Using the petroleum industry's adjoint-free ensemble methods for sequential data assimilation

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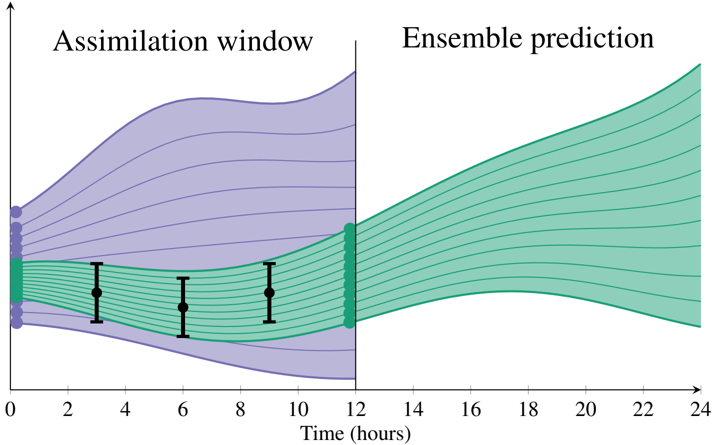
Outline

- Explain ES, IES, ESMDA and relate them to En4DVar.
- Introduce a new chaotic and coupled multiscale test model.
- DA experiments.

Duality of parameter estimation and sequential DA



We start from Bayes' theorem

Bayes' formula

$$f(\mathbf{z}|\mathbf{d}) \propto f(\mathbf{d}|\mathbf{z}) f(\mathbf{z}). \tag{1}$$

Gaussian prior and likelihood gives

$$f(\mathbf{z}|\mathbf{d}) \propto \exp\left\{-\mathcal{J}(\mathbf{z})\right\}, \tag{2}$$

with cost function defined as

$$\mathcal{J}(\mathbf{z}) = \frac{1}{2}\left(\mathbf{z} - \mathbf{z}^{\mathrm{f}}\right)^{\mathrm{T}} \mathbf{C}_{zz}^{-1} \left(\mathbf{z} - \mathbf{z}^{\mathrm{f}}\right) + \frac{1}{2}\left(\mathbf{g}(\mathbf{z}) - \mathbf{d}\right)^{\mathrm{T}} \mathbf{C}_{dd}^{-1} \left(\mathbf{g}(\mathbf{z}) - \mathbf{d}\right). \tag{3}$$

RML approximately samples the posterior Bayes'

Randomized maximum likelihood sampling by Kitanidis (1995)

Define prior realizations

$$\mathbf{z}_j^{\mathrm{f}} \sim \mathcal{N}(\mathbf{z}^{\mathrm{f}}, \mathbf{C}_{zz}) \quad \text{and} \quad \mathbf{d}_j \sim \mathcal{N}(\mathbf{d}, \mathbf{C}_{dd}). \tag{4}$$

RML minimizes the ensemble of cost functions:

$$\mathcal{J}(\mathbf{z}_j) = \frac{1}{2}\left(\mathbf{z}_j - \mathbf{z}_j^{\mathrm{f}}\right)^{\mathrm{T}} \mathbf{C}_{zz}^{-1}\left(\mathbf{z}_j - \mathbf{z}_j^{\mathrm{f}}\right) + \frac{1}{2}\left(\mathbf{g}(\mathbf{z}_j) - \mathbf{d}_j\right)^{\mathrm{T}} \mathbf{C}_{dd}^{-1}\left(\mathbf{g}(\mathbf{z}_j) - \mathbf{d}_j\right). \tag{5}$$

Minima are defined by ensemble of cost-function gradients set to zero

$$\mathbf{C}_{zz}^{-1}\left(\mathbf{z}_j - \mathbf{z}_j^{\mathrm{f}}\right) + \nabla_{\mathbf{z}}\mathbf{g}\left(\mathbf{z}_j\right)\mathbf{C}_{dd}^{-1}\left(\mathbf{g}(\mathbf{z}_j) - \mathbf{d}_j\right) = 0. \tag{6}$$

Solutions methods

Ensemble of GN iterations

$$\mathbf{z}_j^{i+1} = \mathbf{z}_j^i - \gamma\left(\mathbf{C}_{zz}^{-1} + \mathbf{G}_j^{i\,\mathrm{T}}\mathbf{C}_{dd}^{-1}\mathbf{G}_j^i\right)^{-1}\left(\mathbf{C}_{zz}^{-1}\left(\mathbf{z}_j^i - \mathbf{z}_j^{\mathrm{f}}\right) + \mathbf{G}_j^{i\,\mathrm{T}}\mathbf{C}_{dd}^{-1}\left(\mathbf{g}\left(\mathbf{z}_j^i\right) - \mathbf{d}_j\right)\right), \tag{7}$$

Ensemble of incremental 4DVars: $\mathbf{z}_j^{i+1} = \mathbf{z}_j^i + \delta\mathbf{z}_j$

$$\mathcal{J}\left(\delta\mathbf{z}_j\right) = \frac{1}{2}\left(\delta\mathbf{z}_j - \boldsymbol{\xi}_j^i\right)^{\mathrm{T}}\mathbf{C}_{zz}^{-1}\left(\delta\mathbf{z}_j - \boldsymbol{\xi}_j^i\right) + \frac{1}{2}\left(\mathbf{G}_j^i\delta\mathbf{z}_j - \boldsymbol{\eta}_j^i\right)^{\mathrm{T}}\mathbf{C}_{dd}^{-1}\left(\mathbf{G}_j^i\delta\mathbf{z}_j - \boldsymbol{\eta}_j^i\right). \tag{8}$$

A linearization leads to an ensemble of Kalman-smoother updates

$$\mathbf{z}_j^{\mathrm{a}} = \mathbf{z}_j^{\mathrm{f}} + \mathbf{C}_{zz}\mathbf{G}_j^{\mathrm{T}}\left(\mathbf{G}_j\mathbf{C}_{zz}\mathbf{G}_j^{\mathrm{T}} + \mathbf{C}_{dd}\right)^{-1}\left(\mathbf{d}_j - \mathbf{g}\left(\mathbf{z}_j^{\mathrm{f}}\right)\right). \tag{9}$$

Replace the tangent-linear model $\mathbf{G}$ by covariances

Interpret $\mathbf{G}_j^i$ as the best-fit model sensitivity by the linear regression

$$\mathbf{G}_j \approx \mathbf{G} \triangleq \mathbf{C}_{yz}\mathbf{C}_{zz}^{-1}. \tag{10}$$

Introduce an ensemble representation of covariances

Represent the covariance matrices by low-rank ensembles of realizations:

$$\mathbf{Z} = \left(\mathbf{z}_1,\ \mathbf{z}_2,\ \dots\ ,\ \mathbf{z}_N\right), \tag{11}$$

$$\mathbf{D} = \left(\mathbf{d}_1,\ \mathbf{d}_2,\ \dots\ ,\ \mathbf{d}_N\right), \tag{12}$$

$$\boldsymbol{\Upsilon} = \mathbf{g}(\mathbf{Z}). \tag{13}$$

The update becomes a linear combination of the prior ensemble

$$\mathbf{Z}^{\mathrm{a}} = \mathbf{Z}^{\mathrm{f}}\mathbf{T} \tag{14}$$

Ensemble methods

- ES (ensemble smoother) applies linearization to solve gradient Eq. (6).
- IES (iterative ensemble smoother) uses gradient Eq. (6) in GN iterations (7).
- ESMDA (ES with multiple DA) gradually introduce measurements in a sequence of ES steps.

$$\begin{aligned} f\left(\mathbf{z}|\mathbf{d}\right) &\propto f\left(\mathbf{d}|\mathbf{g}(\mathbf{z})\right) f\left(\mathbf{z}\right) \\ &= f\left(\mathbf{d}|\mathbf{g}(\mathbf{z})\right)^{\left(\sum_{i=1}^{\mu}\frac{1}{\alpha_i}\right)} f\left(\mathbf{z}\right) \quad \text{with} \quad \sum_{i=1}^{\mu}\frac{1}{\alpha_i} = 1, \end{aligned} \tag{15}$$

Example with $\mu = 2$ and $\alpha_1 = \alpha_2 = 2$

$$f_1\left(\mathbf{z}|\mathbf{d}\right) \propto f\left(\mathbf{d}|\mathbf{g}(\mathbf{z})\right)^{\frac{1}{2}} f\left(\mathbf{z}\right), \tag{16}$$

$$f\left(\mathbf{z}|\mathbf{d}\right) \propto f\left(\mathbf{d}|\mathbf{g}(\mathbf{z})\right)^{\frac{1}{2}} f_1\left(\mathbf{z}|\mathbf{d}\right). \tag{17}$$

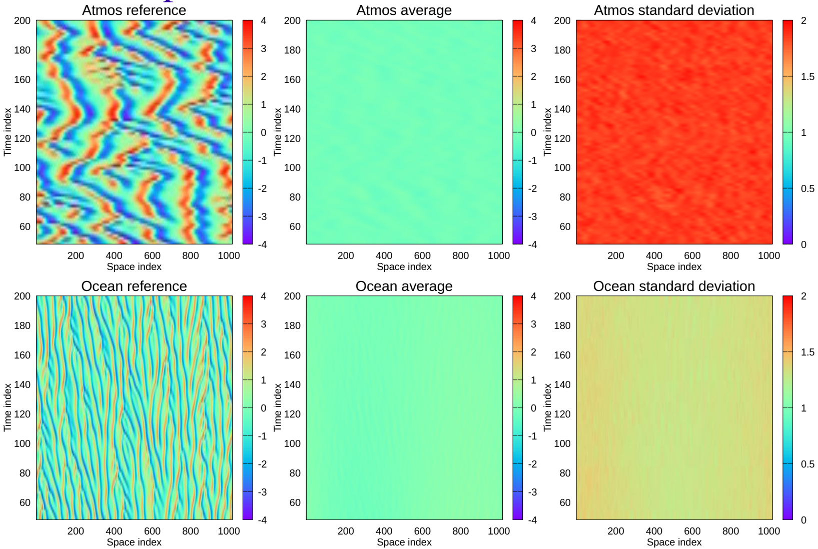
Coupled multiscale Kuramoto-Sivashinsky model

$$\frac{\partial A}{\partial t} = -A\frac{\partial A}{\partial x} - \frac{\partial^2 A}{\partial x^2} - \frac{1}{2}\frac{\partial^4 A}{\partial x^4} + 0.003\left(O - A\right), \tag{18}$$

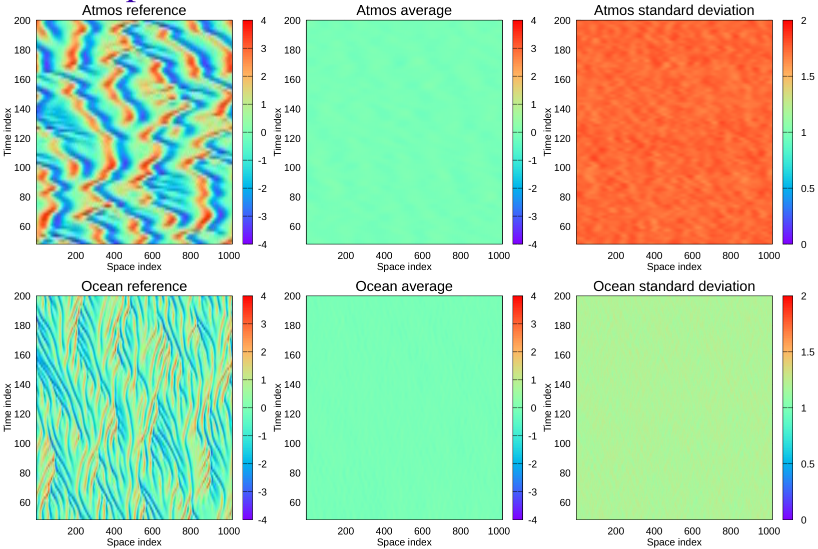
$$\frac{\partial O}{\partial t} = -O\frac{\partial O}{\partial x} - \frac{\partial^2 O}{\partial x^2} - \frac{\partial^4 O}{\partial x^4} + 0.003\left(A - O\right). \tag{19}$$

Scale difference by setting domain size of 32 for Atmos and 256 for Ocean on a 1024 nodes grid.

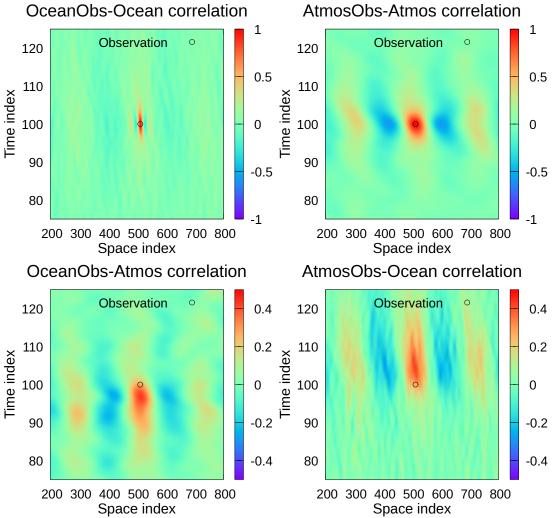
Uncoupled ensemble prediction



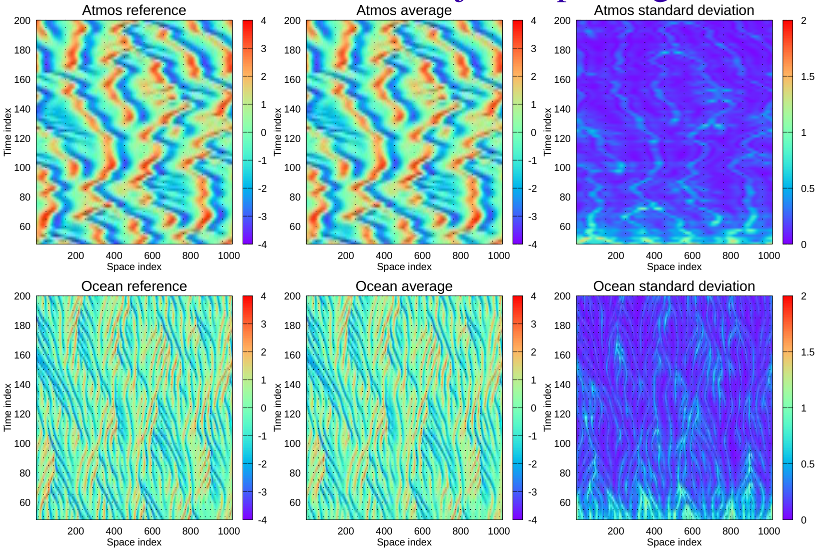
Coupled ensemble prediction



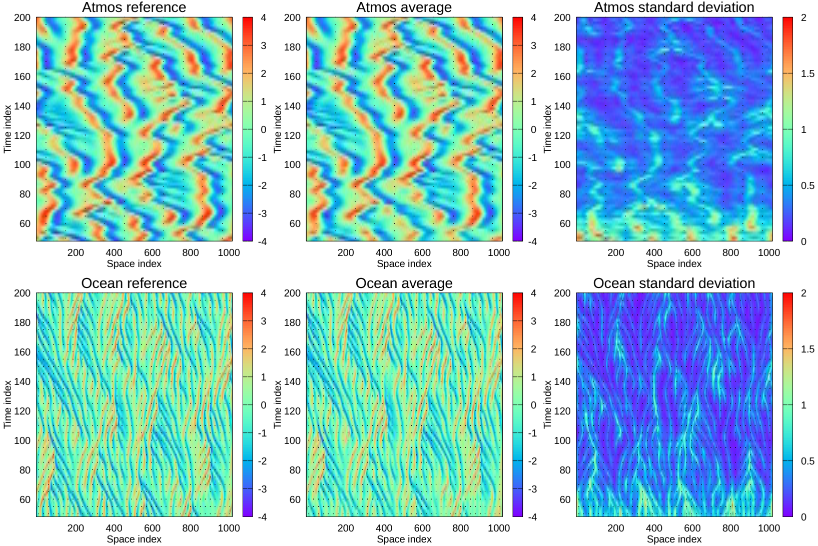
Covariances for coupled model



KS-MDA-5: Ocean and Atmos data and joint updating



KS-MDA-5sep: Ocean and Atmos data and separate updating

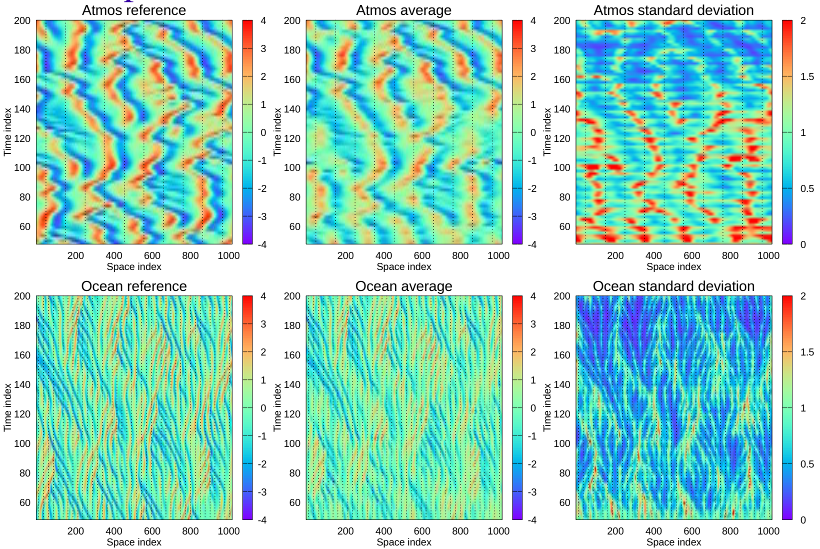


Conclusion

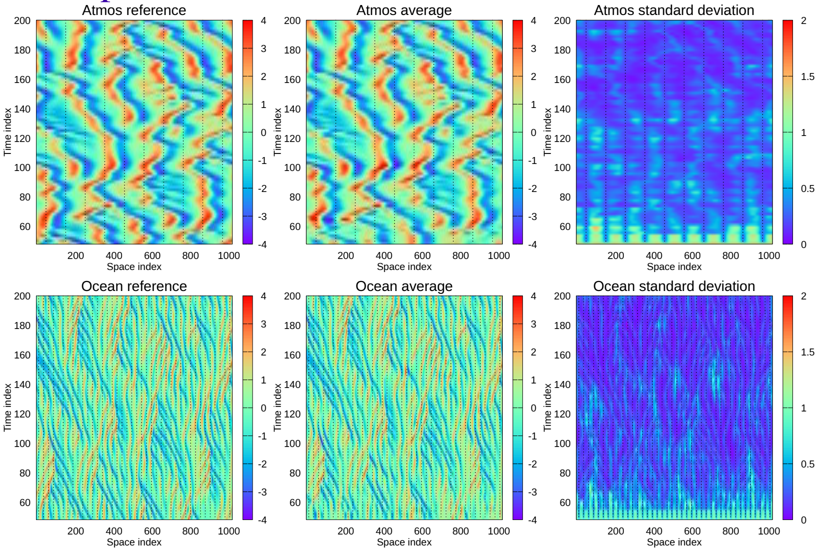
- We recommend combined and simultaneous assimilation of all data in both models.

Next we will discuss update strategies for the DA window.

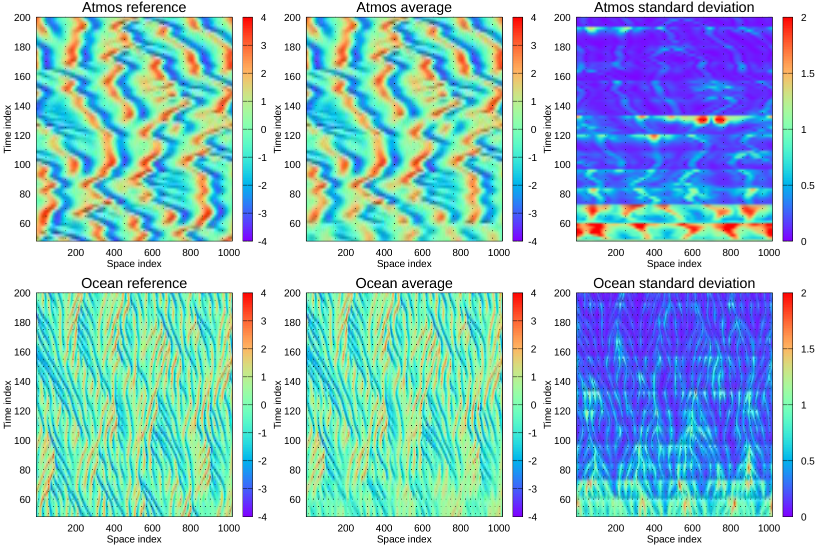
KS-ES-6-2X: ES update of ensemble initial conditions



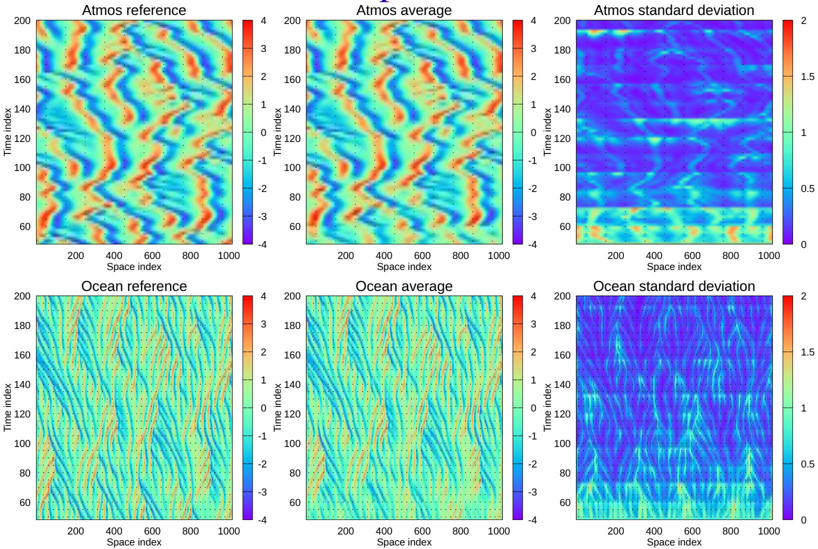
KS-ES-6-2: ES update of ensemble over DA window



KS-MDA-12-5X: ESMDA with update of ensemble initial conditions



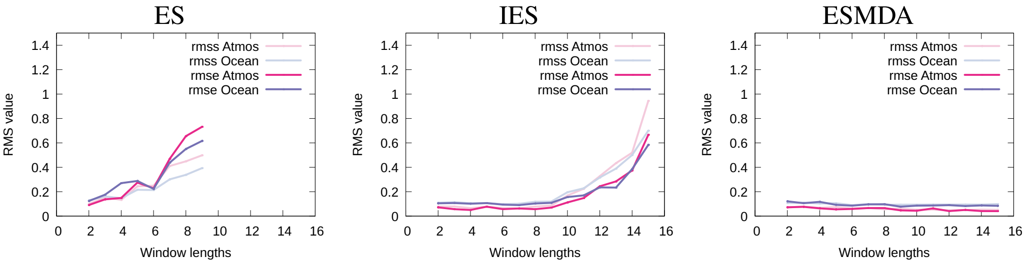
KS-MDA-12-5: ESMDA with ES update over window in final step



Conclusion

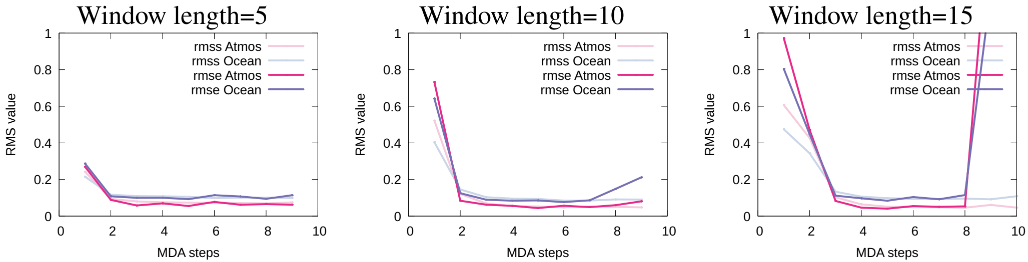
- We recommend combined and simultaneous assimilation of all data in both models.
- ES updates the ensemble over the DA window.
- ESMDA updates the ensemble over the DA window in the final step.
- IES updates the DA window's ensemble initial conditions.

Residuals as a function of the window length



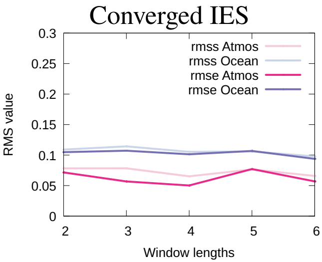
- Iterative methods improve the ES estimate significantly and extends window length.

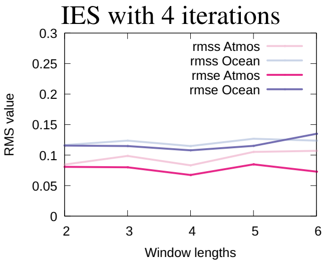
ESMDA sensitivity to number of MDA steps

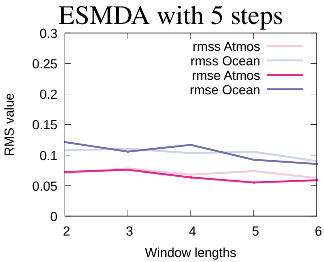


- ESMDA converges in two to five MDA steps for the KS model.

Residuals with increasing window lengths







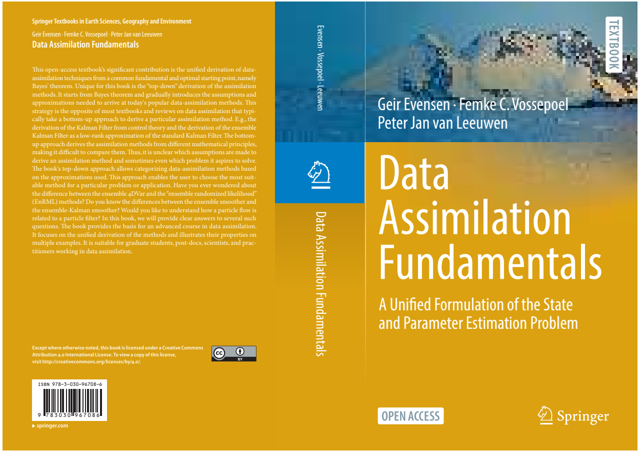
- IES with four iterations gives similar results as ESMDA with five steps (same cost).

Conclusions

- We recommend combined and simultaneous assimilation of all data in both models.
- ES updates the ensemble over the DA window.
- ESMDA updates the ensemble over the DA window in the final step.
- IES updates the DA window's ensemble initial conditions.
- Iterative methods improve the ES estimate significantly and extends window length.
- ESMDA converges in three to five MDA steps for the KS model.
- IES with four iterations gives similar results as ESMDA with five steps (same cost).

- Adjoint-free iterative ensemble smoothers show great potential for sequential data assimilation in high-dimensional and non-linear chaotic coupled dynamical systems.

Data assimilation fundamentals



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