PDAF Parallel Data Assimilation Framework

ALFRED-WEGENER-INSTITUT HELMHOLTZ-ZENTRUM FÜR POLAR- UND MEERESFORSCHUNG

A hybrid nonlinear-Kalman ensemble transform filter with regulation following the system nonlinearity

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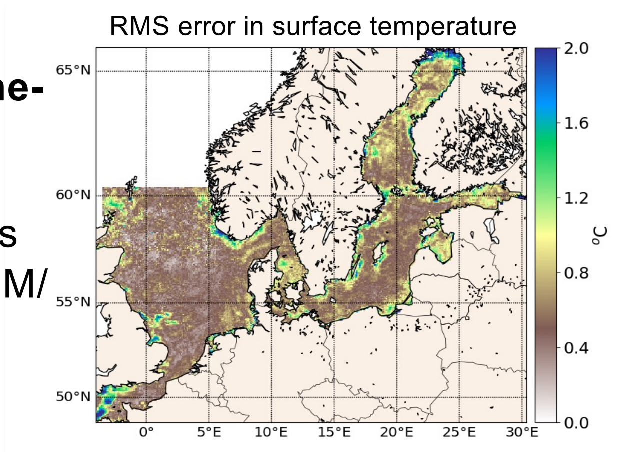
Overview

- Linear and nonlinear ensemble filters
- Hybrid nonlinear-Kalman filter
- Application tests

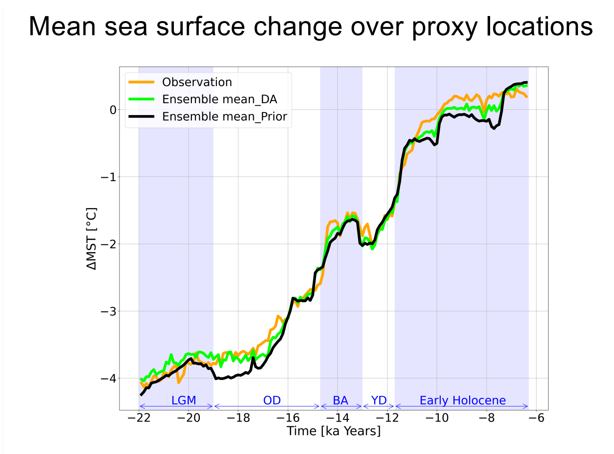
Application Examples (different models utilizing PDAF)

PDAF Parallel Data Assimilation Framework

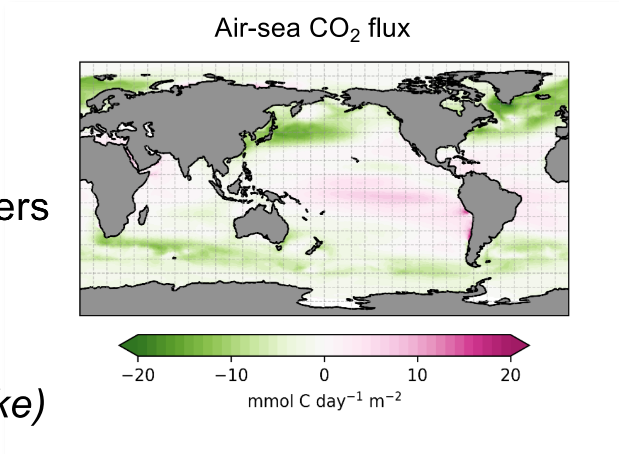
Coastal coupled physics/biogeochemistry DA: CMEMS/BSH - Improving forecasts with NEMO-ERGOM/ HBM-ERGOM: *(S. Vliegen, A. Sathanarayanan)*



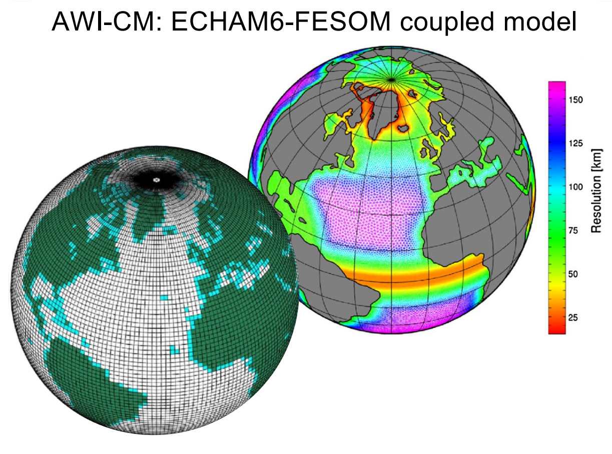
Paleo-climate DA: improve simulation of last deglaciation with CLIMBER-X *(A. Masoum)*



Coupled physics/biogeochemistry DA: Improving parameters & carbon flux in REcoM *(N. Mamnun, F. Bunsen, A. Broschke)*



Coupled ocean-atmosphere DA: Assimilate ocean observations into atmosphere with AWI-CM *(Q. Tang)*



Motivation

Data Assimilation (DA) into non-linear models (e.g. nonhydrostatic dynamics)

- Nonlinearity in DA → non-Gaussianity of error distributions
- For Gaussian distributions: (Ensemble) Kalman filter is optimal
- For non-Gaussian distributions:
  - → Kalman filter suboptimal or failing
  - → Non-linear DA methods (e.g. particle filters): possibly better estimates, but higher sampling errors than KFs

Non-linear model dynamics lead to different degree of non-Gaussianity

→ Aim for DA method that

- adapts to non-Gaussianity
- Allows to utilize optimality of KF for Gaussian distributions

→ **Utilize hybrid combination of KF and nonlinear filter**

Linear and Nonlinear Ensemble Filters

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 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)

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

The Kalman Filter

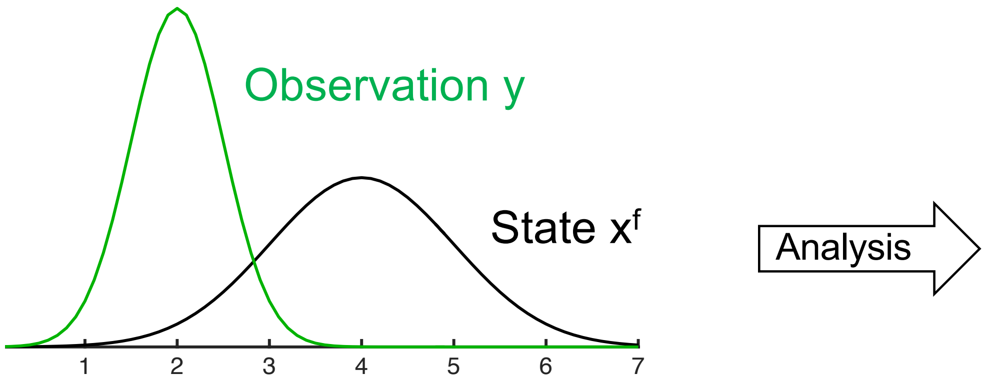
Assume Gaussian distributions
fully described by

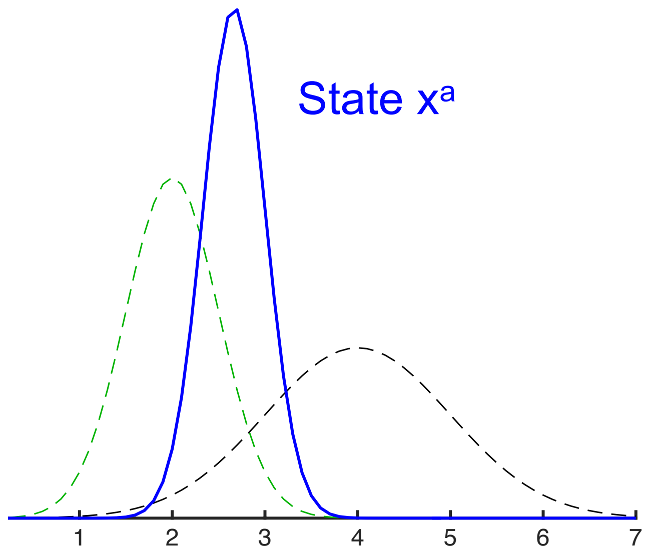
- mean state estimate
- covariance matrix

→ Strong simplification of estimation problem

Analysis is combination auf two Gaussian distributions computed as

- Correction of state estimate
- Update of covariance matrix





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 $\mathbf{y}$

Optimality of the Kalman Filter

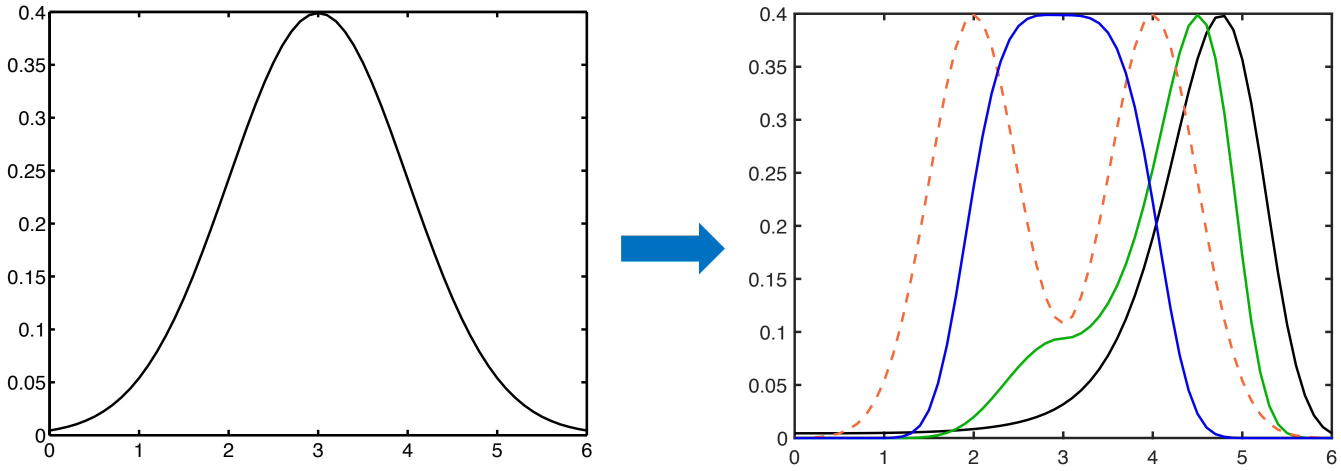
Kalman filter was derived to minimize variance

Kalman filter is optimal only if

- Covariance matrices are known
  (they are not in high-dimensional systems)
- Errors have normal distribution

With a nonlinear model

- Initial Gaussianity not preserved by nonlinear transformation



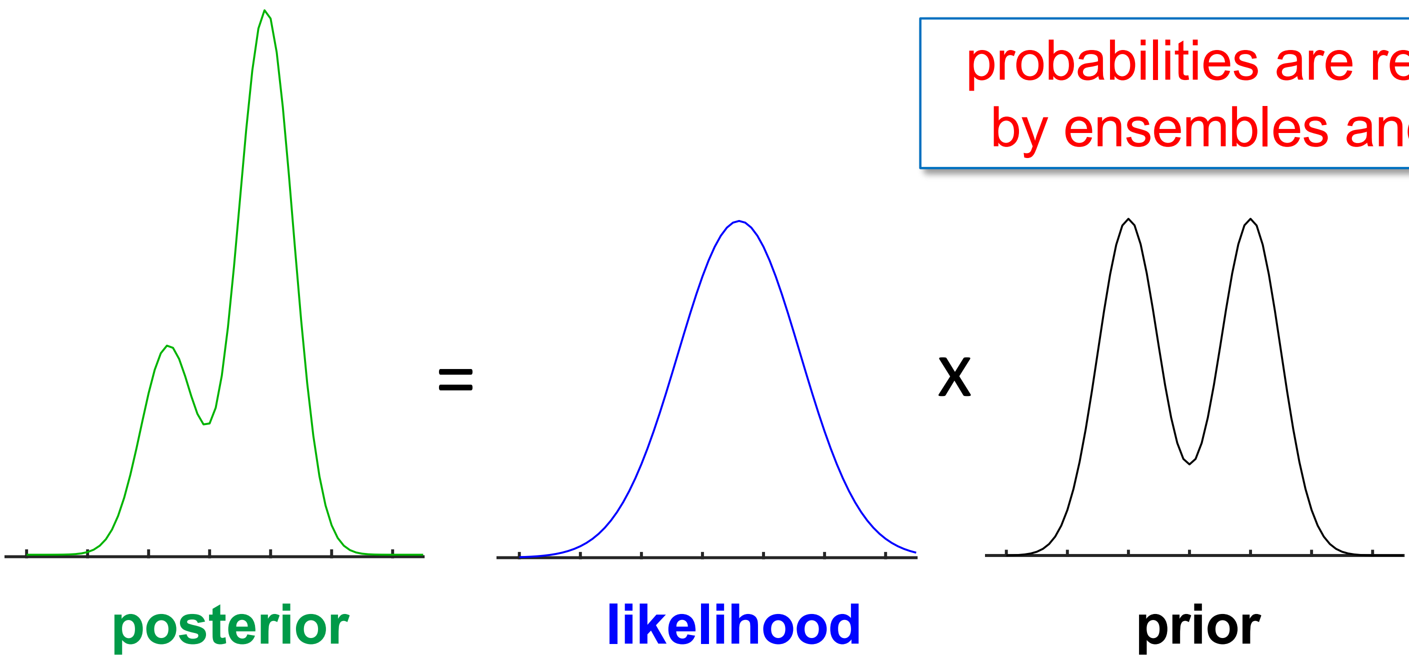
Particle filters: fully nonlinear

Just multiply probabilities:

$$p(x|y) \propto p(y|x)p(x)$$

… and normalize

probabilities are represented by ensembles and weights



Alternative uses of Bayes law

Bayes law: Probability density of $\mathbf{x}$ given $\mathbf{y}$

$$p\left(\mathbf{x}_i|\mathbf{y}_i\right) = \frac{p\left(\mathbf{y}_i|\mathbf{x}_i\right) p\left(\mathbf{x}_i\right)}{p\left(\mathbf{y}_i\right)}$$

Represent $p(\mathbf{x}_i)$ by ensemble: $p(\mathbf{x}_i) = \frac{1}{N}\sum_{j=1}^{N}\delta(\mathbf{x}_i - \mathbf{x}_i^{(j)})$

$$p(\mathbf{x}_i|\mathbf{y}_i) = \sum_{j=1}^{N}\delta(\mathbf{x}_i - \mathbf{x}_i^{(j)})\,\frac{p(\mathbf{y}_i|\mathbf{x}_i^{(j)})}{p(\mathbf{y}_i)}$$

Kalman filter:
assume normal distributions
compute new ensemble states

$$\mathbf{x}_i^{a(j)}; j = 1, \ldots, N$$

Particle Filter:
keep ensemble states
but assign weights

$$w^{(j)} = \frac{p(\mathbf{y}_i|\mathbf{x}_i^{(j)})}{p(\mathbf{y}_i)}$$

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)

NETF is a second-order exact particle filter

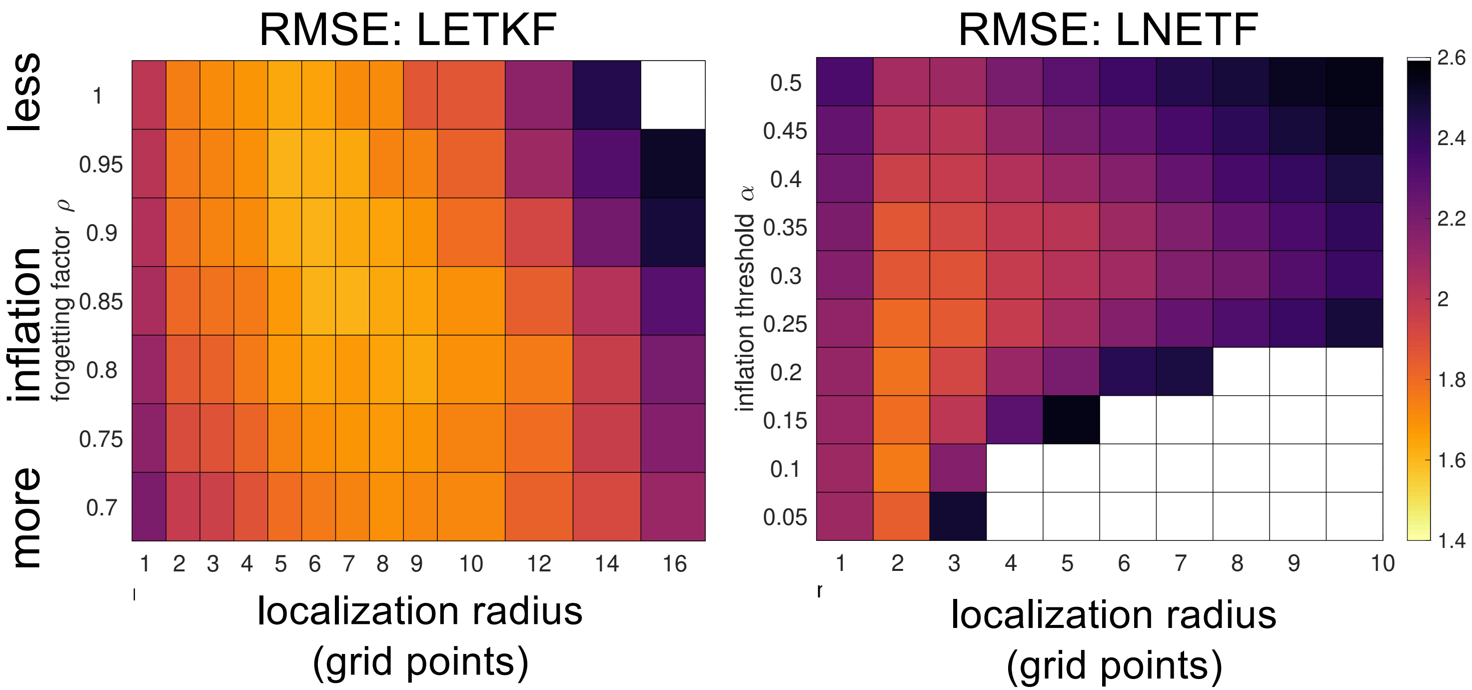
Tödter, J. and Ahrens, B. (2015) *Mon. Wea. Rev.* **143**,1347–1367

ETKF & NETF

- Analogous update schemes
- Both filters can be localized (LETKF and LNETF)

- But
  - ETKF
    - very stable, even in nonlinear cases
    - Optimal for Gaussian / sub-optimal for nonlinear cases
  - NETF
    - accounts for nonlinearity (non-Gaussianity)
    - higher sampling errors than LETKF
    - needs very small localization radii

Test with Lorenz-96 model

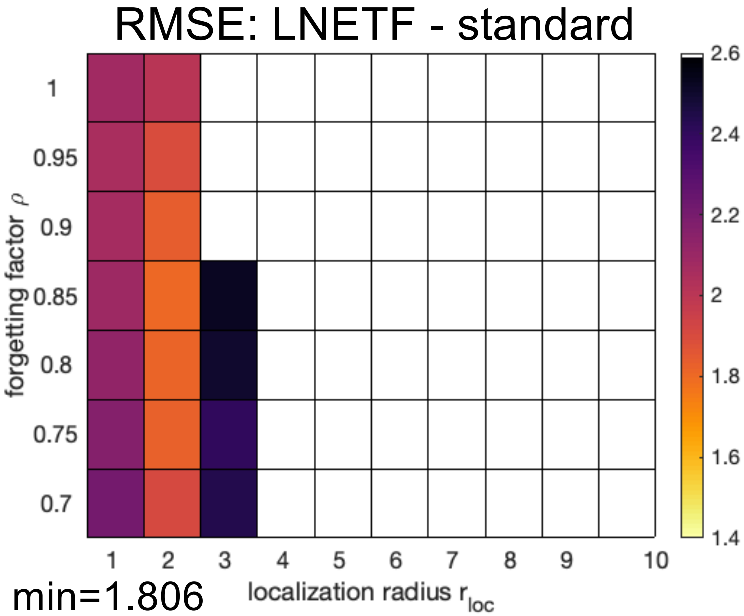


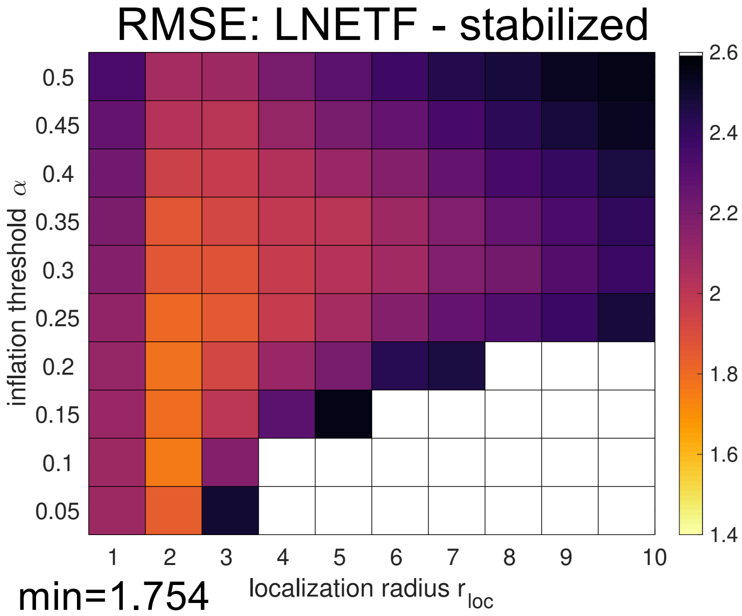
RMSE min=1.606

RMSE min=1.754

- State dimension 40
- Ensemble size N_{ens}=15
- Forecast: 8 time steps (strongly nonlinear DA case)
- 20 observations, obs. error 1.0
- LETKF better than LNETF at this N_{ens}

Stabilizing LNETF – Lorenz-96 model





- State dimension 40
- Ensemble size 15
- Forecast: 8 time steps
- 20 observations

- Standard LNETF needs very small localization radius ('curse of dimensionality' also holds with localization)

Inflation:
- forgetting factor

Inflation:
- fixed inflation (ρ=0.85)
- Minimum effective sample size

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

Hybrid – LETKF-LNETF

Combine the stability of LETKF with nonlinear features of LNETF

ETKF-NETF – Hybrid Filter Variants

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

1-step update (*HSync*)

$$\mathbf{X}^a_{HSync} = \overline{\mathbf{X}}^f + (1-\gamma)\Delta\mathbf{X}_{NETF} + \gamma\Delta\mathbf{X}_{ETKF}$$

- $\Delta\mathbf{X}$: assimilation increment of a filter
- 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

Choosing hybrid weight γ

- Hybrid weight shifts filter behavior

Some possibilities:

- Fixed value
- Adaptive - According to which condition?

  - Frei & Künsch (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)

Issue: Using N_{eff}
- only ensures non-collapsing ensemble
- does not ensure good analysis result

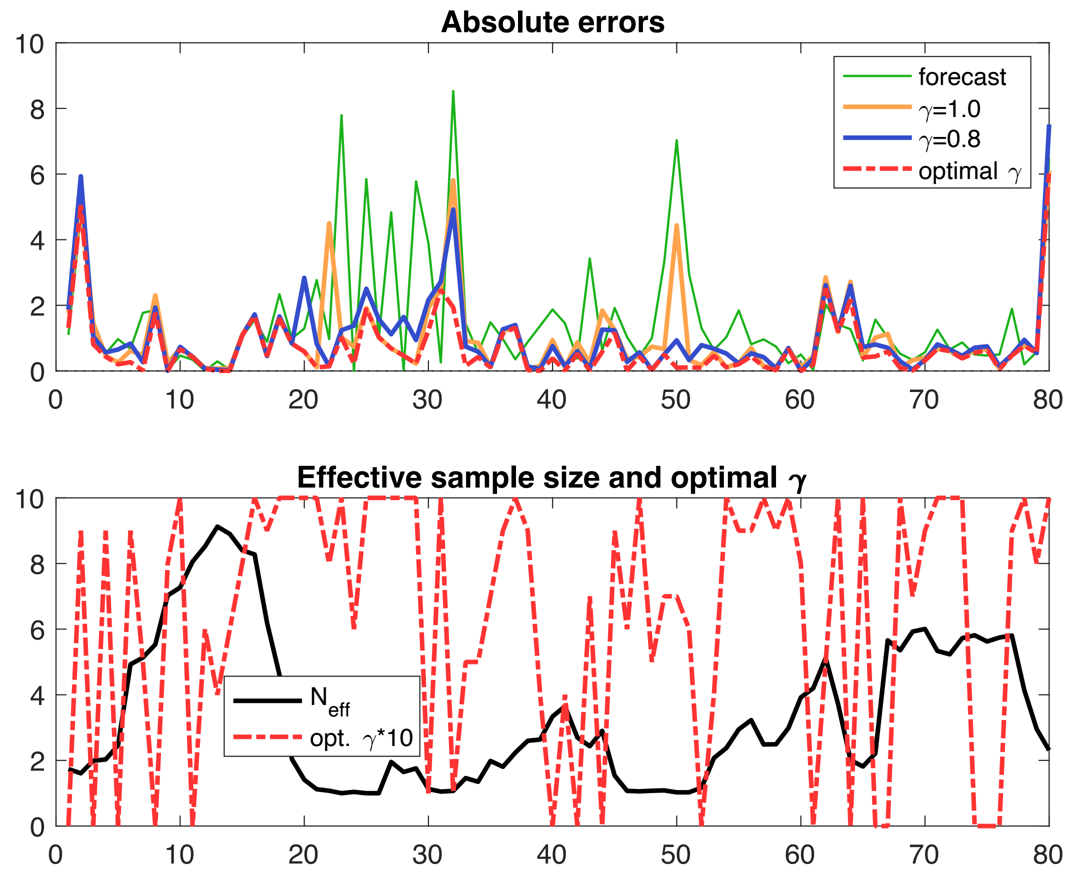
Effect of hybrid weight γ

- 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!

Other works using hybrid filters

Frei & Künsch, 2013 (*FK13*)

- Derived combined KF with resampling PF; KF before PF (with covariance localization)
- Hybrid weight from $N_{eff}/N_e \geq a$

Chustagulprom/Reich/Reinhardt, 2016

- Ensemble square-root filter (ESRF) + ensemble transform PF solving linear transport problem
- KF before PF, PF before KF (better results if PF before KF); hybrid weight from *FK13*

Robert/Leuenberger/Künsch, 2018

- Update of FK13 using ETKF; application to convective-scale setup of COSMO
- KF before PF; hybrid weight from *FK13*

Grooms & Robinson, 2021

- EnSRF + SIR-PF without localization; PF before KF; hybrid weight from *FK13*

Poterjoy, 2022; Kurosawa & Poterjoy, 2023

- Multi-step (tempered) Local PF + final EnKF step
- Poterjoy(2022): Hybrid weight using *FK13*; Kurosawa/Poterjoy(2023): Shapiro-Wilk test

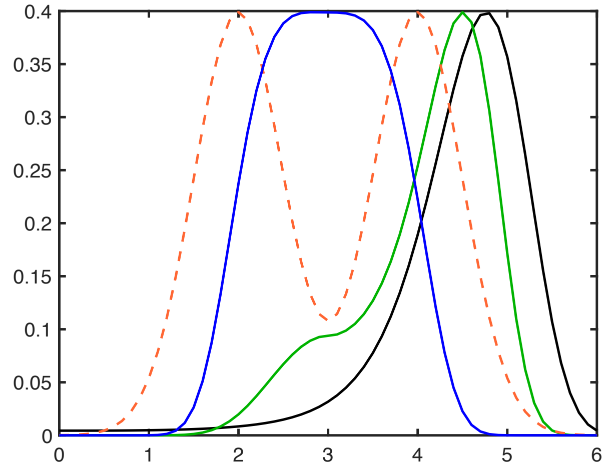
Account for non-Gaussianity: Skewness and Kurtosis

- **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

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

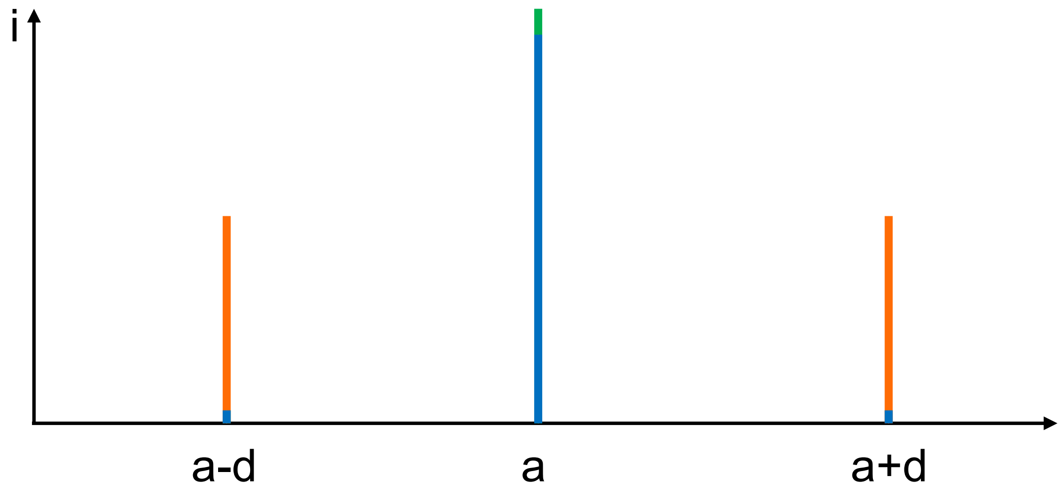


- Skewness and kurtosis
  - generally not bounded
    → but limits depend on ensemble size

Finding bounds: 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

Numerical Experiments

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

Open source:
Code, documentation, and tutorial available at

https://pdaf.awi.de

https://github.com/PDAF/PDAF

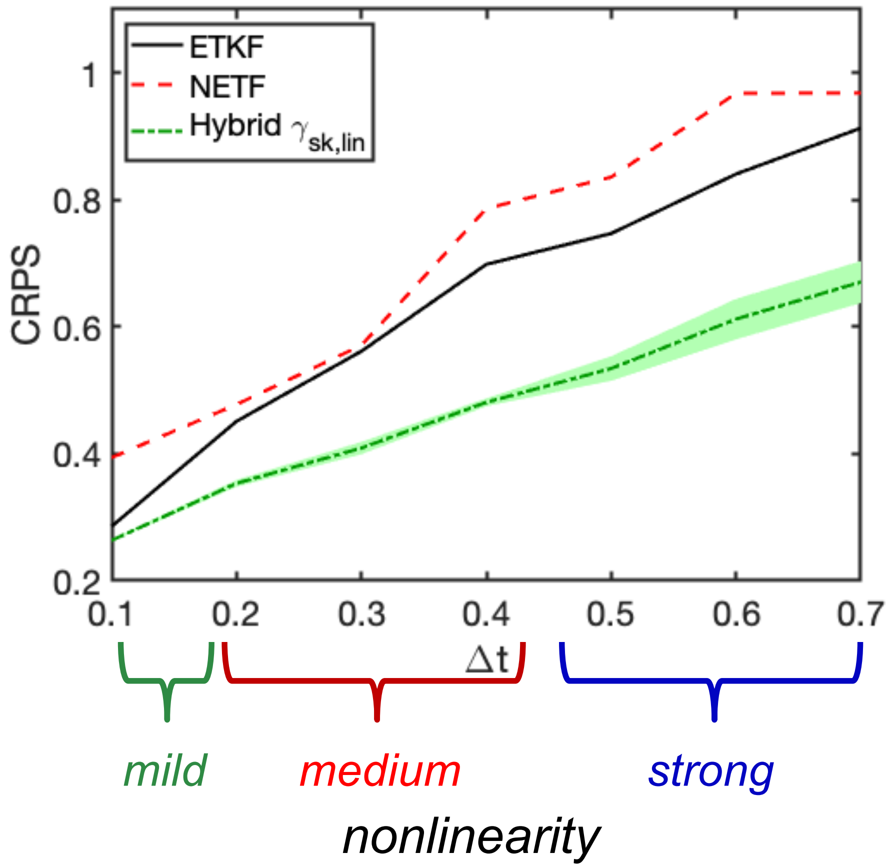
L. Nerger, W. Hiller, Computers & Geosciences 55 (2013) 110-118

AWI

Assimilation with Lorenz-63 model

- Observe full state
- Time step size 0.05
- Vary forecast duration *Δt* to vary nonlinearity
- Ensemble size N_e =25
- HNK filter variant (nonlinear before Kalman)
- Implemented with PDAF

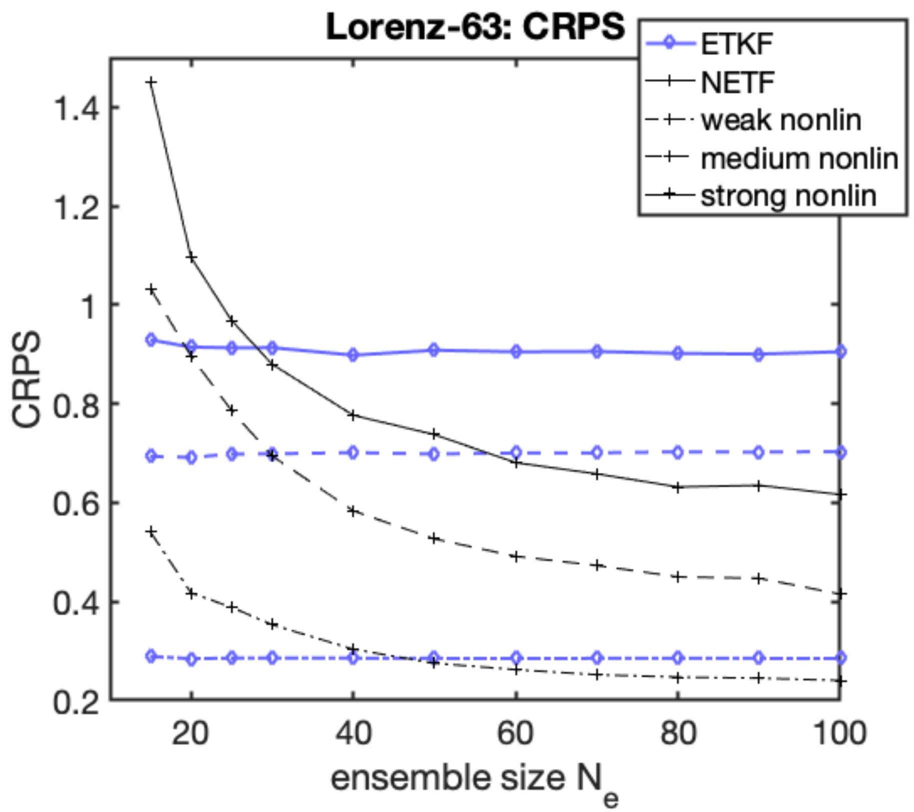
- Error of NETF > ETKF due to sampling errors
- Effect of hybrid filter grows with nonlinearity of assimilation problem (forecast length)
- Hybrid weight $\gamma_{sk,lin}$ yield smallest errors without any tuning
  → Errors are reduced up to 28%
- Note: Hybrid weight $\gamma_{sk,\alpha}$ is suboptimal unless optimally tuned



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

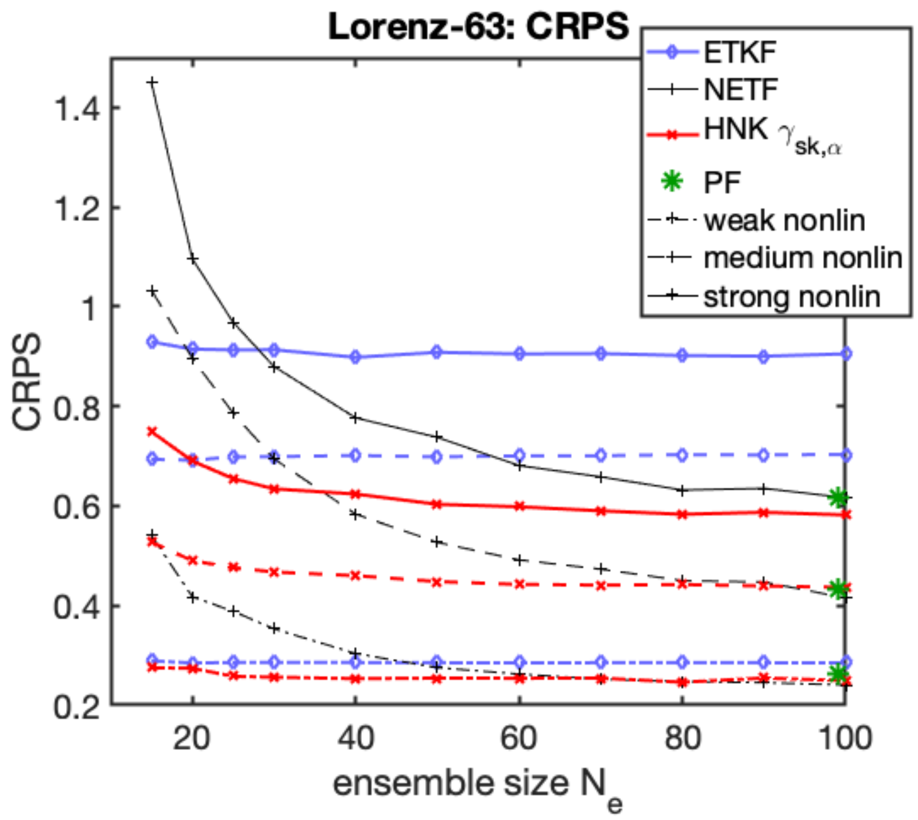


ETKF and NETF for
3 different nonlinearities

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

Assimilation with Lorenz-63 model

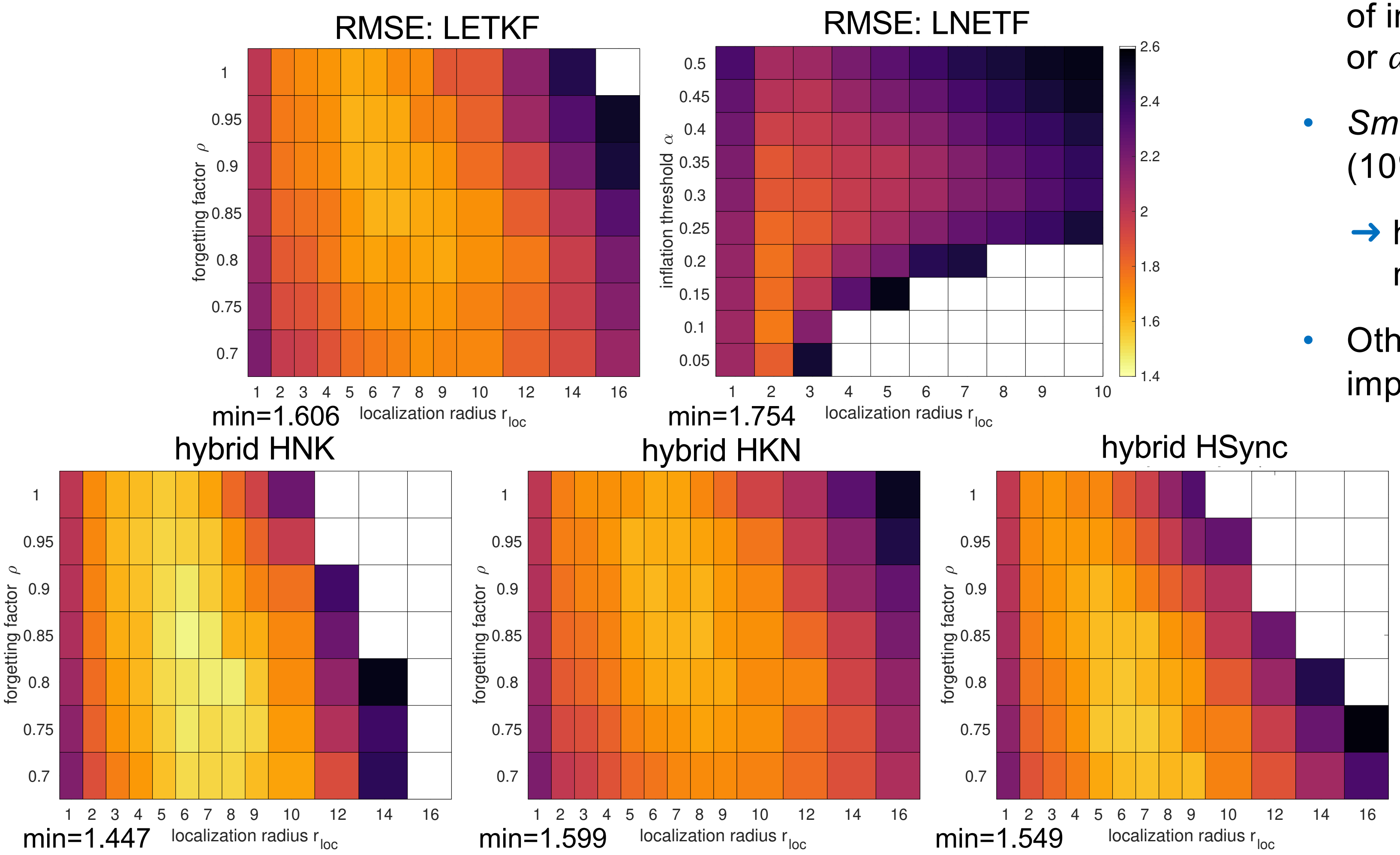
- Hybrid filter HNK
  - particular strong effect for small N_e
  - CRPS from NETF and HNK converge for large N_e
  - errors reduced up to 28%
- Particle Filter
  - comparable CRPS for large N_e
    - PF expected to be superior if N_e sufficiently large (the full nonlinear filter)



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

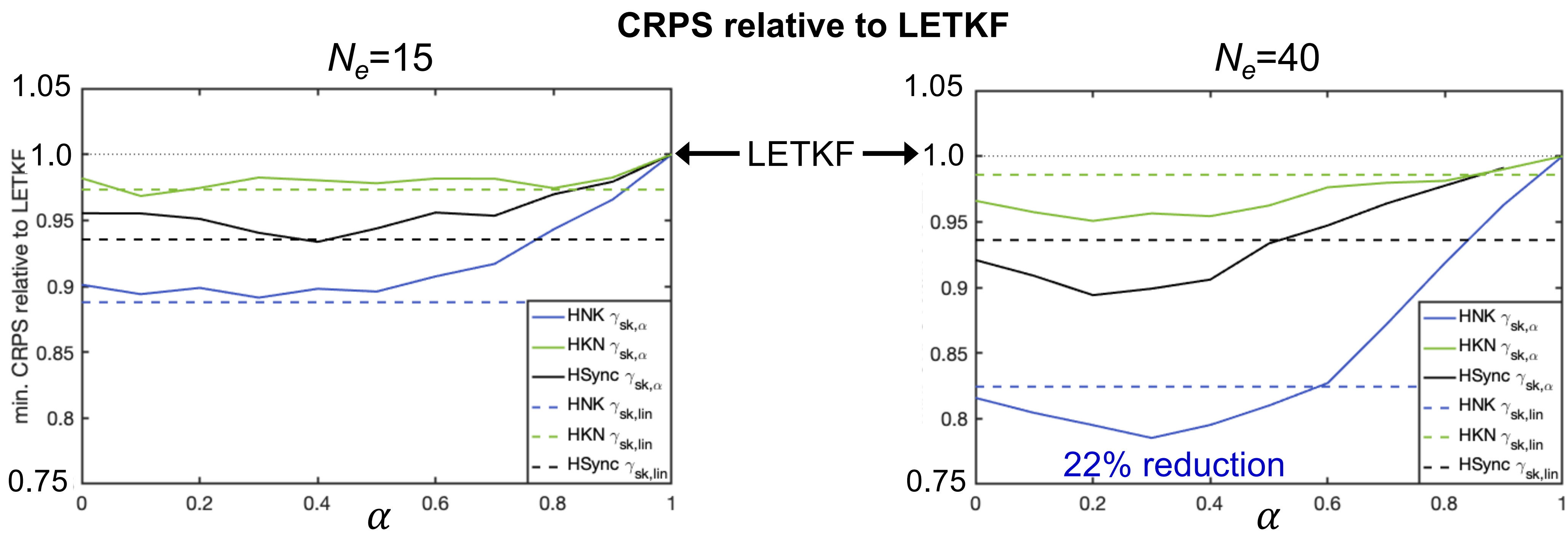
Test with Lorenz-96 model

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



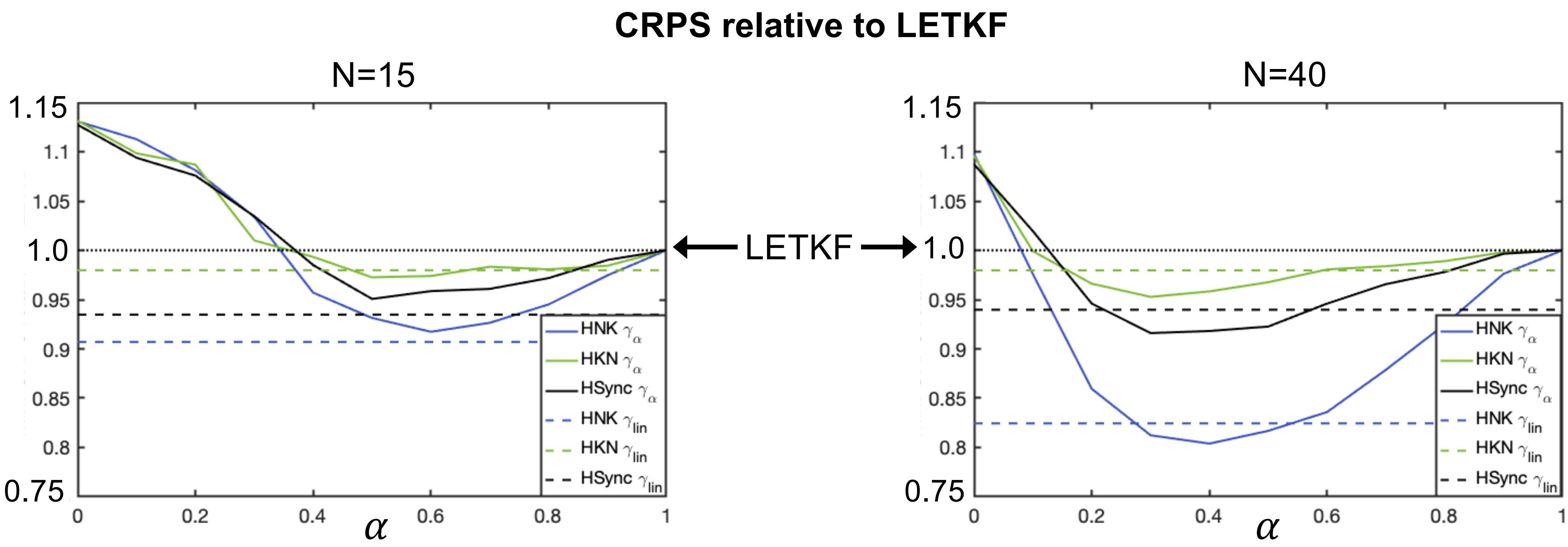
- Show RMS errors as function of inflation (forgetting factor or α) and localization radius
- *Smallest errors:* Hybrid HNK (10% error reduction)
  - → hybrid filter able to utlize non-Gaussian information
- Other hybrid variants also improve the state estimate

Lorenz-96: Influence of γ – using skewness and kurtosis



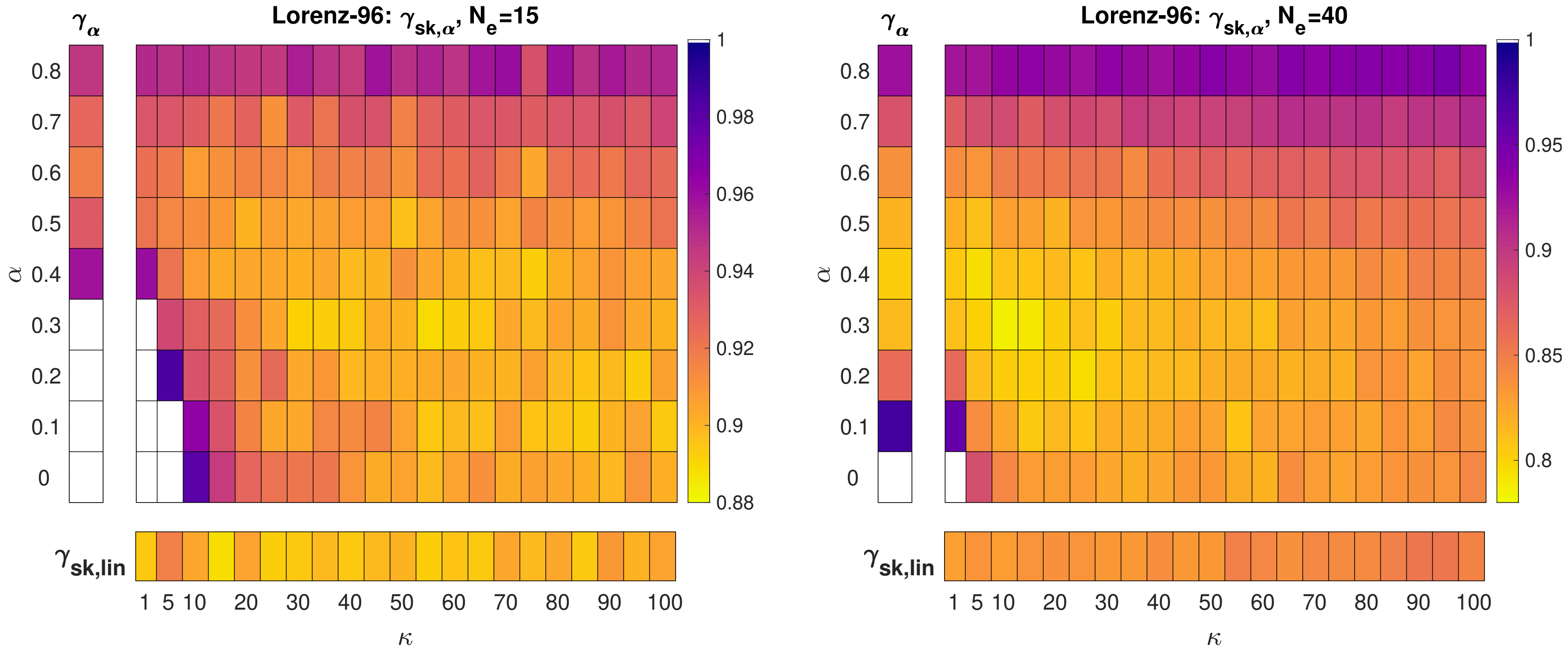
- When accounting for skewness/kurtosis filter is more stable
- $\gamma_{sk,lin}$ yields smallest (N_e=15) or nearly smallest (N_e=40) errors
- smallest errors with $\gamma_{sk,\alpha}$ for optimal tuning

Lorenz-96: Influence of γ – cases γ_α and γ_{lin} (account only for N_{eff})



- Stronger effect of hybrid filter for N_e=40
- γ_{lin} yields optimal (N=15) or nearly optimal (N=40) errors
- γ_α requires tuning; increased errors for small α compared to γ_{sk}

Lorenz-96, Hybrid HNK, dependence on κ



CRPS relative to LETKF

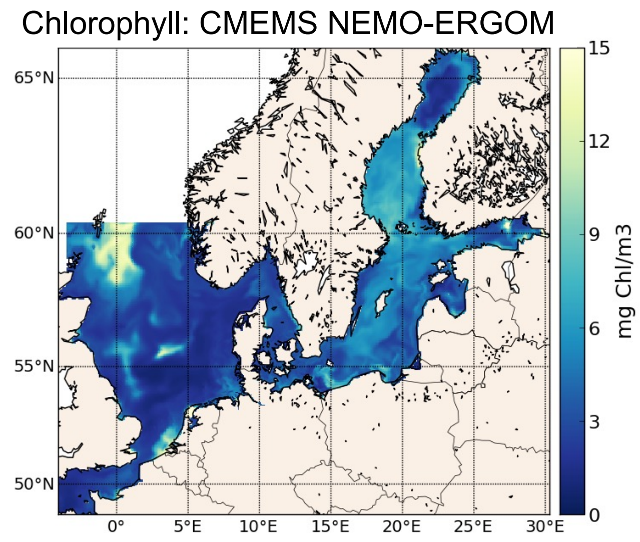
κ can be chosen dependent on ensemble size

- 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

PDAF Parallel Data Assimilation Framework

- 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

SEAMLESS

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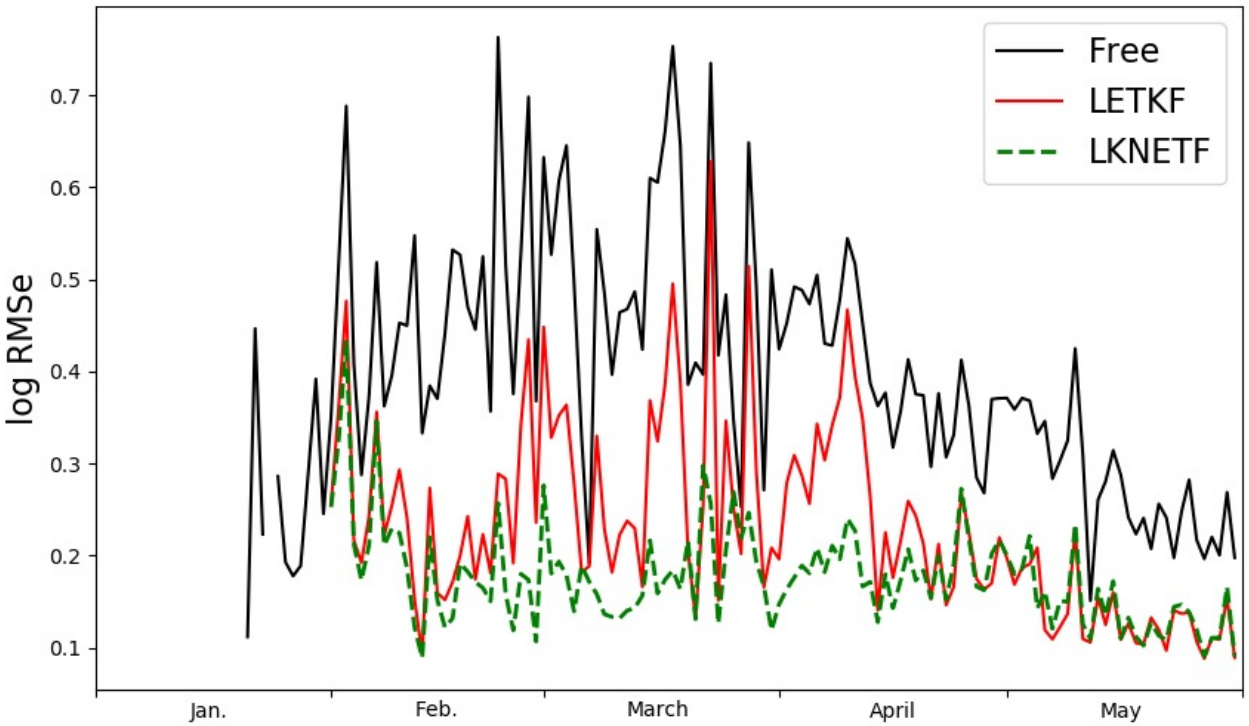
Effect of hybrid filter in high-dimensional application

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

RMS deviation for log-Chlorophyll



Regional model setup

Only assimilate chlorophyll observations

Stronger assimilation effect of LKNETF

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

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}

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

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Next steps

PDAF Parallel Data Assimilation Framework

Need to

- improve understanding of effect of γ
  - mathematical basis
  - Are skewness & kurtosis good choices?
  - Is linear dependence of skewness & kurtosis right?

- asses for which nonlinear cases hybrid filter is superior
  - only 3% lower errors in test with ocean physics at 0.25° resolution

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

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