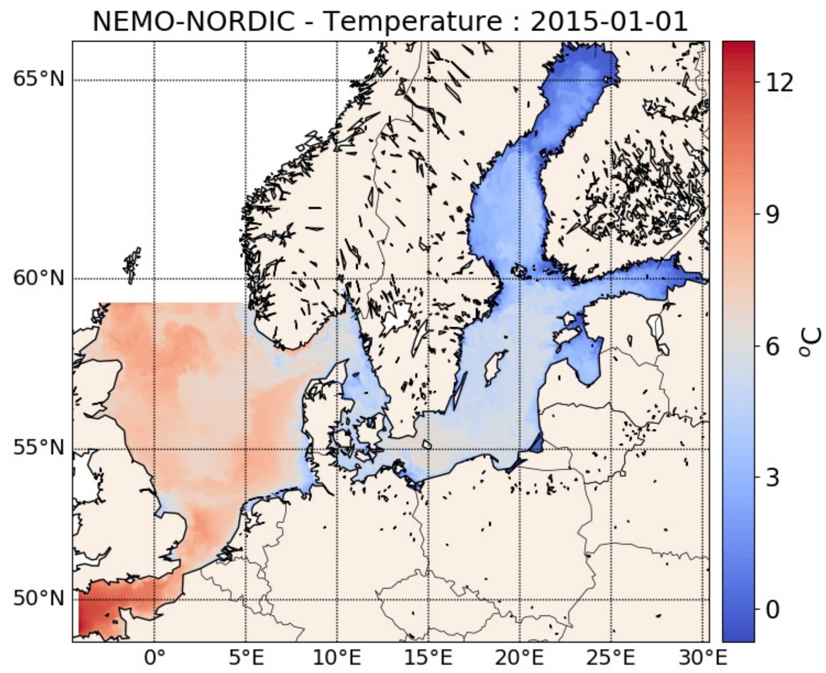
- Example of high-dimensional data assimilation application
- Methods
- Computational challenges
- Software
- Open points

High-dimensional Data Assimilation Application

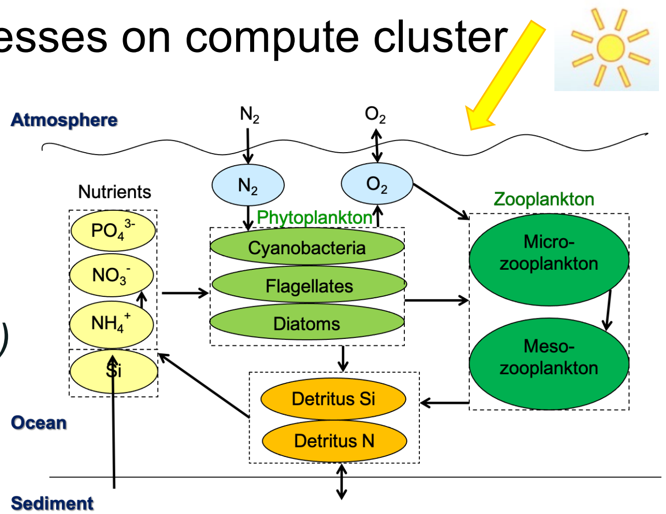
Model: NEMO-ERGOM

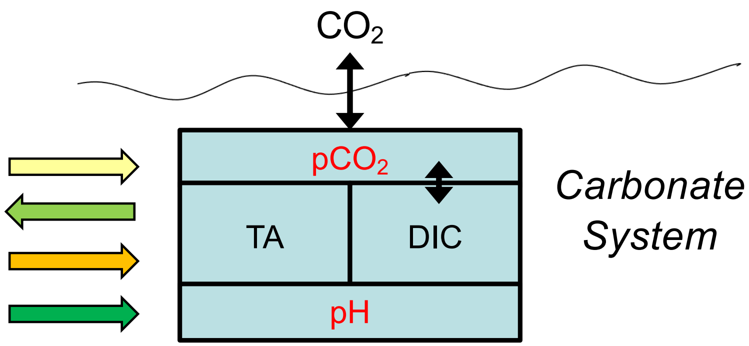
Operational configuration of Copernicus Marine Forecasting Center for Baltic Sea (BAL-MFC)

- Model setup
  - Ocean model NEMO
  - Coupled to ecosystem/carbon model ERGOM
  - 1.8 km resolution, 56 layers
  - Time step 90 sec
  - 192 processes on compute cluster



Ecosystem (biogeochemistry)





Carbonate System

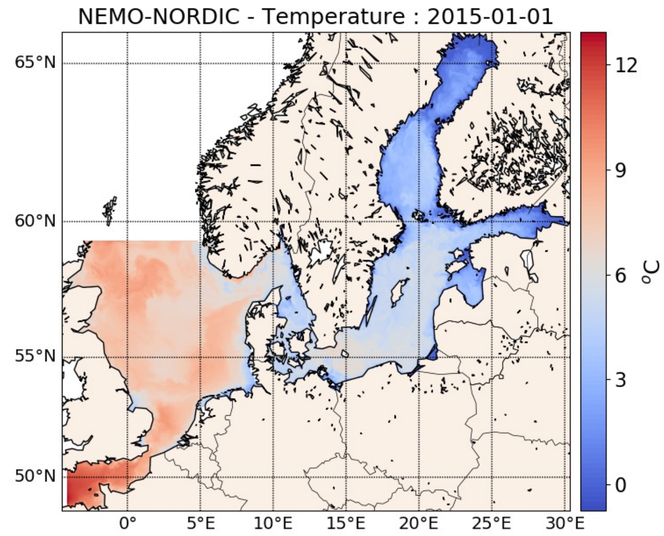
NEMO-ERGOM Coupled Data Assimilation

Ensemble States

- 5 physics variables
- 20 ecosystem variables
- State vector dimension: $704 \cdot 10^6$

Assimilation setup

- ensemble Kalman filter LESTKF
- ensemble size: 30
- Daily assimilation for 1 year
  - Observation data:
    surface temperature and chlorophyll concentration
- Localization: 20 km, Gaspari/Cohn function
- 186 x 30 = 5580 processors on compute cluster
- 12 days computing time
- Output approx. 900 GB (after compression)



Costly to run, store and analyze outputs

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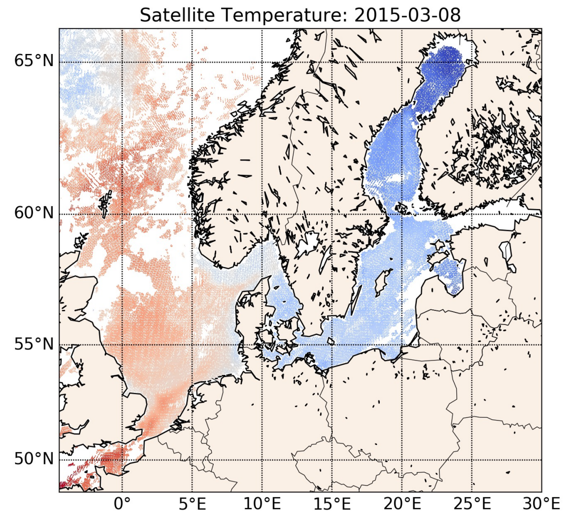
Observations

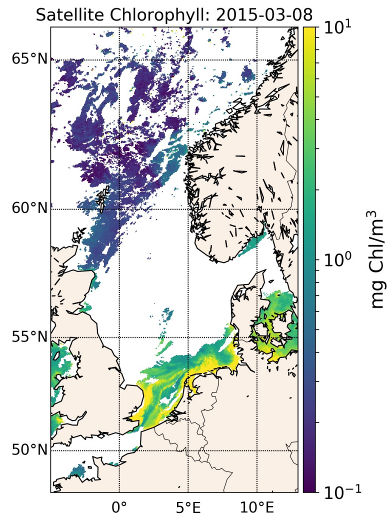
Sea Surface Temperature

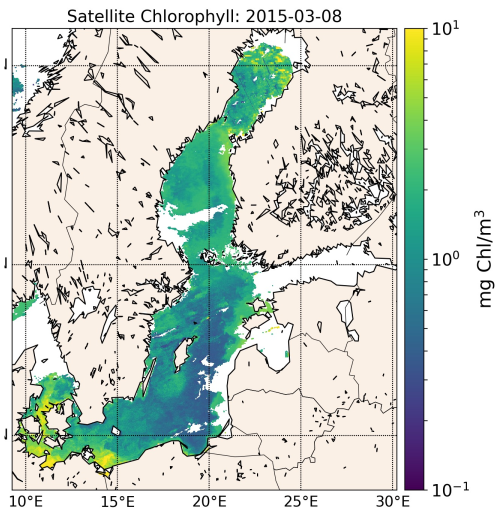
- Level 3 data from Copernicus Marine service (CMEMS)
- resolution 0.02°
- available daily
- No data in cloudy regions
- Number of observations: 17,000 – ~150,000
- observation error for DA: 0.8 °C
  (provided error fields not fully realistic)



Chlorophyll

- Level 3 data from CMEMS
- separate data products for North Sea and Baltic Sea
- resolution 1 km
- available daily
- No data in cloudy regions
- Number of observations: 0 – ~500,000
- observation error: relative error of 0.3





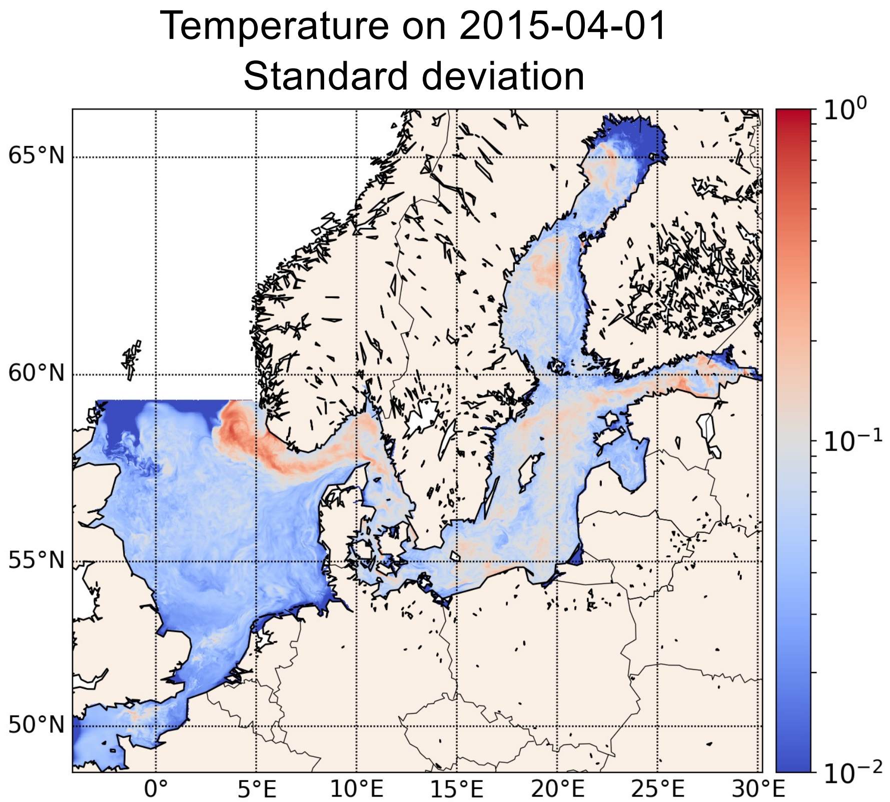
Methods

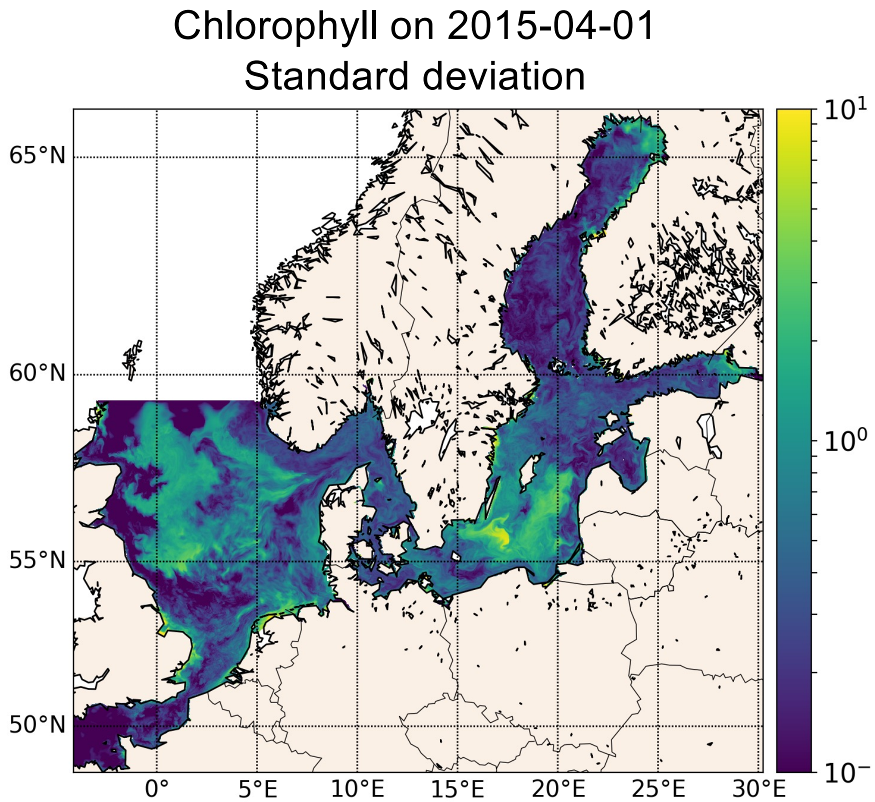
Ensemble-based data assimilation

Estimation by joining model and observational data

Uncertainty Estimates

Dynamic ensembles provide uncertainties (and covariances) for each day





Linear and Nonlinear Ensemble Filters

- Represent state and its error by ensemble $\mathbf{X}$ of N states (use ensemble perturbation matrix $\mathbf{X}^{'} = \mathbf{X} - \bar{\mathbf{X}}$)
- **Forecast**:
  - Integrate ensemble size N with numerical model
- **Analysis step:**
  - update ensemble mean $\overline{\mathbf{x}}^a = \overline{\mathbf{x}}^f + \mathbf{X}'^f \tilde{\mathbf{w}}$
  - update ensemble perturbations $\mathbf{X}'^a = \mathbf{X}'^f \mathbf{W}$

  (both can be combined in a single step)

Dimension of correction (error) space : N-1

- Ensemble Kalman & nonlinear filters: Different definitions of
  - weight vector $\tilde{\mathbf{w}}$ (dimension N)
  - Transform matrix $\mathbf{W}$ (dimension $N \times N$)

ETKF (Bishop et al., 2001)

- Ensemble Transform Kalman filter
  - Assume Gaussian distributions
  - Transform matrix

$$\mathbf{A}^{-1} = (N-1)\mathbf{I} + (\mathbf{H}\mathbf{X}'^f)^T\mathbf{R}^{-1}\mathbf{H}\mathbf{X}'^f$$

  - Mean update weight vector

$$\tilde{\mathbf{w}} = \mathbf{A}(\mathbf{H}\mathbf{X}'^f)^T\mathbf{R}^{-1}\left(\mathbf{y} - \mathbf{H}\overline{\mathbf{x}^f}\right)$$

(depends linearly on observation vector $\mathbf{y}$)

  - Transformation of ensemble perturbations

$$\mathbf{W} = \sqrt{N-1}\ \mathbf{A}^{1/2}\mathbf{\Lambda}$$

$\mathbf{\Lambda}$: mean-preserving random matrix or identity

Note: $\mathbf{W}$ depends only on $\mathbf{R}$, not observation $\mathbf{y}$

Algorithm designed for maximum computational efficiency

Excellent parallelization possibility when combined with localization

Linear filter:
- Gaussian distributions assumed
- Linear in effect of $\mathbf{y}$

NETF (Tödter & Ahrens, 2015)

- Nonlinear Ensemble Transform Filter
  - Mean update from Particle Filter weights:
    for Gaussian observation errors for all particles *i*

$$\tilde{w}^i \sim \exp\left(-0.5(\mathbf{y} - \mathbf{H}\mathbf{x}_i^f)^T \mathbf{R}^{-1} (\mathbf{y} - \mathbf{H}\mathbf{x}_i^f)\right)$$

(nonlinear function of observations $\mathbf{y}$)

  - Ensemble update
    - Transform ensemble to fulfill analysis covariance (like ETKF, but not assuming Gaussianity)
    - Derivation gives

$$\mathbf{W} = \sqrt{N}\left[\mathrm{diag}(\tilde{\mathbf{w}}) - \tilde{\mathbf{w}}\tilde{\mathbf{w}}^T\right]^{1/2} \Lambda$$

($\mathbf{\Lambda}$: mean-preserving random matrix; useful for stability)

Similar computational efficiency as ETKF

Excellent parallelization possibility when combined with localization

Nonlinear filter:
- No assumption of Gaussian distributions
- Nonlinear in $\mathbf{y}$

NETF is a second-order exact particle filter

 Tödter, J. and Ahrens, B. (2015) *Mon. Wea. Rev.* **143**,1347–1367

ETKF-NETF – Hybrid Filter Variants

Factorize the likelihood: ('tempering') $p(\mathbf{y}|\mathbf{x}) = p(\mathbf{y}|\mathbf{x})^{\gamma} p(\mathbf{y}|\mathbf{x})^{(1-\gamma)}$

- γ: hybrid weight (between 0 and 1; 1 for fully ETKF)

2-step updates

Variant 1 (*HNK*): NETF followed by ETKF

$$\tilde{\mathbf{X}}^a_{HNK} = \mathbf{X}^a_{NETF}[\mathbf{X}^f, (1-\gamma)\mathbf{R}^{-1}]$$
$$\mathbf{X}^a_{HNK} = \mathbf{X}^a_{ETKF}[\tilde{\mathbf{X}}^a_{HNK}, \gamma\mathbf{R}^{-1}]$$

- Both steps computed with increased $\mathbf{R}$ according to γ

Variant 2 (*HKN*): ETKF followed by NETF

Related methods:
Frei/Kuensch (2013)
Chustagulprom et al. (2016)
Robert et al. (2018)
Grooms/Robinson (2021)

Nerger, L. (2022) Q. J. R. Meteorol. Soc., **148**, 620-640 doi:10.1002/qj.4221

Choosing hybrid weight γ

- Hybrid weight shifts filter behavior

Some possibilities:

- Fixed value
- Adaptive - According to which condition?

Issue: Using N_{eff}
- only ensures non-collapsing ensemble
- does not ensure good analysis result
- Experimentally no obvious relation between N_{eff} and γ

  - Frei & Kuensch (2013) suggested using effective sample size $N_{eff} = \sum \frac{1}{(w^i)^2}$

(Usual choice for 'tempering')

    - γ_α : Choose γ so that N_{eff} is as small as possible but above minimum limit α (done iteratively)

  - Adaptive alternative

$$\gamma_{lin} = 1 - \frac{N_{eff}}{N_e}$$

(close to 1 if N_{eff} small; no iterations)

Effect of hybrid weight γ

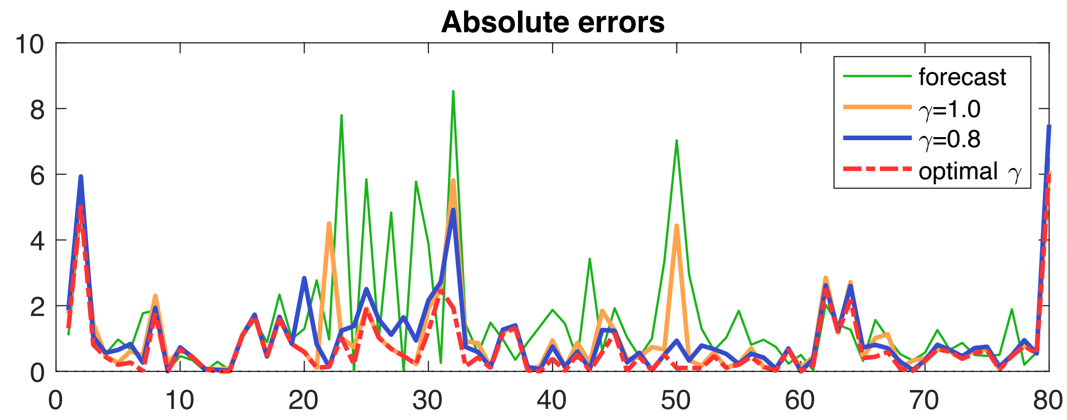
- Lorenz-96 model, size 80
- Examine single analysis step

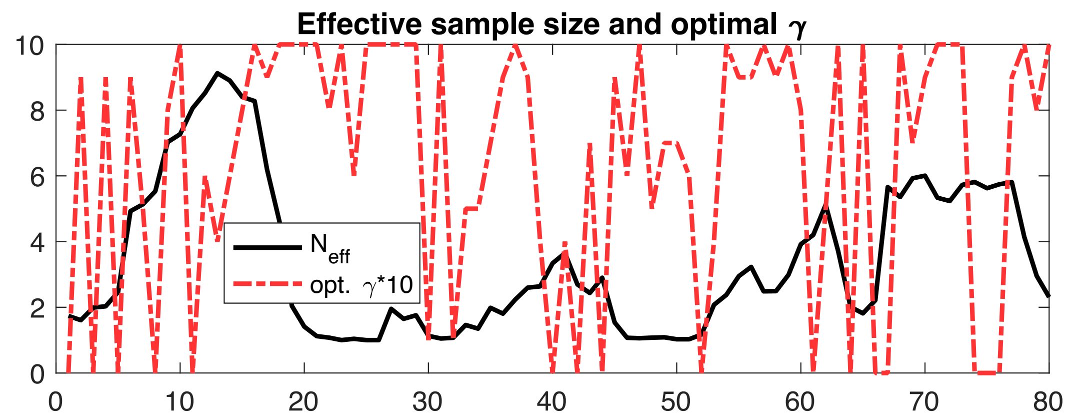
1. Run 33 analysis steps with γ=1 (LETKF)
2. Run analysis step 34 with one of
   a) γ=1
   b) γ=0.8
3. Examine N_{eff} and analysis errors

Additional experiment:

c) Adjust γ at each grid point to get minimum error

No obvious relation between N_{eff} and γ!





Account for non-Gaussianity: Skewness and Kurtosis

- **Mean** – 1st moment
- **Variance** – 2nd moment
- **Skewness** – 3rd moment

$$skew = \frac{\frac{1}{N_e}\sum_{i=1}^{N_e}\left(\mathbf{x}^i - \overline{\mathbf{x}}\right)^3}{\left[\frac{1}{(N_e-1)}\sum_{i=1}^{N_e}\left(\mathbf{x}^i - \overline{\mathbf{x}}\right)^2\right]^{3/2}}$$

- **Kurtosis** – 4th moment

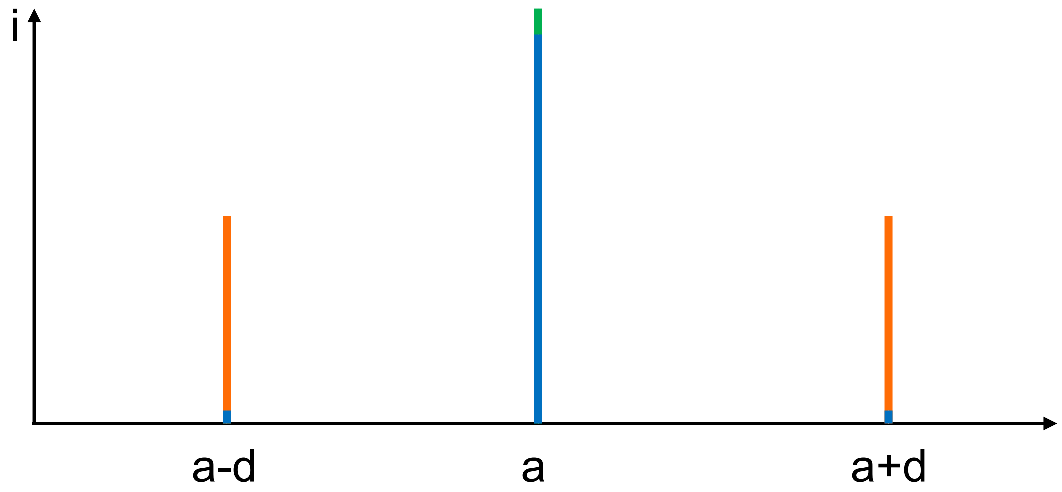
$$kurt = \frac{\frac{1}{N_e}\sum_{i=1}^{N_e}\left(\mathbf{x}^i - \overline{\mathbf{x}}\right)^4}{\left[\frac{1}{(N_e)}\sum_{i=1}^{N_e}\left(\mathbf{x}^i - \overline{\mathbf{x}}\right)^2\right]^{2}} - 3$$

- Skewness and kurtosis
  - generally not bounded
    - → but limits depend on ensemble size

Asymptotic properties of skewness and kurtosis

- Bounds of skewness and kurtosis depend on ensemble size
- Assess extreme cases

Case	Values	*skew* limit	*kurt* limit
max. skew	$x^{(1)} = a - d, \quad x^{(i)} = a,\ i = 2, \ldots, N_e$	$\sqrt{N_e}$	N_e
max. kurt	$x^{(1)} = a - d, \quad x^{(2)} = a + d, \quad x^{(i)} = a,\ i = 3, \ldots, N_e$	0	-2
min. kurt	$x^{(i)} = a - d,\ i = 1, \ldots N_e/2; \quad x^{(j)} = a + d,\ j = N_e/2 + 1, \ldots, N_e$	0	$N_e/2$



AWI

Using skewness and kurtosis to define hybrid weight γ

- Sampling errors are larger in NETF than ETKF
  → Always use ETKF for Gaussian (linear) cases
- Skewness and kurtosis describe deviation from Gaussianity
- mean absolute skewness (mas) and kurtosis (mak) of observed ensemble (with localization: use locally assimilated observations)
- Use normalized means:

$$nmas = \frac{1}{\sqrt{\kappa}} mas \qquad nmak = \frac{1}{\kappa} mak$$

standard value: $\kappa = N_e$

Now define

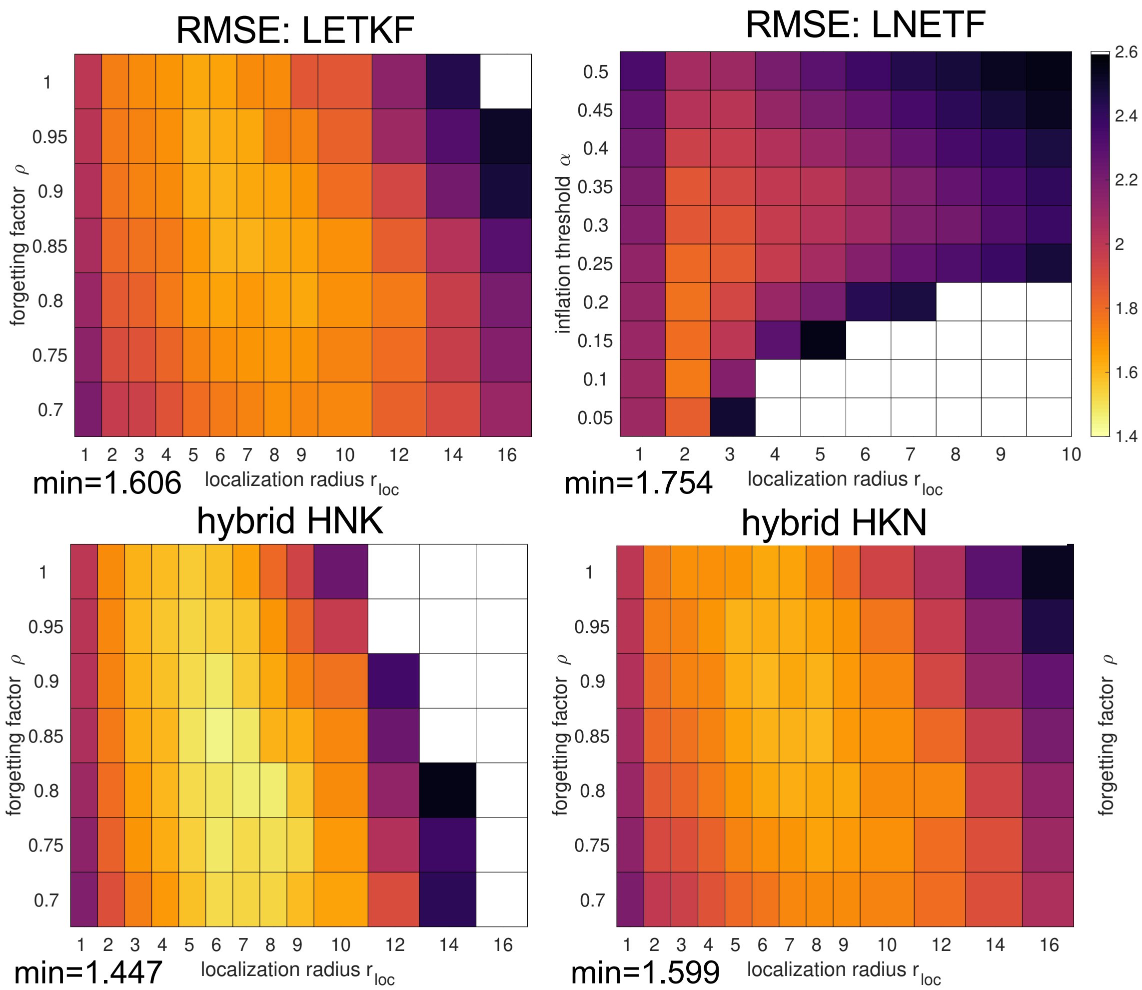
$$\gamma_{sk,\alpha} = \max\left[\min(1 - nmak,\ 1 - nmas),\ \gamma_\alpha\right]$$
$$\gamma_{sk,lin} = \max\left[\min(1 - nmak,\ 1 - nmas),\ \gamma_{lin}\right]$$

stronger influence of $nmas$ and $nmak$ limited by N_{eff}

Note: There are sampling errors, e.g. for skewness $\sigma_{skew} \sim \sqrt{6/N_e}$
→ For N_e=25: ~10% error in γ

Test with Lorenz-96 model

Ensemble size 15; Forecast length: 8 time steps; 20 observations



Strongly nonlinear DA setting

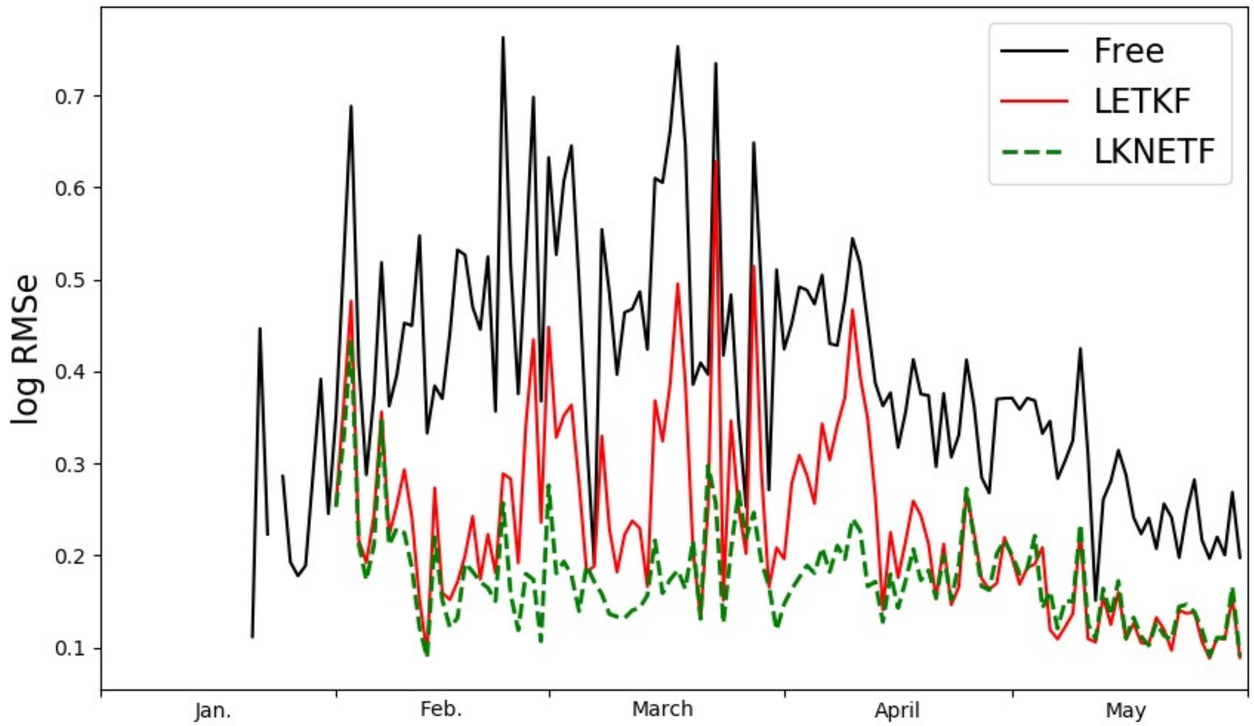
- Show RMS errors as function of inflation (forgetting factor or α) and localization radius
- *Smallest errors:* Hybrid HNK (10% error reduction)

  → hybrid filter able to utlize non-Gaussian information
- Other hybrid variants also improve the state estimate

Effect of hybrid filter in high-dimensional application

Assimilation using rule $\gamma_{sk,\alpha}$

RMS deviation for log-Chlorophyll



Only assimilate chlorophyll observations

Stronger assimilation effect of LKNETF

We still don't know optimal choice of rule for γ

Computational challenges

Computing challenges and features

High-dimensional models

- Costly to compute
- Large amount of output data
- Large size of state vectors
  - Containing all relevant model fields
  - Usually distributed due to parallelization

Ensemble-based data assimilation

- Multiply computing cost (parallel or sequential)
- Full ensemble output would multiply amount of output data
  - Usually only write ensemble mean and variance
- Computing time of model dominates over assimilation method

Software

PDAF: Parallel Data Assimilation Framework

PDAF Parallel Data Assimilation Framework

A unified tool for interdisciplinary data assimilation …

- a program library for data assimilation
- provide support for parallel ensemble forecasts
- provide assimilation methods – fully-implemented & parallelized
- provide tools for observation handling and for diagnostics
- easily useable with (probably) any numerical model
  (coupled to with range of models)
- run from laptops to supercomputers (Fortran, MPI & OpenMP)
- Usable for real assimilation applications and to study assimilation methods
- ensure separation of concerns (model – DA method – observations – covariances)

Open source:
Documentation and tutorial at

http://pdaf.awi.de

github.com/PDAF

Python interface:

https://github.com/yumengch/pyPDAF

L. Nerger, W. Hiller, Computers & Geosciences 55 (2013) 110-118

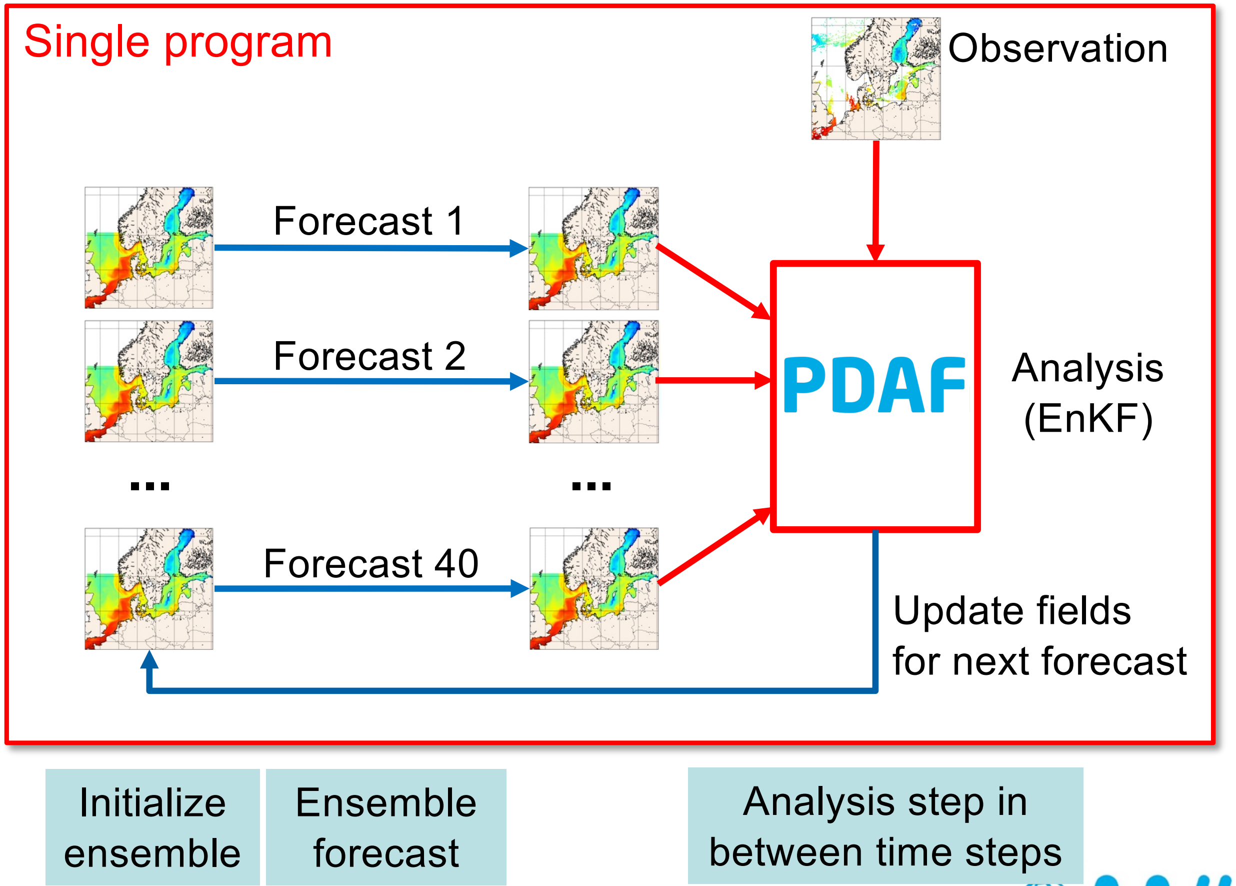
AWI

Online-Coupling – Assimilation-enabled Model

Couple a model with PDAF

- Modify model to simulate ensemble of model states
- Insert analysis step/solver to be executed at prescribed interval
- Run model as usual, but with more processors and additional options

- EnOI and 3D-Var also possible:
  - Evolve single model state
  - Prescribe ensemble perturbations or covariance



Open Points

Open points

Characteristics of problem
– merging observations and models in Geosciences

- Observations
  - High count – O(10^5 - 10^7)
  - Only a few of the model variables
  - Incomplete spatial and temporal coverage
  - Significant errors (measurement and representation)

- Models
  - Large state vectors – (10^6 - 10^9)
  - Costly to run
  - ‘balances’
  - Limited previous model runs available

Open points – linkage a 'modern' ML methods

Potential for improvements with novel ML methods

Reduce execution time

- Dominated by model!
- Faster DA method of little help

Surrogates might help, but

- Costly to build
- Unclear if sufficiently representative (need current representation of error)

Reduce time to tune method

- Tuning required and costly

Do pre-trained neural networks help?

Improve estimates

- Avoid assumptions on distributions (or avoid distributions)
- Avoid sampling errors
- Ensure small state changes to avoid disturbing 'balances'

Summary

PDAF Parallel Data Assimilation Framework

- High-dimensional application in geosciences
  - Costly to compute & large amount of outputs
  - Incompletely observed and with significant errors

- Current standard method basing on optimization or estimation
  - suffer from sampling errors and costly tuning

- Potential of new methods
  - reduce computing time
  - Reduce tuning effort
  - Improve estimates