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High-Dimensional Nonlinear Data Assimilation with the Nonlinear Ensemble Transform Filter (NETF) and its Smoother Extension

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Overview

- Study new Nonlinear Ensemble Transform Filter – NETF (Tödter & Ahrens, MWR, 2015)
- Extend NETF for smoothing
- Test filter and smoother in realistic high-dimensional idealized ocean data assimilation experiments

Kalman and Nonlinear Filters

Ensemble filters – ensemble Kalman filters & NETF

- represent state and its error by ensemble $\mathbf{X}$ of N states
- Forecast:
  - Integrate ensemble with numerical model
- Analysis:
  - 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 filters & NETF: Different definitions of
  - weight vector $\tilde{\mathbf{w}}$
  - Transform matrix $\mathbf{W}$

The Ensemble Kalman Filter (EnKF, Evensen 94)

Ensemble $\{\mathbf{x}_0^{a(l)}, l = 1, \ldots, N\}$

Ensemble covariance matrix

$$\mathbf{P}_k^f := \frac{1}{N-1} \sum_{l=1}^{N} \left(\mathbf{x}_k^{f(l)} - \overline{\mathbf{x}_k^f} \right) \left(\mathbf{x}_k^{f(l)} - \overline{\mathbf{x}_k^f} \right)^T$$

Ensemble mean (state estimate)

$$\mathbf{x}_k^a := \frac{1}{N} \sum_{l=1}^{N} \mathbf{x}_k^{a(l)}$$

Analysis step:

Update each ensemble member

$$\mathbf{x}_k^{a(l)} = \mathbf{x}_k^{f(l)} + \mathbf{K}_k \left(\mathbf{y}_k^{(l)} - \mathbf{H}_k \mathbf{x}_k^{f(l)} \right)$$

$$\mathbf{K}_k = \mathbf{P}_k^f \mathbf{H}_k^T \left(\mathbf{H}_k \mathbf{P}_k^f \mathbf{H}_k^T + \mathbf{R}_k \right)^{-1}$$

Kalman filter

Expensive to compute

moother

Efficient use of ensembles

Kalman gain

$$\tilde{\mathbf{K}}_k = \mathbf{P}_k^f \mathbf{H}_k^T \left(\mathbf{H}_k \mathbf{P}_k^f \mathbf{H}_k^T + \mathbf{R}_k \right)^{-1}$$

Alternative form (Sherman-Morrison-Woodbury matrix identity)

$$\tilde{\mathbf{K}}_k = \left[\left(\mathbf{P}_k^f \right)^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \right]^{-1} \mathbf{H}^T \mathbf{R}^{-1}$$

Looks worse: $n \times n$ matrices need inversion

However: with ensemble $\mathbf{P}_k^f = (N-1)^{-1} \mathbf{X}' \mathbf{X}'^T$

$$\tilde{\mathbf{K}}_k = \mathbf{X}' \left[(N-1)\mathbf{I} + \mathbf{X}'^T \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \mathbf{X}' \right]^{-1} \mathbf{X}'^T \mathbf{H}^T \mathbf{R}^{-1}$$

Inversion of $N \times N$ matrix

(Ensemble perturbation matrix $\mathbf{X}' = \mathbf{X} - \bar{\mathbf{X}}$)

moother

ETKF (Bishop et al., 2001)

- Ensemble Transform Kalman filter:
  - 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 on $\mathbf{R}$ and $\mathbf{y}$)

  - Transformation of ensemble perturbations

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

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

Particle filters – fully nonlinear ensemble filters

- Avoid changing ensemble members ('particles')
- Instead: give particles a weight at change it at the analysis step
  - Initial weight: 1/N for all particles
- Weights are given by statistical likelihood of an observation
- Example: With Gaussian observation errors (for each particle *i*):

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

- Ensemble mean state computed with weights

$$\overline{\mathbf{x}}^a = \overline{\mathbf{x}}^f + \mathbf{X}'^f\tilde{\mathbf{w}} = \mathbf{X}^f\tilde{\mathbf{w}}$$

- This update does not assume any distribution of the state errors (and is not limited to Gaussian distributations)

Nonlinear ensemble transform filter - NETF

- Ensemble Kalman:
  - Transformation according to KF equations
- NETF (Tödter & Ahrens, MWR, 2015)
  - Mean update from Particle Filter weights: for all particles *i*

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

  - Ensemble update
    - Transform ensemble to fulfill analysis covariance (like KF, 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)

(Almost same formulation: Xiong et al., Tellus, 2006)

Derivation of NETF

- Mean state update

$$\overline{\mathbf{x}}^a = \overline{\mathbf{x}}^f + \mathbf{X}'^f \tilde{\mathbf{w}} = \mathbf{X}^f \tilde{\mathbf{w}}$$

- Analysis covariance matrix

$$\mathbf{P}^a = \sum_{i=1,N} \tilde{w}_i \, (\mathbf{x}_i^f - \overline{\mathbf{x}}^a)(\mathbf{x}_i^f - \overline{\mathbf{x}}^a)^T$$

$$\mathbf{P}^a = \frac{1}{N} \mathbf{X}^f \mathbf{W}^2 (\mathbf{X}^f)^T$$

with

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

Difference of ETKF and NETF

- ETKF parameterizes ensemble distribution by a Gaussian distribution
- NETF uses particle filter weights to ensure correct update of ensemble mean and covariance

- Filter update:
  - in ETKF is linear in observations

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

  - in NETF is nonlinear in observations

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

Ensemble Smoothers – ETKS & NETS

- Smoother: Update past ensemble with future observations
- Rewrite ensemble update as
  - Filter:

$$\mathbf{X}^a_{k|k} = \mathbf{X}^f_{k|k-1}\hat{\mathbf{W}}_k$$

analysis time

Observations used up to time

- Smoother at time $i < k$

$$\mathbf{X}^a_{i|k} = \mathbf{X}^f_{i|k-1}\hat{\mathbf{W}}_k$$

➢ works likewise for ETKS and NETS

➢ also possible for localized filters

See, e.g., Nerger, Schulte & Bunse-Gerstner, QJRMS 140 (2014) 2249–2259

Experiments with small Lorenz-96 model

Configuration of Lorenz-96 model experiments

Lorenz-96:

- 1-dimensional period wave
- Chaotic dynamics

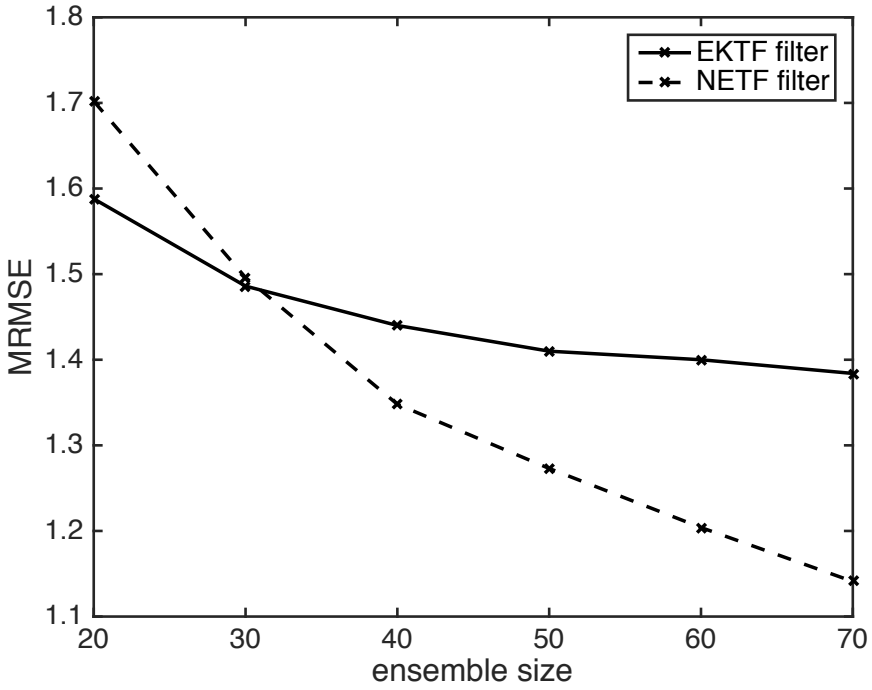
Configuration for assimilation experiments

- State dimension: 80
- Observed: 40 grid points
- Time steps between analysis steps: 8
- Double-exponential observation errors
  (for even stronger nonlinearity)
- Experiment length: 5000 time steps
- Observation error standard deviation: 1

  ➜ this is a difficult case for the assimilation

Performance of NETF – Lorenz-96

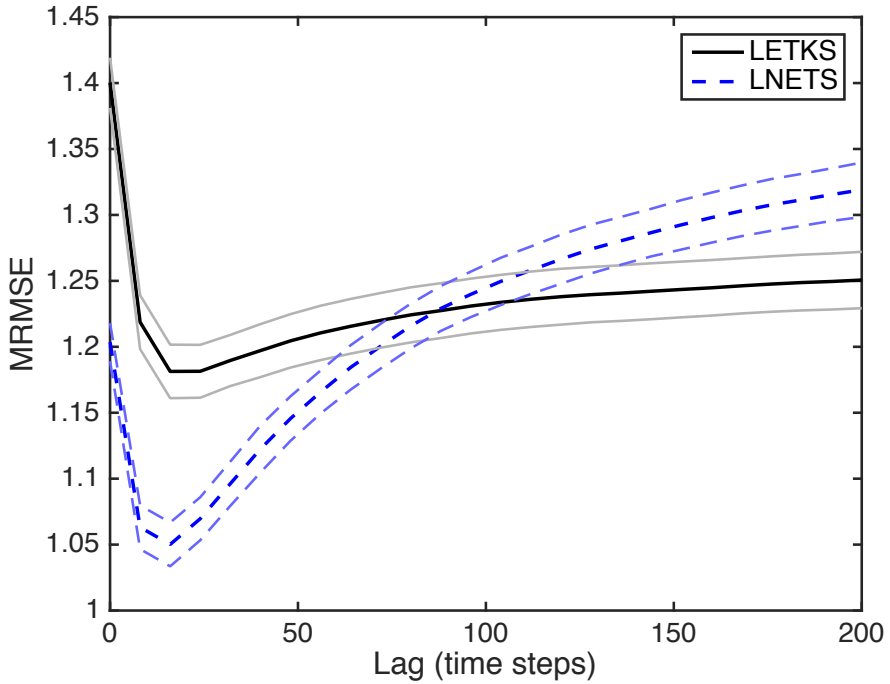
- Performance for small model (Lorenz-96)



- NETF beats ETKF for ensemble size larger 30

Appliction of smoother

- Time period over which smoothing is performed: smoother lag



Typical behavior with nonlinear models

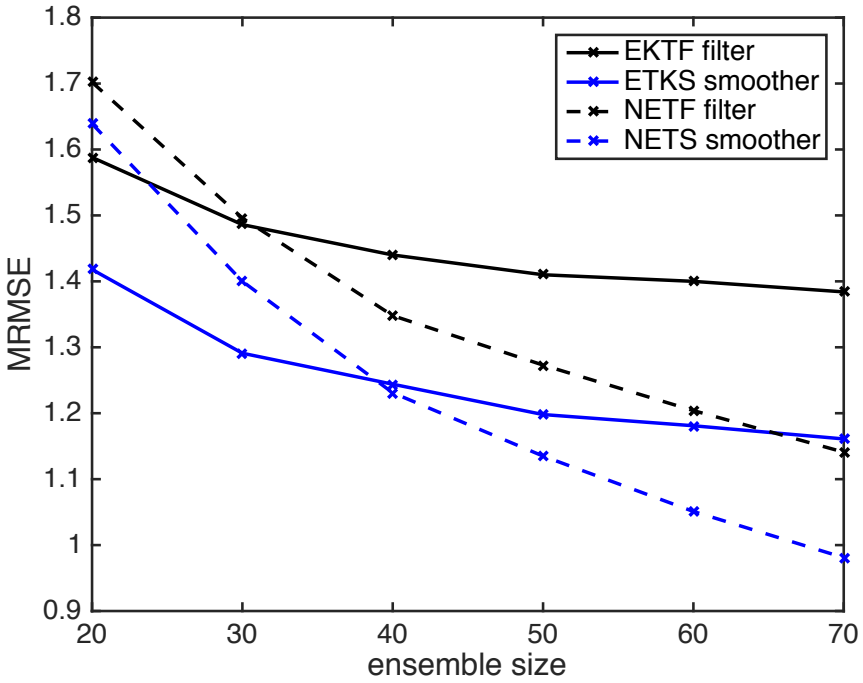
- Fast reduction of error short lag
- Error increase for large lag (caused by nonlinarity)

  ➜ There is an optimal lag with minimum error

L. Nerger, S. Schulte, A. Bunse-Gerstner (2014) QJR. Meteorol. Soc. 140: 2249

Performance of NETF – Lorenz-96

- Performance for small model (Lorenz-96)



- Blue: Smoother
- NETS beats ETKS for ensemble size 40 and larger
  - Smoother slightly stronger for ETKS
  - NETS better than ETKF filter for N=70

Kirchgessner, Toedter, Ahrens, Nerger. (2017) Tellus A 69:1, 1327766

NETF/NETS

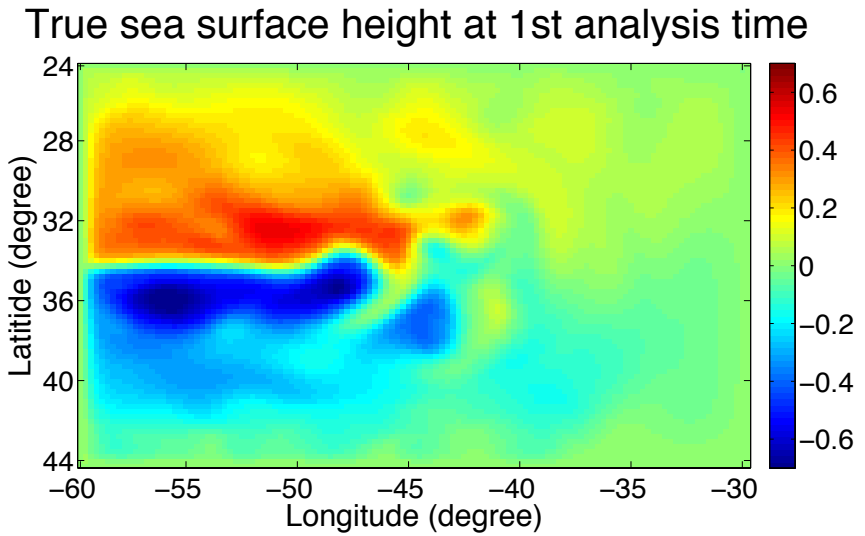
with
high-dimensional ocean model

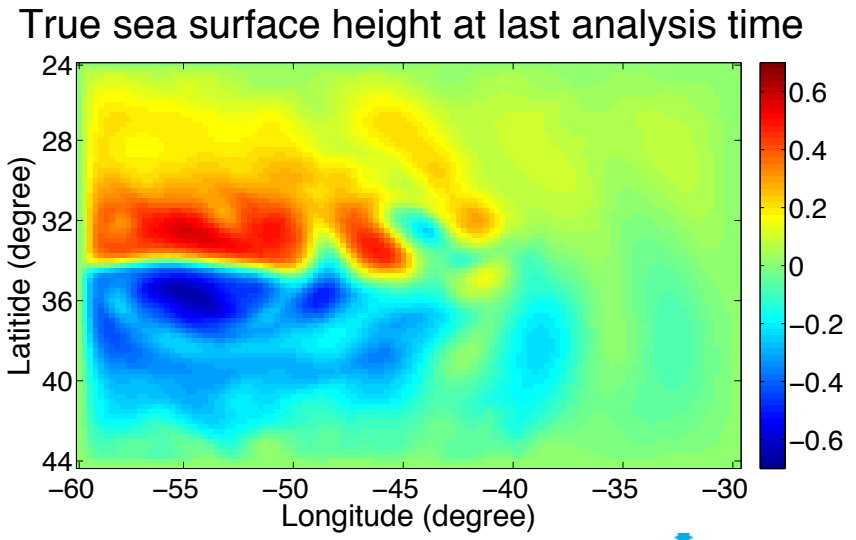
Assimilation into NEMO

European ocean circulation model

Model configuration

- box-configuration “SEABASS”
- ¼° resolution
- 121x81 grid points, 11 layers (state vector ~300,000)
- wind-driven double gyre (a nonlinear jet and eddies)
- medium size SANGOMA benchmark





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www.data-assimilation.net

AWI

PDAF: A tool for data assimilation

PDAF Parallel Data Assimilation Framework

PDAF - Parallel Data Assimilation Framework

- a program library for ensemble data assimilation
- provide support for parallel ensemble forecasts
- provide fully-implemented & parallelized filters and smoothers (EnKF, LETKF, NETF, EWPF … easy to add more)
- easily useable with (probably) any numerical model (applied with NEMO, MITgcm, FESOM, HBM, TerrSysMP, …)
- run from laptops to supercomputers (Fortran, MPI & OpenMP)
- first public release in 2004; continued development
- ~250 registered users; community contributions

Open source:
Code, documentation & tutorials at

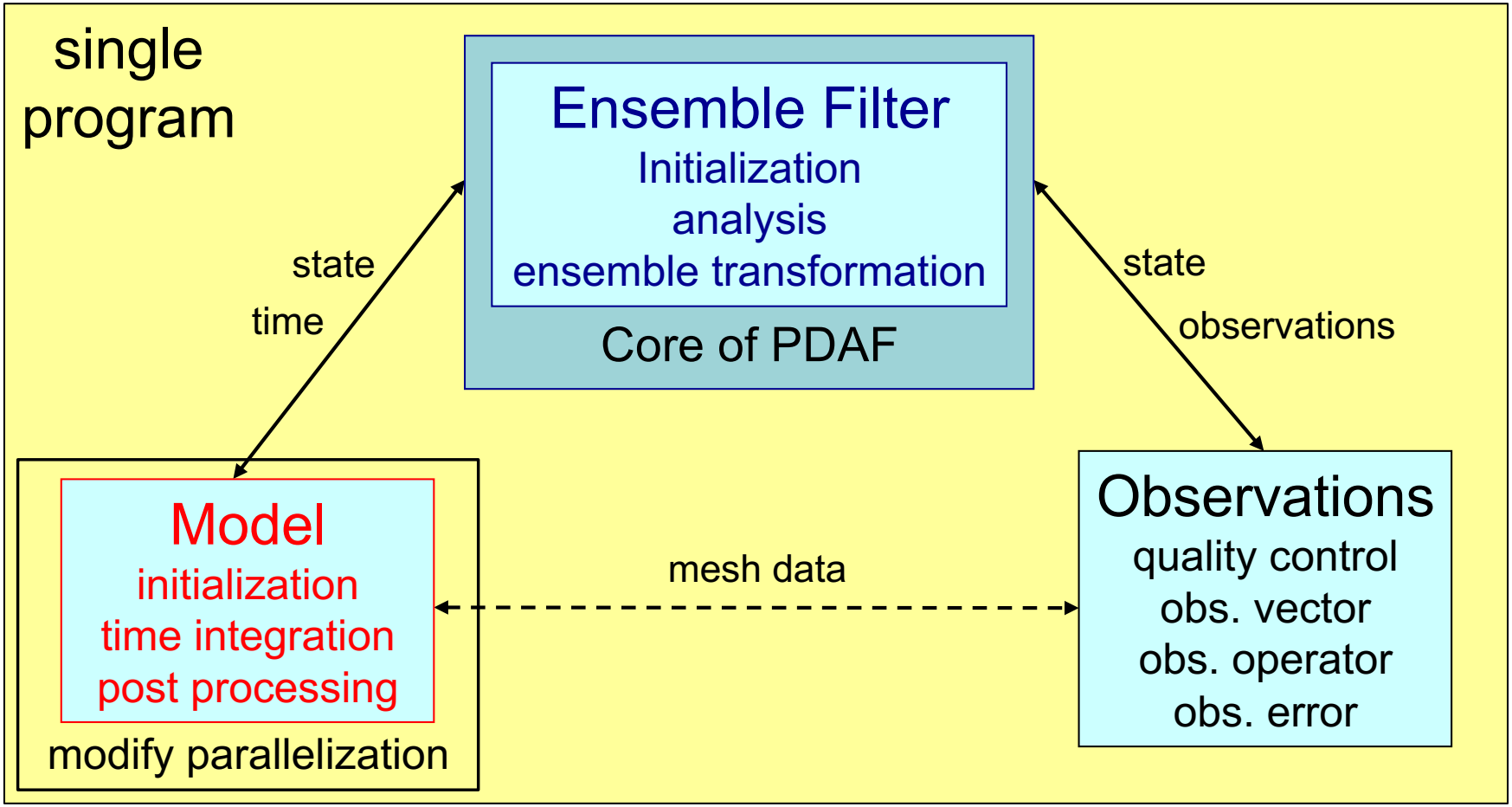
http://pdaf.awi.de

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

AWI

Logical separation of assimilation system

PDAF Parallel Data Assimilation Framework



Explicit interface

Indirect exchange (module/common)

Nerger, L., Hiller, W. Software for Ensemble-based DA Systems – Implementation and Scalability. Computers and Geosciences 55 (2013) 110-118

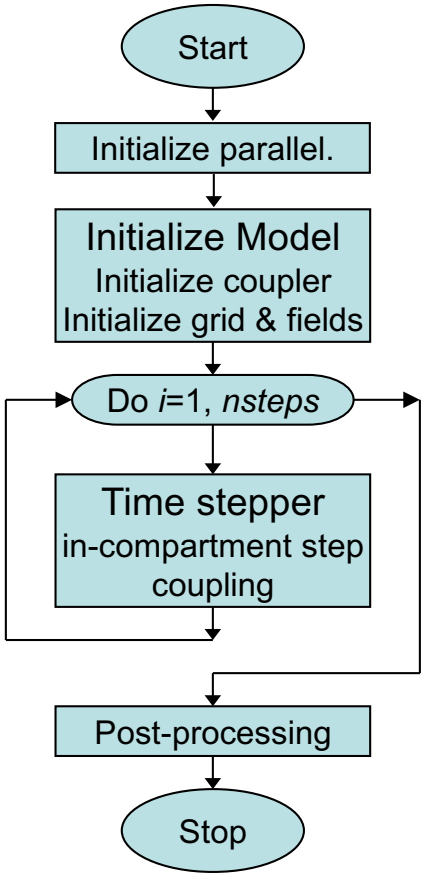
AWI

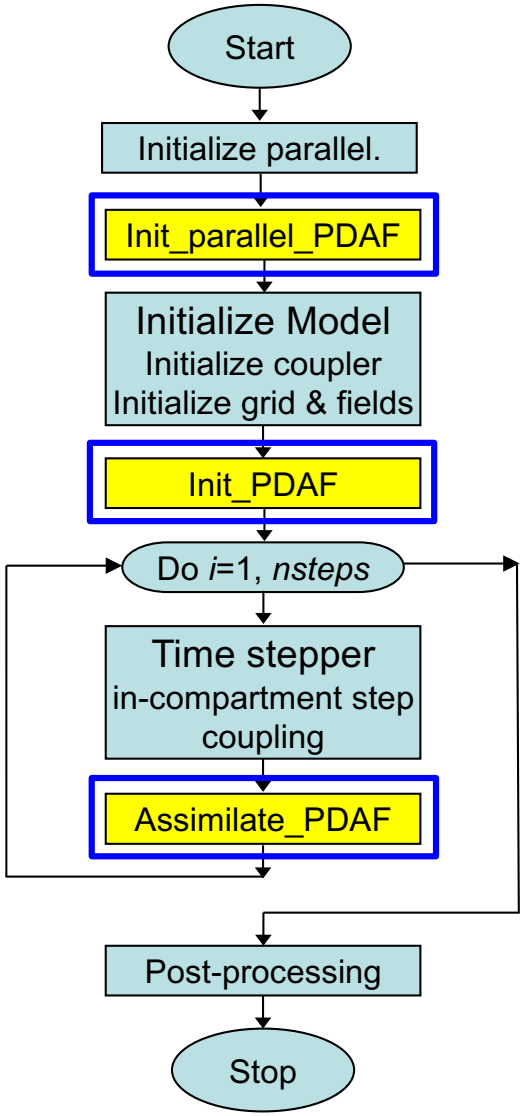
Extending a Model for Data Assimilation

Model

single or multiple executables

coupler might be separate program





Extension for data assimilation

plus:
Possible model-specific adaption:

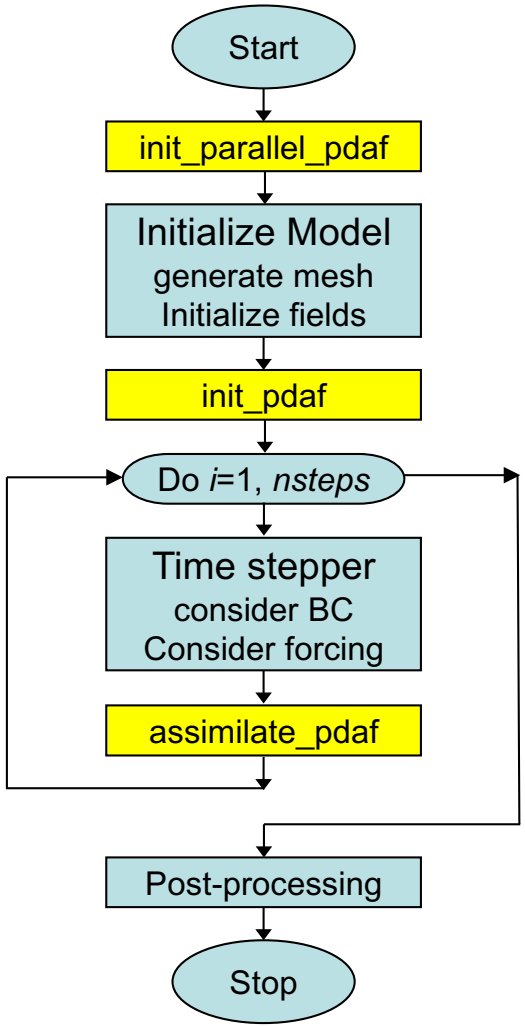
for NEMO: handle leapfrog time stepping

revised parallelization enables ensemble forecast

Features of online-coupled DA program

PDAF Parallel Data Assimilation Framework

- minimal changes to model code when combining model with filter algorithm
- model not required to be a subroutine
- no change to model numerics!
- model-sided control of assimilation program (user-supplied routines in model context)
- observation handling in model-context
- filter method encapsulated in subroutine
- complete parallelism in model, filter, and ensemble integrations



Online coupling: Minimal changes to NEMO

Add to *mynode* (lin_mpp.F90) just before init of myrank

```
#ifdef key_USE_PDAF
   CALL init_parallel_pdaf(0, 1, mpi_comm_opa)
#endif
```

Add to *nemo_init* (nemogcm.F90) at end of routine

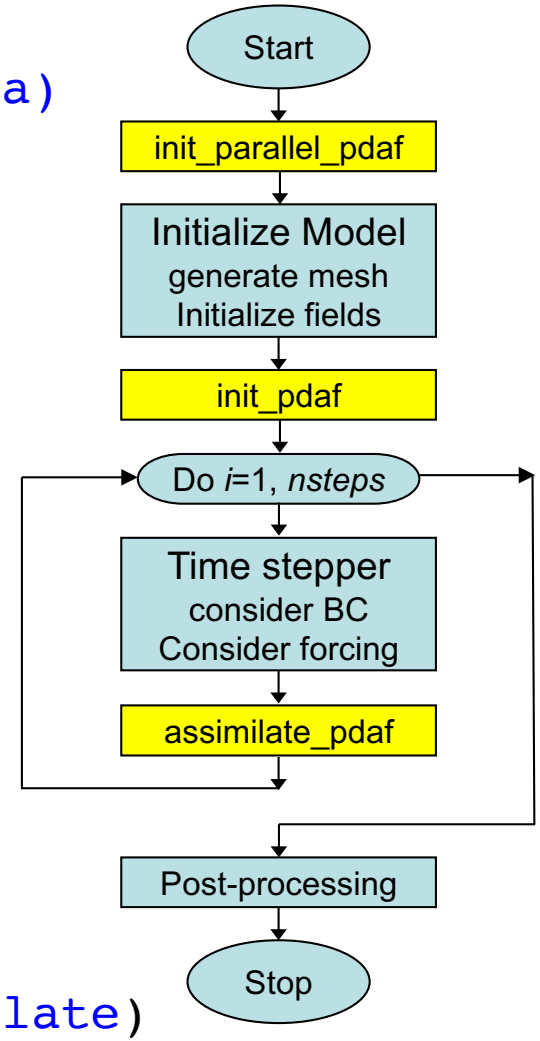
```
#ifdef key_USE_PDAF
   CALL init_pdaf()
#endif
```

Add to *stp* (step.F90) at end of routine

```
#ifdef key_USE_PDAF
   CALL assimilate_pdaf()
#endif
```

Modify *dyn_nxt* (dynnxt.F90)

```
#ifdef key_USE_PDAF
   IF((neuler==0 .AND. kt==nit000).OR.assimilate)
#else
```



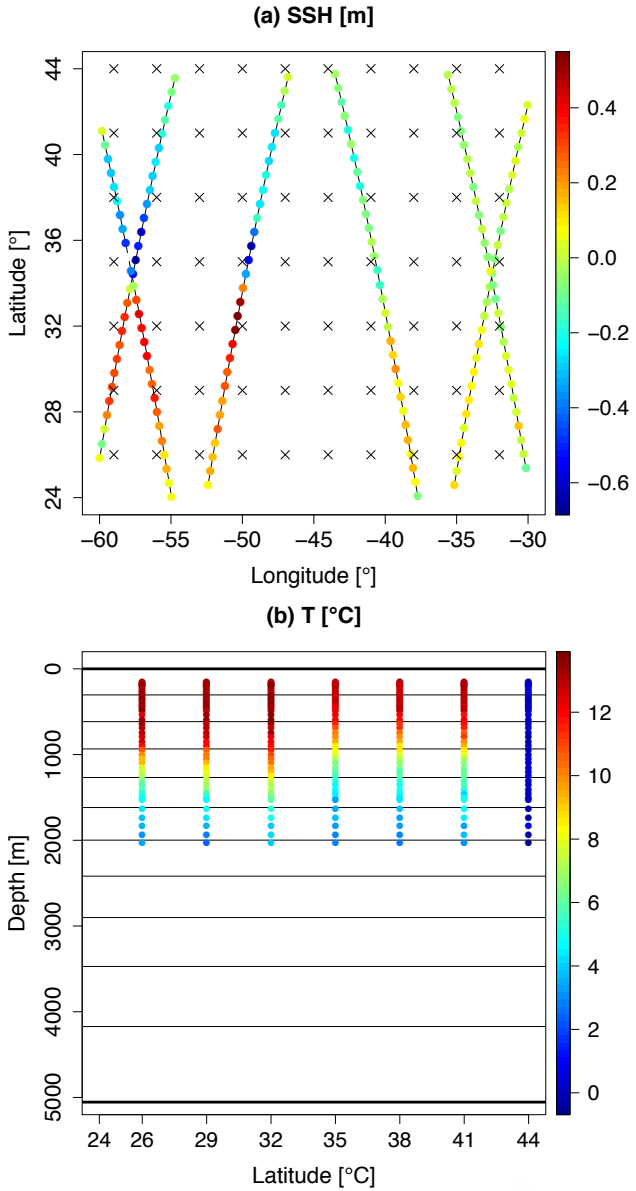
Observations and Assimilation Configuration

Observations

- Simulated satellite sea surface height SSH (Envisat & Jason-1 tracks), 5cm error
- Temperature profiles on 3°x3° grid, surface to 2000m, 0.3°C error

Data Assimilation

- Ensemble size 120
- LETKF, LNETF and smoothers
- Localization: weights on matrix $\mathbf{R}^{-1}$ (Gaspari/Cohn'99 function, 2.5° radius)
- Assimilate each 48h over 360 days

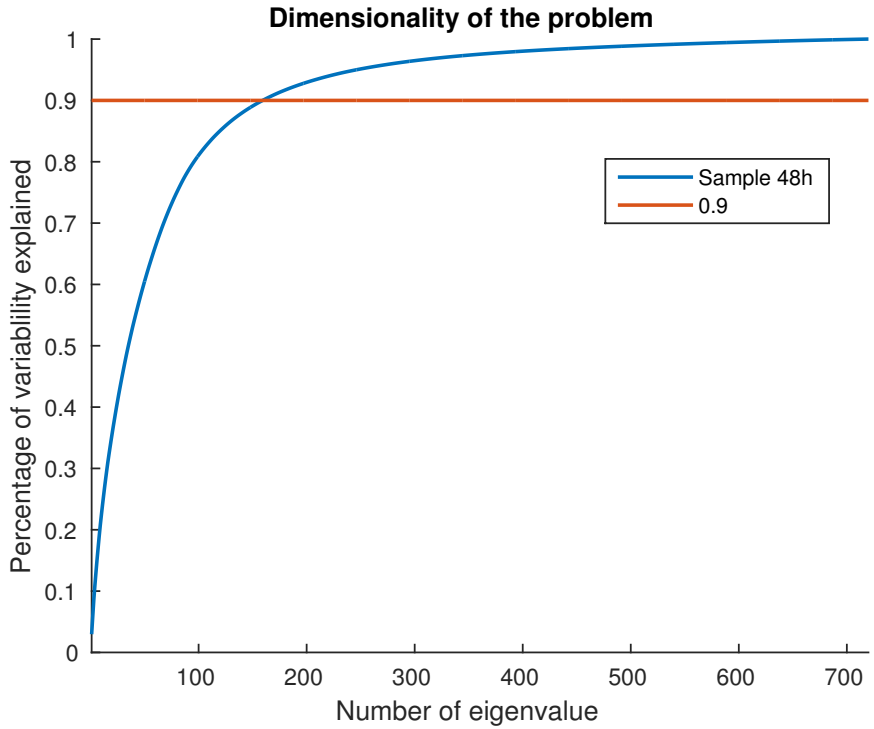


Dimensions of the problem

State vector dimension ~300,000

Dimension of dynamics (error space):

From eigenvalue decompositions (EOFs)

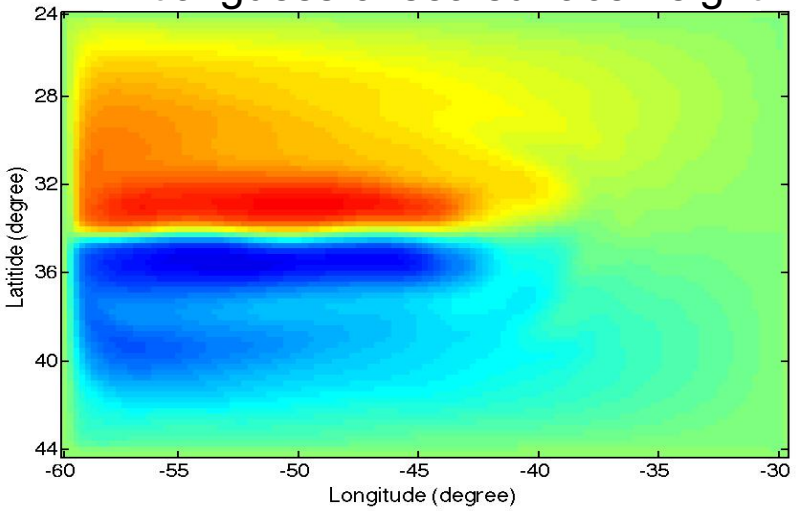


~180 modes for 90% of variability

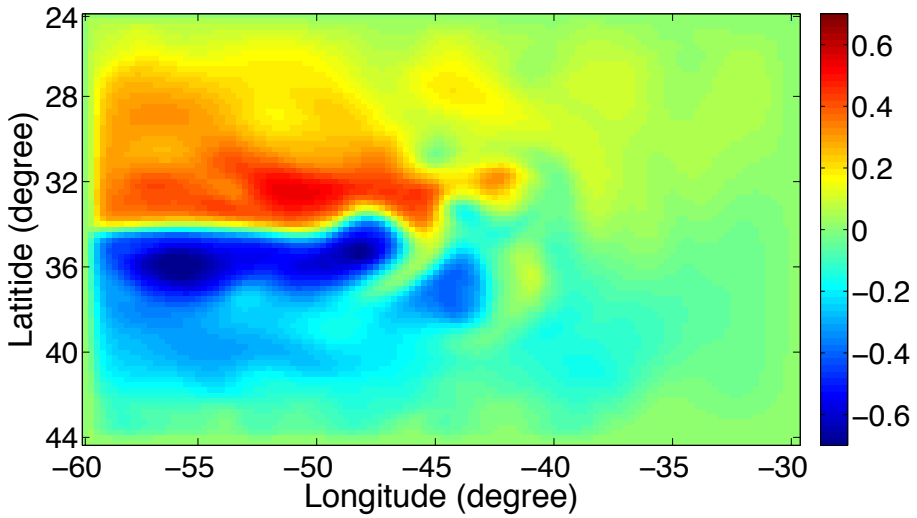
~400 modes for 99.9% of variability

Application of LETKF

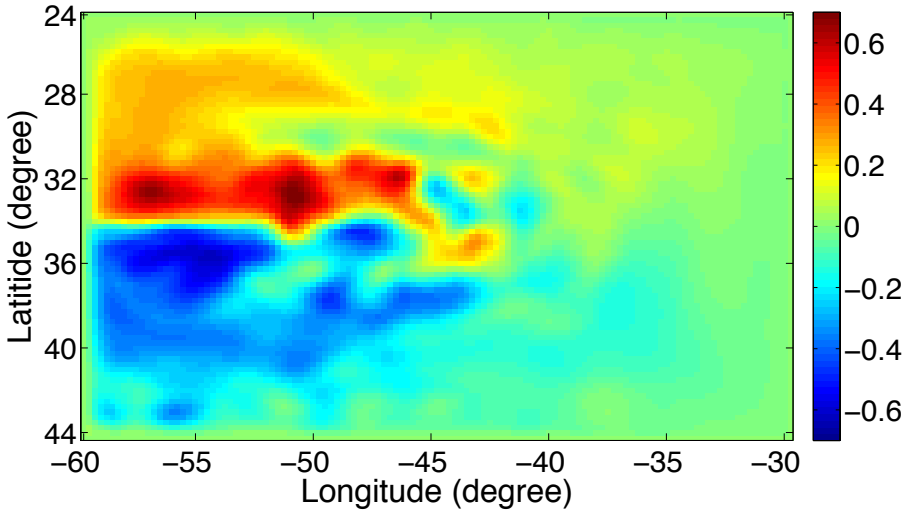
Initial guess of sea surface height



True sea surface height at 1st analysis time



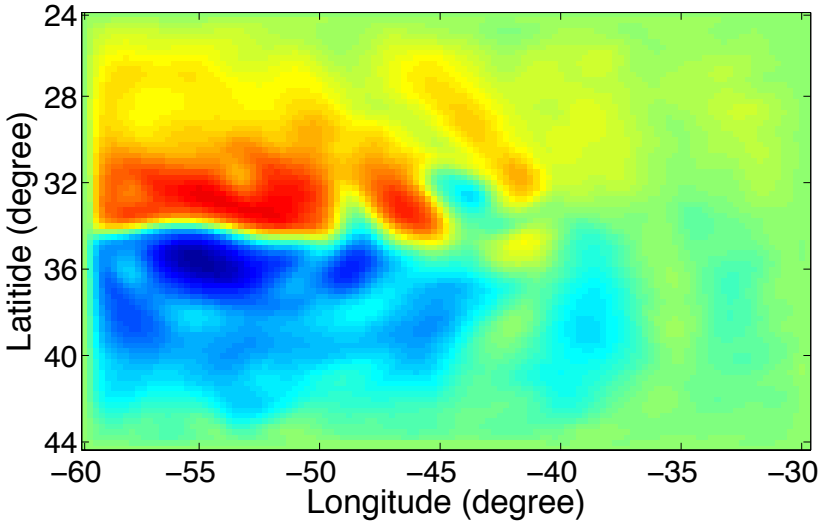
Estimated SSH at 1st analysis time



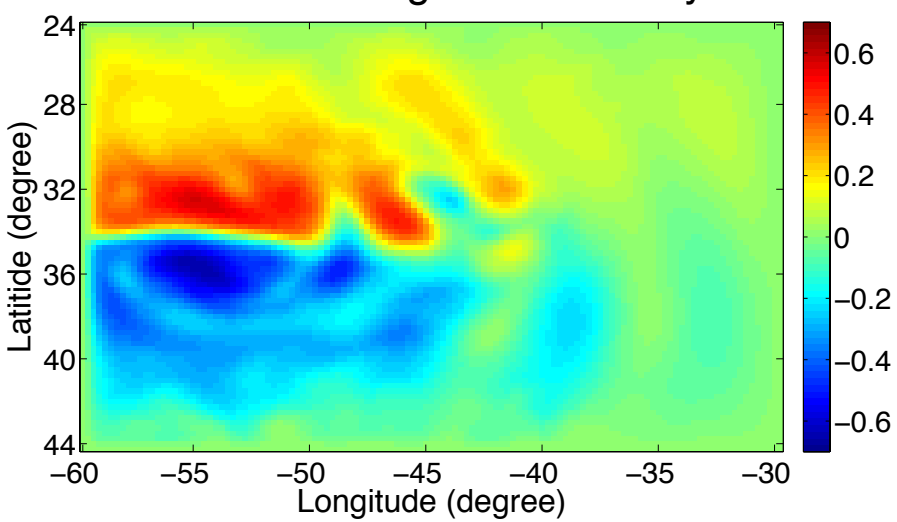
Nonlinear Ensemble Transform Filter & Smoother

Application of LETKF (2)

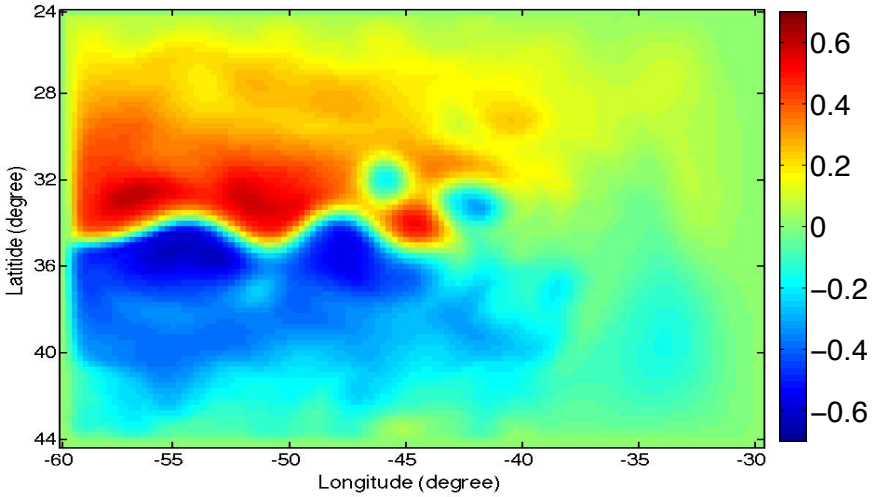
Estimated SSH at last analysis time



True sea surface height at last analysis time



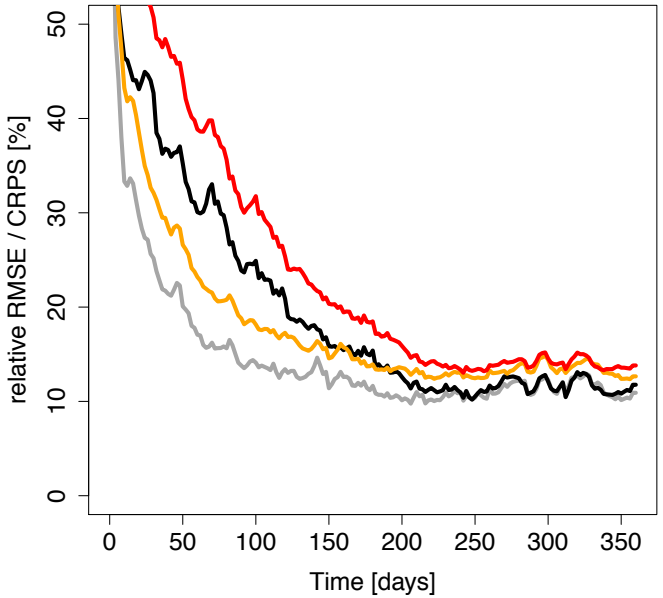
Final SSH without assimilation



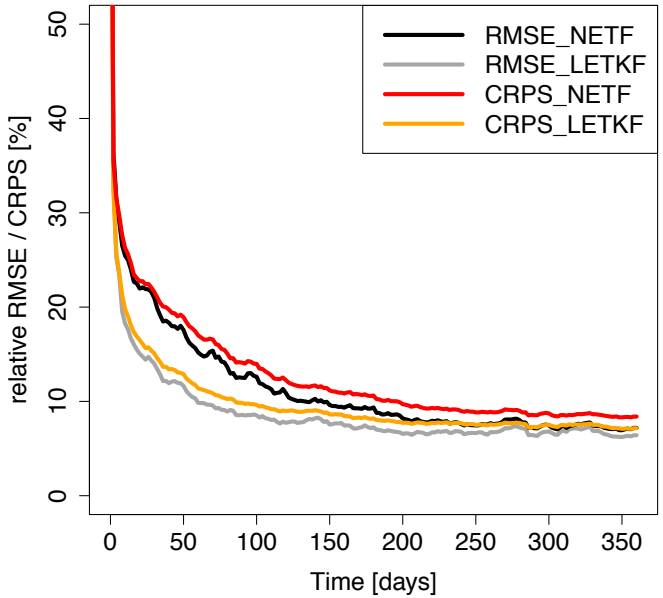
Filter performances in NEMO

- RMS errors reduced to 10% (velocities to 20%) of initial error
- Slower convergence for NETF, but to same error level as LETKF
- CRPS (Continuous Rank Probability Score) shows similar behavior

SSH: Relative error reduction



T: Relative error reduction



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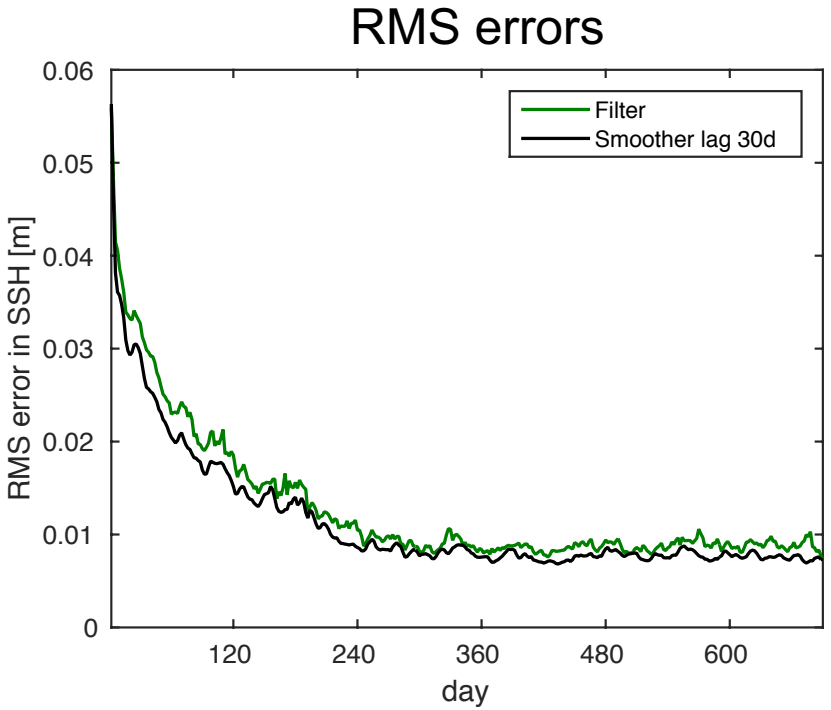
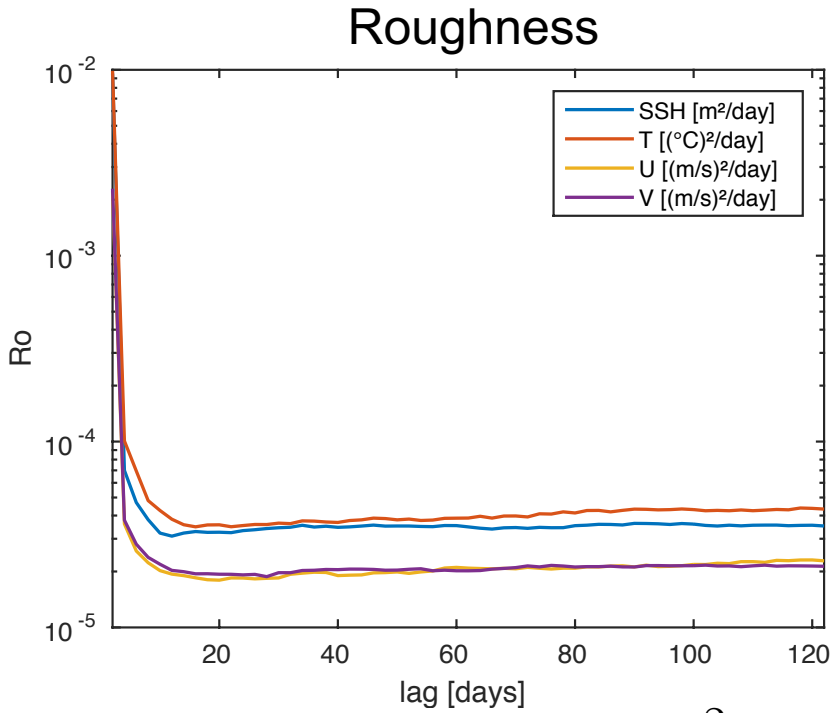
Applying the smoother

- Smoother reduces filter errors by ~10%
- Can be useful as smoothing is cheap to compute
- Roughness of error trajectory is strongly reduced (smoothed)





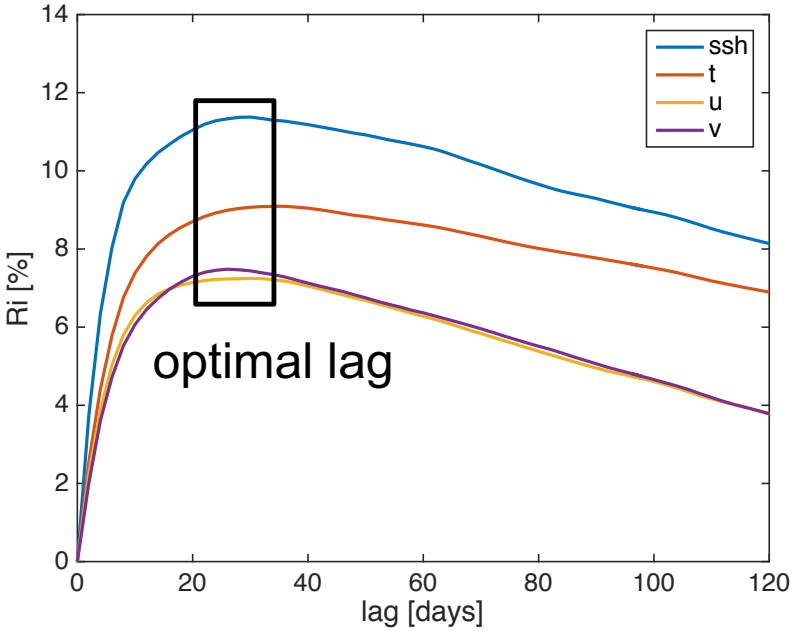
$$Ro = \int \left(\frac{dRMSE}{dt} \right)^2 dt$$

Different smoothing impact

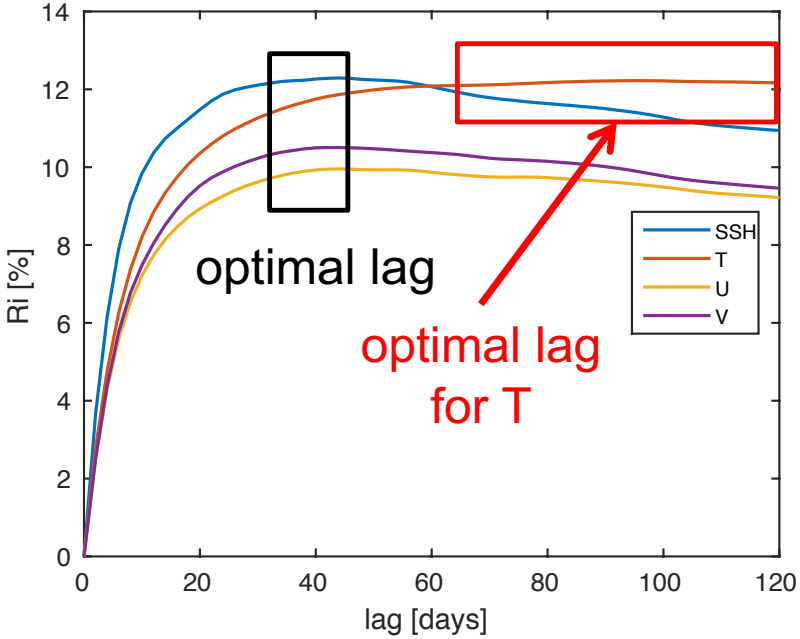
- Consider relative improvement

$$\mathrm{Ri} = 100 \cdot \left(1 - \frac{\mathrm{RMSE}_{smoother}}{\mathrm{RMSE}_{filter}}\right)$$

L-NETF



LETKF

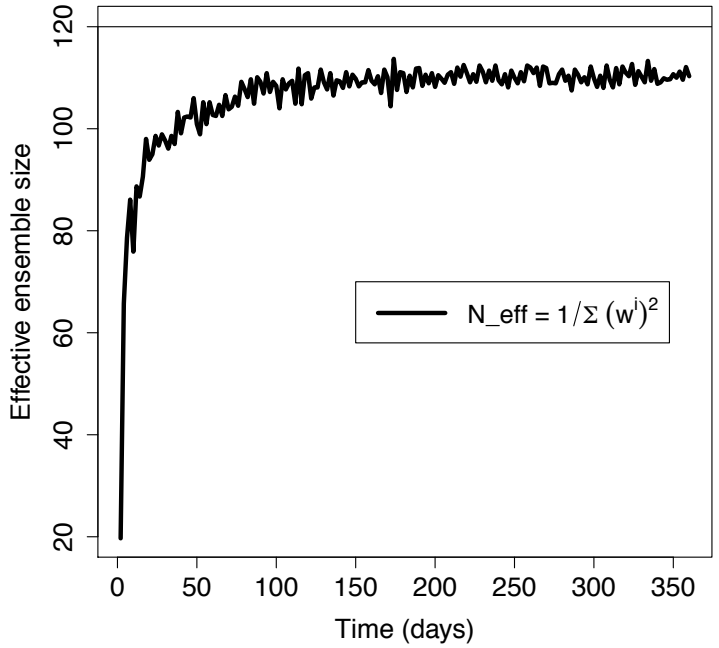


- Similar behavior for ssh (sea surface height)
- Distinct for T
  - ➢ Effect of distinct update schemes (NETF uses observation values for both state and ensemble update)

Ensemble Quality

Effective ensemble size

$$N_{eff} = \frac{1}{\sum_{i=1,N} (w^i)^2}$$



- shows inequality of ensemble weights
- Particle filters need variation in ensemble weights to work
- Extreme cases
  - N_{eff} = 1 (one particle has all weight; degenerate ensemble)
  - N_{eff} = N (all particles has same weight)
- Experiment
  - Strongly variable weights at beginning
  - Lower variability later (but N_{eff} < N)

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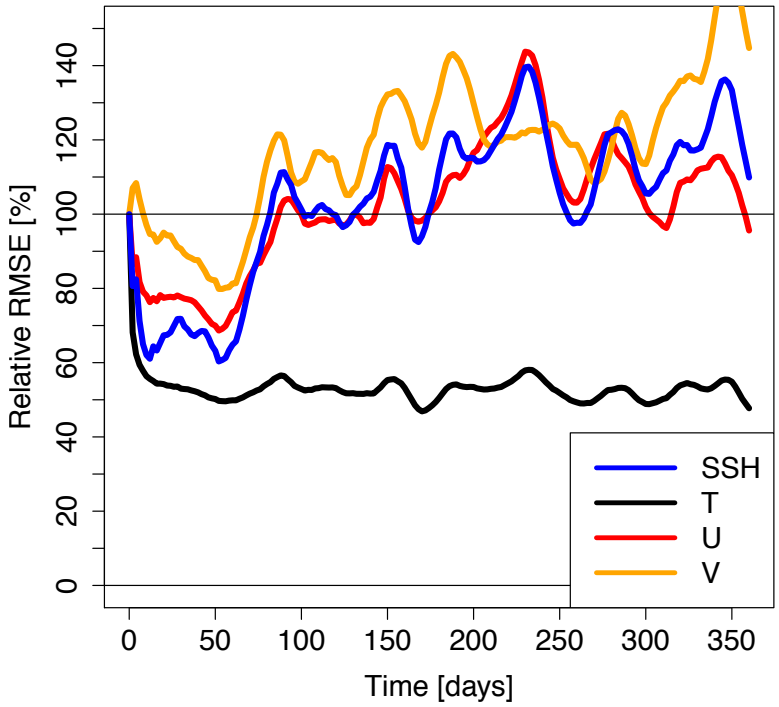
Sensitivity to initial ensemble

- NETF is sensitive to initial ensemble choice
- Using a non-representative ensemble
  (from model variability over 10 years)



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Summary

- Nonlinear ensemble transform filter/smoother (NETF/S)
  - Update state estimate as particle filter
  - Transform ensemble using covariance matrix
- NEMO ocean test case
  - NETF filtering performance similar to LETKF
  - Slower convergence
  - Sensitive on ensemble size
  - Successful smoothing
    - Dependence on lag distinct for LETKS & NETS (due to different update schemes)

Thank you!