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► **To cite this version:**

Marc Bocquet. Finite-size ensemble Kalman filters (EnKF-N) - Iterative ensemble Kalman smoothers (IEnKS). International Conference on Ensemble Methods in Geophysical Sciences, Nov 2012, Toulouse, France. hal-00947750

**HAL Id: hal-00947750**

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Submitted on 21 Feb 2014

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# Finite-size ensemble Kalman filters (EnKF-N) Iterative ensemble Kalman smoothers (IEnKS)

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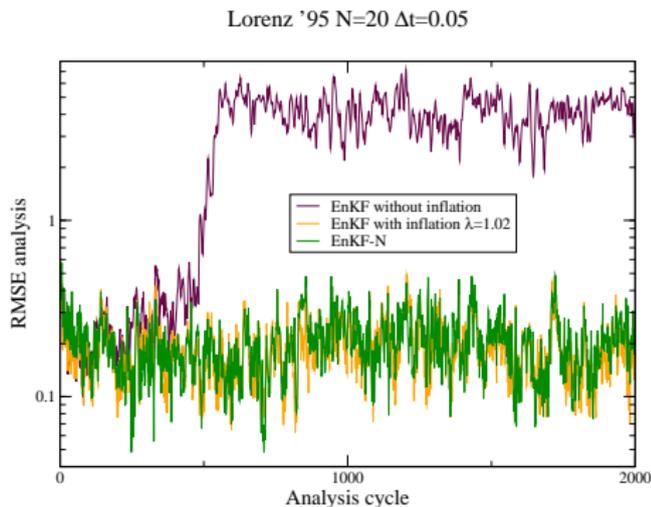
# Outline

- 1 The primal EnKF-N
- 2 The dual EnKF-N
- 3 The iterative ensemble Kalman filter & smoother
- 4 Conclusions

## Failure of the raw ensemble Kalman filter (EnKF)

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

► To properly work, it needs fixes: **localisation** and **inflation**.



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

$$\bar{\mathbf{x}} = \frac{1}{N} \sum_{n=1}^N \mathbf{x}_k, \quad \mathbf{P} = \frac{1}{N-1} \sum_{k=1}^N (\mathbf{x}_k - \bar{\mathbf{x}})(\mathbf{x}_k - \bar{\mathbf{x}})^T. \quad (1)$$

Yet,  $\bar{\mathbf{x}}$  and  $\mathbf{P}$  may not be the true moments of the true filtering distribution (assuming there is one!). Hidden true moments of the true filtering distribution:  $\mathbf{x}_b$  and  $\mathbf{B}$ .

## Getting more from the ensemble

► Idea: even under Gaussian assumptions of the true distribution, the pdf  $p(\mathbf{x}|\mathbf{x}_1, \dots, \mathbf{x}_N)$  extracts more information than  $p(\mathbf{x}|\bar{\mathbf{x}}, \mathbf{P})$ .

► Using Gaussian assumptions, and being only interested in the filtering problem, one can get (hierarchical reasoning):

$$p(\mathbf{x}|\mathbf{x}_1, \dots, \mathbf{x}_N) = \frac{1}{p(\mathbf{x}_1, \dots, \mathbf{x}_N)} \int d\mathbf{x}_b d\mathbf{B} p(\mathbf{x}|\mathbf{x}_b, \mathbf{B}) p(\mathbf{x}_1, \dots, \mathbf{x}_N|\mathbf{x}_b, \mathbf{B}) p(\mathbf{x}_b, \mathbf{B}). \quad (2)$$

- $p(\mathbf{x}|\mathbf{x}_b, \mathbf{B})$ : the standard Gaussian prior but based on the true statistics.
- $p(\mathbf{x}_1, \dots, \mathbf{x}_N|\mathbf{x}_b, \mathbf{B}) = \prod_{k=1}^N p(\mathbf{x}_k|\mathbf{x}_b, \mathbf{B})$
- $p(\mathbf{x}_b, \mathbf{B})$ : prior for the background statistics!

## Choosing priors for the background statistics

- To progress, we need to make assumptions on the background statistics  $p(\mathbf{x}_b, \mathbf{B})$ : **the statistics of the error statistics** or **hyperpriors**.

A very simple choice is a **weakly informative prior**: the Jeffreys' prior [Jeffreys 1961] with an additional assumption of independence for  $\mathbf{x}_b$  and  $\mathbf{B}$ :

$$p(\mathbf{x}_b, \mathbf{B}) \equiv p_J(\mathbf{x}_b, \mathbf{B}) = p_J(\mathbf{x}_b)p_J(\mathbf{B})$$

and

$$p_J(\mathbf{x}_b) = 1, \quad p_J(\mathbf{B}) = |\mathbf{B}|^{-\frac{M+1}{2}}.$$

- With Jeffreys prior, it is possible to perform the integral (with additional complications due to rank-deficiency usually not dealt with by mathematicians).

## Principle of the EnKF-N

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

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

$$p(\mathbf{x}|\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) \propto \left| (\mathbf{x} - \bar{\mathbf{x}})(\mathbf{x} - \bar{\mathbf{x}})^T + \varepsilon_N (N-1) \mathbf{P} \right|^{-\frac{N}{2}}, \quad (3)$$

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

- ▶ Ensemble space decomposition (ETKF version of the filters):  $\mathbf{x} = \bar{\mathbf{x}} + \mathbf{A}\mathbf{w}$ .
- ▶ The variational principle of the analysis (in ensemble space):

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

$$\mathcal{J}(\mathbf{w}) = \frac{1}{2} (\mathbf{y} - H(\bar{\mathbf{x}} + \mathbf{A}\mathbf{w}))^T \mathbf{R}^{-1} (\mathbf{y} - H(\bar{\mathbf{x}} + \mathbf{A}\mathbf{w})) + \frac{N}{2} \ln (\varepsilon_N + \mathbf{w}^T \mathbf{w}). \quad (4)$$

## EnKF-N: algorithm

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

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

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

## The Lorenz '95 model

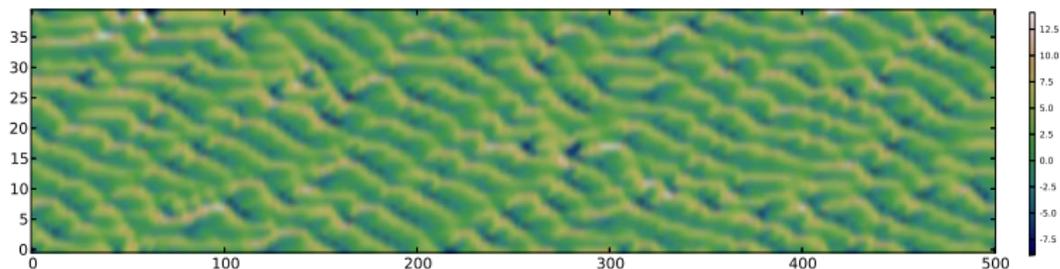
► The toy-model [Lorenz and Emmanuel 1998]:

- It represents a mid-latitude zonal circle of the global atmosphere.
- $M = 40$  variables  $\{x_m\}_{m=1,\dots,M}$ . For  $m = 1, \dots, M$ :

$$\frac{dx_m}{dt} = (x_{m+1} - x_{m-2})x_{m-1} - x_m + F,$$

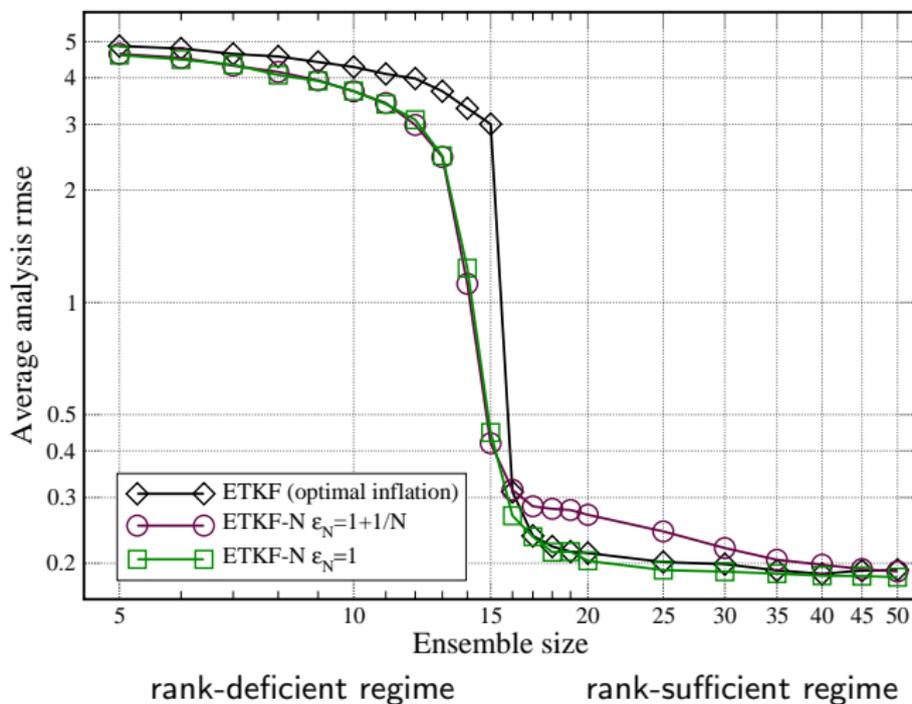
where  $F = 8$ , and the boundary is cyclic.

- 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,  $\mathbf{R} = \mathbf{I}$ .



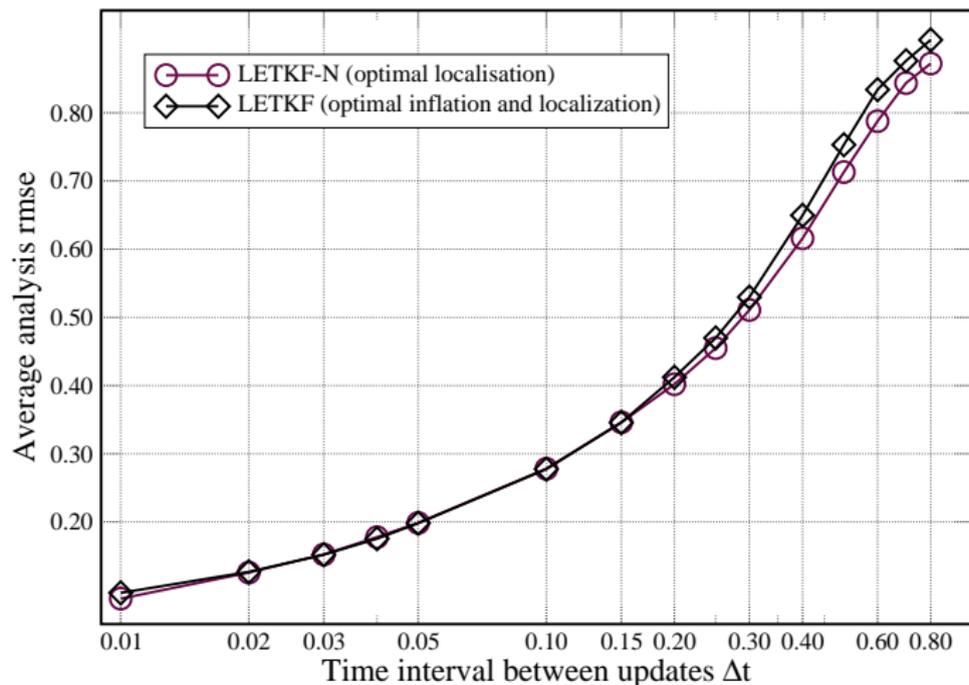
## Application to the Lorenz '95 model

- EnKF-N: analysis rmse versus ensemble size, for  $\Delta t = 0.05$ .



## Application to the Lorenz '95 model

- Local version: LETKF-N, with  $N = 10$  (beware  $\Delta t = 0.01$  requires a correction).



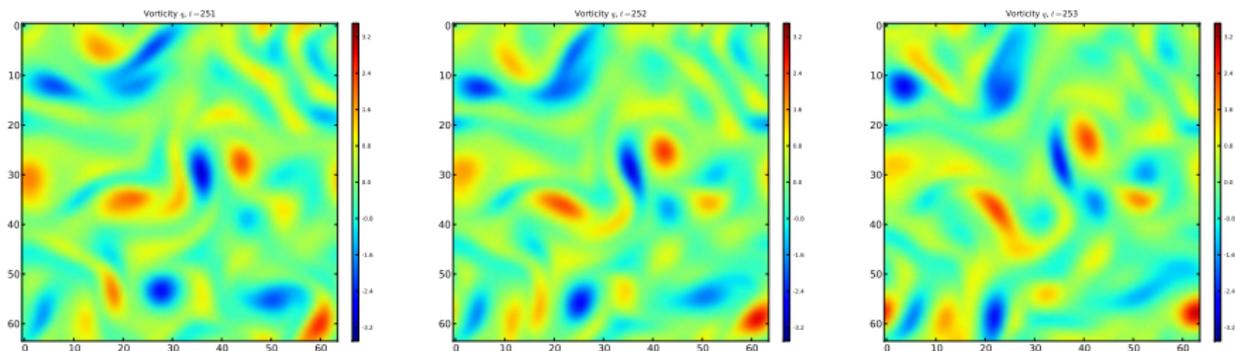
## Forced 2D turbulence model

- Forced 2D turbulence model

$$\frac{\partial q}{\partial t} + J(q, \psi) = \lambda q + \nu \Delta^2 q + F, \quad q = \Delta \psi, \quad (5)$$

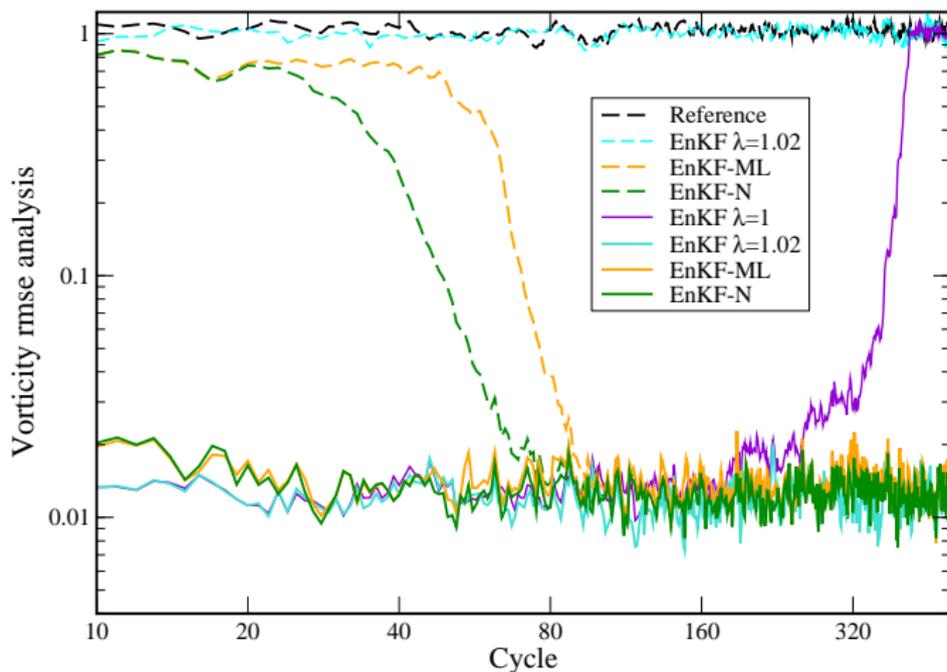
where  $J(q, \psi) = \partial_x q \partial_y \psi - \partial_y q \partial_x \psi$ ,  $q$  is the vorticity 2D field,  $\psi$  is the current function 2D field,  $F$  is the forcing,  $\lambda$  amplitude of the friction,  $\nu$  amplitude of the biharmonic diffusion, grid:  $64 \times 64$  small enough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

- Setup of the experiment: Time-lag between update:  $\Delta_t = 2$ , fully observed,  $\mathbf{R} = 0.1\mathbf{I}$ .



## Application to forced 2D turbulence

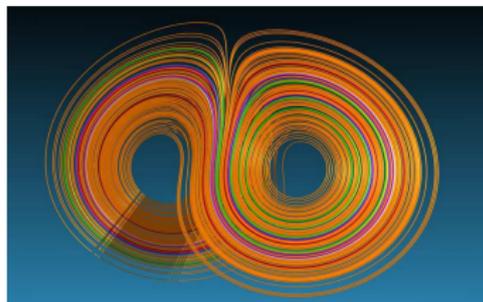
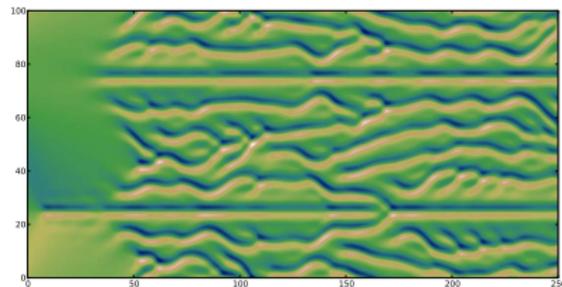
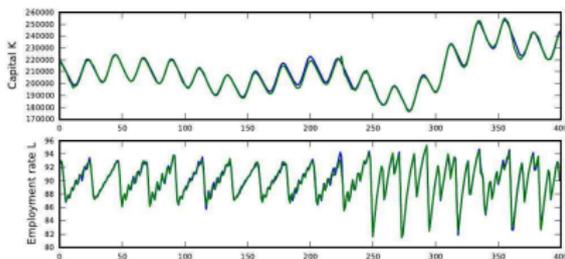
- Comparison of: EnKF with uniform inflation, EnKF-N, adaptive inflation EnKF (EnKF-ML),  $N = 80$  (rank-sufficient regime). Starting away or close from the truth.



## Also tested on ...

## ► EnKF-N also tested on:

- Lorenz '63 model, [Lorenz, 1963]
- Kuramoto-Sivashinski model, [Kuramoto, 1975; Sivashinski, 1977]
- NEDyM economical model, [Hallegatte, Ghil and co-authors, 2008-2012]



Credit: <http://images.math.cnrs.fr>

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- 1 The primal EnKF-N
- 2 The dual EnKF-N**
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## Lagrangian duality

- ▶ The **primal** EnKF-N cost function:

$$\mathcal{J}(\mathbf{w}) = \frac{1}{2}(\mathbf{y} - H(\bar{\mathbf{x}} + \mathbf{X}\mathbf{w}))^T \mathbf{R}^{-1}(\mathbf{y} - H(\bar{\mathbf{x}} + \mathbf{X}\mathbf{w})) + \frac{N}{2} \ln(\varepsilon_N + \mathbf{w}^T \mathbf{w}). \quad (6)$$

- ▶ **Idea:** Split the radial degree of freedom of  $\mathbf{w}$ , that is  $\sqrt{\mathbf{w}^T \mathbf{w}}$ , from its angular degrees of freedom, that is  $\mathbf{w}/\sqrt{\mathbf{w}^T \mathbf{w}}$ .

- ▶ Lagrangian:

$$\mathcal{L}(\mathbf{w}, \rho, \zeta) = \frac{1}{2}(\delta - \mathbf{Y}\mathbf{w})^T \mathbf{R}^{-1}(\delta - \mathbf{Y}\mathbf{w}) + \frac{1}{2}\zeta(\mathbf{w}^T \mathbf{w} - \rho) + \frac{N}{2} \ln(\varepsilon_N + \rho), \quad (7)$$

where  $\delta = \mathbf{y} - \mathbf{H}\bar{\mathbf{x}}$ .

- ▶ Saddle point equations:

$$\begin{cases} \zeta^* = N/(\varepsilon_N + \rho^*) \\ \zeta^* \mathbf{w}^* = -\mathbf{Y}^T \mathbf{R}^{-1}(\delta - \mathbf{Y}\mathbf{w}^*) \end{cases} \Rightarrow \begin{cases} \rho^* = N/\zeta^* - \varepsilon_N \\ \mathbf{w}^* = (\zeta^* + \mathbf{Y}^T \mathbf{R}^{-1} \mathbf{Y})^{-1} \mathbf{Y}^T \mathbf{R}^{-1} \delta \end{cases} \quad (8)$$

## Non-convex strong duality

- **Dual** cost function defined for  $\zeta > 0$  by

$$\begin{aligned} \mathcal{D}(\zeta) &= \inf_{\mathbf{w}} \sup_{\rho \geq 0} \mathcal{L}(\mathbf{w}, \rho, \zeta) \\ &= \frac{1}{2} \delta^T \left( \mathbf{R} + \mathbf{Y} \zeta^{-1} \mathbf{Y}^T \right)^{-1} \delta + \frac{\varepsilon_N \zeta}{2} + \frac{N}{2} \ln \frac{N}{\zeta} - \frac{N}{2}. \end{aligned} \quad (9)$$

- Dual and primal problems:

$$\Delta = \inf_{\zeta > 0} \mathcal{D}(\zeta) \quad \text{and} \quad \Pi = \inf_{\mathbf{w}} \mathcal{J}(\mathbf{w}). \quad (10)$$

- **Strong duality** result (non quadratic, non-convex case!):

$$\Delta = \Pi. \quad (11)$$

## The dual EnKF-N scheme

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

$$\zeta_a = \min_{\zeta \in ]0, N/\varepsilon_N]} \left\{ \delta^T \left( \mathbf{R} + \mathbf{Y}\zeta^{-1}\mathbf{Y}^T \right)^{-1} \delta + \varepsilon_N \zeta + N \ln \frac{N}{\zeta} - N \right\} \quad (12)$$

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

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## Iterative ensemble Kalman filters

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

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- ▶ 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 filters

► A fairly recent idea:

[Gu & Oliver, 2007]: The idea.

[Kalnay & Yang, 2010]: A step in the right direction.

[Sakov, Oliver & Bertino, 2011]: The “*pièce de résistance*”

[Bocquet & Sakov, 2012]: Correction of the bundle scheme + ensemble transform form.

► IEnKF cost function in ensemble space:

$$\begin{aligned} \tilde{\mathcal{J}}(\mathbf{w}) &= \frac{1}{2} (\mathbf{y}_2 - H_2(\mathcal{M}_{1 \rightarrow 2}(\bar{\mathbf{x}}_1 + \mathbf{A}_1 \mathbf{w})))^T \mathbf{R}_2^{-1} (\mathbf{y}_2 - H_2(\mathcal{M}_{1 \rightarrow 2}(\bar{\mathbf{x}}_1 + \mathbf{A}_1 \mathbf{w}))) \\ &\quad + \frac{1}{2} (N-1) \mathbf{w}^T \mathbf{w}. \end{aligned} \quad (13)$$

► Gauss-Newton scheme:

$$\begin{aligned} \mathbf{w}^{(p+1)} &= \mathbf{w}^{(p)} - \tilde{\mathcal{H}}_{(p)}^{-1} \nabla \tilde{\mathcal{J}}(\mathbf{w}^{(p)}) \\ \nabla \tilde{\mathcal{J}}_{(p)} &= -\mathbf{Y}_{(p)}^T \mathbf{R}_2^{-1} \left( \mathbf{y}_2 - H_2 \mathcal{M}_{1 \rightarrow 2}(\bar{\mathbf{x}} + \mathbf{A}_1 \mathbf{w}^{(p)}) \right) + (N-1) \mathbf{w}^{(p)}, \\ \tilde{\mathcal{H}}_{(p)} &= (N-1) \mathbf{I}_N + \mathbf{Y}_{(p)}^T \mathbf{R}_2^{-1} \mathbf{Y}_{(p)}, \quad \mathbf{Y}_{(p)} = [H_2 \mathcal{M}_{2 \leftarrow 1} \mathbf{A}_1]_{(p)}', \end{aligned} \quad (14)$$

## Iterative ensemble Kalman filters

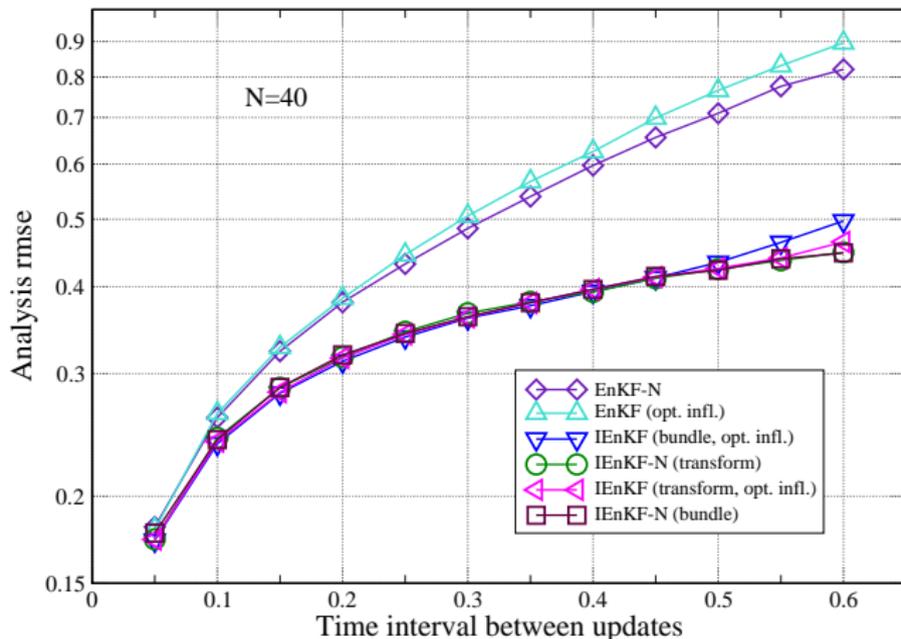
- ▶ Sensitivities  $\mathbf{Y}_{(p)}$  computed by ensemble propagation without TLM and adjoint.
- ▶ Finite-size versions of the filter are just defined by substituting the prior:

$$\frac{N-1}{2} \mathbf{w}^T \mathbf{w} \longrightarrow \frac{N}{2} \ln \left( \varepsilon_N + \mathbf{w}^T \mathbf{w} \right). \quad (15)$$

- ▶ As a variational **reduced** method, one can use Gauss-Newton [Sakov et al., 2012], Levenberg-Marquardt [Bocquet and Sakov, 2012; Chen and Oliver, 2012], etc, minimisation schemes (not limited to quasi-Newton).
- ▶ Essentially a lag-one smoother. Does the job of a lag-one 4D-Var, with dynamical error covariance matrix and without **the use of the TLM and adjoint!** Very efficient in very nonlinear conditions if one can afford the multiple ensemble propagations.

## Finite-size iterative ensemble Kalman filters

- ▶ Setup: Lorenz '95,  $M = 40$ ,  $N = 40$ ,  $\Delta t = 0.05 - 0.60$ ,  $\mathbf{R} = \mathbf{I}$ .
- ▶ Comparison of EnKF-N, EnKF (optimal inflation), IEnKF-N (bundle and transform), IEnKF (bundle and transform, optimal inflation)

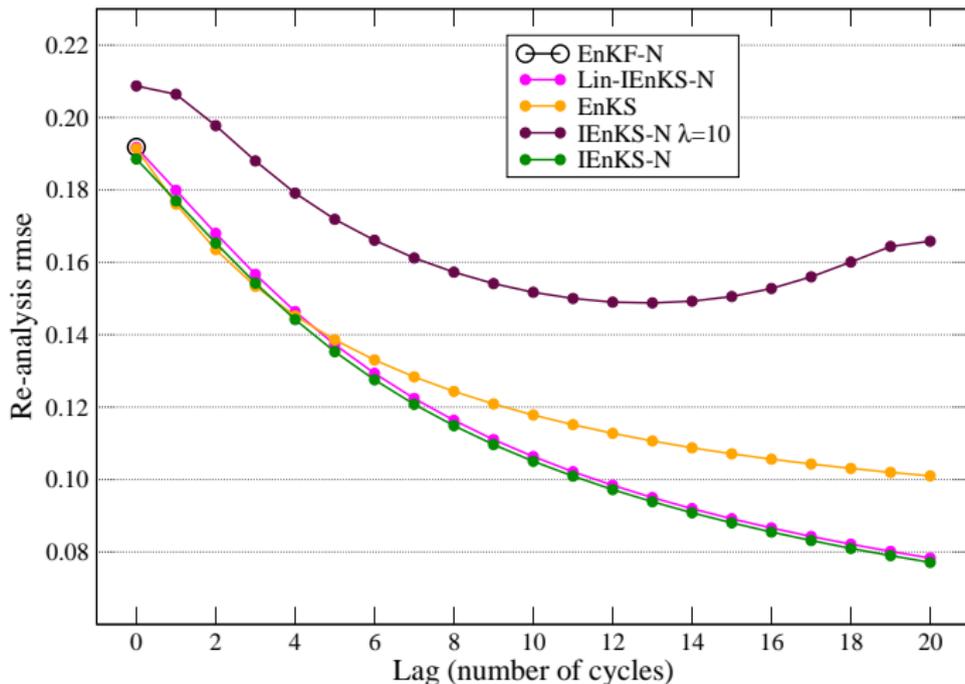


## Iterative ensemble Kalman smoothers

- ▶ In a mildly nonlinear context (built on linear and Gaussian hypotheses)  
Many earlier studies, see [Cosme et al., 2012] for a review, and [Cosme et al., 2010] for an application to oceanography.
  
- ▶ In a non-sequential but very non-linear context  
Many earlier studies, for instance [Evensen and van Leeuwen, 2000]  
[Chen & Oliver, 2012] in the context of reservoir modelling
  
- ▶ Sequential nonlinear context: [This talk]  
The IEnKS cost function is just the extension of the IEnKF cost function for a temporal window of  $L$  cycles.

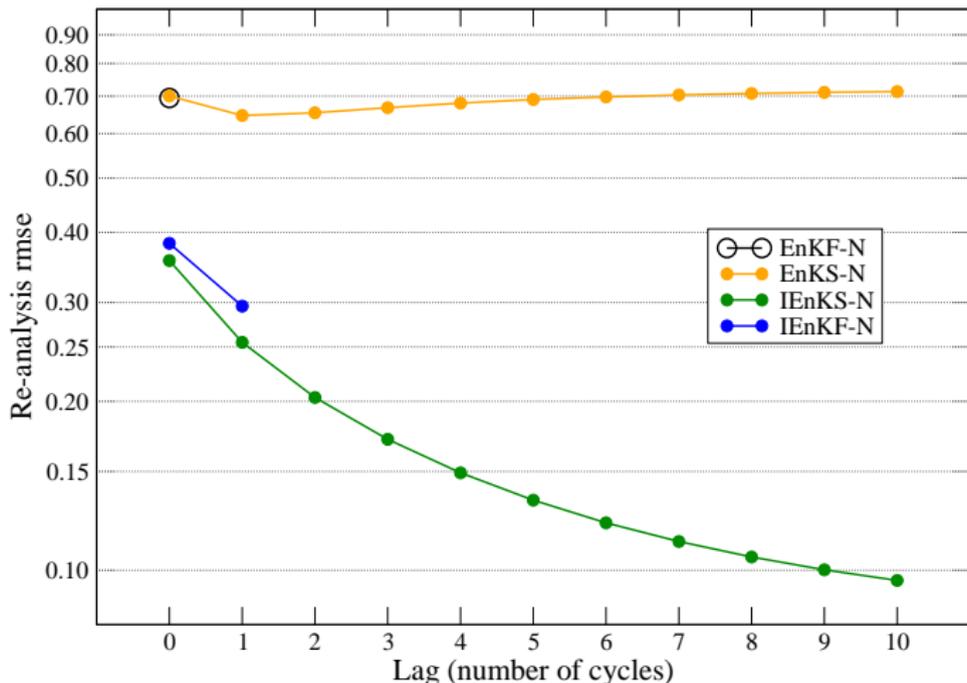
## Finite-size iterative ensemble Kalman smoothers

- ▶ Setup: Lorenz '95,  $M = 40$ ,  $N = 20$ ,  $\Delta t = 0.05$ ,  $\mathbf{R} = \mathbf{I}$ .
- ▶ Comparison of EnKF-N, IEnKS-N, Lin-IEnKS-N, EnKS-N, IEnKS-N with a large inflation (reduced-rank 4D-Var?), with  $L = 20$ .



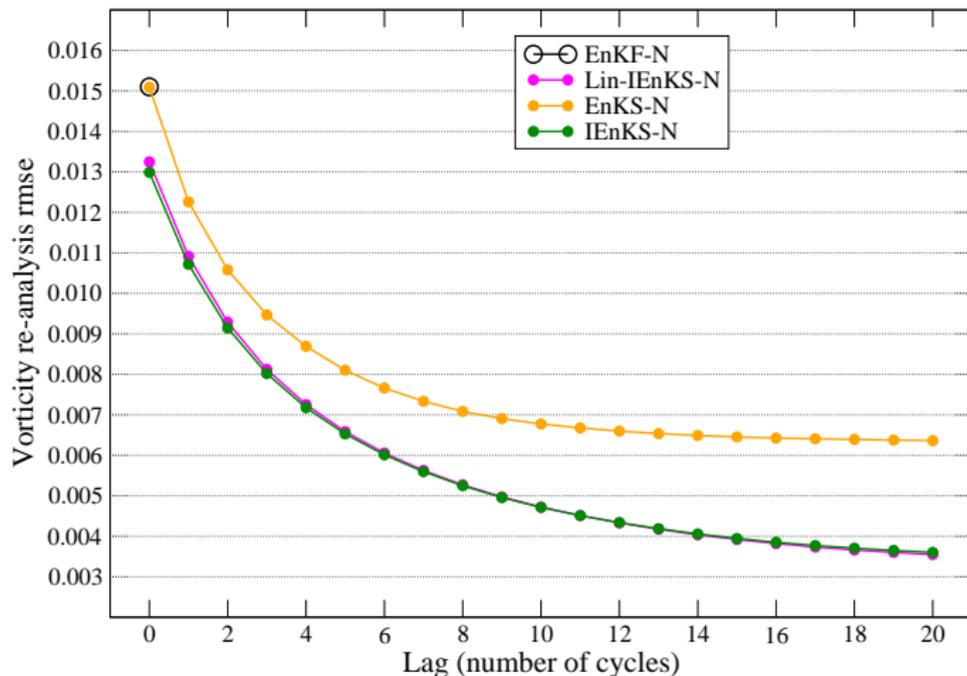
## Finite-size iterative ensemble Kalman smoothers

- ▶ Setup: Lorenz '95,  $M = 40$ ,  $N = 20$ ,  $\Delta t = 0.30$ ,  $\mathbf{R} = \mathbf{I}$ .
- ▶ Comparison of EnKF-N, IEnKF-N, IEnKS-N, ETKS-N, with  $L = 10$ .
- ▶ Lin-IEnKS-N has (understandably) diverged.



## Finite-size iterative ensemble Kalman smoothers

- ▶ Setup: 2D turbulence,  $64 \times 64$ ,  $N = 40$ ,  $\Delta t = 2$ ,  $\mathbf{R} = 0.1\mathbf{I}$ .
- ▶ Comparison of EnKF-N, IEnKF-N, IEnKS-N, ETKS-N, with  $L = 20$ .



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## Conclusions

- A new prior for the ensemble forecast meant to be used in an EnKF analysis has been built. It takes into account **sampling errors**.
- It yields a new class of filters **EnKF-N**, that **does not seem to require inflation** supposed to account for sampling errors.
- Local variants (both LA and CL) available.
- Dual variant EnKF-N is an EnKF with built-in *optimal* inflation (accounting for sampling errors).
- Almost linear regime more problematic because of Jeffreys' prior. Another hyperprior is needed.
- The iterative ensemble Kalman filter has been generalised to an iterative ensemble Kalman smoother (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 better retrospective analysis than standard Kalman smoothers in mildly nonlinear conditions.
- When affordable, it beats other Kalman filter/smoothers in strongly non-linear conditions.

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