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

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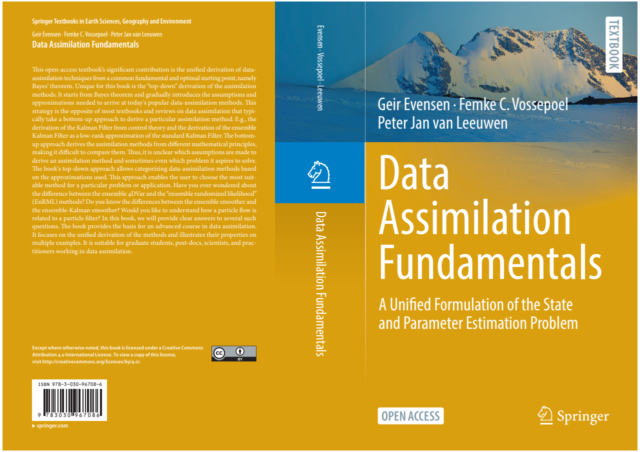
NORCE

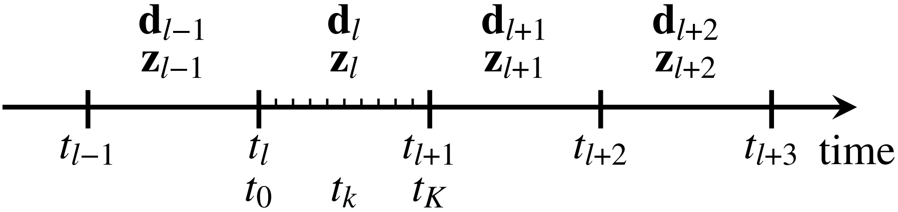
Outline

- Explain ES, IES (EnRML), ESMDA and relate them to En4DVar.
- Introduce a new coupled multiscale test model.
- Sequential DA experiements.

Data assimilation fundamentals



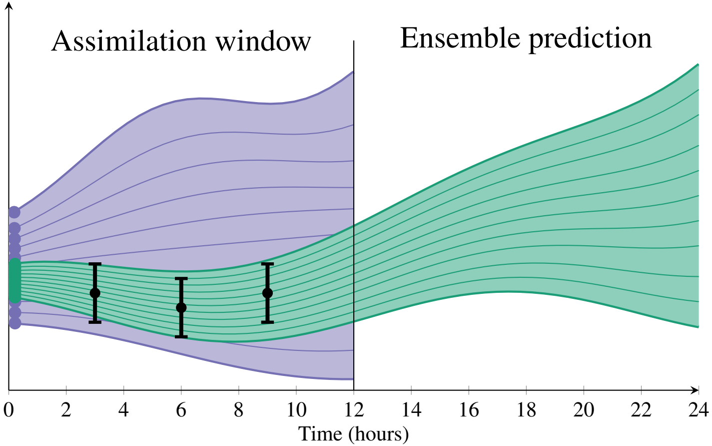
Split time into data-assimilation windows



Assumes:

- Model is a Markov process.
- Independent measurenments between windows.
- A filtering assumption.
- Errors propagate from one window to the next.

Smoother for perfect models and parameter estimation



Formulation from Bayes' theorem

Bayes' theorem

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

Approximation 1 (Gaussian prior and likelihood)

We assume that the prior distributions of the state vector's components $\mathbf{z}$ *and observation errors* $\boldsymbol{\epsilon}$ *are both Gaussian distributed.*

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

We wish to sample the posterior Bayes'

Approximation 2 (Randomized Maximum Likelihood sampling)
In the weakly nonlinear case, we can approximately sample the posterior pdf with Gaussian priors by minimizing the ensemble of cost functions defined by Eq. (4).

ps: it's really Randomized MAP sampling, or rather just approximate sampling of the posterior pdf.

RML minimizes an ensemble of cost functions

We define realizations

$$\mathbf{z}_j^{\mathrm{f}} \leftarrow \mathcal{N}(\mathbf{z}^{\mathrm{f}}, \mathbf{C}_{zz}) \quad \text{and} \quad \mathbf{d}_j \leftarrow \mathcal{N}(\mathbf{d}, \mathbf{C}_{dd}) \tag{3}$$

Ensemble of cost functions

$$\mathcal{J}(\mathbf{z}_j) = \frac{1}{2}\left(\mathbf{z}_j - \mathbf{z}_j^{\mathrm{f}}\right)^{\mathrm{T}} \mathbf{C}_{zz}^{-1}\left(\mathbf{z}_j - \mathbf{z}_j^{\mathrm{f}}\right) + \frac{1}{2}\left(\mathbf{g}(\mathbf{z}_j) - \mathbf{d}_j\right)^{\mathrm{T}} \mathbf{C}_{dd}^{-1}\left(\mathbf{g}(\mathbf{z}_j) - \mathbf{d}_j\right), \tag{4}$$

Ensemble of gradients set to zero

$$\mathbf{C}_{zz}^{-1}\left(\mathbf{z}_j - \mathbf{z}_j^{\mathrm{f}}\right) + \nabla_{\mathbf{z}}\mathbf{g}(\mathbf{z}_j)\mathbf{C}_{dd}^{-1}\left(\mathbf{g}(\mathbf{z}_j) - \mathbf{d}_j\right) = 0. \tag{5}$$

Thus, we must solve N independent minimizations.

Linearization leads to an approximate explicit solution

Approximation 3 (Linearization)

Linearize $\mathbf{g}(\mathbf{z})$ *around the prior estimate* $\mathbf{z}^{\mathrm{f}}$,

$$\mathbf{g}(\mathbf{z}) \approx \mathbf{g}(\mathbf{z}^{\mathrm{f}}) + \mathbf{G}(\mathbf{z} - \mathbf{z}^{\mathrm{f}}), \tag{6}$$

and approximate the gradient evaluated at the prior estimate

$$\mathbf{G}^{\mathrm{T}} = \nabla_{\mathbf{z}} \mathbf{g}(\mathbf{z})\big|_{\mathbf{z}=\mathbf{z}^{\mathrm{f}}}. \tag{7}$$

$\mathbf{G}$ *is the tangent-linear operator of* $\mathbf{g}(\mathbf{z})$ *and* $\mathbf{G}^{\mathrm{T}}$ *is its adjoint.*

- Used to derive EKF, ES, EnKF etc.
- We will avoid linearization by using iterative methods.

Solutions methods using the tangent linear model $\mathbf{G}$

Ensemble of incremental 4DVars

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

Ensemble of GN iterations

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

The linear Approximation 3 leads to an Ensemble of Kalman-filter updates

$$\mathbf{z}_j^{\mathrm{a}} = \mathbf{z}_j^{\mathrm{f}} + \mathbf{C}_{zz}\mathbf{G}_j^{\mathrm{T}} \left(\mathbf{G}_j \mathbf{C}_{zz} \mathbf{G}_j^{\mathrm{T}} + \mathbf{C}_{dd}\right)^{-1} \left(\mathbf{d}_j - \mathbf{g}\left(\mathbf{z}_j^{\mathrm{f}}\right)\right). \tag{10}$$

Use an averaged model sensitivity to avoid adjoints

Approximation 4 (Best-fit averaged model sensitivity)

Interpret $\mathbf{G}_j$ *in Eq. (10) and* $\mathbf{G}_j^i$ *in Eq. (9) as the sensitivity matrix in linear regression and represent them using the definition*

$$\mathbf{G}_j \approx \mathbf{G} \triangleq \mathbf{C}_{yz}\mathbf{C}_{zz}^{-1}. \tag{11}$$

We approximate the individual model sensitivities with a common averaged sensitivity used for all realizations.

Ensemble representation of covariances

Approximation 5 (Ensemble approximation)

It is possible to approximately represent a covariance matrix by a low-rank ensemble of states with fewer realizations than the state dimension.

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

$$\mathbf{D} = \left(\mathbf{d}_1,\ \mathbf{d}_2,\ \dots\ ,\ \mathbf{d}_N\right), \tag{13}$$

$$\boldsymbol{\Upsilon} = \mathbf{g}(\mathbf{Z}). \tag{14}$$

The update becomes a linear combination of the prior ensemble

$$\mathbf{Z}^{\mathrm{a}} = \mathbf{Z}^{\mathrm{f}}\mathbf{T} \tag{15}$$

Iterative smoother algorithm (subspace EnRML)

Input: $\mathbf{Z} \in \Re^{n\times N}$ ▹ Prior state-vector ensemble

Input: $\mathbf{D} \in \Re^{m\times N}$ ▹ Perturbed measurements

$\mathbf{W}^{(0)} = 0$ ▹ $\mathbf{W} \in \Re^{N\times N}$

$\mathbf{\Pi} = \left(\mathbf{I} - \frac{1}{N}\mathbf{1}\mathbf{1}^{\mathrm{T}}\right) / \sqrt{N-1}$ ▹ $\mathbf{\Pi} \in \Re^{N\times N}$

$\mathbf{E} = \mathbf{D}\mathbf{\Pi}$ ▹ $\mathbf{E} \in \Re^{m\times N}$

$i = 0$

repeat

$\quad \mathbf{Y}^i = \mathbf{g}(\mathbf{Z}^i)\mathbf{\Pi}$ ▹ $\mathbf{Y} \in \Re^{m\times N}$

$\quad$ **if** $(n < N-1) \quad \mathbf{Y}^i = \mathbf{Y}^i \mathbf{A}^{i\dagger}\mathbf{A}^i$

$\quad \mathbf{\Omega}^i = \mathbf{I} + \mathbf{W}^i\mathbf{\Pi}$ ▹ $\mathbf{\Omega} \in \Re^{N\times N}$

$\quad \mathbf{S}^i = \mathbf{Y}^i \mathbf{\Omega}^{i\,-1}$ ▹ $\mathbf{S} \in \Re^{m\times N}$

$\quad \mathbf{W}^{i+1} = \mathbf{W}^i - \gamma\left(\mathbf{W}^i - \mathbf{S}^{i\mathrm{T}}\left(\mathbf{S}^i\mathbf{S}^{i\mathrm{T}} + \mathbf{E}\mathbf{E}^{\mathrm{T}}\right)^{-1}\left(\mathbf{S}^i\mathbf{W}^i + \mathbf{D} - \mathbf{g}(\mathbf{Z}^i)\right)\right)$

$\quad \mathbf{T}^i = \left(\mathbf{I} + \mathbf{W}^{i+1} \big/ \sqrt{N-1}\right)$ ▹ $\mathbf{T} \in \Re^{N\times N}$

$\quad \mathbf{Z}^{i+1} = \mathbf{Z}\mathbf{T}^i$

$\quad i = i + 1$

until convergence

Ensemble methods

- ES (ensemble smoother) applies linearization to solve gradient Eq. (5).
- IES (iterative ensemble smoother) uses gradient Eq. (5) in GN iterations (9).
- ESMDA (ES with Multiple DA) uses tapering of likelihood to gradually introduce the measurements using ES in each step.

$$\begin{aligned} f\left(\mathbf{z}|\mathbf{d}\right) &\propto f\left(\mathbf{d}|\mathbf{g}(\mathbf{z})\right) f\left(\mathbf{z}\right) \\ &= f\left(\mathbf{d}|\mathbf{g}(\mathbf{z})\right)^{\left(\sum_{i=1}^{\mu} \frac{1}{\alpha^i}\right)} f\left(\mathbf{z}\right) \end{aligned} \tag{16}$$

with

$$\sum_{i=1}^{\mu} \frac{1}{\alpha^i} = 1, \tag{17}$$

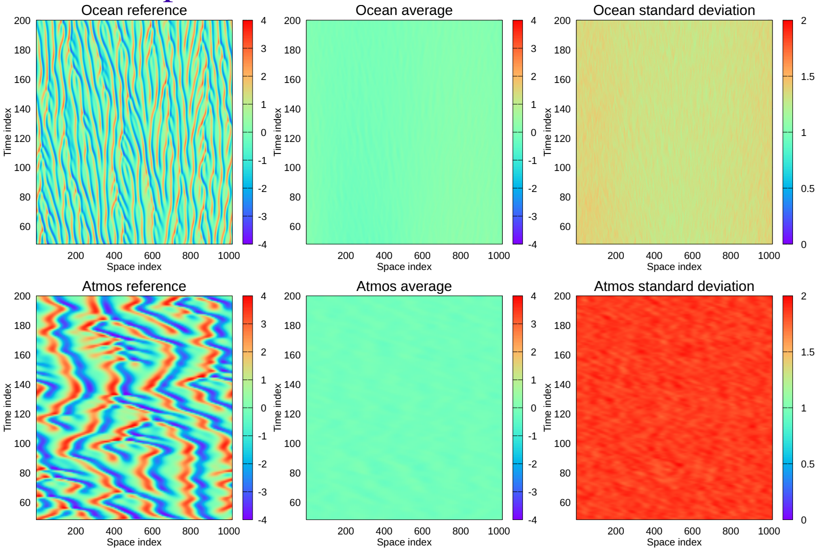
Coupled multiscale Kuramoto-Sivashinsky model

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

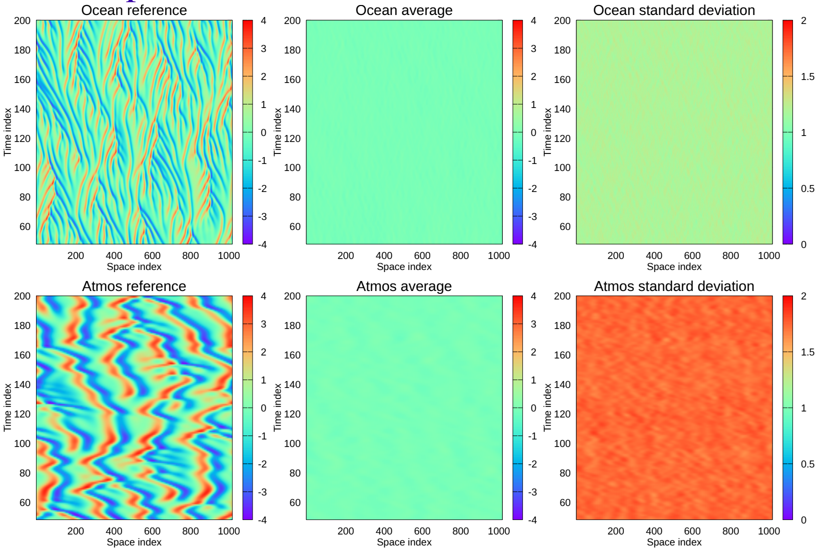
$$\frac{\partial O}{\partial t} = -O\frac{\partial O}{\partial x} - \frac{\partial^2 O}{\partial x^2} - \frac{\partial^4 O}{\partial x^4} + 0.003\left(A - O\right). \tag{19}$$

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

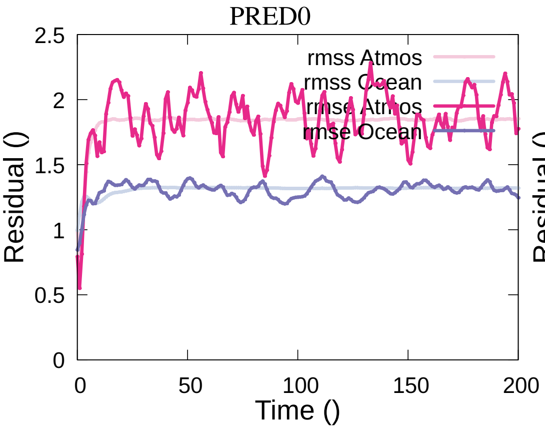
Uncoupled ensemble prediction

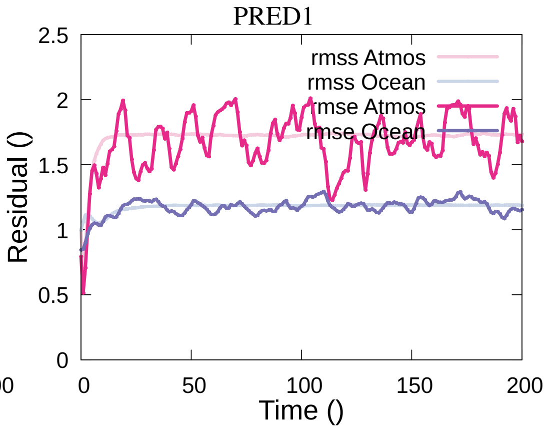


Coupled ensemble prediction

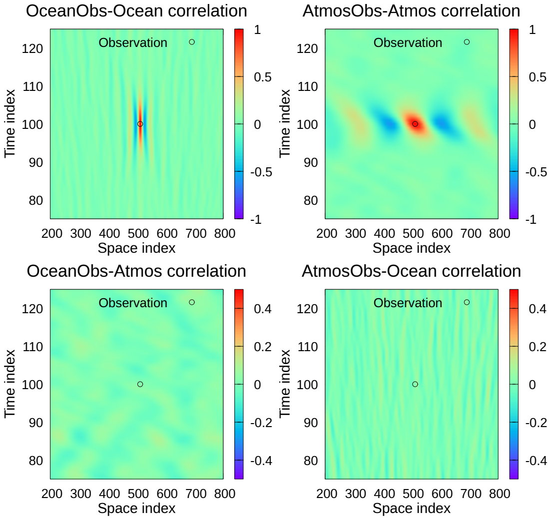


Resduals and estimated standard deviations

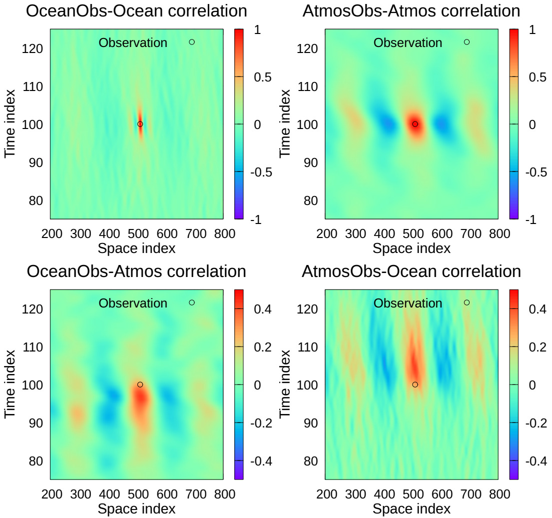




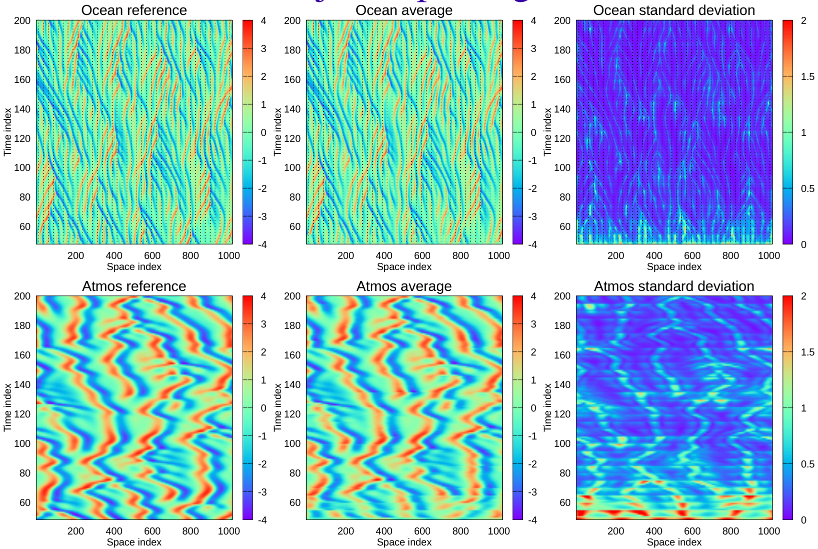
Covariances for uncoupled model



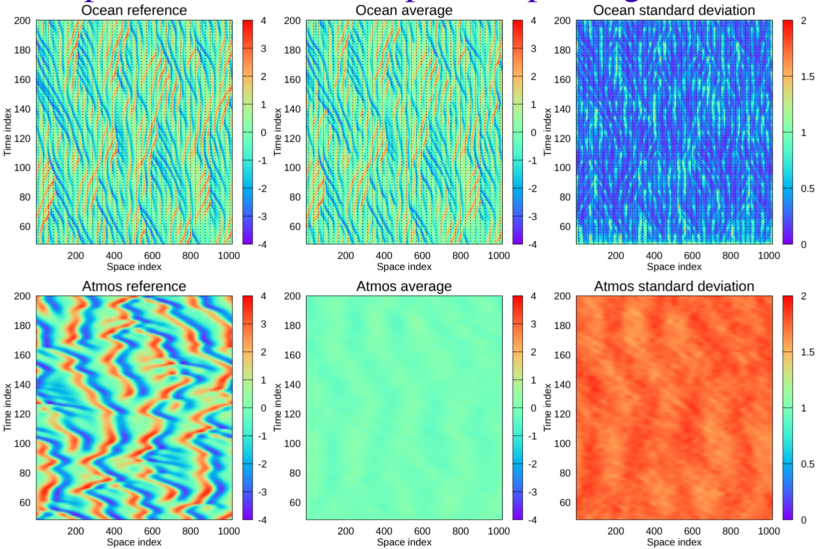
Covariances for uncoupled model



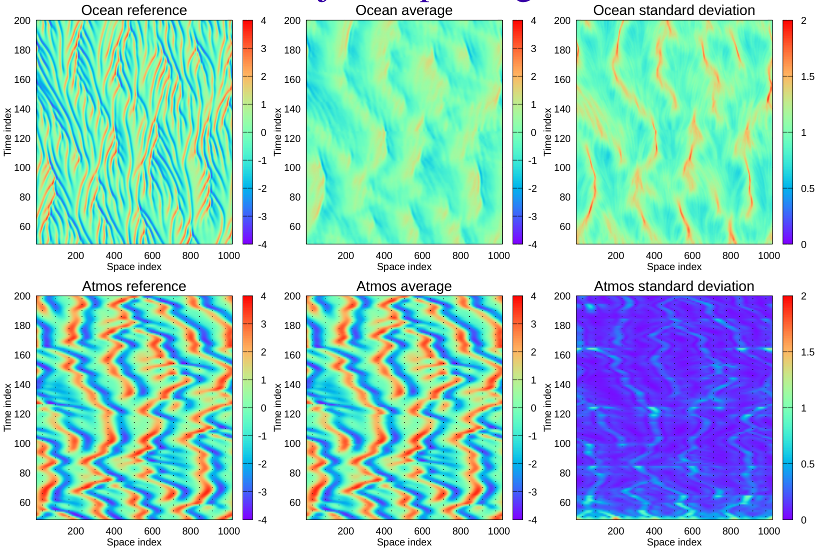
KS-MDA-5-O: Ocean data and joint updating



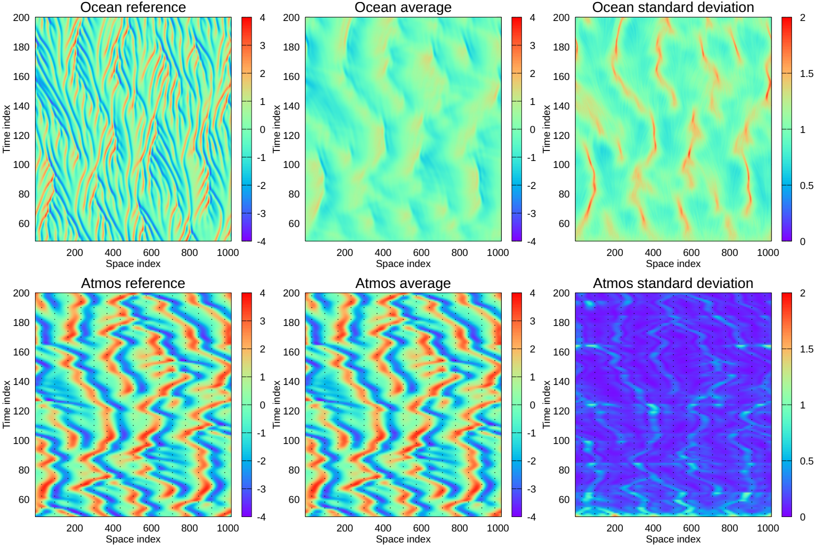
KS-MDA-5-Osep: Ocean data and separate updating



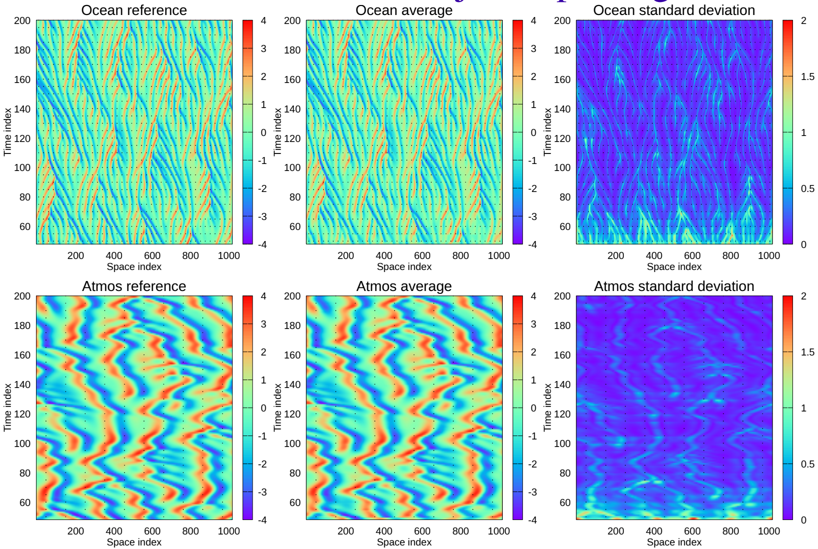
KS-MDA-5-A: Atmos data and joint updating



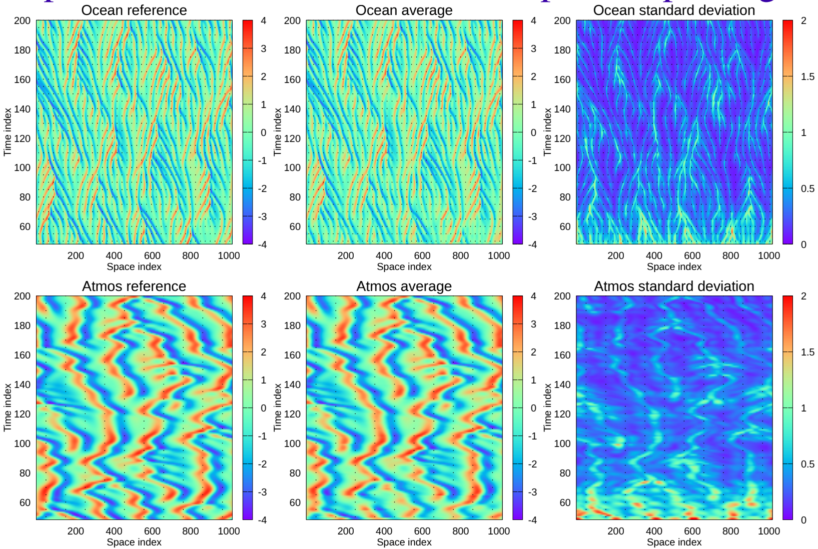
KS-MDA-5-Asep: Atmos data and separate updating



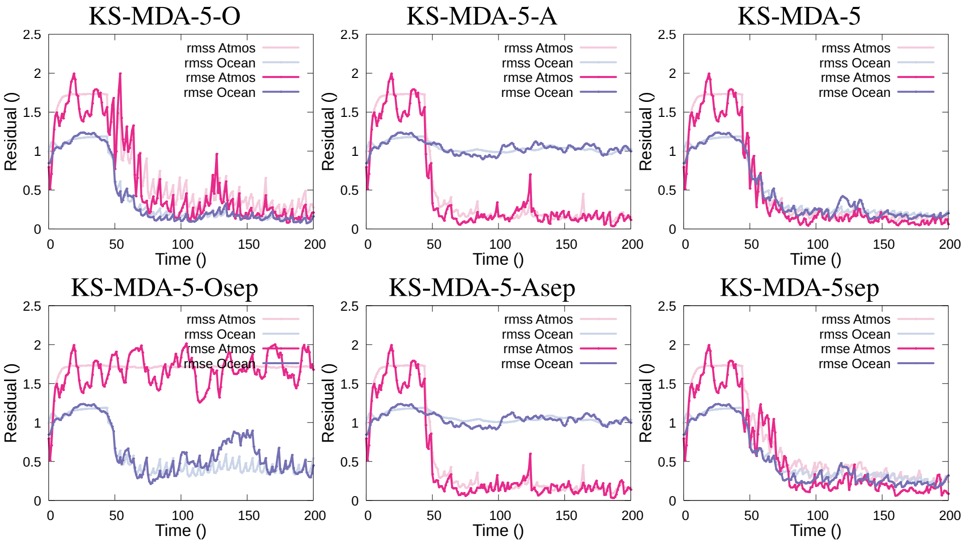
KS-MDA-5: Ocean and Atmos data and joint updating



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



Residuals

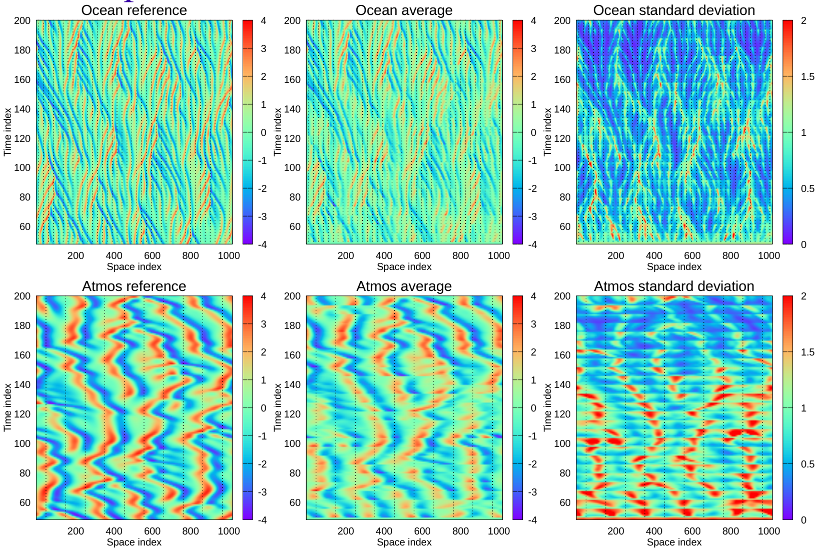

KS-MDA-5-O
KS-MDA-5-A
KS-MDA-5
KS-MDA-5-Osep
KS-MDA-5-Asep
KS-MDA-5sep
rmss Atmos
rmss Ocean
rmse Atmos
rmse Ocean
Residual ()
Time ()
0
0.5
1
1.5
2
2.5
0
50
100
150
200

Conclusion

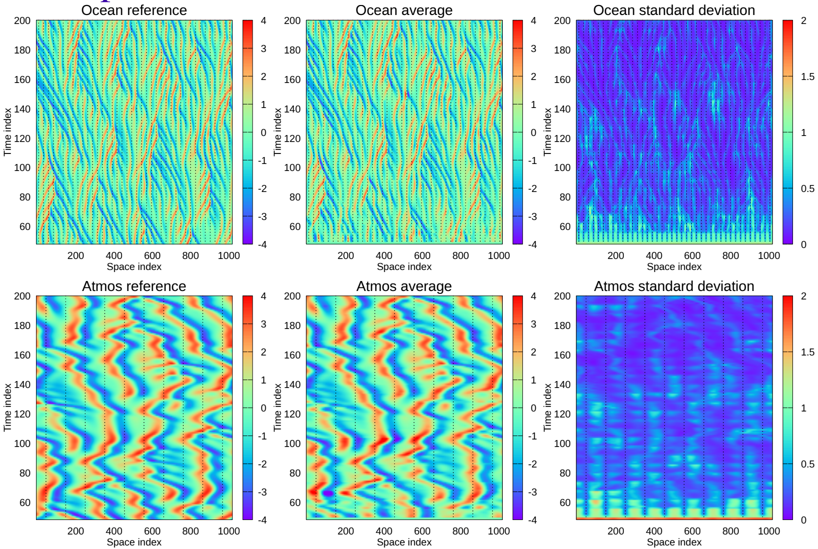
- We recommend combined and simultaneous assimilation of all data in both models.

Next we will discuss update strategies for the DA window.

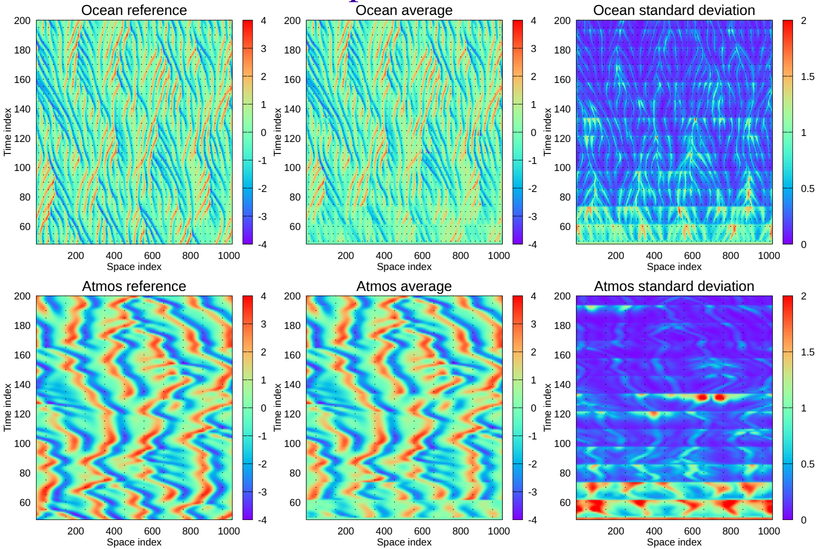
KS-ES-6-2X: ES update of ensemble initial conditions



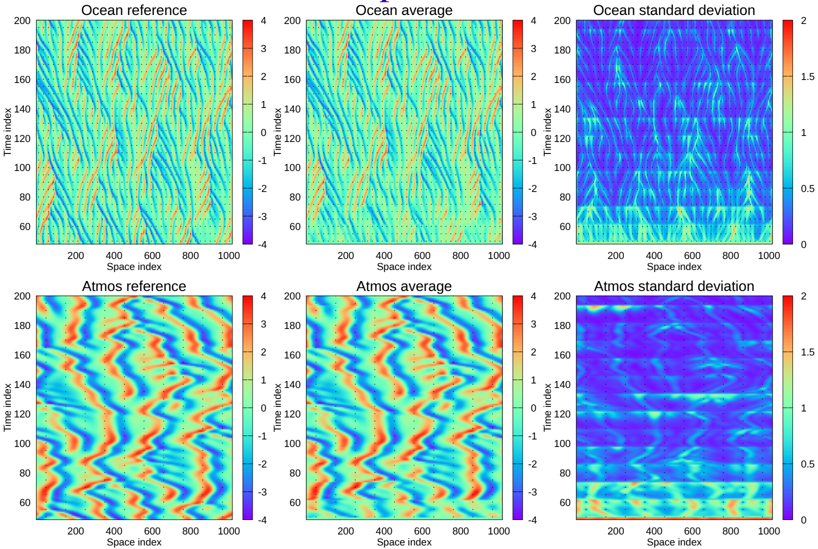
KS-ES-6-2: ES update of ensemble over DA window



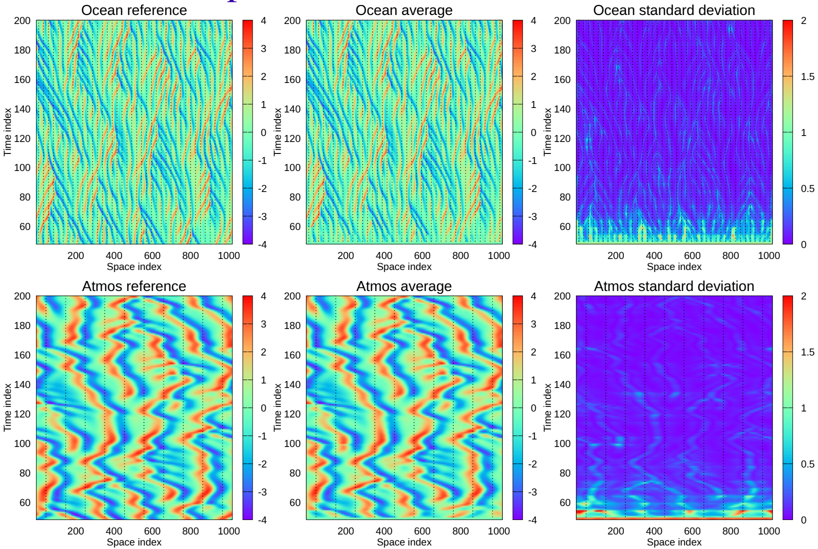
KS-MDA-12-5X: ESMDA with update of ensemble initial conditions



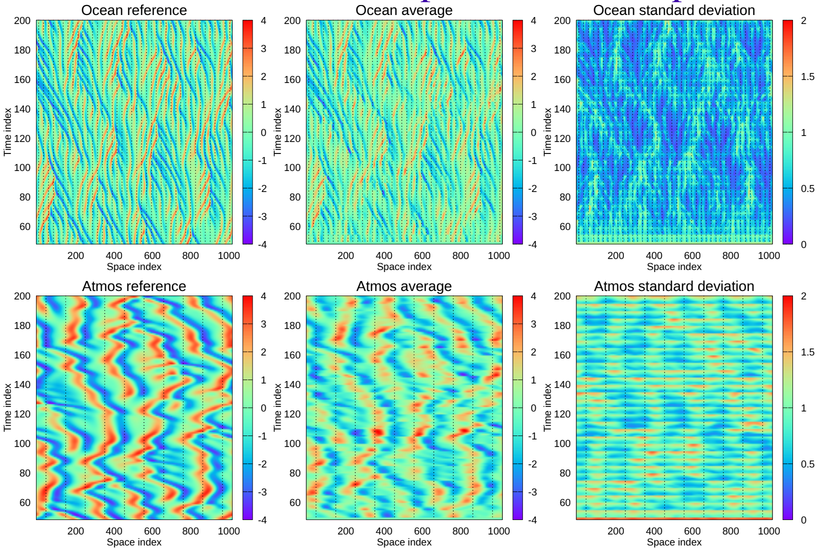
KS-MDA-12-5: ESMDA with ES update over window in final step



KS-IES-5-2X: IES with update of ensemble initial conditions



KS-IES-5-2: IES with full ensemble update in final step



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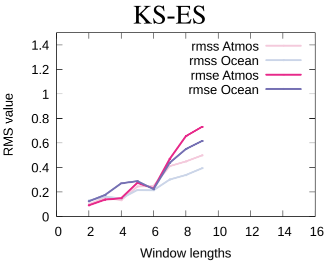
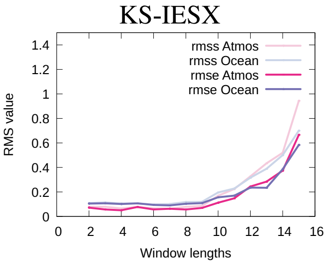
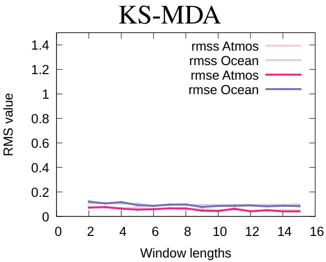
- Recommend combined and simultaneous assimilation of all data in both models.
- ES updates the ensemble over the DA window.
- ESMDA updates the ensemble over the DA window in the final step.
- IES (EnRML) updates the ensemble initial conditions.

Sensitivity to window lengths







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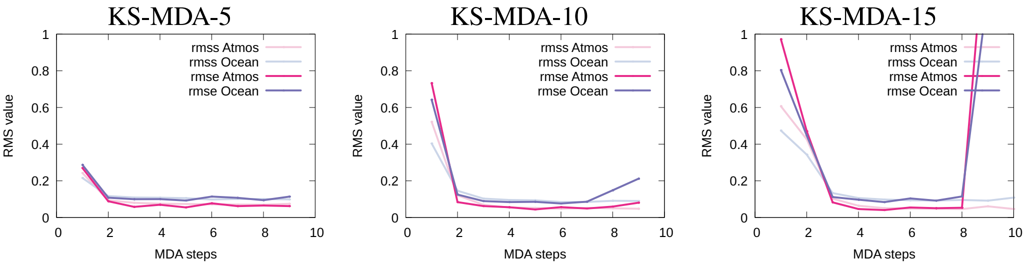
- Iterative methods improve the estimate quality significantly and extends window length.

ESMDA sensitivity to MDA steps



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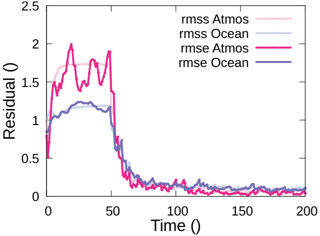
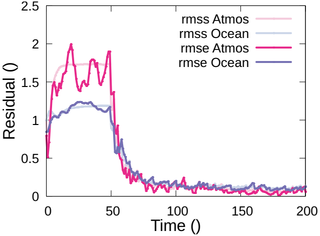
- ESMDA converges in three to five MDA steps for the KS model.

Residuals as function of time for IES, IES4, MDA5

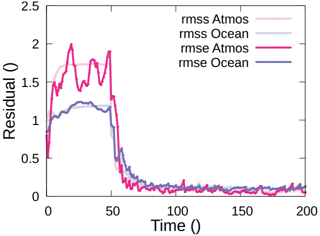
KS-IES-3-2X



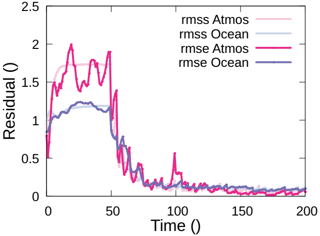
KS-IES4-3-2X



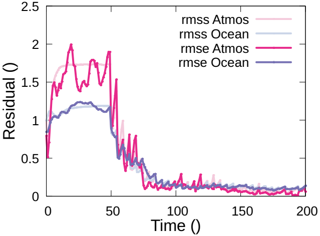
KS-MDA5-3-2



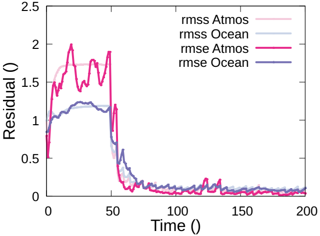
KS-IES-5-2X



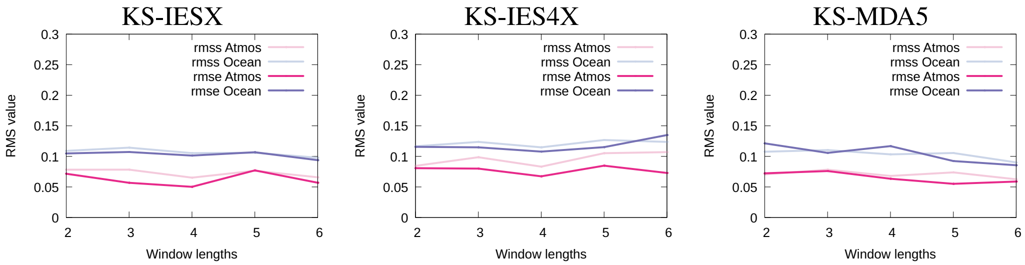
KS-IES4-5-2X



KS-MDA5-5-2



Residuals



KS-IESX
KS-IES4X
KS-MDA5
rmss Atmos
rmss Ocean
rmse Atmos
rmse Ocean
RMS value
Window lengths
0
0.05
0.1
0.15
0.2
0.25
0.3
2
3
4
5
6

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- ESMDA updates the ensemble over the DA window in the final step.
- IES (EnRML) updates the ensemble initial conditions.
- Iterative methods improve the estimate quality significantly and extends window length.
- ESMDA converges in three to five MDA steps for the KS model.
- IES with four iteration gives similar results as ESMDA with five steps (same cost).

A final conclusion

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

Bibliography

Evensen, G., P. N. Raanes, A. S. Stordal, and J. Hove. Efficient implementation of an iterative ensemble smoother for data assimilation and reservoir history matching. *Frontiers in Applied Mathematics and Statistics*, 5:47, 2019. doi:10.3389/fams.2019.00047.

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Raanes, P. N., A. S. Stordal, and G. Evensen. Revising the stochastic iterative ensemble smoother. *Nonlin. Processes Geophys*, 26:325–338, 2019. doi:10.5194/npg-2019-10.