Ensemble-based data assimilation for complex models of the Earth system

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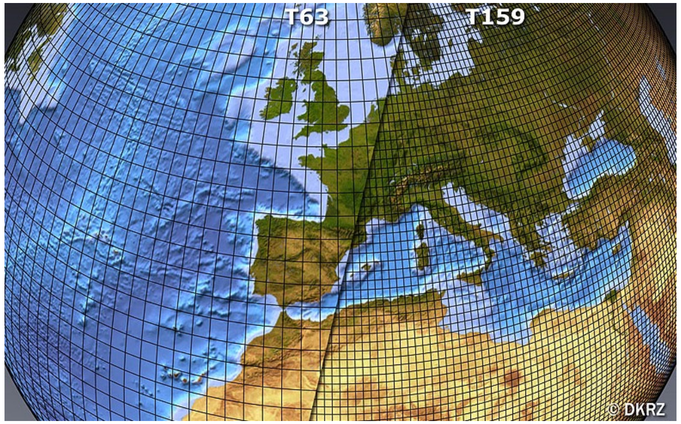
Overview

- High-dimensional data assimilation applications
- Software
- Methods
- Open points

Data Assimilation – Combining Models and Observations

Models



Observations

Combine both sources of information

quantitatively and optimally by computer algorithm

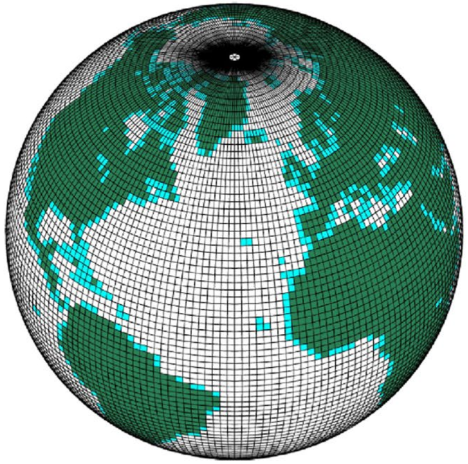
→ Data Assimilation

High-dimensional
Data Assimilation Applications

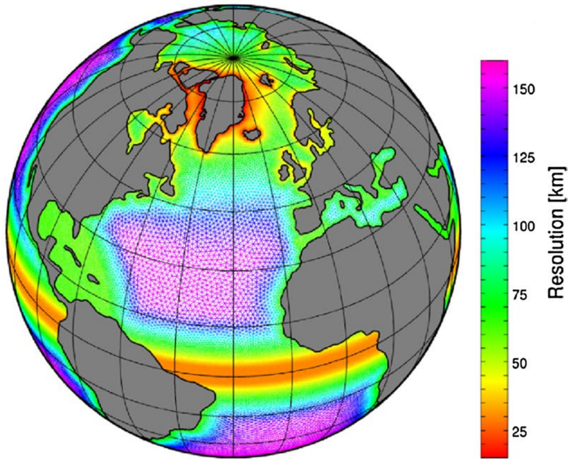
improving model predictions

Assimilation into atmosphere-ocean coupled model: AWI-CM

Atmosphere



Ocean



OASIS3-MCT

fluxes

ocean/ice state

Atmosphere
+ land surface
96 processor cores

Coupler library
OASIS3-MCT

Ocean
+ sea ice
192 processor cores

Two separate programs for atmosphere and ocean

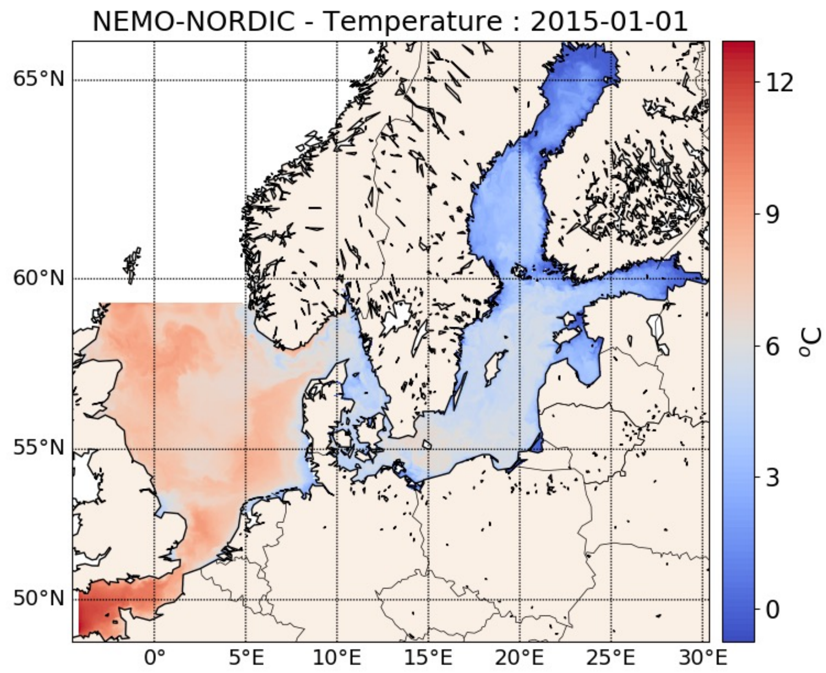
Goal: Develop data assimilation methodology for
cross-component assimilation ("strongly-coupled")
"assimilate ocean observations into the atmosphere"
for improved model simulations

Nerger et al. (2020). Geoscientific Model Development, 13, 4305–4321, doi:10.5194/gmd-13-4305-2020

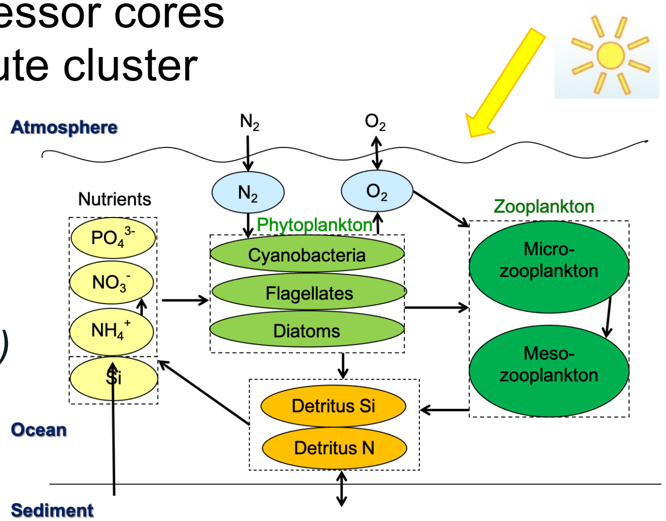
Regional ocean forecasting

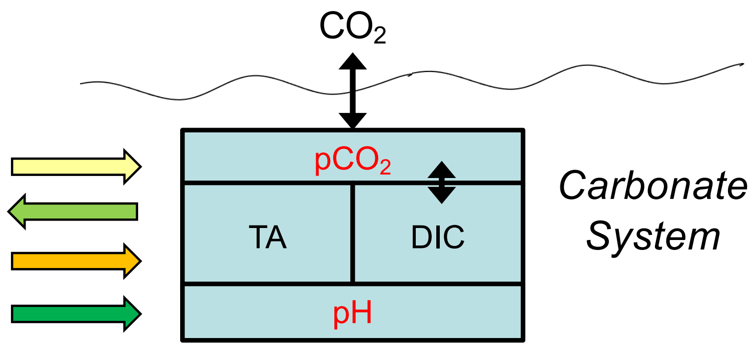
Operational configuration of Copernicus Marine Forecasting Center for Baltic Sea (BAL-MFC)

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



Ecosystem (biogeochemistry)



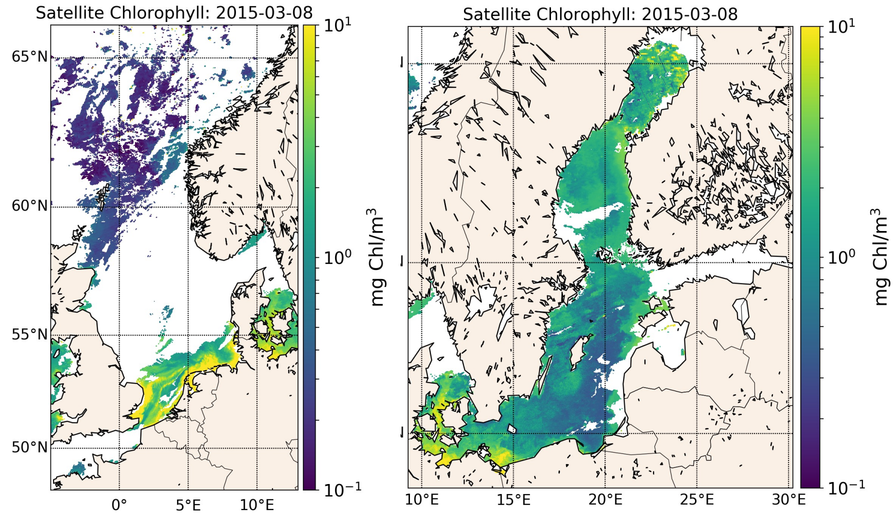


Carbonate System

Observations - Ocean

Remote sensing (satellites, radar, planes)

- Only observe ocean surface
- E.g. temperature, sea surface height, chlorophyll

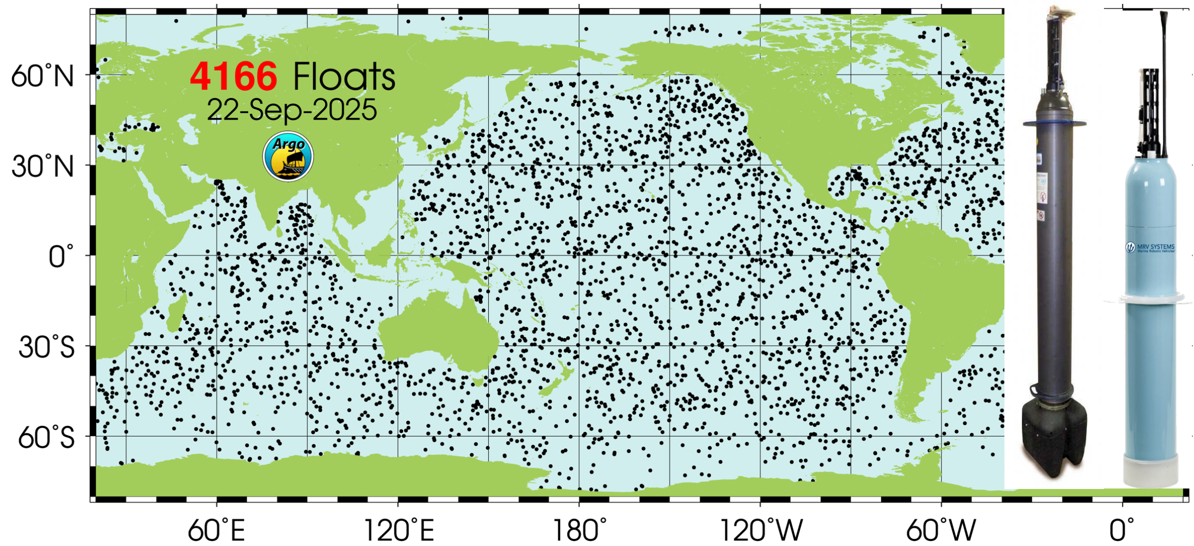


Ships / stations / drifters / floats ('in situ')

- Measurements inside the ocean
- Very sparse data

Example 'ARGO floats'

- Observations of temperature, salinity
- down to 2000m
- Velocities from displacement
- World ocean covered by 4166 devices - very sparse



Applying data assimilation

Integrate observations and models

- Models provide dynamical information
- Observations provide sparse data on real world
- Need uncertainty estimates for model state and observations
  - variances and error-correlations

→ Apply ensemble-based data assimilation
  - Using O(10) – O(100) model states (more not feasible)
    - Costly to compute (O(10^3) – O(10^3) processor cores
    - Large amount of output data (tera-bytes)

  - Small sample of probability distribution of model state
    - Large sampling errors

Data Assimilation - Possibilities

"Observation-constrained (ensemble) modeling"

Aims

1. Optimal estimation of some modelled system:
   - initial conditions (forecasting - weather/ocean/etc)
   - state trajectory (reanalysis - temperature, concentrations, …)
   - process parameters (ice strength, plankton growth, …)
   - fluxes (heat, primary production, …)
   - boundary conditions and 'forcing' (wind stress, …)

2. More advanced: Improvement of model formulation and observations
   - detect systematic errors (bias)
   - revise parameterizations based on parameter estimates
   - detect relevant observations for observation system design

Software

How we realize DA applications

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
  - Assimilation often only 1-5% of total run time

PDAF – Parallel Data Assimilation Framework

PDAF Parallel Data Assimilation Framework

A unified tool for interdisciplinary data assimilation …

- provide support for parallel ensemble forecasts
- provide DA methods (EnKFs, smoothers, PFs, 3D-Var) - fully-implemented & parallelized
- provide tools for observation handling and for diagnostics
- easy implementation with (probably) any numerical model (<1 month)
- a program library (PDAF-core) plus additional functions & templates
- run from notebooks to supercomputers (Fortran, MPI & OpenMP – model compatibility)
- ensure separation of concerns (model – DA method – observations – covariances)
- first release in year 2004; continuous further development

Focus on

- Easy implementation
- Performance for complex models
- Flexibility to extend system

Open source:
Code, documentation, and tutorial available at

https://pdaf.awi.de

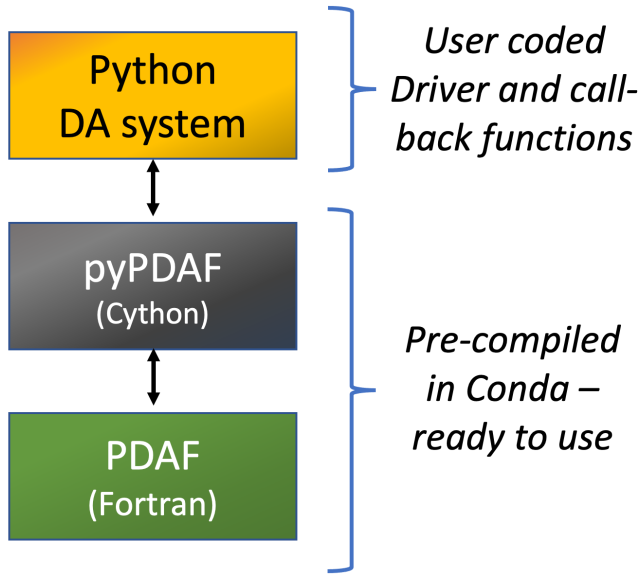
github.com/PDAF/PDAF

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

pyPDAF

Python interface to PDAF

- allows to code all application-specific functionality in Python
  (not touching Fortran!)
- assimilation analysis computed inside PDAF
  (excellent performance due to compiled Fortran code)
- supports all functionality of PDAF including MPI-parallelization
  - online coupling (e.g. for Python-coded models)
  - offline coupling (using files from model runs)
- demonstrated low overhead for localized ensemble filters
- installation using Conda



github.com/yumench/pyPDAF

Y. Chen et al. (2024). Geoscientific Model Development, submitted

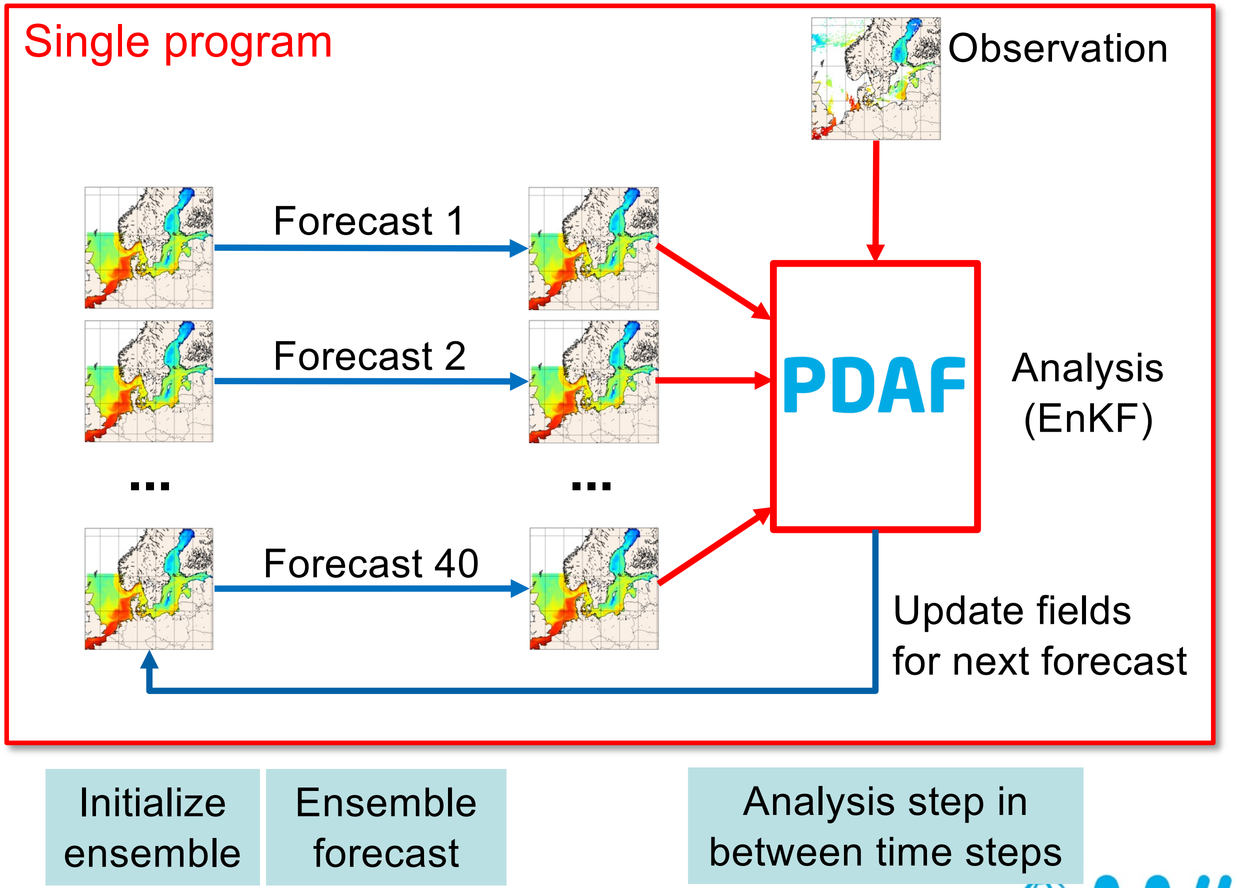
Online-Coupling – Assimilation-enabled Model

PDAF Parallel Data Assimilation Framework

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



Methods

Ensemble-based data assimilation

Estimation by joining model and observational data

Data Assimilation – Model and Observations

Two components:

1. **State**: $\mathbf{x} \in \mathbb{R}^n$ (contains different model variables)

   Dynamical model

   $$\mathbf{x}_i = M_{i-1,i}\left[\mathbf{x}_{i-1}\right]$$

2. **Observations**: $\mathbf{y} \in \mathbb{R}^m$ (contains different observed fields)

   Observation equation (relation of observation to state $\mathbf{x}$):

   $$\mathbf{y} = H\left[\mathbf{x}\right]$$

Dimensions:

state	n: $10^6 - 10^9$
observations	m: $10^4 - 10^6$

Linear and Nonlinear Ensemble Filters

- Represent state and its error by ensemble $\mathbf{X}$ of N_e states
  (use ensemble perturbation matrix $\mathbf{X}' = \mathbf{X} - \bar{\mathbf{X}}$)

- **Forecast**:
  - Integrate ensemble size N_e with numerical model

Dimension of correction (error) space : $N_e - 1$

- **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)

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

ETKF (Bishop et al., 2001) / ESTKF (Nerger et al., 2012)

- Ensemble Transform Kalman filter / Error Subspace Transform Kalman filter
  - Assume Gaussian distributions
  - Transform matrix ($\mathbf{L}_{ETKF} = \mathbf{X}'^f$ or $\mathbf{L}_{ESTKF} = \mathbf{X}^f\mathbf{T}$)

$$\mathbf{A}^{-1} = (N_e - 1)I + (\mathbf{HL})^T\mathbf{R}^{-1}\mathbf{HL}$$

  - Mean update weight vector

$$\tilde{\mathbf{w}} = \mathbf{A}(\mathbf{HL})^T\mathbf{R}^{-1}\left(\mathbf{y} - \mathbf{H}\overline{\mathbf{x}^f}\right)$$

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

  - Transformation of ensemble perturbations

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

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

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

Algorithms designed for maximum computational efficiency

Excellent parallelization possibility when combined with localization

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

Covariance inflation and localization

- Inflation
  - sampling errors in ensemble result in too low variance
  - counter by increasing ensemble variance before analysis
  - Efficient utilizing factor ρ in transform matrix

- Localized Ensemble Transform Kalman filter
  - Loop through model grid and update 'local domains'
  - Utilize only observations within 'influence radius' around updated grid point
  - Local transform matrix with inflation

$$\hat{\mathbf{A}}^{-1} = \rho\,(N_e - 1)I + (\hat{\mathbf{H}}\mathbf{L})^T\hat{\mathbf{R}}^{-1}\hat{\mathbf{H}}\mathbf{L}$$

  - update weight vector and matrix

$$\hat{\bar{\mathbf{w}}} = \hat{\mathbf{A}}(\hat{\mathbf{H}}\mathbf{L})^T\hat{\mathbf{R}}^{-1}\left(\hat{\mathbf{y}} - \hat{\mathbf{H}}\overline{\mathbf{x}^f}\right)$$

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

- Localization is empirical
- Optimal values for ρ and influence radius are unknown
- Some adaptive methods exist (most without theretical basis)

Improving beyond Ensemble Kalman

- Nonlinear filtering
  - Particle filters
    - replace ensemble transformation by weights and resampling
    - Difficult due to degenerate weights
    - Localization can help
  - Iterative filters
    - Iterative KFs (Bocquet et al.)
    - Particle flow filter (Stein variational descent) (Pulido, van Leeuwen, Hu)
  - Hybrid particle-Kalman filters
    - Combine linear (Gaussian) Kalman with particle filters
      - Localized PF (Poterjoy)
      - Local hybrid Kalman-nonlinear transform filter

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

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

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

Similar computational efficiency as ETKF/ESTKF

Localization analogous to ETKF/ESTKF

Excellent parallelization possibility when combined with localization

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

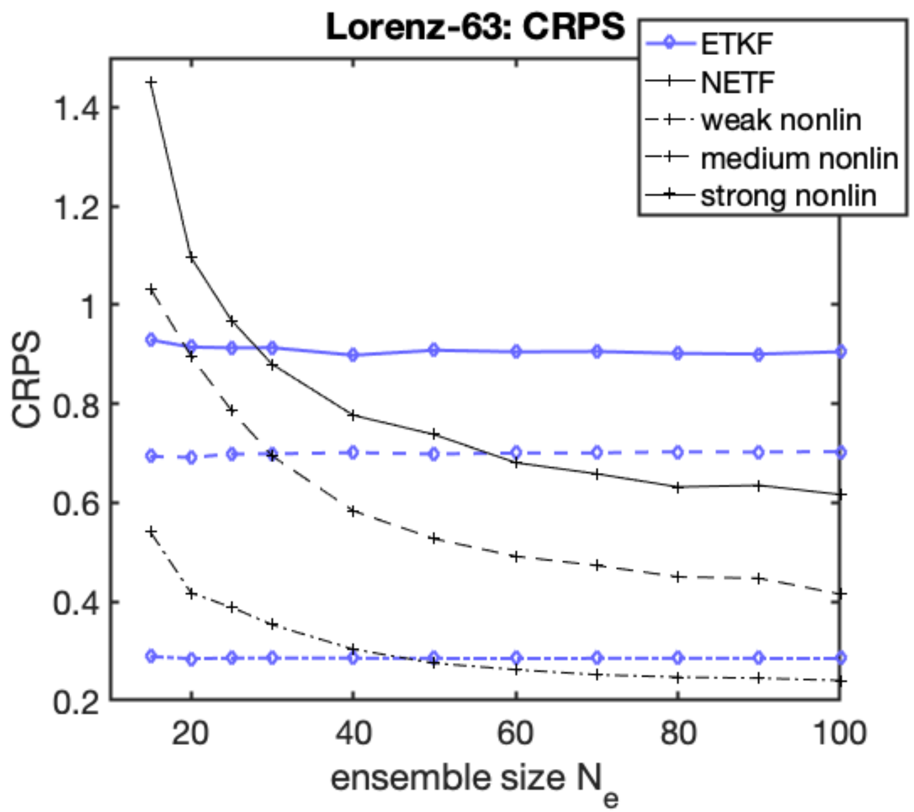
NETF is a second-order exact particle filter

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

EKTF & NETF with Lorenz-63 model

Dependence on ensemble size

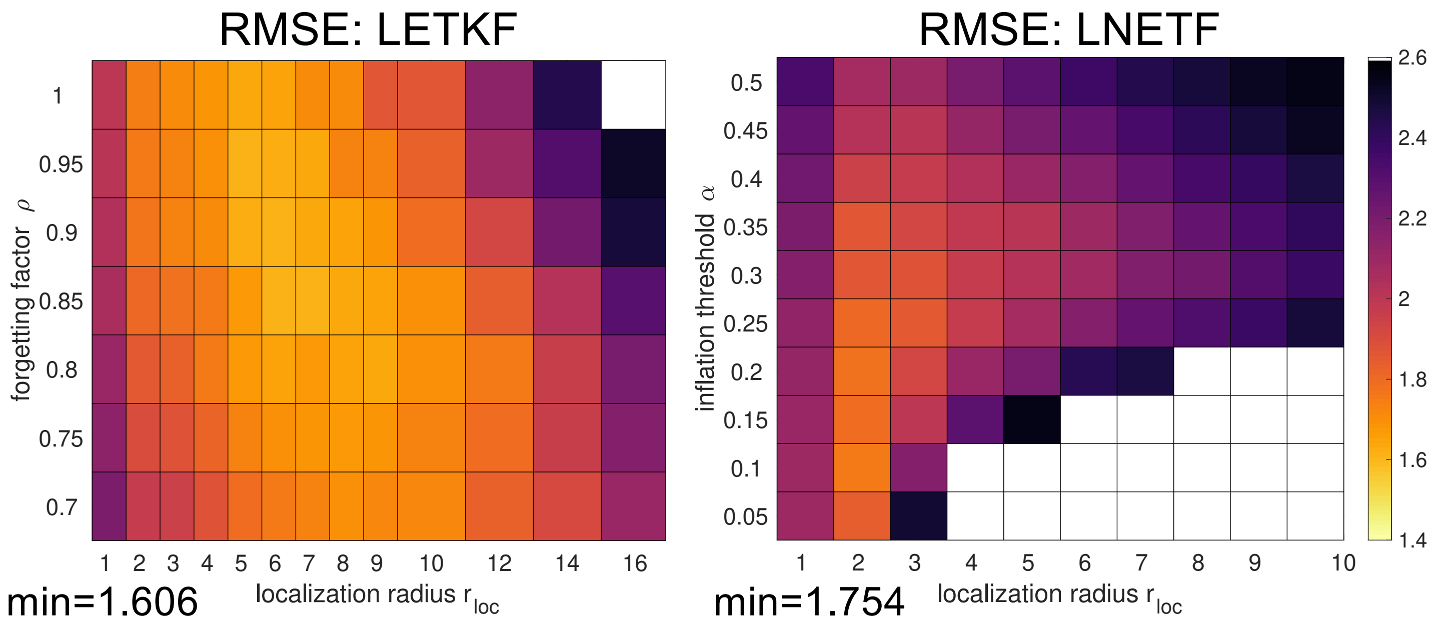
- NETF yields smaller errors than ETKF if ensemble size large enough
  - → Size limit decreases for larger nonlinearity
  - → Improvement by NETF stronger for higher nonlinearity



ETKF and NETF for
3 different nonlinearities

(weak Δt=0.1, medium Δt=0.4, strong Δt=0.7)

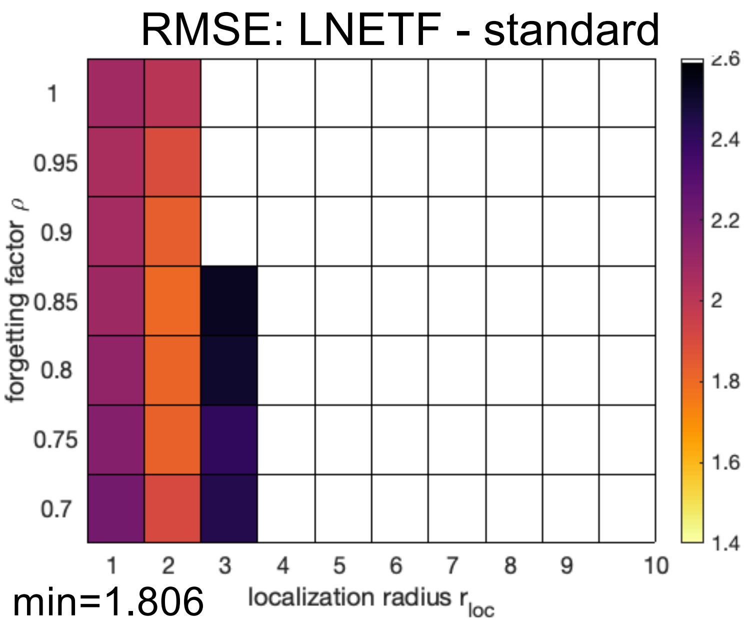
Test with Lorenz-96 model

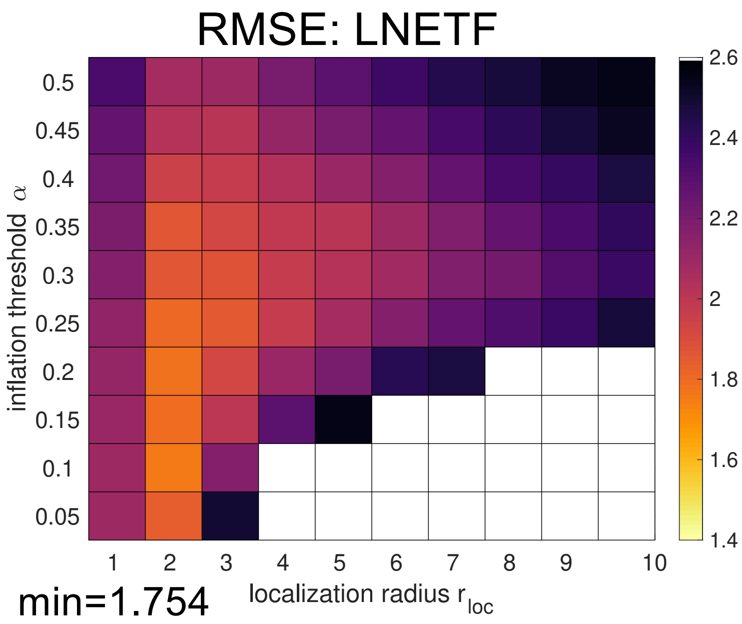


- State dimension 40
- Ensemble size 15
- Forecast: 8 time steps
- 20 observations
- Show RMS errors as function of inflation (forgetting factor or inflation theshold α) and localization radius

- LNETF worse than LETKF

Stabilizing LNETF – Lorenz-96 model





Inflation:
- forgetting factor

Inflation:
- forgetting factor (ρ=0.85)
- Minimum effective sample size

$$N_{eff} = \sum \frac{1}{(w^i)^2} > \alpha$$

- State dimension 40
- Ensemble size 15
- Forecast: 8 time steps
- 20 observations
- Show RMS errors as function of inflation (forgetting factor or inflation theshold α) and localization radius

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)

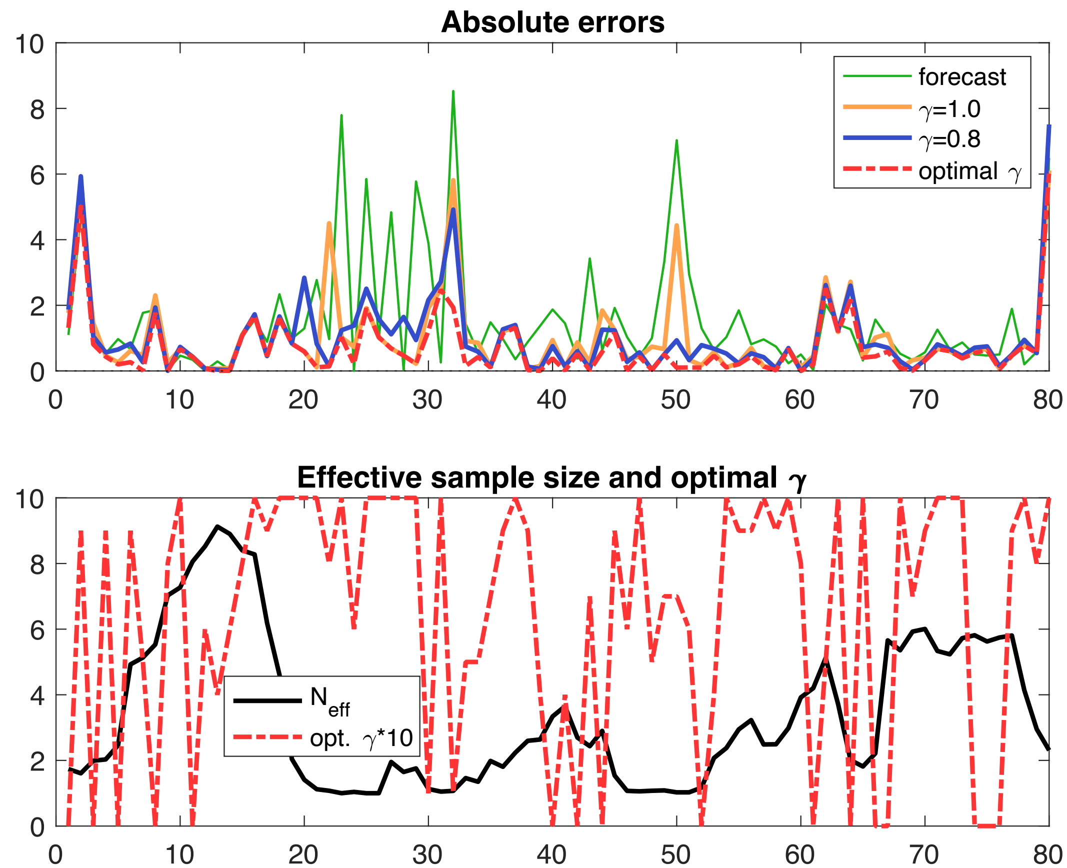
Effect of hybrid weight γ

- 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

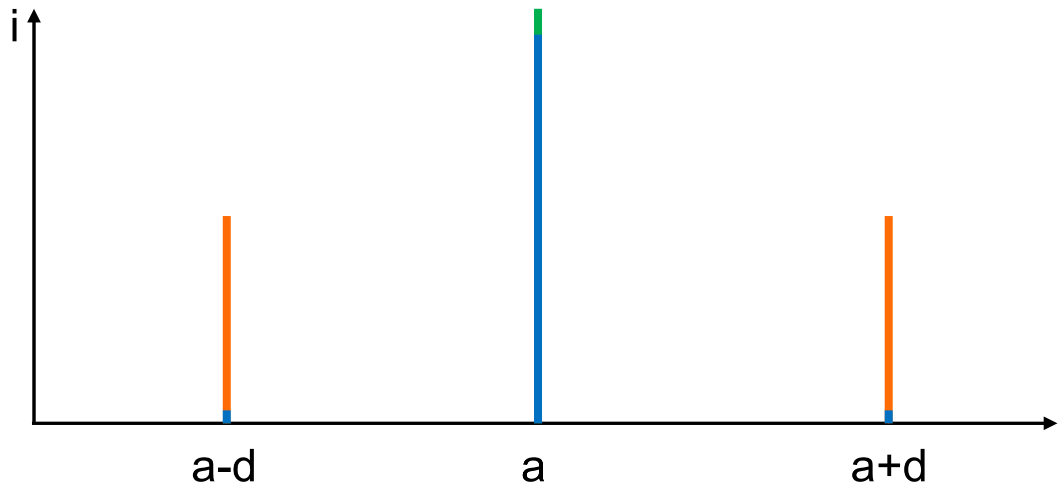
$$kurt = \frac{\frac{1}{N_e}\sum_{i=1}^{N_e}\left(\mathbf{x}^i - \overline{\mathbf{x}}\right)^4}{\left[\frac{1}{(N_e)}\sum_{i=1}^{N_e}\left(\mathbf{x}^i - \overline{\mathbf{x}}\right)^2\right]^{2}} - 3$$

- 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	$N_e/2$



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

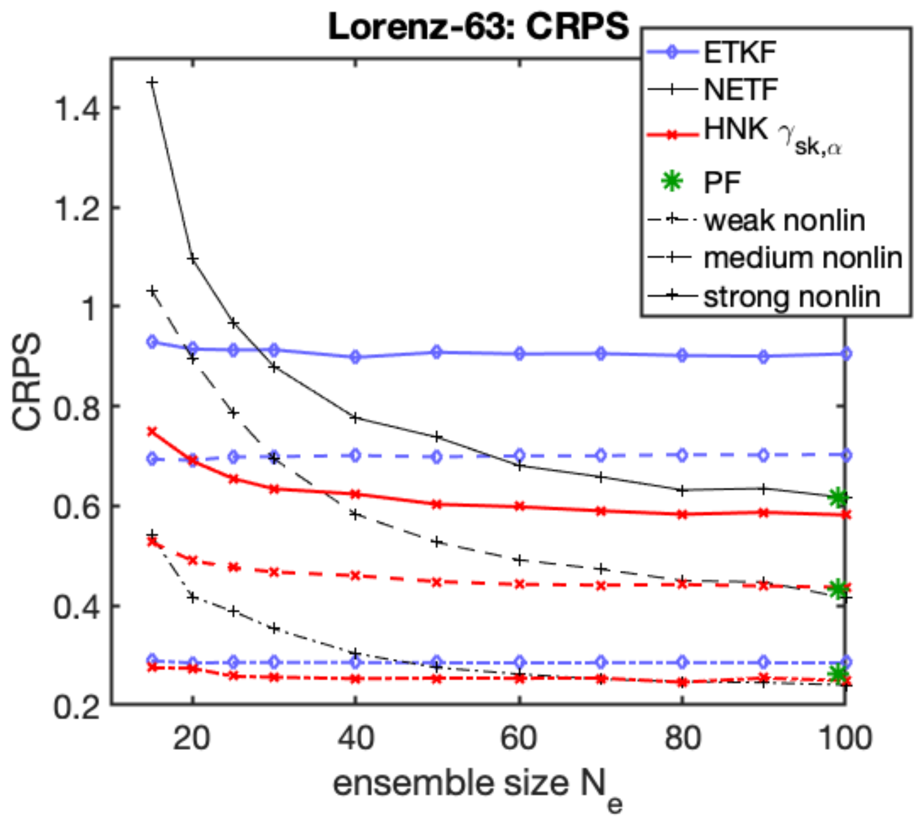
$$\gamma_{sk,\alpha} = \max\left[\min(1 - nmak,\ 1 - nmas),\ \gamma_\alpha\right]$$
$$\gamma_{sk,lin} = \max\left[\min(1 - nmak,\ 1 - nmas),\ \gamma_{lin}\right]$$

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

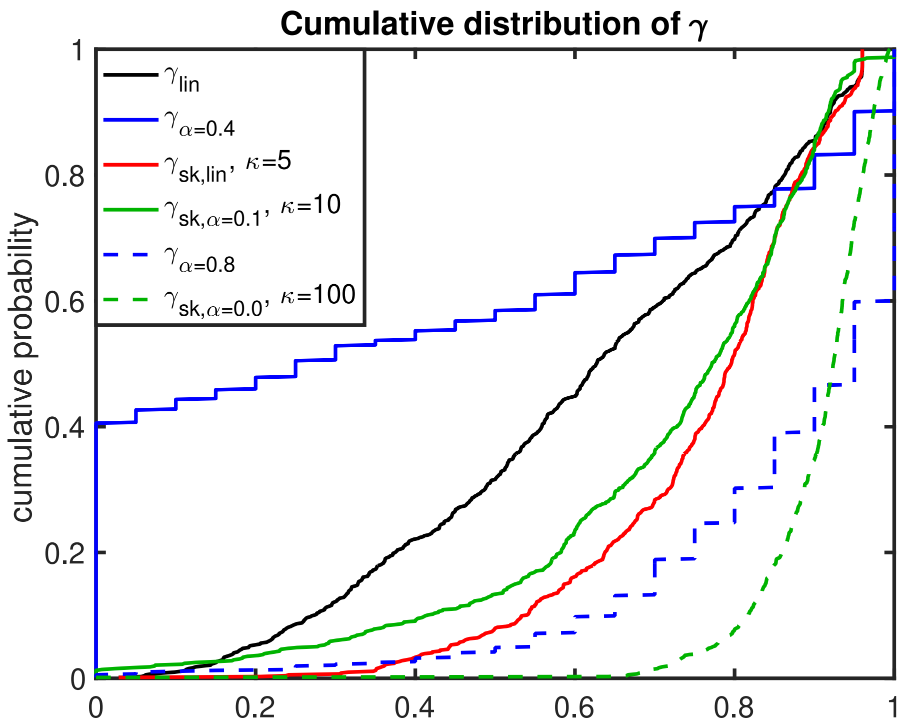
Assimilation with Lorenz-63 model

- Lorenz-63 3-variable model ('Butterfly')
- Hybrid filter HNK
  - particular strong effect for small N_e
  - CRPS from NETF and HNK converge for large N_e
  - errors reduced up to 28%
- Particle Filter
  - comparable CRPS for large N_e
    - PF expected to be superior if N_e sufficiently large (the full nonlinear filter)



- Note: Easy to use large ensemble for Lorenz-63, difficult for higher dimensional models

Lorenz-63, distribution of γ for different cases



Filter:	γ_{lin}	$\gamma_{\alpha=0.4}$	$\gamma_{sk,lin}$	$\gamma_{sk,\alpha=0.1}$	$\gamma_{\alpha=0.8}$	$\gamma_{sk,\alpha=0.0}$
κ	-	-	5	10	-	100
CRPS	0.673	0.707	0.671	0.639	0.826	0.873
RMSE	1.125	1.178	1.113	1.105	1.372	1.575

Results for N_e=25, Δt=0.7

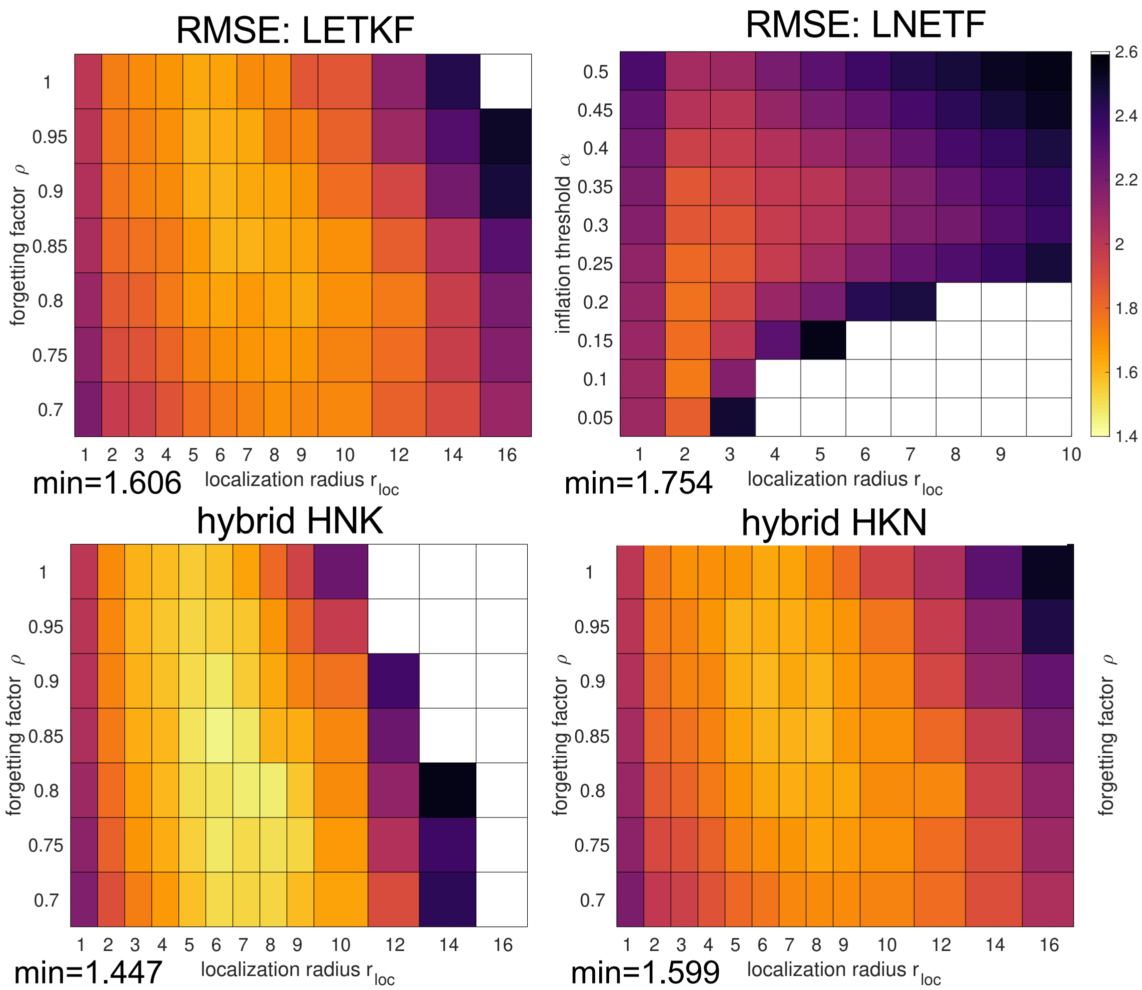
Low-CRPS cases obtained for different distributions of $\boldsymbol{\gamma}$

→ non-unique solution

→ sometimes lowering $\boldsymbol{\gamma}$ does not change result at an analysis time

Test with Lorenz-96 model

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

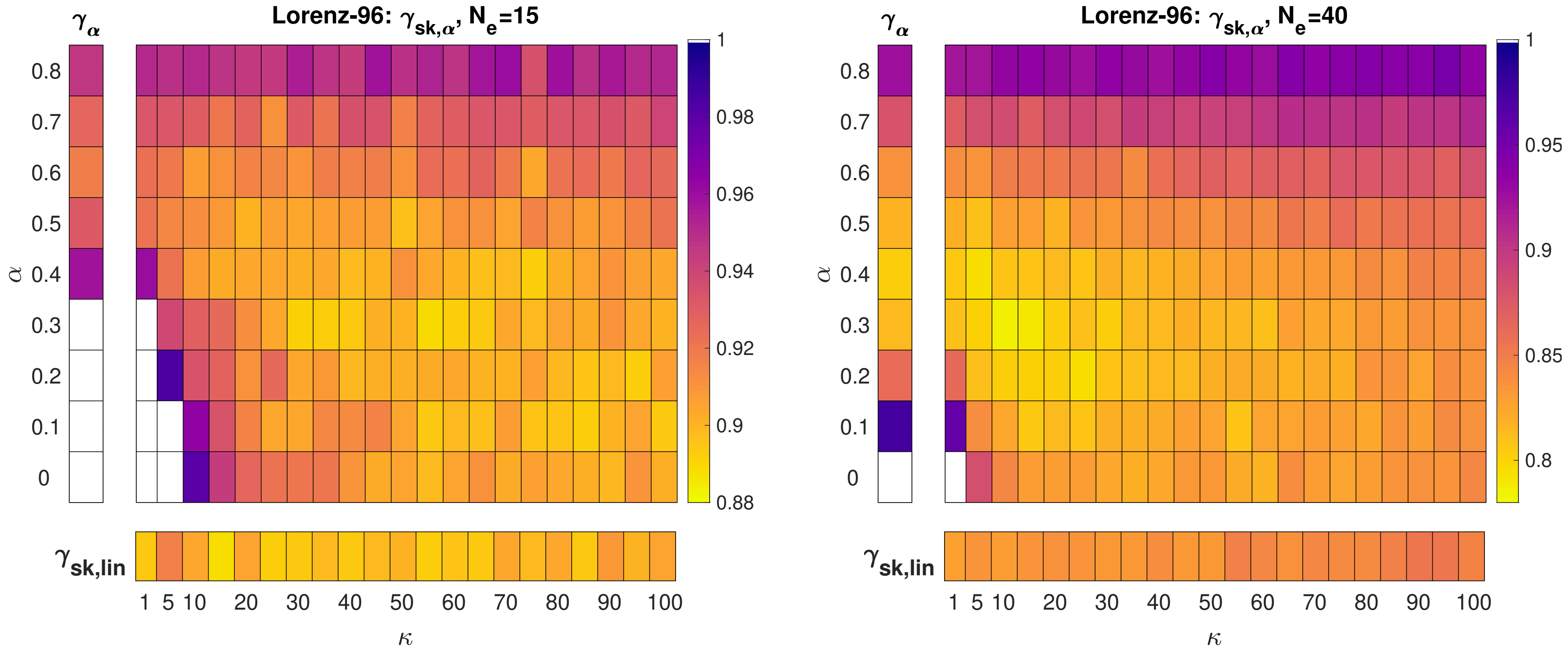


Strongly nonlinear DA setting

- 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

Lorenz-96, Hybrid HNK, dependence on κ



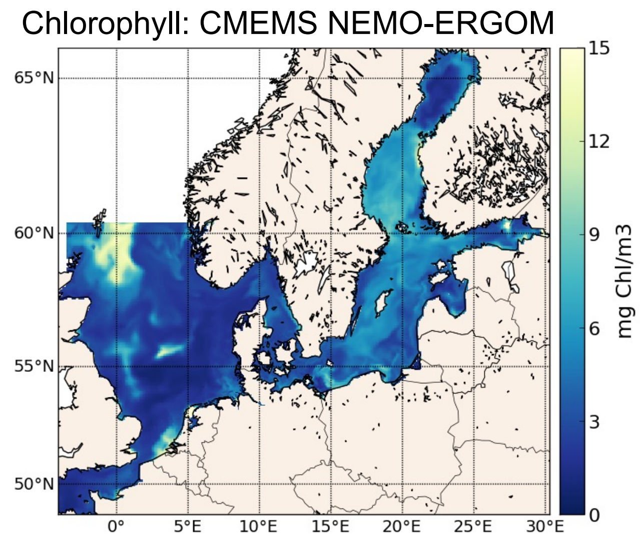
CRPS relative to LETKF

κ can be chosen dependent on ensemble size

- Limits of skewness and kurtosis depend on N_e
  - but actual skewness and kurtosis do not depend on system, not on N_e
- Standard value $=N_e$, but smaller large large N_e

Application example

- Ocean-biogeochemical model:
  - NEMO + ERGOM
- Configuration: NORDIC 2.0
  - 1.8km resolution, 56 layers, 90s time step
  - North Sea & Baltic Sea
  - Operational use in CMEMS for the Baltic Sea
- DA implementation
  - augment NEMO-ERGOM with DA functionality by PDAF (online-coupling in memory)
  - State vector:
    - physics + biogeochemistry
      State vector size ~153 million
  - Assimilate satellite chlorophyll data

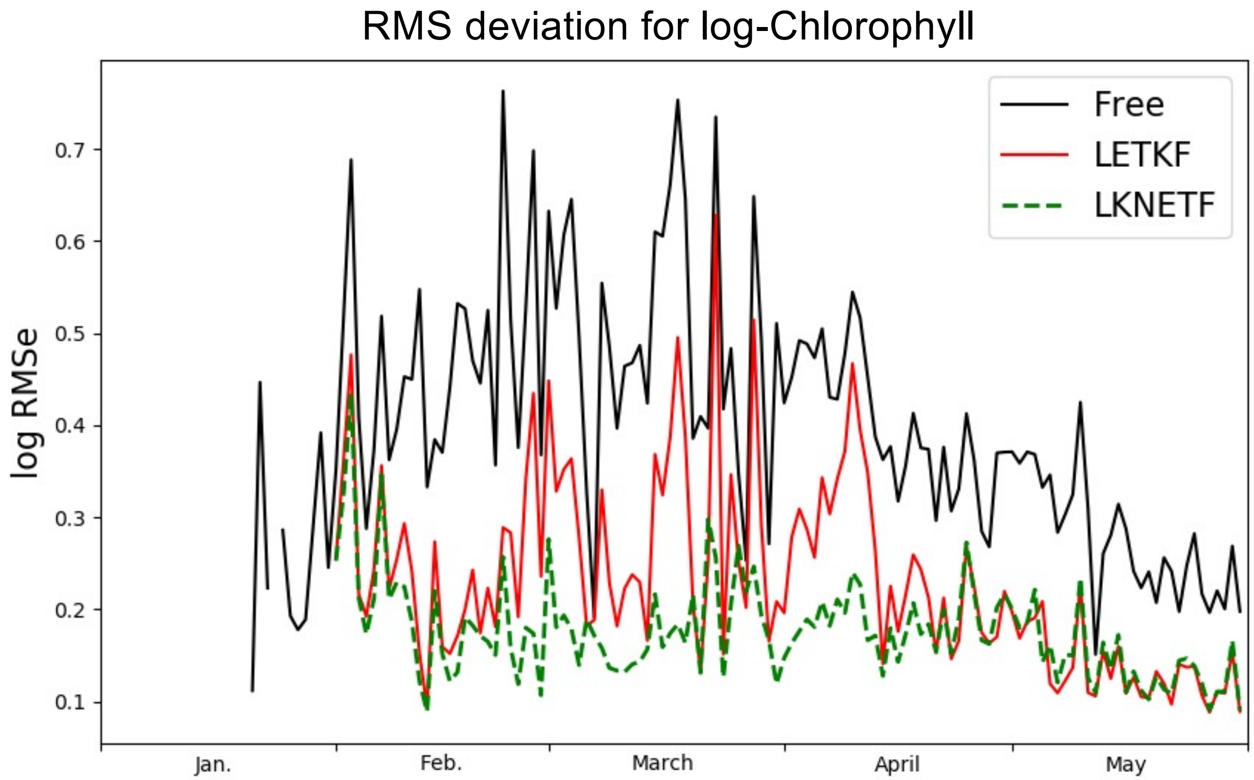


ocean and biogeochemical dynamics are nonlinear and distributions non-Gaussian

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 776480

Effect of hybrid filter in high-dimensional application

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



Regional model setup

Only assimilate chlorophyll observations

Stronger assimilation effect of LKNETF

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

Potential further steps

Particularities

- High-dimensional systems with relations governed by physics
- Very sparsely observed

Potential for improvements

Reduce execution time

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

Reduce time to tune method

- Tuning required and costly

Improve estimates

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

Surrogates might help, but

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

Do pre-trained neural networks help?

Summary

- 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

- hybrid nonlinear-Kalman ensemble transform filter
  - Combine LETKF and LNETF methods
  - hybrid weight γ shifts filter behavior using skewness & kurtosis (but no theory)
  - Cost of analysis step ~2x LETKF

Summary

PDAF Parallel Data Assimilation Framework

Introduced hybrid nonlinear-Kalman ensemble transform filter

- Combine LETKF and LNETF methods
- hybrid weight γ shifts filter behavior
- Cost of analysis step ~2x LETKF

Experiments with Lorenz models

- Hybrid filter successfully reduces errors compared to LETKF and LNETF
- Best results for variant HNK: LNETF applied before LETKF
- Can compute γ from skewness and kurtosis
  - → allows to control nonlinearity of filter based on non-Gaussianity
  - → Improved stability & reduced errors compared to tempering rule on N_{eff}

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