An iterative ensemble Kalman smoother

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The IEnKS: at the crossroad between the EnKF and 4D-Var

- The IEnKS follows the scheme of the EnKF:

Deterministic analysis → Posterior ensemble generation → Ensemble forecast

- Except that:
  - The analysis in ensemble space is variational [e.g. Zupanski, 2005] over a finite time windows. It may require several iterations in strongly nonlinear conditions [Gu & Oliver, 2007; Sakov et al., 2012; Bocquet and Sakov, 2012-2014].
  - The gradient of the 4D cost function is computed with the ensemble [Gu & Oliver, 2007; Liu et al., 2008; Buehner et al. 2010]: no need for the tangent linear/adjoint.

- It generalises the iterative extended Kalman filter/smoother [Wishner et al., 1969; Jazwinski, 1970; Bell, 1994] to ensemble methods.

- It is a unified/straightforward scheme (no hybridisation so to speak).

- The IEnKS belongs to the class of ensemble variational (EnVar) methods. Other members of the family are: Hybrid methods, 4D-Var-Ben, 4DEnVar, Ensemble of data assimilation (EDA), etc.

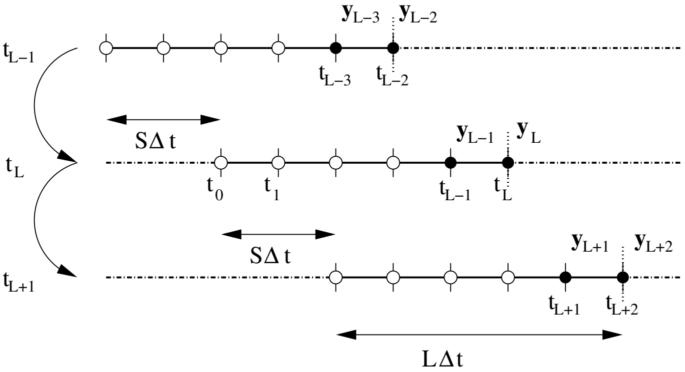
- The IEnKF/IEnKS differ from the other ones in that they stem from a convincing (heuristic) Bayesian derivation.
This derivation says that, under the conditions that:
- the prior is assumed Gaussian,
- the statistics of the errors are modeled by an ensemble,
and without worying about practical implementation, the solution is unique.

- Besides, and very importantly, the complete cycle (i.e. including posterior ensemble generation) has been including from the very beginning (EnKF inheritance).

- The IEnKS has potential for parameter estimation, as it is variational but avoids the derivation of the adjoint.

The IEnKS: the cycling

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



The IEnKS: a variational standpoint

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

$$\mathscr{J}(\mathbf{x}_0) = \sum_{k=1}^{L} \frac{1}{2}\left(\mathbf{y}_k - H_k \circ \mathscr{M}_{k\leftarrow 0}(\mathbf{x}_0)\right)^{\mathrm{T}} \beta_k \mathbf{R}_k^{-1}\left(\mathbf{y}_k - H_k \circ \mathscr{M}_{k\leftarrow 0}(\mathbf{x}_0)\right) + \frac{1}{2}\left(\mathbf{x}_0 - \overline{\mathbf{x}}_0\right)\mathbf{P}_0^{-1}\left(\mathbf{x}_0 - \overline{\mathbf{x}}_0\right). \tag{1}$$

$\{\beta_0, \beta_1, \ldots, \beta_L\}$ weight the observations impact within the window.

- 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:

$$\widetilde{\mathscr{J}}(\mathbf{w}) = \mathscr{J}\left(\overline{\mathbf{x}}_0 + \mathbf{A}_0\mathbf{w}\right). \tag{2}$$

- IEnKS cost function in ensemble space [Hunt et al., 2007; Bocquet and Sakov, 2012-2014]:

$$\widetilde{\mathscr{J}}(\mathbf{w}) = \frac{1}{2}\sum_{k=1}^{L}\left(\mathbf{y}_k - H_k \circ \mathscr{M}_{k\leftarrow 0}\left(\overline{\mathbf{x}}_0 + \mathbf{A}_0\mathbf{w}\right)\right)^{\mathrm{T}} \beta_k \mathbf{R}_k^{-1}\left(\mathbf{y}_k - H_k \circ \mathscr{M}_{k\leftarrow 0}\left(\overline{\mathbf{x}}_0 + \mathbf{A}_0\mathbf{w}\right)\right) + \frac{1}{2}(N-1)\mathbf{w}^{\mathrm{T}}\mathbf{w}. \tag{3}$$

The 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], quasi-Newton, etc., minimisation schemes.
- Gauss-Newton scheme (the Hessian is approximate):

$$
\begin{aligned}
\mathbf{w}^{(p+1)} &= \mathbf{w}^{(p)} - \widetilde{\mathscr{H}}_{(p)}^{-1} \nabla \widetilde{\mathscr{J}}_{(p)}(\mathbf{w}^{(p)}) , \\
\mathbf{x}_0^{(p)} &= \mathbf{x}_0^{(0)} + \mathbf{A}_0 \mathbf{w}^{(p)} , \\
\nabla \widetilde{\mathscr{J}}_{(p)} &= - \sum_{k=1}^{L} \mathbf{Y}_{k,(p)}^{\mathrm{T}} \beta_k \mathbf{R}_k^{-1} \left(\mathbf{y}_k - H_k \circ \mathscr{M}_{k\leftarrow 0}(\mathbf{x}_0^{(p)}) \right) + (N-1)\mathbf{w}^{(p)} , \\
\widetilde{\mathscr{H}}_{(p)} &= (N-1)\mathbf{I}_N + \sum_{k=1}^{L} \mathbf{Y}_{k,(p)}^{\mathrm{T}} \beta_k \mathbf{R}_L^{-1} \mathbf{Y}_{(p)} , \\
\mathbf{Y}_{k,(p)} &= [H_k \circ \mathscr{M}_{k\leftarrow 0}]'_{|\mathbf{x}_0^{(p)}} \mathbf{A}_0 .
\end{aligned}
\tag{4}
$$

- One solution to compute the 4D sensitivities: the bundle scheme. It simply mimics the action of the tangent linear by finite difference:

$$
\mathbf{Y}_{k,(p)} \approx \frac{1}{\varepsilon} H_k \circ \mathscr{M}_{k\leftarrow 0} \left(\mathbf{x}^{(p)} \mathbf{1}^{\mathrm{T}} + \varepsilon \mathbf{A}_0 \right) \left(\mathbf{I}_N - \frac{\mathbf{1}\mathbf{1}^{\mathrm{T}}}{N} \right) . \tag{5}
$$

The IEnKS: ensemble update and the forecast step

- Generate an updated ensemble from the previous analysis:

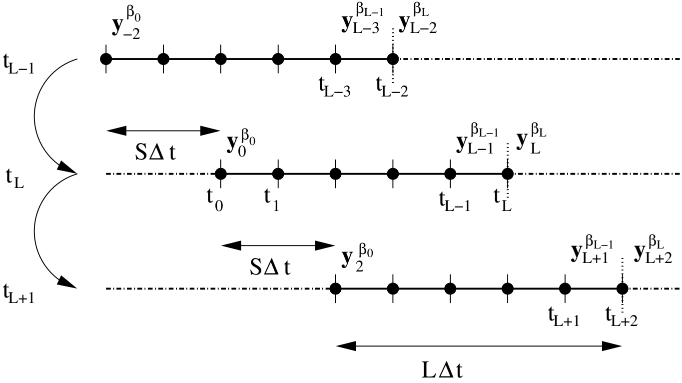
$$\mathbf{E}_0^\star = \mathbf{x}_0^\star \mathbf{1}^\mathrm{T} + \sqrt{N-1}\mathbf{A}_0 \widetilde{\mathscr{H}}_\star^{-1/2}\mathbf{U} \quad \text{where} \quad \mathbf{U1} = \mathbf{1}, \quad \mathbf{u} = (1, 1, \ldots, 1)^\mathrm{T}. \tag{6}$$

- Just propagate the updated ensemble from t_0 to t_S:

$$\mathbf{E}_S = \mathscr{M}_{S \leftarrow 0}(\mathbf{E}_0). \tag{7}$$

- In the quasi-static, most efficient but costly case: $S = 1$.

IEnKS: single vs multiple data assimilation



- SDA IEnKS: The observation vector are assimilated once and for all. Exact scheme.

- MDA IEnKS: The observation vector are assimilated several times and weighted by β_k within the window. Approximate scheme in nonlinear conditions.

IEnKS: single vs multiple data assimilation

- 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 [Emerick and Reynolds, 2012]. Maybe more stable over long windows.
  - The multiple assimilation of each observation with its original weights. It is (heuristically) 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 reweights the observations within the data assimilation window, and perform a final analysis.

Iterative ensemble Kalman filter: accounting for sampling errors

- Finite-size versions of the iterative filter are just defined by substituting the prior:

$$\frac{N-1}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} \longrightarrow \frac{N}{2}\ln\left(\varepsilon_N + \mathbf{w}^{\mathrm{T}}\mathbf{w}\right). \tag{8}$$

- It implicitly (primal) or explicitly (dual) defines an optimal multiplicative inflation meant to compensate for sampling errors, related to the argmin of a dual cost function

$$\lambda^\star = \sqrt{\frac{N-1}{\zeta^\star}}, \qquad \zeta^\star = \operatorname{argmin} \mathscr{D}(\zeta). \tag{9}$$

$$\mathscr{D}(\zeta) = \frac{1}{2}\delta^{\mathrm{T}}\left(\mathbf{R}+\mathbf{Y}\zeta^{-1}\mathbf{Y}^{\mathrm{T}}\right)^{-1}\delta + \frac{\varepsilon_N\zeta}{2} + \frac{N}{2}\ln\frac{N}{\zeta} - \frac{N}{2}. \tag{10}$$

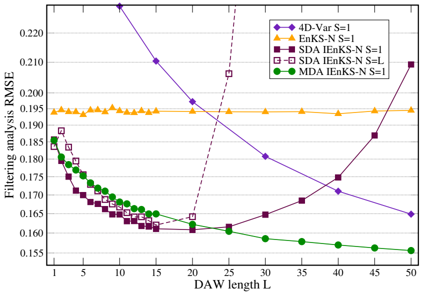
- This adaptive scheme is quite useful since the IEnKS may require substantial inflation in strongly nonlinear regimes (because of subsequent sampling errors).

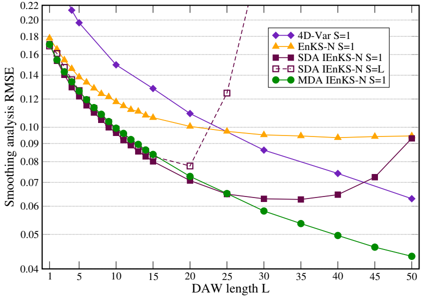
- Also (very) useful for extensive numerical experiments (no need to tune the inflation!).

Application to the Lorenz-95 model

- Weakly nonlinear case: Lorenz-95, $M = 40$, $N = 20$, $\Delta t = 0.05$, $\mathbf{R} = \mathbf{I}$.

- Comparison of 4D-Var $S = 1$, EnKS $S = 1$, SDA IEnKS $S = 1$, SDA IEnKS $S = L$, and MDA IEnKS $S = 1$.

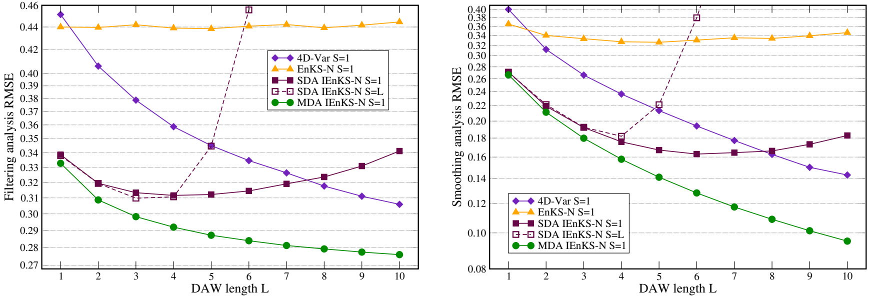




Application to the Lorenz-95 model

- Strongly nonlinear case: Lorenz-95, $M = 40$, $N = 20$, $\Delta t = 0.20$, $\mathbf{R} = \mathbf{I}$.

- Comparison of 4D-Var $S = 1$, EnKS $S = 1$, SDA IEnKS $S = 1$, SDA IEnKS $S = L$, and MDA IEnKS $S = 1$.

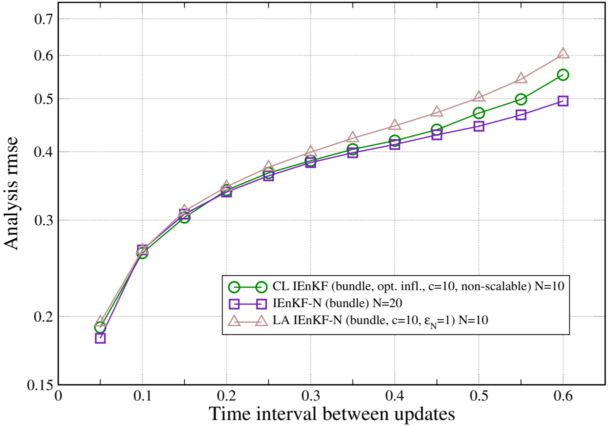


IEnKF/IEnKS: Localisation

- Localisation in an EnVar context is non-trivial because localisation and the evolution model do not commute:

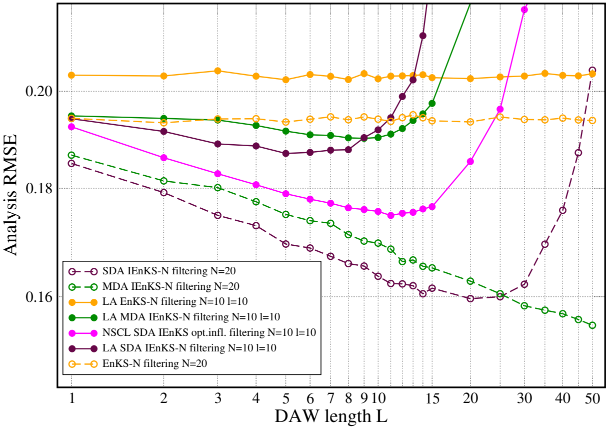
$$\mathbf{M}_{k\leftarrow 0}\left(\mathbf{C}\circ\mathbf{B}_0\right)\mathbf{M}_{k\leftarrow 0}^{\mathrm{T}} \neq \mathbf{C}\circ\left(\mathbf{M}_{k\leftarrow 0}\mathbf{B}_0\mathbf{M}_{k\leftarrow 0}^{\mathrm{T}}\right). \quad (11)$$

- Local analysis of the IEnKF, and comparison with a non-scalable optimal approach.



IEnKF/IEnKS: Localisation

- Local analysis of the IEnKS, and comparison with a non-scalable optimal approach (filtering performance).



IEnKF/IEnKS: Augmented state formalism

- IEnKS treats parameters the way both 4D-Var and EnKF treat them.

- The state space is augmented from $\mathbf{x} \in \mathbb{R}^M$ to a vector

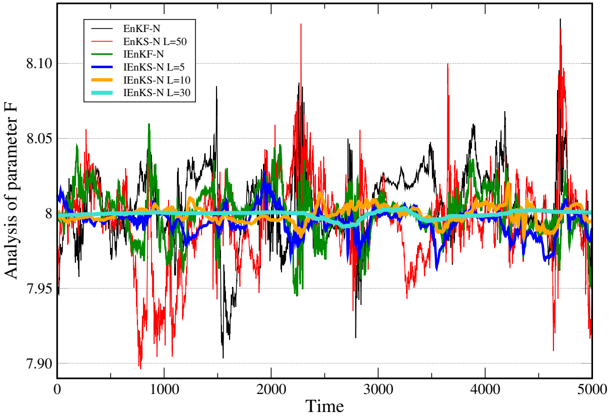
$$\mathbf{0} = \begin{pmatrix} \mathbf{x} \\ \theta \end{pmatrix} \in \mathbb{R}^{M+P}, \tag{12}$$

Technically, there is nothing more to the joint state and parameter IEnKS than in the state IEnKS.

- A forward model needs to be introduced for the parameters:
  - For instance, the persistence model ($\theta_{k+1} = \theta_k$),
  - or some jittering such as a Brownian motion ($\theta_{k+1} = \theta_k + \varepsilon_k$).

Estimation of the Lorenz-95 forcing parameter F

- F is static but unknown.

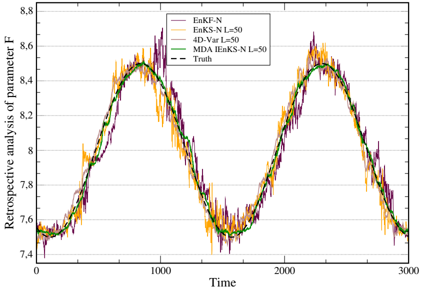


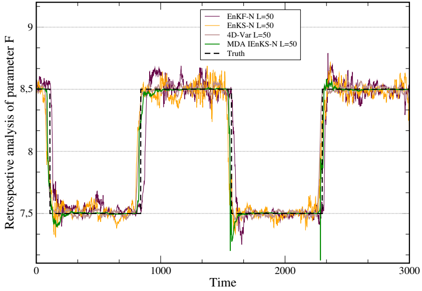
- Augmented state vector $\in \mathbb{R}^{41}$, $N = 20$. The forcing of the true model is $F = 8$.
- Evolution model for F: persistence assumption.

Estimation of the Lorenz-95 forcing parameter F

- The forcing parameter F is time-varying and unknown.
- Internalised model error (F is in the augmented state) + unaccounted external model error (the true F is time-varying $\neq$ persistence assumption).

Method / F profile	Sinusoidal	Step-wise
EnKF-N	0.063	0.079
EnKS-N L=50	0.040	0.063
4D-Var L=50	0.030	0.045
MDA IEnKS-N L=50	0.020	0.031





Weak constraint IEnKS

- Weak constraint 4D-Var analysis cost function:

$$\mathscr{L} = \frac{1}{2}\sum_{k=1}^{K} ||\mathbf{y}_k - H_k(\mathbf{x}_k)||^2_{\mathbf{R}_k^{-1}} + \frac{1}{2}\sum_{k=1}^{K} ||\mathbf{x}_k - M_{k\leftarrow k-1}(\mathbf{x}_{k-1})||^2_{\mathbf{Q}_k^{-1}} + \frac{1}{2}||\mathbf{x}_0 - \mathbf{x}_b||^2_{\mathbf{B}^{-1}} \quad (13)$$

- Gauss-Newton (non-incremental) iteration of the weak constraint 4D-Var analysis (dual, i.e. PSAS way):

$$\underline{\mathbf{x}}^{j+1} = \underline{\mathbf{x}}^{j} - \mathbf{L}^{-1}\underline{\eta} + \mathbf{L}\mathbf{D}\mathbf{L}^{\mathrm{T}}\mathbf{H}^{\mathrm{T}}\left(\mathbf{H}\mathbf{L}\mathbf{D}\mathbf{L}^{\mathrm{T}}\mathbf{H}^{\mathrm{T}} + \mathbf{R}\right)^{-1}\left(\underline{\delta} - \mathbf{H}\mathbf{L}^{-1}\underline{\eta}\right). \quad (14)$$

All objects are 4-dimensional.
$\underline{\delta}$, $\underline{\eta}$ are perturbations around the reference trajectory.
Using Fisher/Desroziers' notations:

$$\mathbf{D} = \begin{bmatrix} \mathbf{B} & & & & \\ & \mathbf{Q}_1 & & & \\ & & \mathbf{Q}_2 & & \\ & & & \ddots & \\ & & & & \mathbf{Q}_K \end{bmatrix} \qquad \mathbf{L} = \begin{bmatrix} \mathbf{I} & & & & \\ \mathbf{M}_{1\leftarrow 0} & \mathbf{I} & & & \\ \mathbf{M}_{2\leftarrow 0} & \mathbf{M}_{2\leftarrow 1} & \mathbf{I} & & \\ \vdots & & \ddots & \ddots & \\ \mathbf{M}_{K\leftarrow 0} & \mathbf{M}_{K\leftarrow 1} & \cdots & \mathbf{M}_{K\leftarrow K-1} & \mathbf{I} \end{bmatrix} \quad (15)$$

Weak constraint IEnKS

▶ Weak constraint IEnKS analysis cost function: many options. But not many practical with potential. One elegant option is to perform the analysis in the following subspace:

$$k = 0, \ldots, K : \qquad \mathbf{x}_k = \mathbf{x}_k^j + \mathbf{A}_k^j \mathbf{w}_k \tag{16}$$

where the ensemble anomalies are defined as $\mathbf{A}_k^j = \mathbf{M}_{k\leftarrow k-1}^j \mathbf{A}_{k-1}^j$, $\mathbf{w} \in \mathbb{R}^{(K+1)\times N}$.

▶ Choice for the weak constraint IEnKS and comparison with the weak constraint 4D-Var and 4DEnVar:

- Weak constraint 4D-Var: $\mathbf{B} = \mathbf{L}\mathbf{D}\mathbf{L}^{\mathrm{T}}$
- Weak constraint 4DEnVar: $\mathbf{B} = \mathbf{Z}\mathbf{Z}^{\mathrm{T}}$, with $\mathbf{Z}^{\mathrm{T}} = [\mathbf{Z}_0^{\mathrm{T}}, \mathbf{Z}_1^{\mathrm{T}}, \ldots, \mathbf{Z}_K^{\mathrm{T}}]$
- Weak constraint IEnKS: $\mathbf{B} = \mathbf{A}\boldsymbol{\Xi}\mathbf{A}^{\mathrm{T}}$, with $\boldsymbol{\Xi} = \mathbf{G}\boldsymbol{\Gamma}\mathbf{G}^{\mathrm{T}}$
  - $\mathbf{A} = \bigoplus_{k=0}^{K} \mathbf{A}_k$ (direct sum)
  - $\mathbf{G} = \mathbf{L}$ but with $\mathbf{M}_{k\leftarrow l} = \mathbf{I}$
  - $\boldsymbol{\Gamma} = (N-1)^{-1}\mathbf{I} \oplus \bigoplus_{k=1}^{K} q_k \left(\mathbf{A}_k \mathbf{A}_k^{\mathrm{T}} + \mathbf{u}\mathbf{u}^{\mathrm{T}}\right)$

▶ Weak constraint IEnKS somehow in-between weak constraint 4D-Var and weak constraint 4DEnVar.

Weak constraint IEnKS

- The weak constraint IEnKS has the proper limit when $\mathbf{Q}_k \longrightarrow \mathbf{0}$, i.e., the IEnKS.

- Shares the same mathematical structure as 4DEnVar but with the anomalies of the weak constraint 4D-Var $\mathbf{Z} = \mathbf{L}\mathbf{B}^{1/2}\mathbf{A}$ with $\mathbf{A}$ a matrix of normal i.i.d., albeit in an ensemble space

- Convergence not proven yet.

- Trade-off between the singularity/smoothness of the $\mathbf{Q}_k \rightarrow \mathbf{0}$ limit (call it conditioning) and the use of $\mathbf{L}/\mathbf{L}^{-1}$ depending on whether the analysis is primal or dual. Mike Fisher's saddle point must be the right approach to follow. . . .

- Numerics so far relatively disappointing (but work in progress) on Lorenz-95. Not as performing as one would have expected. The adaptive inflation of IEnKS-N of its finite-size variant is correcting for most errors!

- If correct, then I might become sceptical about the interest of the weak-constraint formalism in general (temporal localisation better than weak constraint formalism ?)

Conclusions

- The iterative ensemble Kalman smoother (IEnKS) is a method to seamlessly combine the advantages of variational and ensemble Kalman filtering.
- The IEnKS is a generalisation of the iterative ensemble Kalman filter (IEnKF). It is an EnVar method. It is flow-dependent, tangent linear and adjoint free.
- The IEnKF/IEnKS have the potential to (significantly) outperform both the EnKF and the 4D-Var in all regimes. IEnKS already does so with toy-models.
- IEnKS is very well suited for parameter (or joint state/parameter) estimation, and does so in a very simple way via the augmented state formalism.
- Weak constraint IEnKS formalism in between weak constraint 4D-Var and weak constraint 4DEnVar.
- More complex reactive air quality toy-model under development in order to test the IEnKS on challenging atmospheric chemistry problems. $\longrightarrow$ see Jean-Matthieu Haussaire's poster.

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