PDAF Parallel Data Assimilation Framework

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Hybrid nonlinear-Kalman ensemble transform filtering for data assimilation in systems with different degrees of nonlinearity

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Motivation

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

- Nonlinearity in DA → non-Gaussianity of error distributions
  - → Non-linear model dynamics lead to different degree of non-Gaussianity
- 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

→ Aim for DA method that

- adapts to non-Gaussianity
- Allows to utilize optimality of Kalman filter for Gaussian distributions
  - → **Utilize hybrid combination of Kalman and nonlinear filters**

Linear and Nonlinear Ensemble Filters

- Represent state and its error by ensemble $\mathbf{X}$ of N states
- **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 $N \times N$)

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 $\mathbf{y}$)

  - Transformation of ensemble perturbations

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

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

($\mathbf{W}$ depends only on $\mathbf{R}$, not $\mathbf{y}$)

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

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)

Note: $\mathbf{W}$ depends on $\mathbf{y}$ and $\mathbf{R}$ (higher sampling errors than ETKF)

NETF: second-order exact particle filter using transformation rather than resampling

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

ETKF-NETF – Hybrid Filter Variants

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

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 & 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)

Issue: Using N_{eff}

- only ensures non-collapsing ensemble
- does not ensure good analysis result

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

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

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

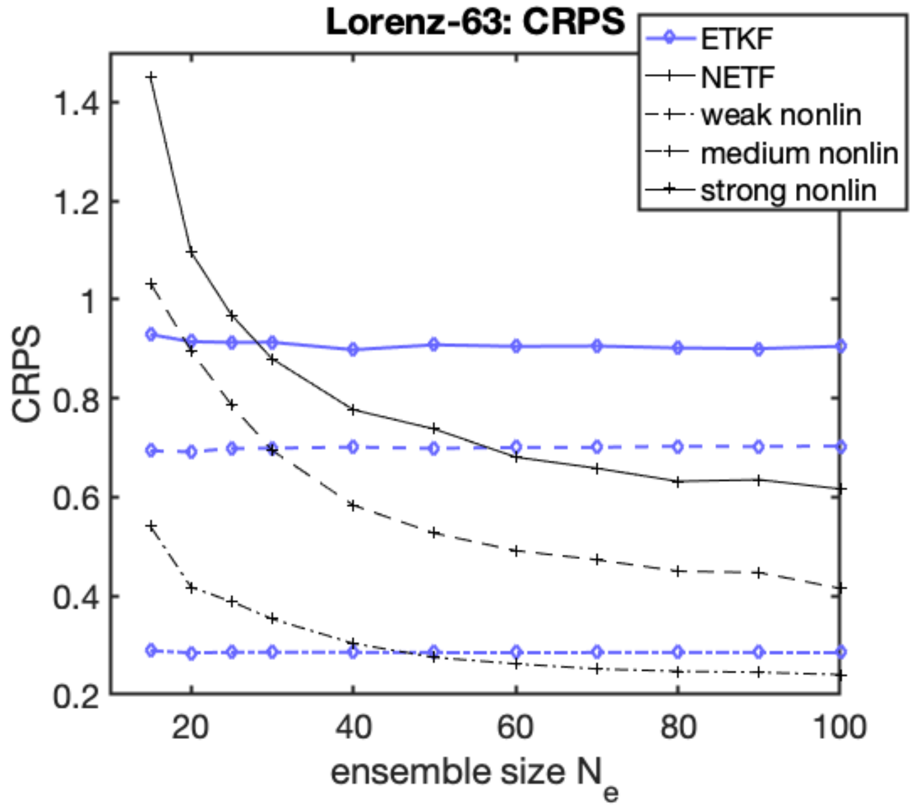
Note: There are sampling errors, e.g. for skewness $\sigma_{skew} \sim \sqrt{6/N_e}$

→ For N_e=25: ~10% error in γ

Numerical experiments

- Lorenz-63 and Lorenz-96 models
- Configurations that ensure high nonlinearity
  - long forecast times
  - Lorenz-96 also incomplete observations
- Assimilation implemented using PDAF (https://pdaf.awi.de)

- NETF yields smaller errors than ETKF if ensemble size large enough
  - → Size 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)

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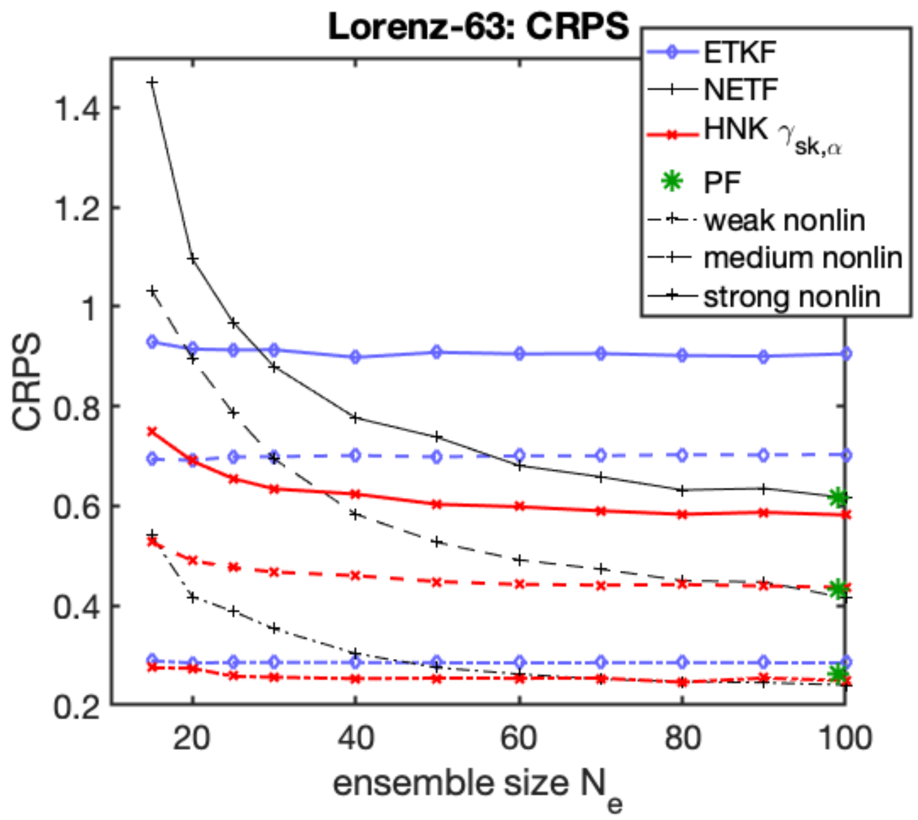
AWI

Assimilation with Lorenz-63 model

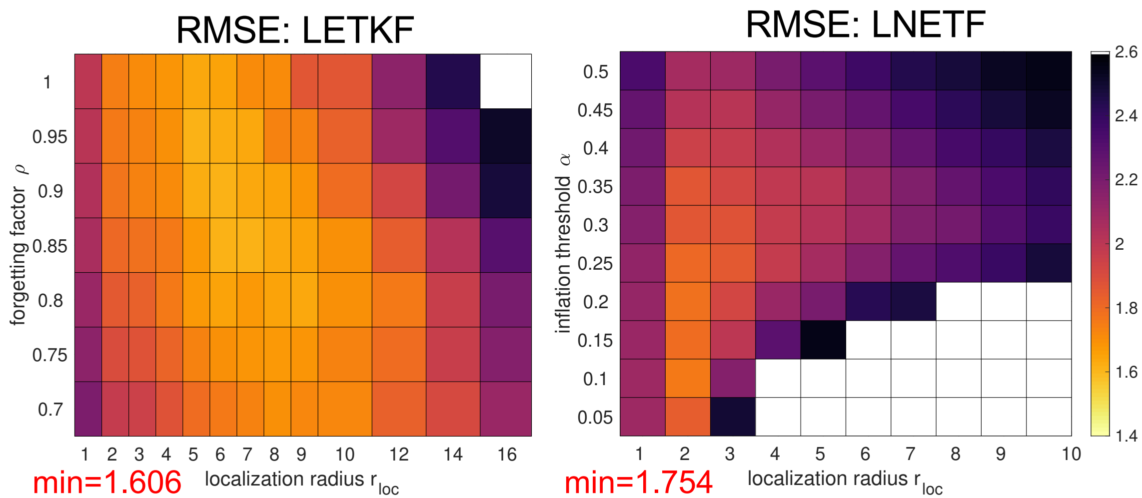
- **Hybrid filter HNK**
  - particular strong effect for small N_e
  - CRPS from NETF and HNK converge for large N_e
  - errors reduced up to 28%
- **Particle Filter** $*$
  - comparable CRPS for large N_e
    - PF expected to be superior if N_e sufficiently large (the full nonlinear filter)

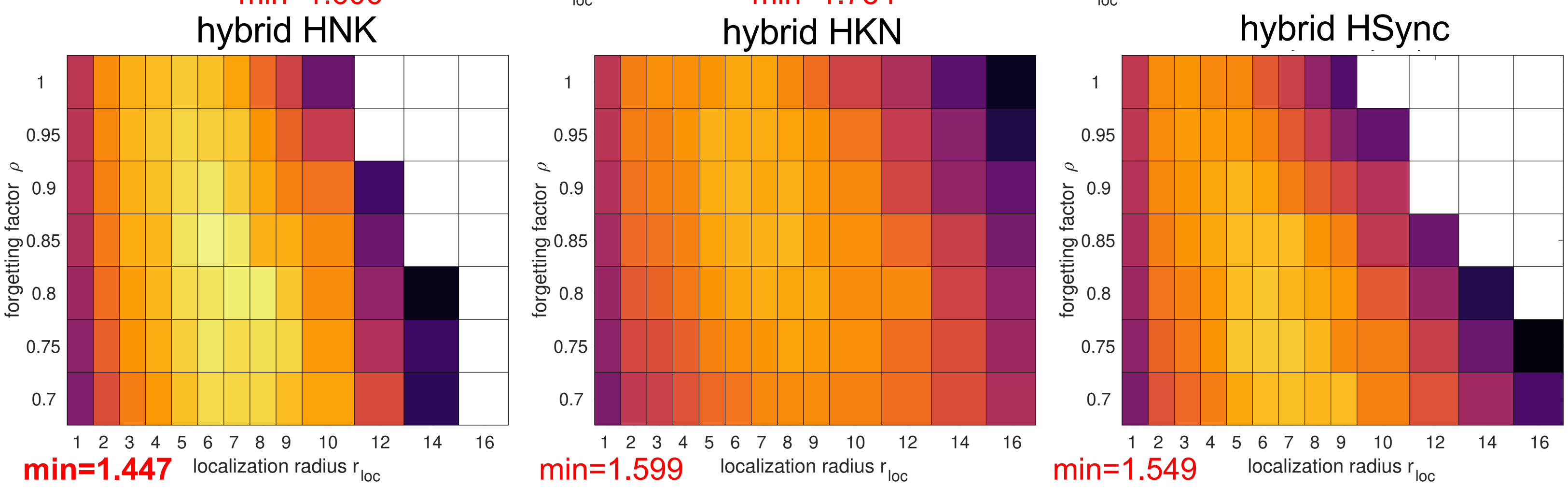


- Note: Easy to get large ensemble for Lorenz-63, difficult for higher dimensional models

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
- LNETF worse than LETKF
- All hybrid variants improve the state estimate
- *Smallest errors:* Hybrid HNK (10% error reduction)

Summary

PDAF Parallel Data Assimilation Framework

Hybrid nonlinear-Kalman ensemble transform filter (LKNETF)

- Combine LETKF and LNETF methods
- hybrid weight γ shifts between both methods

Experiments with Lorenz models

- Hybrid filter reduces errors compared to both LETKF and LNETF
- Best results for particle filter applied before LETKF
- Compute γ based on skewness and kurtosis
  → allows to control nonlinearity of filter based on non-Gaussianity

Ongoing work

- more applications to complex models to understand performance (Tests: ocean 1/4°: little effect; marine biogeochemistry: large effect; PM2.5 components modeling: large effect)
- mathematical consistent description for hybrid weight