An iterative ensemble Kalman smoother

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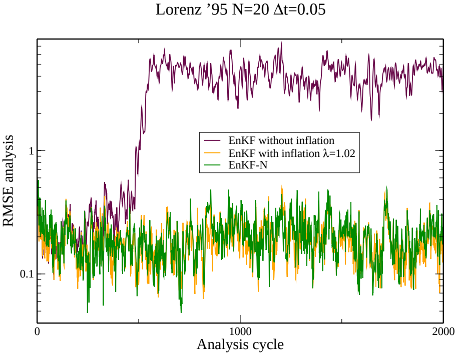
Reminder: failure of the raw ensemble Kalman filter (EnKF)

- EnKF relies for its analysis on the first and second-order empirical moments:

$$\overline{\mathbf{x}} = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_k\,, \qquad \mathbf{P} = \frac{1}{N-1}\sum_{k=1}^{N}(\mathbf{x}_k - \overline{\mathbf{x}})(\mathbf{x}_k - \overline{\mathbf{x}})^{\mathrm{T}}\,. \tag{1}$$

- With the exception of Gaussian and linear systems, the EnKF fails to provide a proper estimation on most systems.

- To properly work, it needs clever but *ad hoc* fixes: localisation and inflation.



- In a perfect model context, the finite-size EnKF (EnKF-N) avoids tuning inflation.

Reminder: principle of the EnKF-N

- The prior of EnKF and the prior of EnKF-N:

$$p(\mathbf{x}|\overline{\mathbf{x}},\mathbf{P}) \propto \exp\left\{-\frac{1}{2}(\mathbf{x}-\overline{\mathbf{x}})^{\mathrm{T}}\mathbf{P}^{-1}(\mathbf{x}-\overline{\mathbf{x}})\right\}$$

$$p(\mathbf{x}|\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N) \propto \left|(\mathbf{x}-\overline{\mathbf{x}})(\mathbf{x}-\overline{\mathbf{x}})^{\mathrm{T}}+\varepsilon_N(N-1)\mathbf{P}\right|^{-\frac{N}{2}}, \quad (2)$$

with $\varepsilon_N = 1$ (mean-trusting variant), or $\varepsilon_N = 1+\frac{1}{N}$ (original variant).

- Ensemble space decomposition (ETKF version of the filters): $\mathbf{x} = \overline{\mathbf{x}} + \mathbf{A}\mathbf{w}$.

- The variational principle of the analysis (in ensemble space):

$$\mathscr{J}(\mathbf{w}) = \frac{1}{2}(\mathbf{y}-H(\overline{\mathbf{x}}+\mathbf{A}\mathbf{w}))^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{y}-H(\overline{\mathbf{x}}+\mathbf{A}\mathbf{w})) + \frac{N-1}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}$$

$$\mathscr{J}(\mathbf{w}) = \frac{1}{2}(\mathbf{y}-H(\overline{\mathbf{x}}+\mathbf{A}\mathbf{w}))^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{y}-H(\overline{\mathbf{x}}+\mathbf{A}\mathbf{w})) + \frac{N}{2}\ln\left(\varepsilon_N+\mathbf{w}^{\mathrm{T}}\mathbf{w}\right). \quad (3)$$

Reminder: the EnKF-N algorithm

1. Requires: The forecast ensemble $\{\mathbf{x}_n\}_{n=1,\ldots,N}$, the observations $\mathbf{y}$, and error covariance matrix $\mathbf{R}$
2. Compute the mean $\overline{\mathbf{x}}$ and the anomalies $\mathbf{A}$ from $\{\mathbf{x}_k\}_{k=1,\ldots,N}$.
3. Compute $\mathbf{Y} = \mathbf{HA}$, $\delta = \mathbf{y} - \mathbf{H}\overline{\mathbf{x}}$
4. Find the minimum:

$$\mathbf{w}_a = \min_{\mathbf{w}} \left\{ (\delta - \mathbf{Yw})^{\mathrm{T}} \mathbf{R}^{-1} (\delta - \mathbf{Yw}) + N \ln \left(\varepsilon_N + \mathbf{w}^{\mathrm{T}}\mathbf{w} \right) \right\}$$

5. Compute $\mathbf{x}^a = \overline{\mathbf{x}} + \mathbf{A}\mathbf{w}_a$.
6. Compute $\mathbf{\Omega}_a = \left(\mathbf{Y}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{Y} + N \frac{(\varepsilon_N + \mathbf{w}_a^{\mathrm{T}}\mathbf{w}_a)\mathbf{I}_N - 2\mathbf{w}_a\mathbf{w}_a^{\mathrm{T}}}{(\varepsilon_N + \mathbf{w}_a^{\mathrm{T}}\mathbf{w}_a)^2} \right)^{-1}$
7. Compute $\mathbf{W}^a = \{(N-1)\mathbf{\Omega}_a\}^{1/2}\,\mathbf{U}$
8. Compute $\mathbf{x}_k^a = \mathbf{x}^a + \mathbf{A}\,\mathbf{W}_k^a$

Iterative Kalman filters: context

- The iterative extended Kalman filter [Wishner et al., 1969; Jazwinski, 1970] IEKF
- The iterative extended Kalman smoother [Bell, 1994] IEKS

Much too costly + needs the TLM and the adjoint $\longrightarrow$ ensemble methods

- The iterative ensemble Kalman filter [Sakov et al., 2012; Bocquet and Sakov, 2012] IEnKF
- The iterative ensemble Kalman smoother [This talk. . .] IEnKS

It's TLM and adjoint free!

Don't want to be bothered by inflation tuning?

- The finite-size iterative ensemble Kalman filter [Bocquet and Sakov, 2012] IEnKF-N
- The finite-size iterative ensemble Kalman smoother [This talk. . .] IEnKS-N

Iterative ensemble Kalman smoother (IEnKS): context

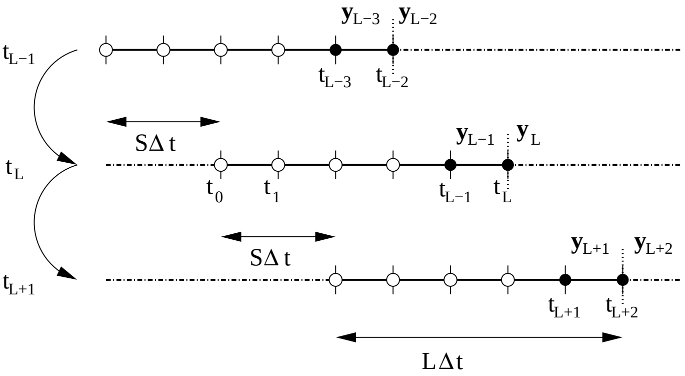
- An extension of the iterative ensemble Kalman filter (IEnKF), a fairly recent idea:
  - [Gu & Oliver, 2007]: Initial idea.
  - [Kalnay & Yang, 2010-2012]: A closely related idea.
  - [Sakov, Oliver & Bertino, 2012]: The "pièce de résistance"
  - [Bocquet & Sakov, 2012]: Bundle scheme + ensemble transform form.

- Related but not to be confused with the iterative ensemble Smoother (IEnS) in the oil reservoir modelling smoothers, where cycling is not an issue.

- Assumptions of the present study:
  - Perfect model.
  - In the rank-sufficient regime. Localisation is more challenging (but possible) in this context (Pavel's talk).
  - Looking for the best performance. Numerical cost secondary.

Iterative ensemble Kalman smoother: the cycling

- L: length of the data assimilation window; S: shift of the data assimilation window in between two updates.



- This may or may not lead to overlapping windows. Here, we study the case $S = 1$, which is close to quasi-static conditions [Pires et al., 1996].

- Let us first focus on the single data assimilation (SDA) scheme.

SDA IEnKS: a variational standpoint

- Analysis IEnKS cost function in state space $p(\mathbf{x}_0|\mathbf{y}_L) \propto \exp\left(-\mathscr{J}(\mathbf{x}_0)\right)$:

$$\mathscr{J}(\mathbf{x}_0) = \frac{1}{2}\left(\mathbf{y}_L - H_L \circ \mathscr{M}_{L\leftarrow 0}(\mathbf{x}_0)\right)^{\mathrm{T}} \mathbf{R}_L^{-1} \left(\mathbf{y}_L - H_L \circ \mathscr{M}_{L\leftarrow 0}(\mathbf{x}_0)\right) + \frac{1}{2}\left(\mathbf{x}_0 - \overline{\mathbf{x}}_0\right) \mathbf{P}_0^{-1} \left(\mathbf{x}_0 - \overline{\mathbf{x}}_0\right). \quad (4)$$

- Reduced scheme in ensemble space, $\mathbf{x}_0 = \overline{\mathbf{x}}_0 + \mathbf{A}_0\mathbf{w}$, where $\mathbf{A}_0$ is the ensemble anomaly matrix:

$$\widetilde{\mathscr{J}}(\mathbf{w}) = \mathscr{J}\left(\overline{\mathbf{x}}_0 + \mathbf{A}_0\mathbf{w}\right). \quad (5)$$

- IEnKS cost function in ensemble space:

$$\widetilde{\mathscr{J}}(\mathbf{w}) = \frac{1}{2}\left(\mathbf{y}_L - H_L \circ \mathscr{M}_{L\leftarrow 0}\left(\overline{\mathbf{x}}_0 + \mathbf{A}_0\mathbf{w}\right)\right)^{\mathrm{T}} \mathbf{R}_L^{-1} \left(\mathbf{y}_L - H_L \circ \mathscr{M}_{L\leftarrow 0}\left(\overline{\mathbf{x}}_0 + \mathbf{A}_0\mathbf{w}\right)\right) + \frac{1}{2}(N-1)\mathbf{w}^{\mathrm{T}}\mathbf{w}. \quad (6)$$

SDA IEnKS: minimisation scheme

- As a variational reduced method, one can use Gauss-Newton [Sakov et al., 2012], Levenberg-Marquardt [Bocquet and Sakov, 2012; Chen and Oliver, 2013], etc, minimisation schemes (not limited to quasi-Newton).

- Gauss-Newton scheme:

$$\begin{aligned}
\mathbf{w}^{(p+1)} &= \mathbf{w}^{(p)} - \widetilde{\mathscr{H}}_{(p)}^{-1} \nabla \widetilde{\mathscr{J}}_{(p)}(\mathbf{w}^{(p)}) \, , \\
\mathbf{x}_0^{(p)} &= \mathbf{x}_0^{(0)} + \mathbf{A}_0 \mathbf{w}^{(p)} \, , \\
\nabla \widetilde{\mathscr{J}}_{(p)} &= -\mathbf{Y}_{(p)}^{\mathrm{T}} \mathbf{R}_L^{-1} \left(\mathbf{y}_L - H_L \circ \mathscr{M}_{L\leftarrow 0}(\mathbf{x}_0^{(p)}) \right) + (N-1)\mathbf{w}^{(p)} \, , \\
\widetilde{\mathscr{H}}_{(p)} &= (N-1)\mathbf{I}_N + \mathbf{Y}_{(p)}^{\mathrm{T}} \mathbf{R}_L^{-1} \mathbf{Y}_{(p)} \, , \\
\mathbf{Y}_{(p)} &= [H_L \circ \mathscr{M}_{L\leftarrow 0} \mathbf{A}_0]'_{(p)} \, .
\end{aligned} \tag{7}$$

- One alternative to compute the sensitivities: the bundle scheme. It simply mimics the action of the tangent linear by finite difference:

$$\mathbf{Y}_{(p)} \approx \frac{1}{\varepsilon} H_L \circ \mathscr{M}_{1\leftarrow 0} \left(\mathbf{x}^{(p)} \mathbf{1}^{\mathrm{T}} + \varepsilon \mathbf{A}_0 \right) \left(\mathbf{I}_N - \frac{\mathbf{1}\mathbf{1}^{\mathrm{T}}}{N} \right) . \tag{8}$$

IEnKS: ensemble update and the forecast step

- Generate an updated ensemble from the previous analysis:

$$\mathbf{E}_0^\star = \mathbf{x}_0^\star \mathbf{1}^{\mathrm{T}} + \sqrt{N-1}\mathbf{A}_0 \widetilde{\mathscr{H}}_\star^{-1/2}\mathbf{U} \quad \text{where} \quad \mathbf{U1} = \mathbf{1}\,. \tag{9}$$

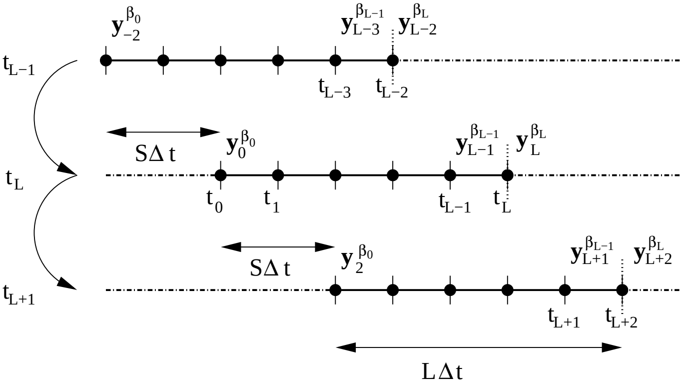
- Just propagate the updated ensemble from t_0 to t_S:

$$\mathbf{E}_S = \mathscr{M}_{S\leftarrow 0}(\mathbf{E}_0)\,. \tag{10}$$

In the quasi-static case: $S = 1$.

IEnKS: introducing the MDA scheme

- Suppose we could assimilate the observation vectors several times...



- This leads to overlapping windows. Here, we study the quasi-static case $S = 1$.
- This is called multiple data assimilation (MDA) scheme.

IEnKS: the MDA approach

- Two flavours of Multiple Data Assimilation:
  - The splitting of observations: Following the partition $1 = \sum_{k=1}^{L} \beta_k$, the observation vector $\mathbf{y}$ with prior error covariance matrix is split into L partial observation $\mathbf{y}^{\beta_k}$, with prior error covariance matrix $\beta_k^{-1}\mathbf{R}$.
    It is a consistent approach in the Gaussian/linear limit, and one hopes it is still so in nonlinear conditions.
  - The multiple assimilation of each observation with its original weights. It is correct but the filtering/smoothing pdf (essentially) becomes a power of the searched pdf!

- An extra step in the analysis.
  - MDA IEnKS does not approximate *per se* the filtering pdf, but a more complex pdf.
  - To approach the correct filtering/smoothing pdf, one needs an extra step, that we called the balancing step which re-weights the observations within the data assimilation window, and perform a final analysis.

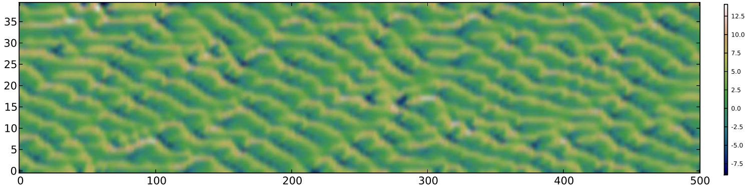
The Lorenz '95 model

- The toy-model [Lorenz and Emmanuel 1998]:
  - It represents a mid-latitude zonal circle of the global atmosphere.
  - $M = 40$ variables $\{x_m\}_{m=1,\ldots,M}$. For $m = 1,\ldots,M$:

$$\frac{\mathrm{d}x_m}{\mathrm{d}t} = (x_{m+1} - x_{m-2})x_{m-1} - x_m + F\,,$$

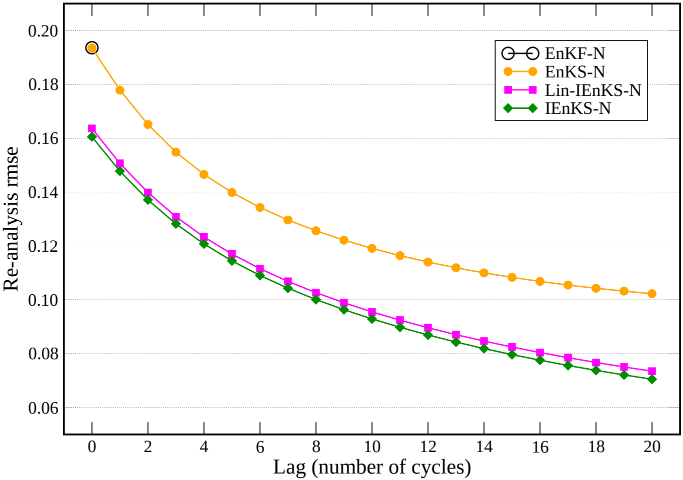
    where $F = 8$, and the boundary is cyclic.
  - Chaotic dynamics, topological dimension of 13, a doubling time of about 0.42 time units, and a Kaplan-Yorke dimension of about 27.1.

- Setup of the experiment: Time-lag between update: $\Delta_t = 0.05$ (about 6 hours for a global model), fully observed, $\mathbf{R} = \mathbf{I}$.



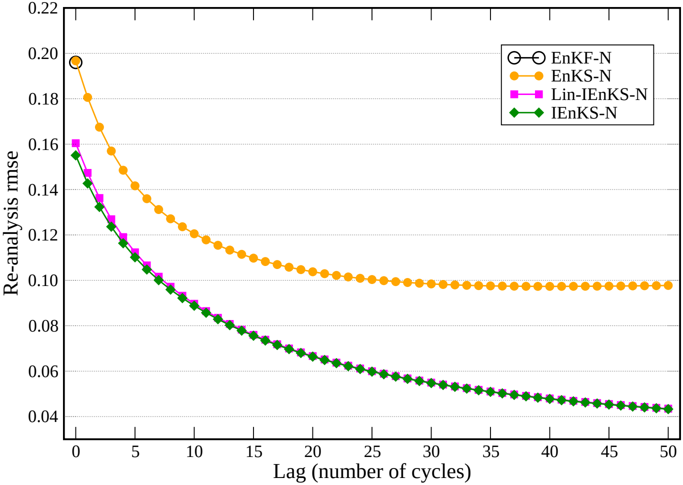
Application to the Lorenz '95 model

- Setup: Lorenz '95, $M = 40$, $N = 20$, $\Delta t = 0.05$, $\mathbf{R} = \mathbf{I}$.
- Comparison of EnKF-N, SDA IEnKS-N, SDA Lin-IEnKS-N, EnKS-N, with $L = 20$.



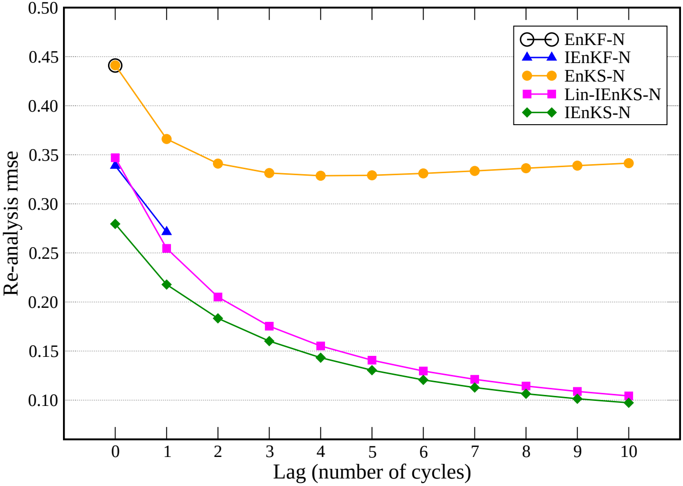
Application to the Lorenz ’95 model

- Beyond $L > 25$, the performance of the SDA IEnKS slowly degrades.
- Setup: Lorenz ’95, $M = 40$, $N = 20$, $\Delta t = 0.05$, $\mathbf{R} = \mathbf{I}$.
- Comparison of EnKF-N, MDA IEnKS-N, MDA Lin-IEnKS-N, EnKS-N, with $L = 50$.



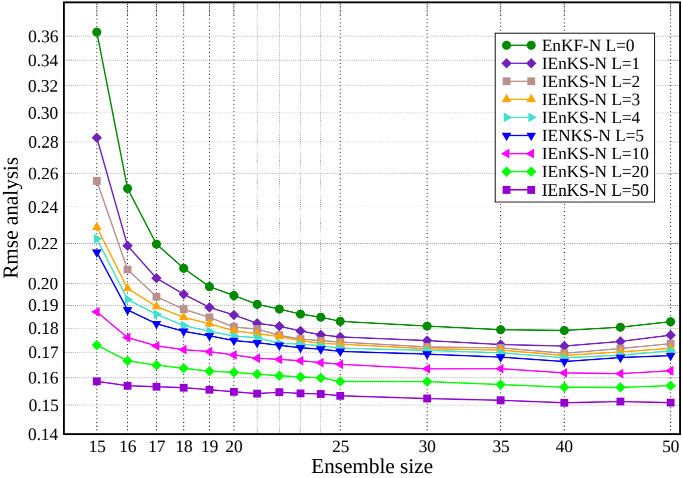
Application to the Lorenz '95 model

- Setup: Lorenz '95, $M = 40$, $N = 20$, $\Delta t = 0.20$, $\mathbf{R} = \mathbf{I}$.
- Comparison of EnKF-N, IEnKF-N, MDA IEnKS-N, ETKS-N, with $L = 10$.
- Lin-IEnKS-N has (understandably) diverged.



Application to the Lorenz '95 model

- Setup: Lorenz '95, $M = 40$, $\Delta t = 0.05$, $\mathbf{R} = \mathbf{I}$.
- Filtering performance of the EnKF-N, IEnKF-N, MDA IEnKS-N for an increasing L.



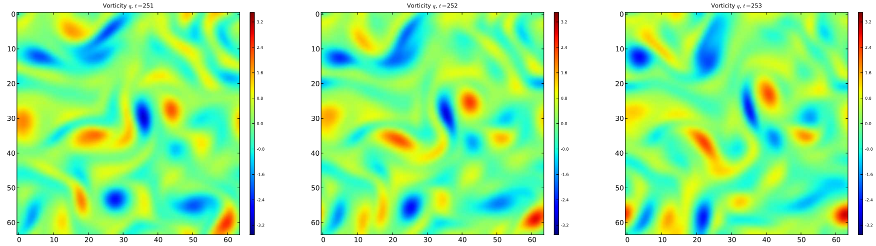
Forced 2D turbulence model

- Forced 2D turbulence model

$$\frac{\partial q}{\partial t} + J(q,\psi) = -\xi q + \nu \Delta^2 q + F\,, \qquad q = \Delta\psi\,, \tag{11}$$

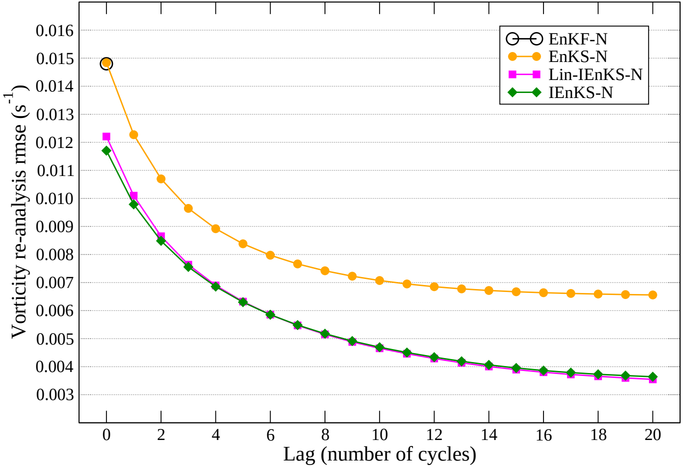
where $J(q,\psi) = \partial_x q \partial_y \psi - \partial_y q \partial_x \psi$, q is the vorticity 2D field, ψ is the current function 2D field, F is the forcing, ξ amplitude of the friction, ν amplitude of the biharmonic diffusion, grid: 64×64 small enough to be in the sufficient-rank regime.

- Setup of the experiment: Time-lag between update: $\Delta_t = 2$, decorellation of 0.82, fully observed, $\mathbf{R} = 0.09\mathbf{I}$.



Application to 2D turbulence

- Setup: 2D turbulence, 64×64, $N = 40$, $\Delta t = 2$, $\mathbf{R} = 0.09\mathbf{I}$.
- Comparison of EnKF-N, MDA Lin-IEnKS-N, MDA IEnKS-N, EnKS-N, with $L = 20$, with balancing.



Conclusions

- The iterative ensemble Kalman smoother (IEnKS) is a way to elegantly combine the advantages of variational and ensemble Kalman filtering, and avoids some of their drawbacks.
- The IEnKS is a generalisation of the iterative ensemble Kalman filter (IEnKF). It is an En-Var method. It is tangent linear and adjoint free. It is, by construction, flow-dependent.
- Though based on Gaussian assumptions, it can offer (much) better retrospective analysis than standard Kalman smoothers in mildly nonlinear conditions.
- When affordable, it beats other Kalman filter/smoothers in strongly non-linear conditions.
- (Properly defined) multiple assimilation of observations can stabilise the smoother over very large data assimilation window (20 days of Lorenz '95).
- More generally the IEnKF/IEnKS have the potential to beat both the EnKF and the 4D-Var (IEnKS already does so with toy-models).
- Localisation remains a fundamental issue in this context (a glimpse onto it in Pavel's talk).

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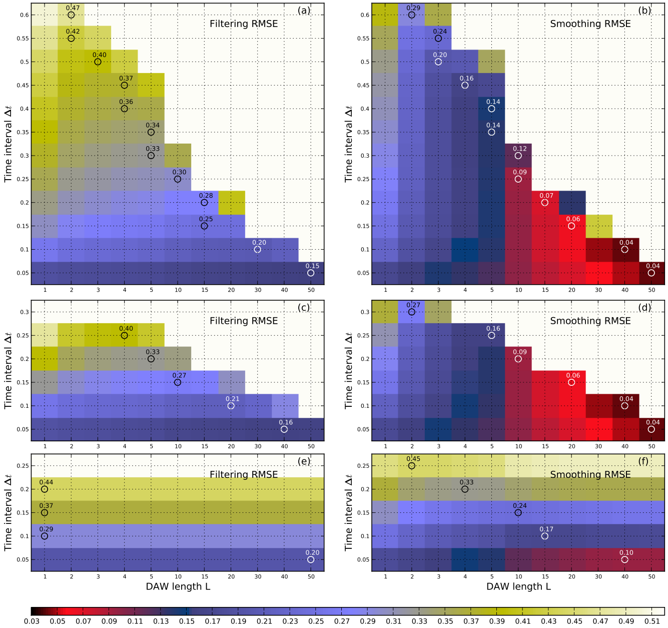
MDA
IEnKS-N

MDA
Lin-IEnKS-N

EnKS-N



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