

Data assimilation for chaotic dynamics

From model-driven to data-driven

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With: **A. Aydogdu, L. Bertino, M. Bocquet, J. Brajard, S. Cheng, Y. Chen, J. Demaeeyer, G. Evensen, C. Grudzien, C. Jones, P. Raanes, P. Rampal, C. Sampson, M. Tondeur, S. Vannitsem**

EnKF workshop 2021

DA from model-driven to (*a bit more*) data-driven

- ▶ In geosciences we possess a “good knowledge” of the laws governing the system.
- ▶ The DA ability to combine model and data has been pivotal to the success of DA from the early time.
- ▶ Using the model, information propagates from observed to unobserved regions.

Part I

Model-driven DA *or How shaping the DA algorithm to the model in hands*

- ▶ But models are not perfect and neither complete.
- ▶ Recently, machine learning tools have shown formidable in retrieving hidden dynamics only from data.

Part II

Data-driven DA *or How making DA and ML joining forces*

Outline

1 Part I: Model-driven data assimilation

- DA for chaotic models
- DA with adaptive mesh models

2 Data driven DA - Combining data assimilation and machine learning

- DA-ML to emulate an hidden dynamics
- DA-ML to infer unresolved scales parametrization

3 Forward looking

4 Bibliography

DA for chaotic models: *key challenges*

- ▶ Atmosphere and ocean, are examples of chaotic dissipative dynamics \Rightarrow Highly state-dependent error growth.
- ▶ DA must track and incorporate this flow-dependency in the quantification of the uncertainty (*i.e.* error covariance).
- ▶ Dissipation induces an “effective” dimensional reduction \Rightarrow The error dynamics is confined to a subspace of much smaller dimension, $n_0 \ll m$: the **unstable subspace**
- ▶ The existence of the underlying *unstable-stable splitting of the phase space* expected to have enormous impact on DA.

Questions

- ❶ Is there any fingerprint of the unstable subspace on the fate of (En)KF and (En)KS?
- ❷ Can dynamical properties be used to design computationally cheap DA strategies?

Deterministic linear case: behaviour of the KF and KS

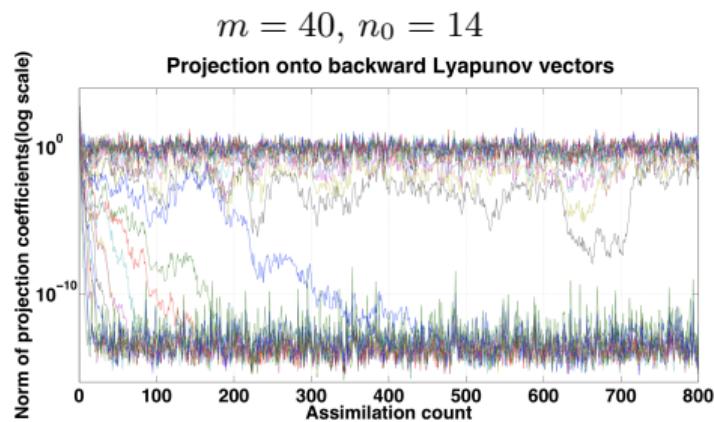
(Some) key **analytic results** (without controllability):

- ▶ **Collapse of the uncertainty:** KF error covariance asymptotically in the span of the unstable-neutral backward Lyapunov vectors (BLVs^u) [Gurumoorthy *et al* 2017]
- ▶ **Convergence of the covariance:** Low rank, n_0 , KF covariance, initialized in the span of BLVs^u, converges to the true KF one

$$\lim_{k \rightarrow \infty} \|\mathbf{P}_k - \hat{\mathbf{P}}_k\| = 0$$

if the unstable-neutral subspace is observed [Bocquet *et al* 2017]. **Warning:** *neutral modes are tricky!*

- ▶ Likewise demonstrated for Kalman smoother [Bocquet & Carrassi 2017].

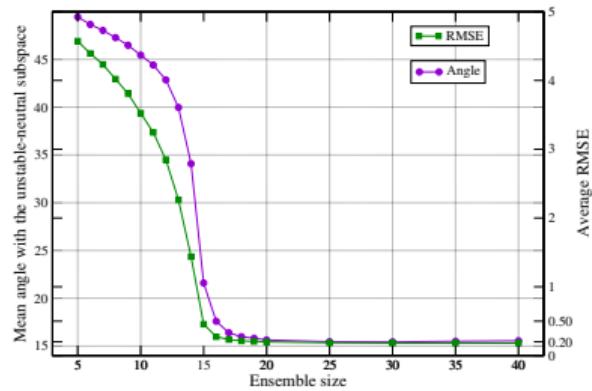
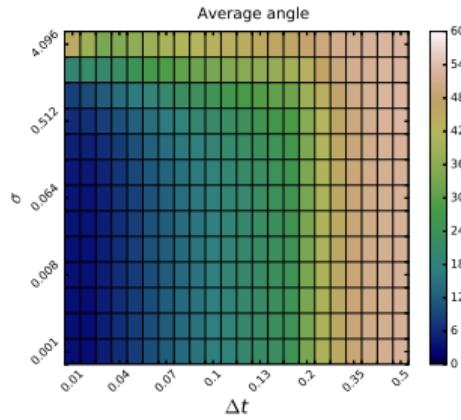


KF/KS reduced rank surrogates based on BLVs are possible.

Deterministic nonlinear case: behaviour of the EnKF and EnKS

- ▶ Asymptotic rank of EnKF covariances related to multiplicity and strength of unstable Lyapunov exponents (LEs) [Carrassi *et al* 2009; Gonzalez-Tokman & Hunt 2013].
- ▶ When the EnKF/EnKS ensemble subspace recovers the unstable subspace the unknown system state is estimated with high accuracy (sudden drop of RMSE) [Bocquet & Carrassi, 2017].

- Lorenz 96 model, $m = 40$, $n_0 = 14$
- **Left** - Angle Unstable/Ensemble subspaces vs $(\Delta t^{obs}, \sigma^{obs})$.
- **Right** - EnKF RMSE (green) and Angle (purple) vs N .



Nonlinear systems, with “weakly nonlinear” error dynamics, need only n_0 members!

What is the picture in *multiscale systems* with *coupled DA*?

► **MAOOAM:** Modular arbitrary-order ocean-atmosphere model [Vannitsem *et al*, 2016]

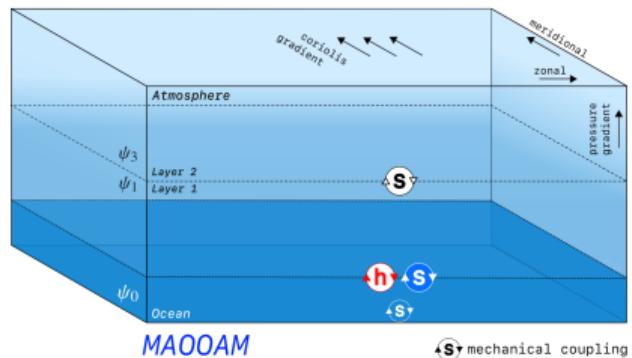
► A two-layer QG atmosphere coupled, thermally and mechanically, to a QG shallow-water ocean layer in the β -plane.

► MAOOAM is resolved in spectral space, for streamfunction and potential temperature, with adjustable resolution.

Selected model configurations

Coupling	k [adim]	k_p [adim]	λ [$\frac{W}{m^2 K}$]	d [s^{-1}]	T_0^{atm} [K]	T_0^{oce} [K]	m^{atm}	m^{oce}	
36wk							20	16	
52wk	Weak	0.010	0.020	10	6×10^{-8}	289	20	32	
56wk							24	32	
36st							20	16	
52st	Strong	0.0145	0.029	15.06	9×10^{-8}	290.20	299.35	20	32
56st							14	32	

- a) 2-layer atmosphere coupled to 1-layer ocean configuration
 b) includes friction at boundaries for atmosphere and wind stress at A-O boundary



- a) includes thermal and radiative heat transport between atmosphere and ocean as function of T_a and T_o .

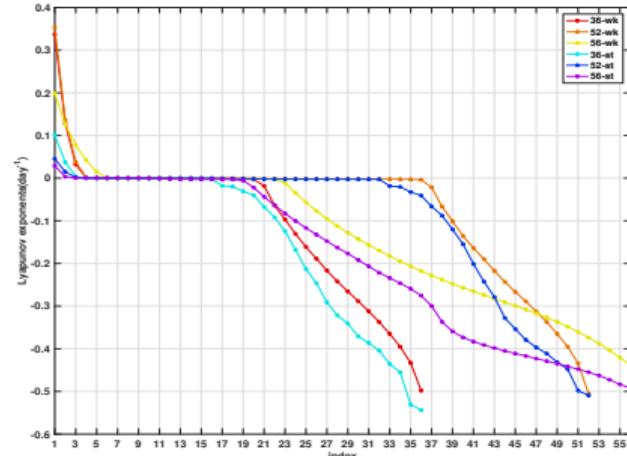
Mechanical component

Thermal component

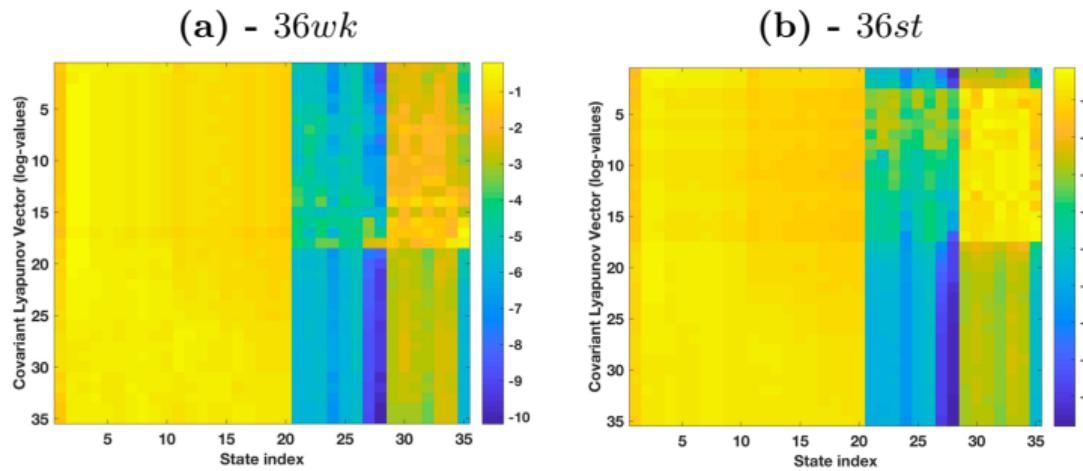
Stability analysis and the effect of the coupling

Model configuration	36wk	52wk	56wk	36st	52st	56st
# Positive $\lambda_i \in [10^{-2}, 1]$	3	3	4	2	2	1
# Near-neutral ⁺ $\lambda_i \in [10^{-5}, 10^{-2}]$	3	7	3	2	4	4
# Neutral $\lambda_i \in [-10^{-5}, 10^{-5}]$	1	1	2	1	1	1
# Near-neutral ⁻ $\lambda_i \in [-10^{-2}, -10^{-5}]$	13	25	12	11	25	13
# Negative $\lambda_i \in [-1, -10^{-2}]$	16	16	34	20	20	37
Kolmogorov entropy	0.498	0.528	0.459	0.139	0.060	0.029
Kaplan–Yorke dimension	25.06	41.03	28.42	20.29	33.35	19.32

- ▶ Many “quasi-neutral” LEs.
- ▶ The strongly coupled configurations are “less chaotic”.
- ▶ The addition of 16 ocean modes from $m = 36$ to $m = 52$ and 56 acts primarily on the “quasi-neutral” LEs ⇒ **Are they related to the coupling?**



Covariant Lyapunov vectors reveal the coupling



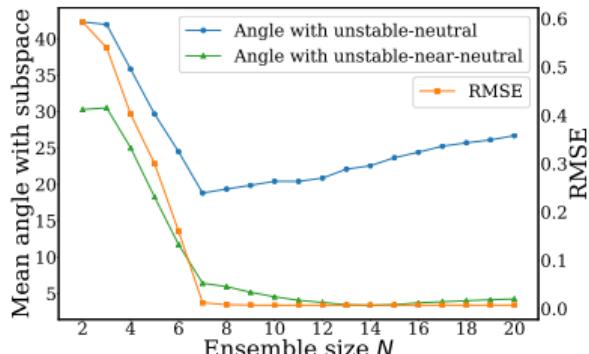
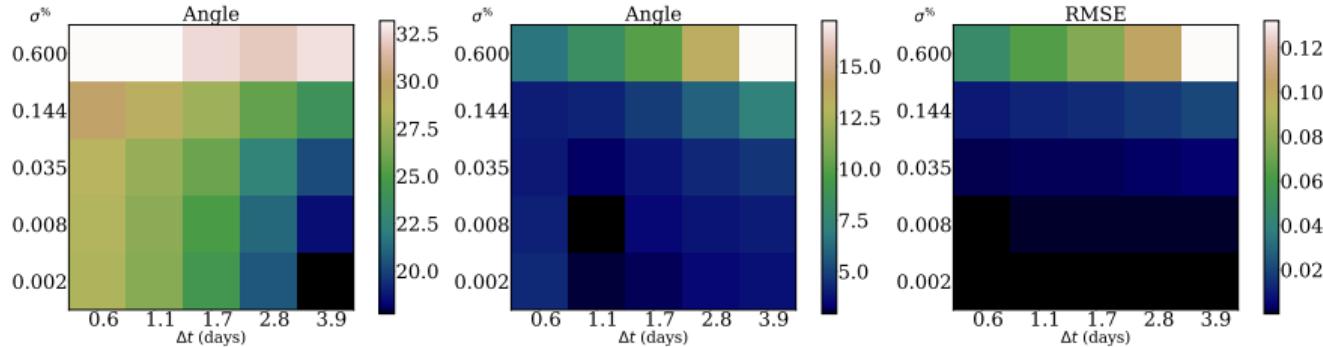
Tondeur, et al, 2020

- Unstable and Stable CLVs show a transition in projections \Rightarrow Instabilities are either originated in the atmosphere or in the ocean.
- However, the “almost neutral” CLVs show comparable projections on both atmosphere and ocean \Rightarrow **They are a manifestation of the coupling.**

Coupled DA should rely on CLVs to propagate information across model components

Strongly coupled EnKF: instabilities tracking & minimum ensemble

- Angle ensemble span with unstable-neutral (left) and unstable plus quasi-neutral modes (center).



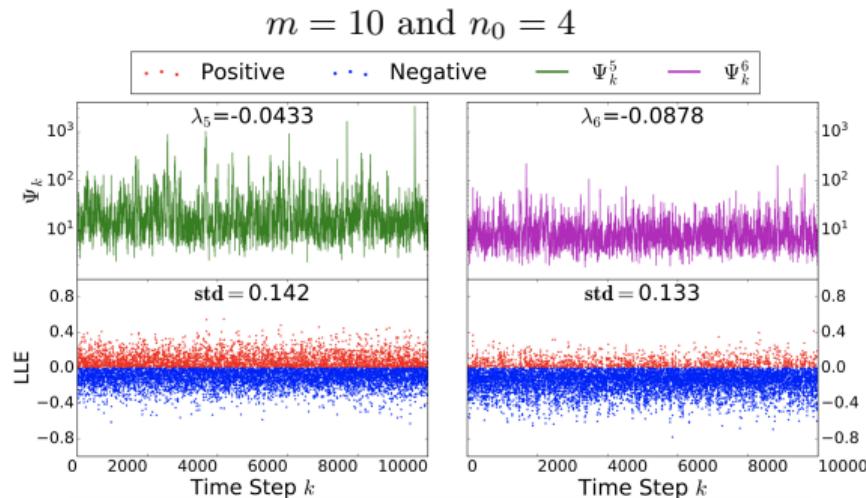
In coupled DA, all “quasi-neutral” modes – related to the coupling – must be taken into account

Carrassi *et al.*, 2021

From deterministic to stochastic models

$$\mathbf{x}_k = \mathcal{M}_{k:k-1}(\mathbf{x}_{k-1}) + \boldsymbol{\eta}_k, \quad \boldsymbol{\eta}_k \in \mathcal{N}(\mathbf{0}, \mathbf{Q}_k)$$

- ▶ Model error injects uncertainties in all directions (\mathbf{Q}_k is usually full rank).
- ▶ Uncertainty in the stable LVs **no longer zero, but still bounded.** \Rightarrow How large?
- ▶ The bounds, Ψ_k^i , depend directly on the variance of the local instabilities [Grudzien *et al* 2018a].
- ▶ For systems with high temporal variability (LLEs with high variance) the error in some stable modes can be bound to impractically large values.



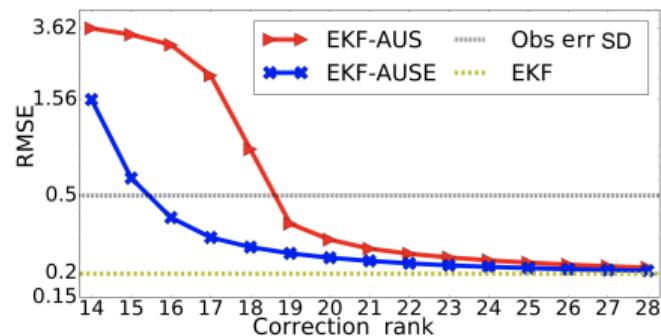
In stochastic systems it is necessary to include weakly stable BLVs of high variance

The interplay among nonlinearity, sampling and model error: *The upwelling effect*

- The error in the filtered space (“seen” by DA) is given recursively by [Grudzien *et al* 2018b]

$$\epsilon_{k+1}^f = (\mathbf{U}_{k+1}^{ff} - \mathbf{U}_{k+1}^{ff} \mathbf{K}_k \mathbf{H}_k \mathbf{E}_k^f) \epsilon_k^f - \mathbf{U}_{k+1}^{ff} \mathbf{K}_k \epsilon_k^{\text{obs}} + \boldsymbol{\eta}_k^f + (\mathbf{U}_{k+1}^{\text{fu}} - \mathbf{U}_{k+1}^{ff} \mathbf{K}_k \mathbf{H}_k \mathbf{E}_k^u) \epsilon_k^u$$

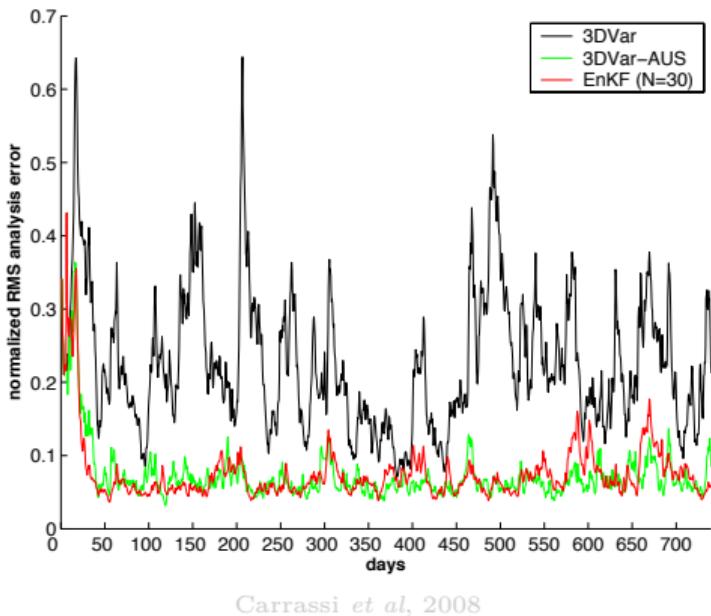
- The terms in black highlight the stabilising effect of the DA . [Carrassi *et al* 2008b].
- The terms in red describe the **dynamical upwelling** of the unfiltered to the filtered variables.
- It causes the filter to underestimate the error and implies the need for inflation.
- It is **driven by sampling error**, $n < m$, but is **exacerbated by stochastic noise**.



- EKF solves the *full-rank* recursion.
- EKF-AUS solves the *low-rank* recursion without upwelling (black terms only).
- EKF-AUSE solves the *low-rank* recursion with upwelling (black+red terms).

How to make use of instabilities in DA - Assimilation in the unstable subspace

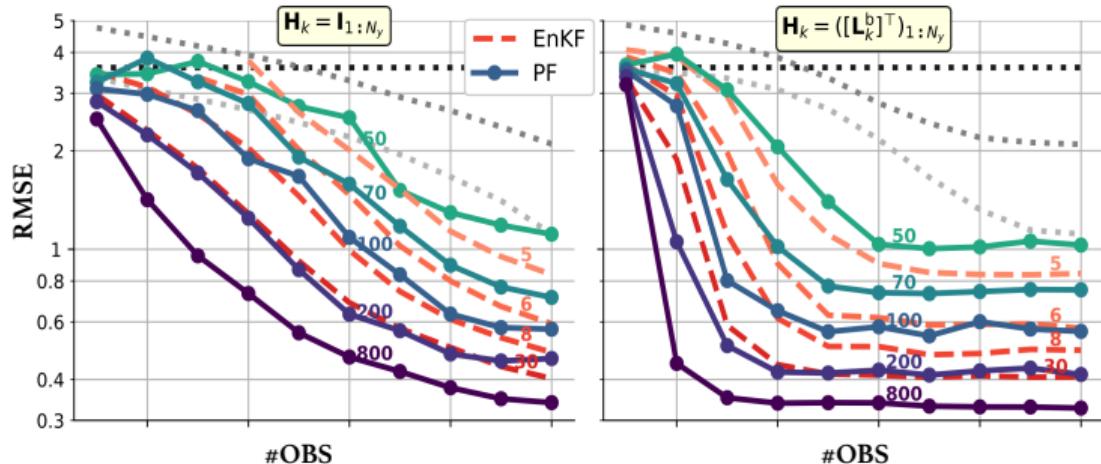
- ▶ The **Assimilation in the Unstable Subspace** uses it to perform the assimilation
 - Reduce problem size to that of the unstable directions.
 - Accurate and computationally efficient.



The roles of instabilities in Bayesian DA: A look at particle filters

- ▶ Can we use in a PF as few data as the number of error growth directions?
- ▶ Revisiting the curse of dimensionality for chaotic dynamics?

- RMSE of EnKF and Particle filter (bootstrap filter) vs #Obs (N_y)
- Observe the first N_y system's components (left) or along the first N_y Lyapunov vectors (right).
- Experiments and figure from *P. Raanes*.



Carrassi et al 2021

Targeting observations to the directions of dynamical growth of the uncertainty is very efficacious

The RMSE never degrades with the inclusion of more observations beyond $N_y > n_0 \implies$ the required #particles depends on the rank of the unstable-neutral subspace.

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DA for *adaptive mesh models*

- ▶ Numerical models using adaptive moving meshes have become increasingly prevalent in recent years.
- ▶ Applications for systems displaying highly localised structures such as shock waves or interfaces \Rightarrow Mesh resolution is increased in the proximity of the localised structure.
- ▶ Or fluids in a Lagrangian frame \Rightarrow Move the nodes of the mesh with the dynamical flow.
- ▶ Mesh adaptation can include **remeshing**: a procedure that adds or removes mesh nodes according to rules reflecting constraints in the numerical solver \Rightarrow Mesh size is not longer conserved.

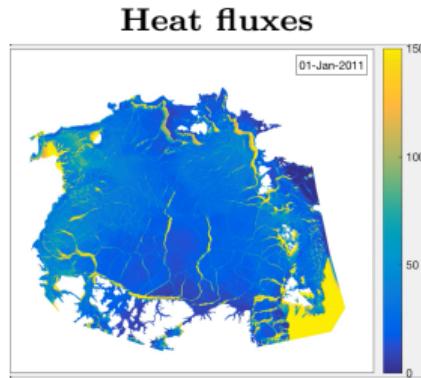
Challenges for DA

- ① Position of nodes change in time \Rightarrow Difficult to compute gradients.
- ② Number of nodes and element of the mesh changes too \Rightarrow Difficult to compute gradients and to connect to couplers.
- ③ Different state space's size for each ensemble members \Rightarrow How do we compute ensemble-based statistics in ensemble-DA?

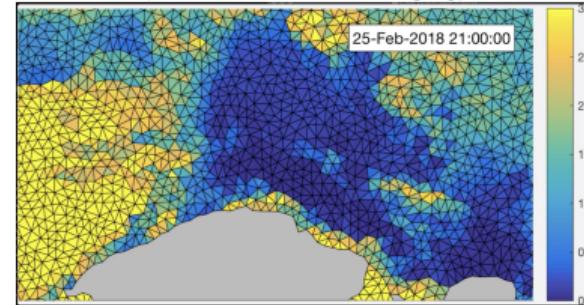
An example of adaptive mesh model: The sea-ice model neXtSIM Rampal et al, 2016

- For navigation purposes \Rightarrow Needs for detailed short-term predictions of sea-ice leaks and opening
- On longer timescales \Rightarrow Spatio-temporal characteristics of sea ice control locations and intensity of energy gas & momentum exchange between ocean, ice and atmosphere

- ▶ neXtSIM treats sea-ice as an elastic solid that can break following a *cohesion parameter*
- ▶ neXtSIM is solved on a 2D unstructured triangular **Lagrangian adaptive moving mesh**.
- ▶ It uses **remeshing** \Leftrightarrow Insert/Remove nodes for computational accuracy/economy.

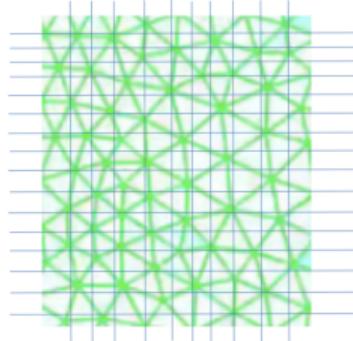


Opening on a polynya north of Greenland
(Sea ice thickness [m])



Proposed strategy: Projected EnKF

- ▶ Introduce a **reference mesh** with given properties (*e.g.* uniformity, regularity) onto which project each members.
- ▶ Perform the analysis update on the reference mesh.
- ▶ Methodology and results in *Aydogdu et al, 2019*.

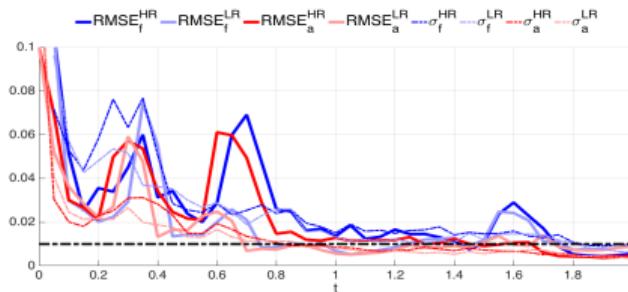
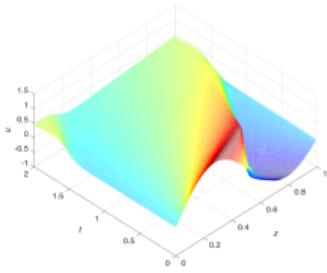


How to choose the reference mesh? Can we do it based on the model?

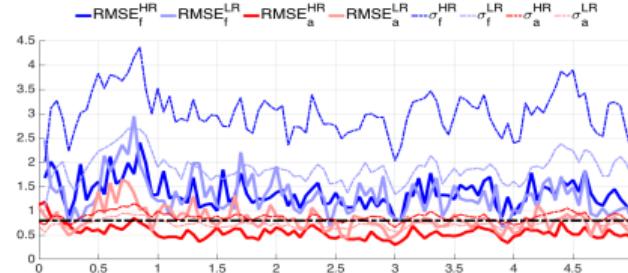
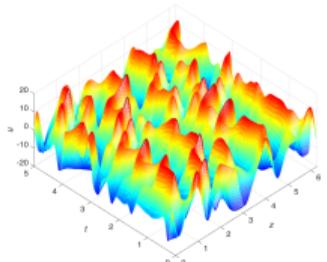
- ▶ The resolution range in the adaptive moving mesh reflects the computational constraints of the physics
- ▶ We use these constraints to define the resolution of the *reference mesh* based on the maximum/minimum possible resolution of the individual adaptive moving meshes in the ensemble. We consider two cases:
 - ① **High resolution** reference mesh (HR): *at most* one node of an adaptive mesh in each of its cells
 - ② **Low resolution** reference mesh (LR): *at least* one node in each cell of the fixed reference mesh.

Projected EnKF: numerical results in 1D

Burgers' equation $\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial z} = \nu \frac{\partial^2 u}{\partial z^2}, z \in [0, 1)$

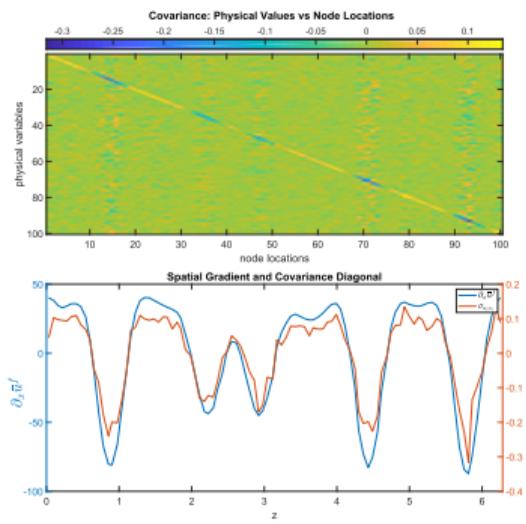
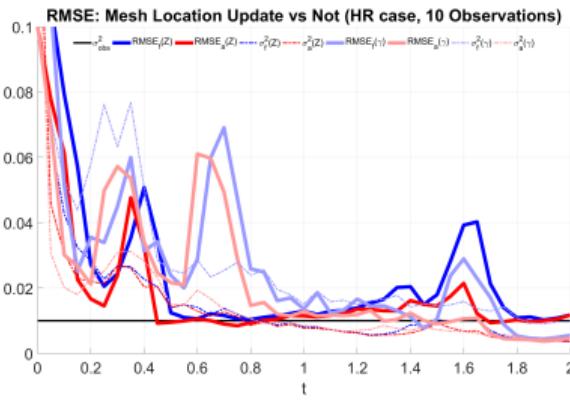


Kuramoto-Shivasinsky $\frac{\partial u}{\partial t} + \nu \frac{\partial^4 u}{\partial z^4} + \frac{\partial^2 u}{\partial z^2} + u \frac{\partial u}{\partial z} = 0, z \in [0, 2\pi)$



Joint physics and mesh update

- If the mesh is dynamic and dependent on the physics, can we update the mesh as well?
- Can we do it from just the physical observations?



► We develop a DA method updating **both** physical variables and the mesh.

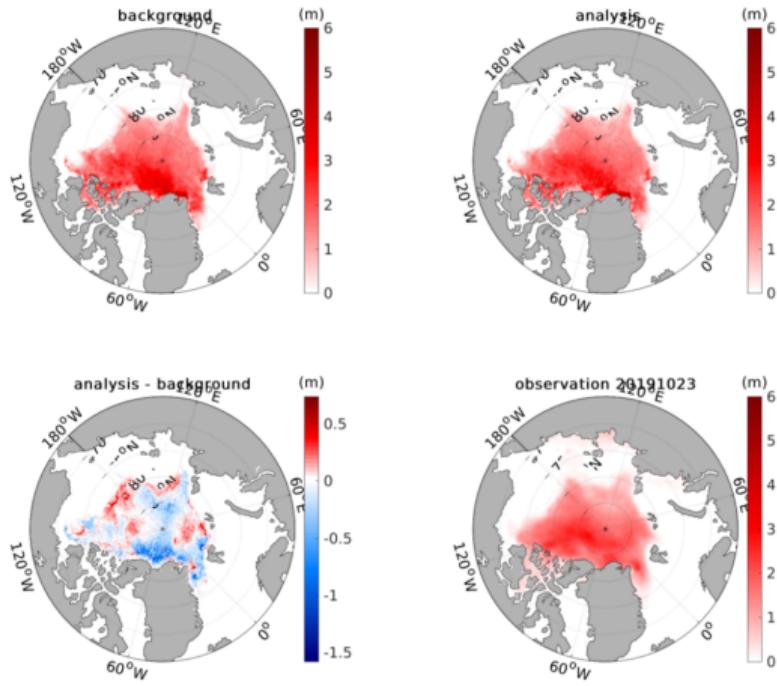
► This leverages the **information carried in the mesh structures** that drive their locations ⇒ Better gradients.

► The shape of ensemble-based variance closely matches that of the gradient ⇒ including the node locations in the state vector encodes a deeper level of information into the DA process.

Sampson *et al*, 2021

neXtSIM : Preliminary results - Cheng, Chen, Aydogdu *et al,*

PEnKF analysis for 22 Oct 2019
N=40 members
Obs = CS2MOS (weekly)



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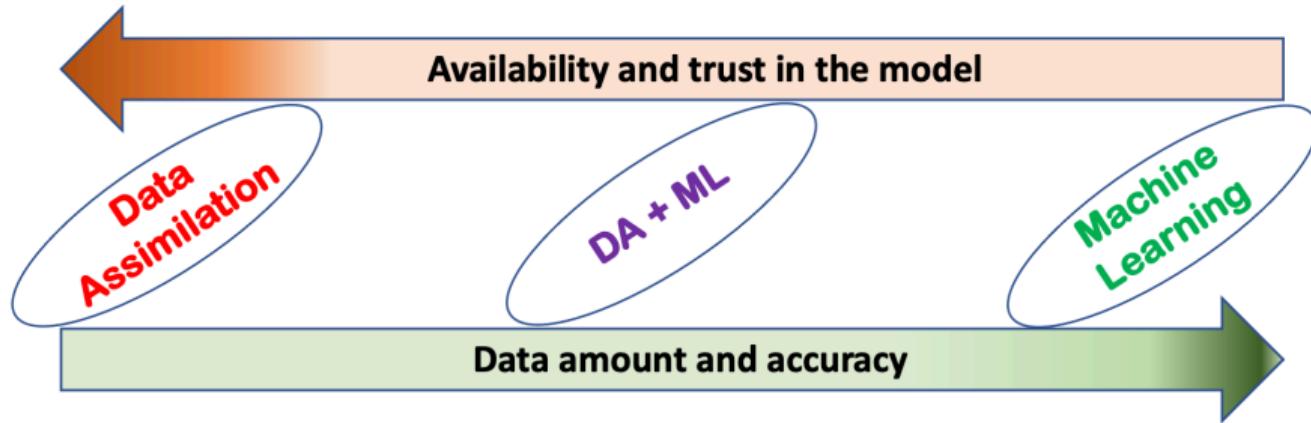
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Part II - Combining DA and ML



- ▶ Many works on data-driven reconstruction of the dynamics in DA and ML: Park and Zhu 1994; Wang and Lin 1998; Paduart et al. 2010; Brunton et al. 2016; Lguensat et al. 2017; Pathak, Lu, et al. 2017; Harlim 2018; Dueben and Bauer 2018; Long et al. 2018; Fablet et al. 2018; Bocquet et al., 2019; Bonavita and Laloyaux, 2020; Vlachas et al. 2020; Brunton et al. 2016; Farchi et al. 2021 and many more...;

Objectives of this work

- Given the dataset $\mathbf{y}_k^{\text{obs}}$ ($1 \leq k \leq K$)

$$\mathbf{y}_k^{\text{obs}} = \mathcal{H}_k(\mathbf{x}_k) + \epsilon_k^{\text{o}} \quad \epsilon_k^{\text{o}} \in \mathcal{N}(0, \mathbf{R})$$

observed from an **underlying dynamical model**:

$$\frac{d\mathbf{x}}{dt} = \phi(\mathbf{x}) \quad \text{with resolvent} \quad \mathbf{x}_{k+1} = \mathcal{M}(\mathbf{x}_k) = \mathbf{x}_k + \int_{t_k}^{t_{k+1}} \phi(\mathbf{x}) dt$$

DA+ML for two complementary goals

- Emulate the full model $\mathcal{M}(\mathbf{x})$.
- Infer the unresolved scale effect and build an hybrid physical/data-driven model.

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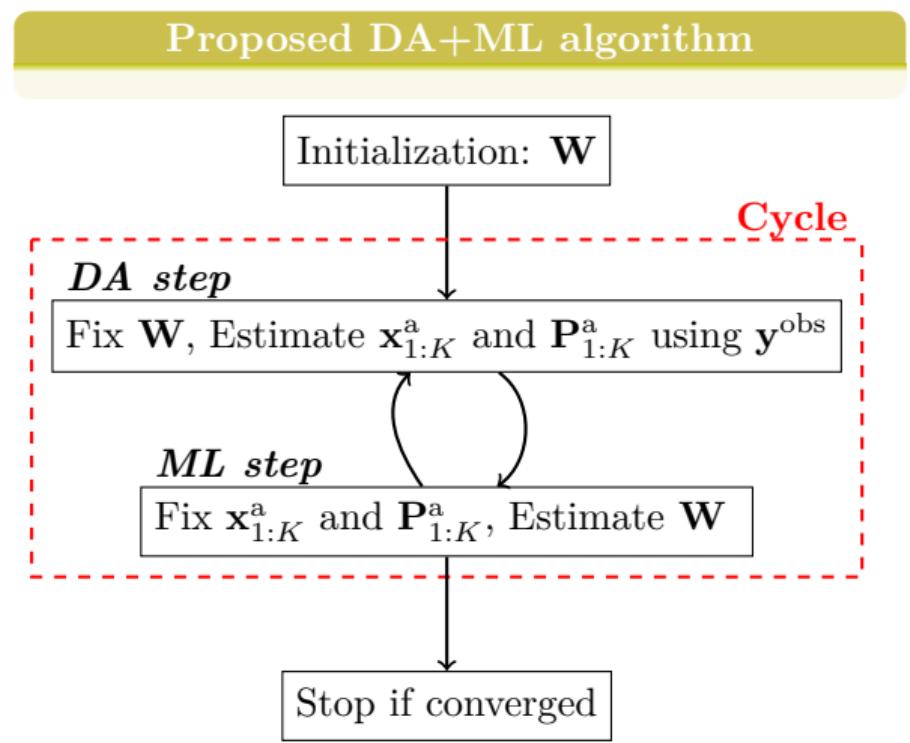
Emulating a model by combining DA and ML [Brajard *et al*, 2020]

Emulation of the resolvent **combining** DA and ML:

$$\mathbf{x}_{k+1} = \mathcal{M}(\mathbf{x}_k) \approx \mathcal{G}_{\mathbf{W}}(\mathbf{x}_k) + \epsilon_k^m,$$

where $\mathcal{G}_{\mathbf{W}}$ is a neural network parameterised by \mathbf{W} and ϵ_k^m is a stochastic noise.

- ▶ For the DA part we use the Finite-Size Ensemble Kalman Filter (EnKF-N).
- ▶ For the ML part we train a neural net



Proposed DA+ML algorithm

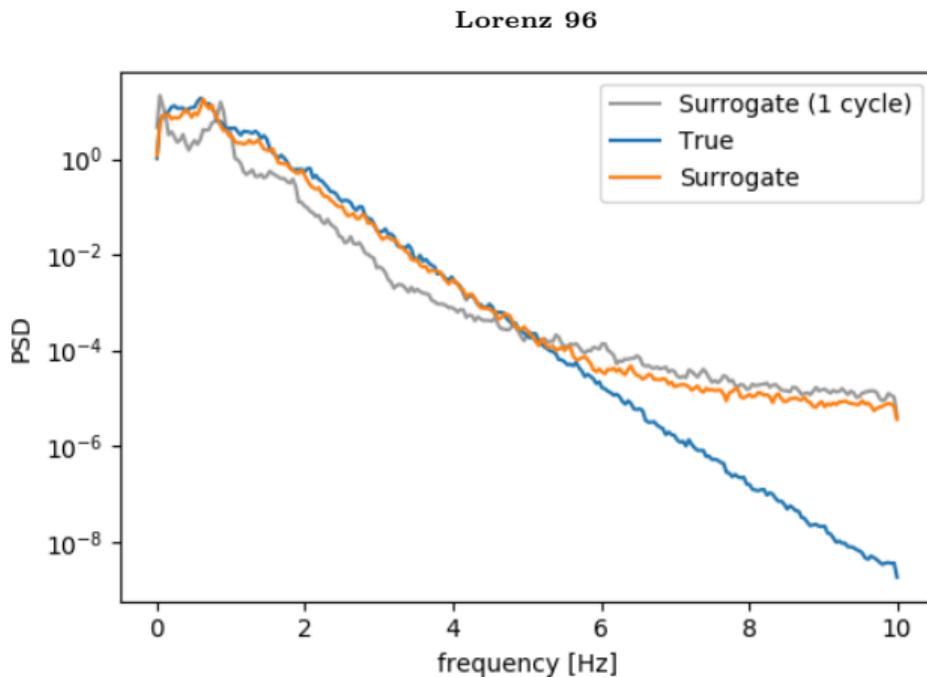
- ▶ Step 1 - Data Assimilation: estimate the state field $\mathbf{x}_{1:K}$ (the analysis) and associated (analysis) error covariance, \mathbf{P}_k , based on the fixed model parameters \mathbf{W} and using sparse and noisy data, \mathbf{y} .
- ▶ Step 2 - Machine learning: using $\mathbf{x}_{1:K}$ and \mathbf{P}_k from DA estimate \mathbf{W}
 - The neural network can be expressed as a parametric function $\mathcal{G}_{\mathbf{W}}(\mathbf{x}_k) = \mathbf{x}_k + f_{\text{nn}}(\mathbf{x}_k, \mathbf{W})$ where f_{nn} is a neural network and \mathbf{W} its weights; f_{nn} is composed of convolutive layers.
 - The determination of the optimal \mathbf{W} is done in the *training phase* by minimising the loss function:

$$L(\mathbf{W}) = \sum_{k=0}^{K-N_f-1} \sum_{i=1}^{N_f} \left\| \mathcal{G}_{\mathbf{W}}^{(i)}(\mathbf{x}_k) - \mathbf{x}_{k+i} \right\|_{\mathbf{P}_k^{-1}}^2,$$

where N_f is the number of time steps corresponding to the forecast lead time on which the error between the simulation and the target is minimised (with “coordinate descent” *Bocquet et al. (2020)*).

- \mathbf{P}_k is a symmetric, semi-definite positive matrix estimated using the *analysis error covariances* from the DA step.
- This time-dependent matrix, \mathbf{P}_k , plays the role of the surrogate model error covariance matrix and gives different weights to each state during the optimisation process.

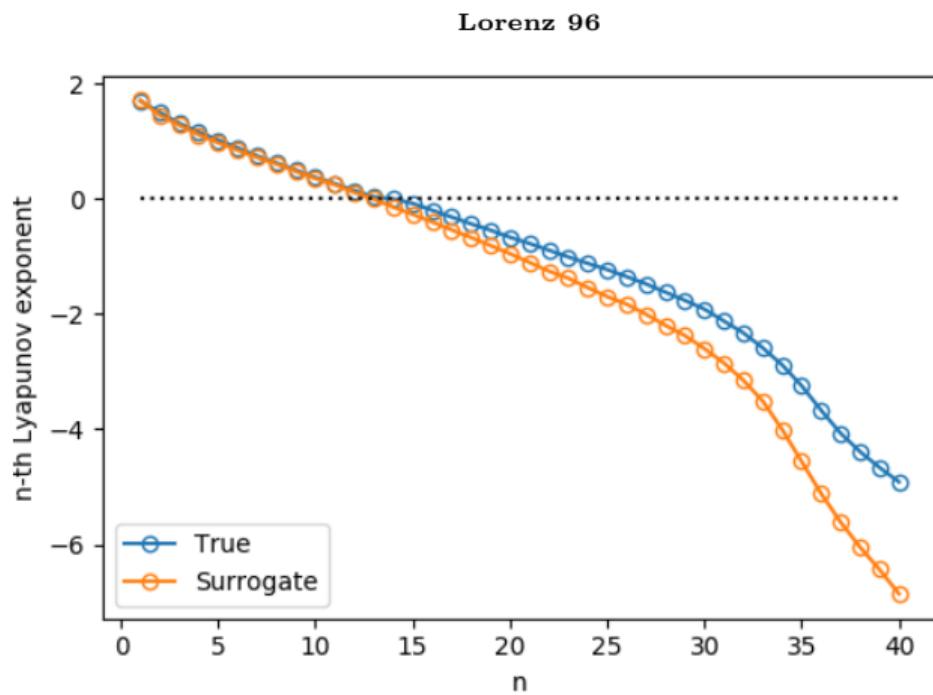
Emulating the underlying dynamics: Power spectrum density



- ▶ After one cycle, some frequencies are favoured (see the peak at $\sim 0.8\text{Hz}$) and indicate that the **periodic signals are learnt first**.
- ▶ At convergence, the surrogate model reproduces the spectrum up to 5 Hz but then **adds high-frequency noise**.
- ▶ **Low frequencies are better observed** and better reproduced after the DA step.
- ▶ The PSD has been computed using a long simulation (16,000 time steps), which means that **the surrogate model is very stable**.

Brajard *et al.*, 2020

Emulating the underlying dynamics: Lyapunov spectrum

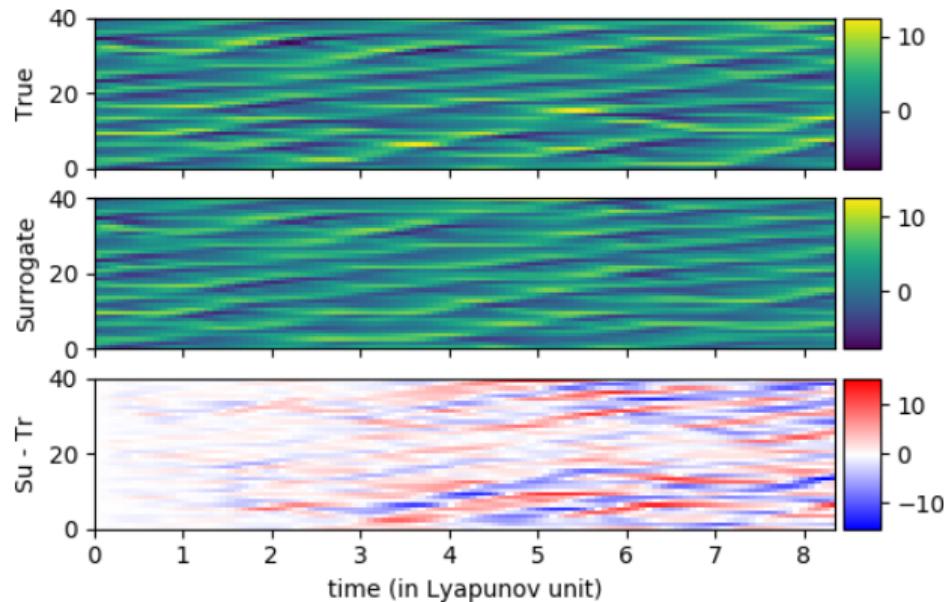


- ▶ Accurate unstable spectrum \Rightarrow Same error growth rate and Kolmogorov entropy, as the true model.
- ▶ Less accurate reconstruction of the neutral and quasi-neutral part of the spectrum.
- ▶ This is similar to what found in *Pathak et al. (2017)*. Maybe due to the slower convergence (linear vs exponential) of the neutral exps *Bocquet et al. (2017)*.
- ▶ The stable part of the spectrum is shifted toward smaller values \Rightarrow PDFs contracts faster than in the true model, *i.e.* surrogate model more dissipative than the truth.

Brajard *et al.*, 2020

Forecast skill

Hovmöller plot of the true and surrogate models (in Lyapunov time*, LT)



- ▶ The simulations start from the same initial conditions.
- ▶ Good prediction until 2 LTs. Error saturation at 4-5 LTs.
- ▶ (*): the time for the error to grow by a factor e .

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Combined DA-ML to infer unresolved scales parametrizations

The objective is to produce a hybrid (physical/data-driven) model

$$\mathbf{x}(t + \delta t) = \mathcal{M}^\varphi[\mathbf{x}(t)] + \mathcal{M}^{\text{UN}}[\mathbf{x}(t)],$$

where:

- $\mathbf{x}(t)$ is the state of the dynamical system
- \mathcal{M}^φ is the physical model (assumed to be known a priori)
- \mathcal{M}^{UN} is the unresolved component of the dynamics to be inferred from data
- δt is the integration time step

\mathcal{M}^{UN} is approximated by a **data-driven model** represented under the form of a neural network whose parameters are $\boldsymbol{\theta}$: $\mathcal{M}_{\boldsymbol{\theta}}[\mathbf{x}(t)]$

Proposed approach

Simplified description of the algorithm:

- ➊ Estimating the state $\mathbf{x}_{1:K}^a$. At each time t_k , we calculate a forecast \mathbf{x}^f :

$$\mathbf{x}_{k+1}^f = \mathbf{x}^f(t_k + \Delta t) = (\mathcal{M}^\varphi)^{N_c}(\mathbf{x}_k^a)$$

An observation \mathbf{y}_{k+1} is assimilated with strongly coupled EnKF to produce an analysis \mathbf{x}_{k+1}^a

- ➋ Determining an estimation of the unknown part of the model. We assume that:

- $\mathbf{x}(t + \Delta t) \approx (\mathcal{M}^\varphi)^{N_c}(\mathbf{x}(t)) + N_c \cdot \mathcal{M}^{\text{UN}}[\mathbf{x}(t)]$
- $\mathbf{x}(t) \approx \mathbf{x}^a(t)$

We consider that $\mathcal{M}^{\text{UN}}(\mathbf{x}_k) \approx \mathbf{z}_{k+1} = 1/N_c \cdot (\mathbf{x}_{k+1}^a - \mathbf{x}_{k+1}^f) \implies$ The “target” (*i.e.* the model error) is estimated using the *analysis increments* (?).

- ➌ Training a neural network \mathcal{M}_θ by minimising the loss $L(\theta) = \sum_{k=0}^{K-1} \|\mathcal{M}_\theta(\mathbf{x}_k^a) - \mathbf{z}_{k+1}\|^2$
- ➍ Using the hybrid model $\mathcal{M}^\varphi + \mathcal{M}_\theta$ to produce new simulations (*e.g.* to make forecasts).

Experiments with MAOOAM

- ➊ **Truth:** $n_a = 20$ and $n_o = 8$ modes for atmosphere and ocean. **Total dimension** $N_x = 56$.
- ➋ **Truncated:** $n_a = 10$ and $n_o = 8$ modes for atmosphere and ocean. **Total dimension** $N_x = 36$.
- ▶ The truncated model is **missing 20 high-order atmospheric variables**
- ▶ There is not locality in spectral space so the NN is made of 3 layers multi-layer perceptrons

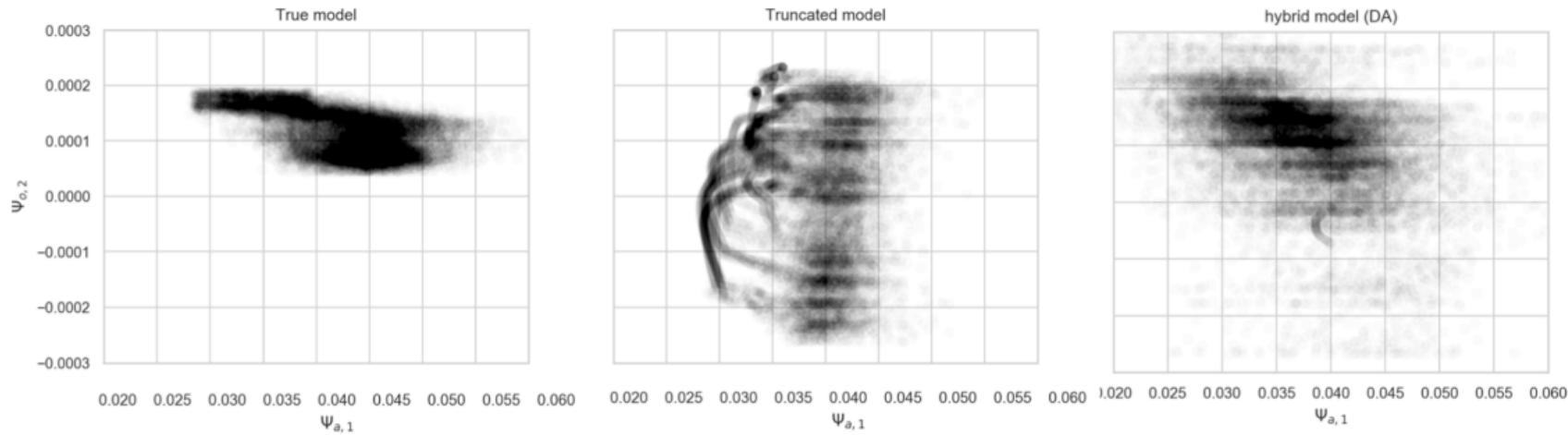
RMSE-f of hybrid and truncated MAOOAM models

RMSE-f(lead time τ)	$\psi_{o,2}$ (2 years)	$\theta_{o,2}$ (2 years)	$\psi_{a,1}$ (1 day)
Truncated	0.23	0.21	0.36
Coupled DA-ML hybrid	0.10	0.06	0.28

- The hybrid models have superior skill to the truncated model.
- The improvement is larger for the ocean that is fully resolved \Rightarrow **Enhanced representation of the atmosphere-ocean coupling processes thanks to coupled DA.**
- The atmosphere is improved less: the hybrid is not very good in representing the fast processes.

Numerical experiments: atmosphere-ocean model MAOOAM

Reconstruction of the model attractor



- The truncated model visits areas of the phase space that are not admitted in the real dynamics.
- Discrepancies are reduced by the hybrid models.

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Forward looking - Some open interesting (to me only?) questions

- ▶ Theory of **DA for multi-scale random and/or non-autonomous climate dynamics** (in relation to random attractor and/or pull-back attractor) (*discussion ongoing with C. Grudzien & others*)
- ▶ Can we use **CLVs to guide strongly coupled DA?**
- ▶ We have used the underlying system's unstable properties to design DA. Can we do the opposite: **use DA to infer key invariant quantities**, e.g. KS, LEs (*ongoing work with Y. Chen & others*).
- ▶ Computing instabilities on-the-fly is too expensive. Can **ML providing a state-dependent map of LLEs/LLVs to be used in DA or in ensemble generation?** (*ongoing work with D. Ayers & others*).
- ▶ Moving mesh models have trouble to be coupled and discontinuous Galerkin methods is becoming an alternative to keep fine features description in an Eulerian mesh. Can we **adapt DA to the node-dependency of the DGM?** (*ongoing work with C. Jones & others*).
- ▶ Sea-ice models calibration is challenging, especially in the Marginal Ice Zone. Can we use combined **DA+ML to infer sub-grid scales parametrization of the sea-ice or to emulate some physical processes?** (*ongoing work with L. Bertino, M. Bocquet, J. Brajard & others*)

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