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Identifying Efficient Ensemble Perturbations for Initializing Probabilistic S2S Prediction

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EMS 5 September 2023

Teaser

- S2S predictions is beyond atmosphere predictability limit

  ➡ Coupled Earth system models must be used

- Usually done with ensemble:

  ➡ How to initialize them consistently to obtain **reliable** results?

- Already tested, use of local properties:
  - Bred vectors (Peña & Kalnay, 2004; Yang et al., 2008; O'Kane et al., 2019)
  - Backward Lyapunov Vectors (BLVs, related to singular vectors) (Vannitsem & Duan, 2020)

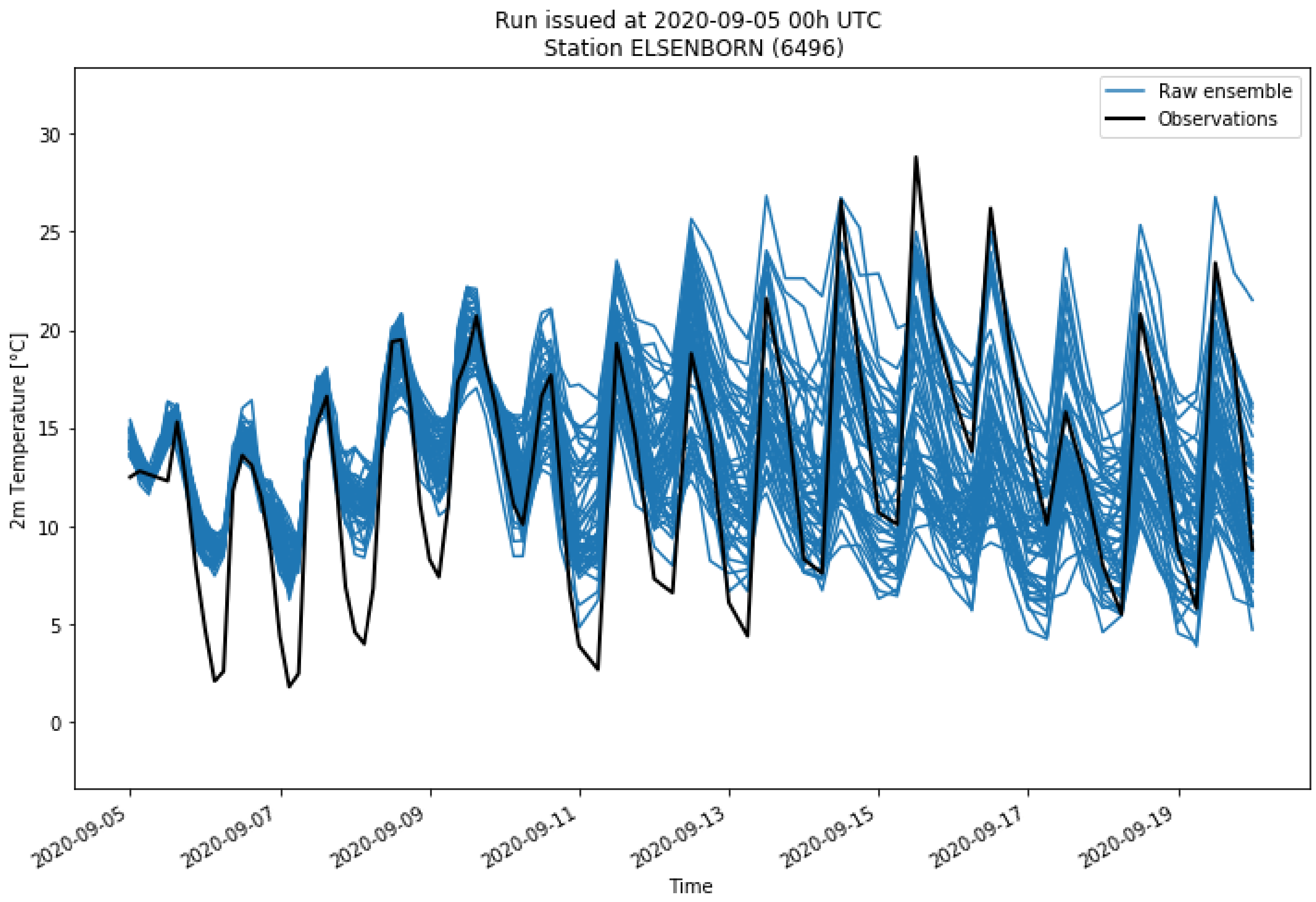
  to tune the initialization of the models.

In the present work, we study the projections of the initial conditions on mainly:

- Lyapunov vectors
- Empirical Orthogonal Functions
- Dynamical Mode Decomposition adjoint modes

Ensemble (probabilistic) forecasting

- Models are chaotic
  → sensitivity to initial conditions
- Statistical estimates: ensemble mean and spread
- Ensemble spread saturates toward the climatological range of values



Probabilistic forecasting - Theoretical basis

The Liouville Equation and Its Potential Usefulness for the Prediction of Forecast Skill. Part I: Theory

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(Manuscript received 7 May 1993, in final form 14 September 1993)

2. The Liouville equation

$$\frac{\partial \rho(\mathbf{X}, t)}{\partial t} + \sum_{k=1}^{N} \frac{\partial}{\partial X_k} [\rho(\mathbf{X}, t)\dot{X}_k(\mathbf{X}, t)] = 0. \quad (2.2)$$

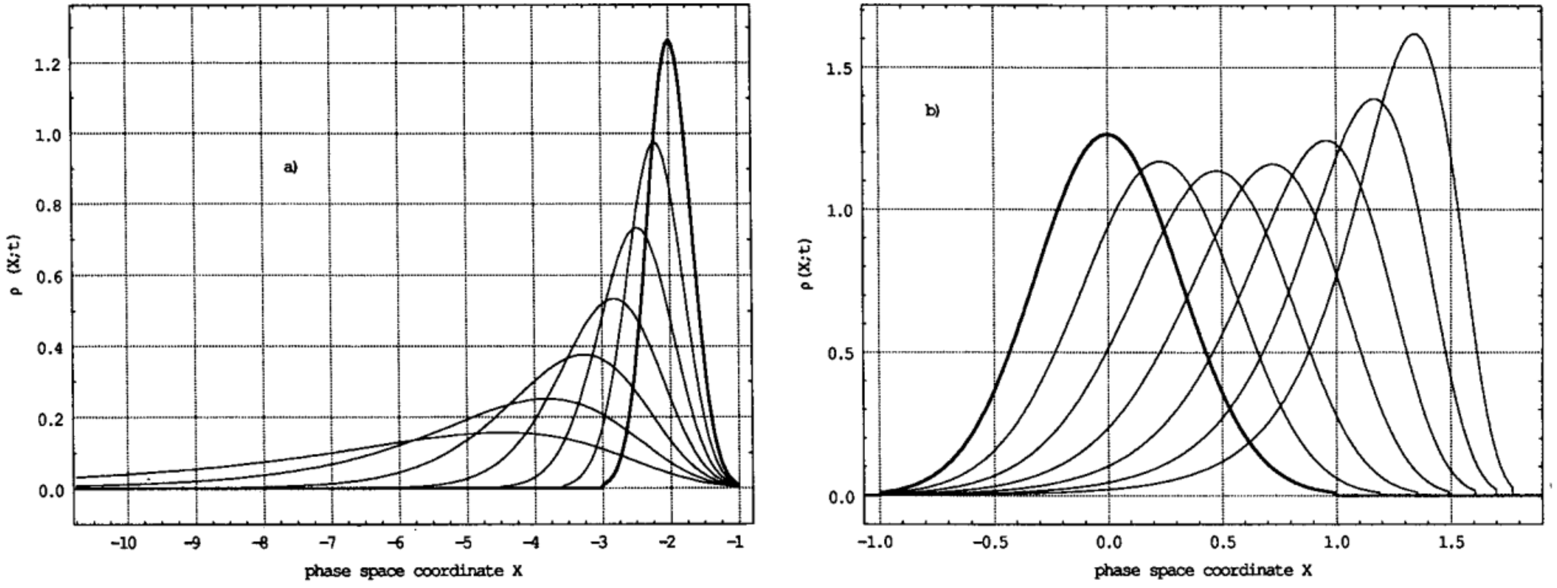


FIG. 1. Display of the analytical solution (4.8) of the LE (4.3) relevant for system (4.1) taking the initial pdf to be Gaussian with mean (a) −2, (b) 0, and variance 0.1 (marked bold). The pdf $\rho(\mathbf{X}, t)$ is plotted as a function of $\mathbf{X}$ with parameter t, taking on the values (a) 0.0–0.3 (step 0.05), and (b) 0.0–0.6 (step 0.1), respectively. For the values of the system parameters a, b, and c, see section 4.

See also Leith (1978).

Verification - What is a reliable ensemble?

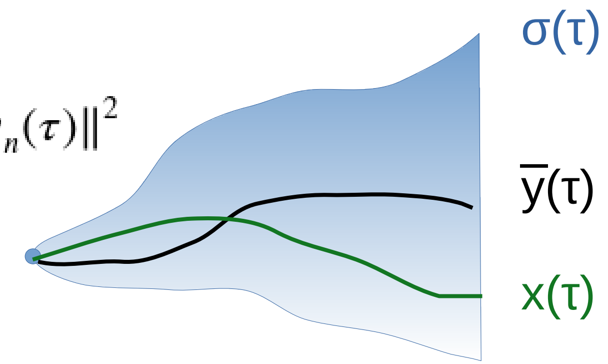
All ensemble members and the true state of a variable are independent draws from the same distribution P(x).

Score to measure this

→ Compare the <MSE of ensemble mean> and the <ensemble variance> sampled over N forecasts.

For the ensemble to be reliable, we must then have:

$$\mathrm{MSE}(\tau) = \frac{1}{N}\sum_{n=1}^{N} \|\boldsymbol{x}_n(\tau) - \bar{\boldsymbol{y}}_n(\tau)\|^2 \quad \approx \quad \mathrm{Spread}^2(\tau) = \frac{1}{N}\sum_{n=1}^{N}\frac{1}{M-1}\sum_{m=1}^{M}\|\boldsymbol{y}_{m,n}(\tau) - \bar{\boldsymbol{y}}_n(\tau)\|^2$$



where

$$\bar{\boldsymbol{y}}_n(\tau) = \frac{1}{M}\sum_{m=1}^{M} \boldsymbol{y}_{m,n}(\tau)$$

is the ensemble mean over the members $\boldsymbol{y}_{m,n}(\tau)$ of the nth ensemble forecast and $\boldsymbol{x}_n(\tau)$ is the corresponding reference solution.

Because if an ensemble is reliable then both MSE and Spread² converge for large N to the variance of P(x).

Leutbecher & Palmer (2007)

Verification - What is a reliable ensemble?

All ensemble members and the true state of a variable are independent draws from the same distribution P(x).

Another score to measure this: Dawid-Sebastiani score (based on ignorance score)

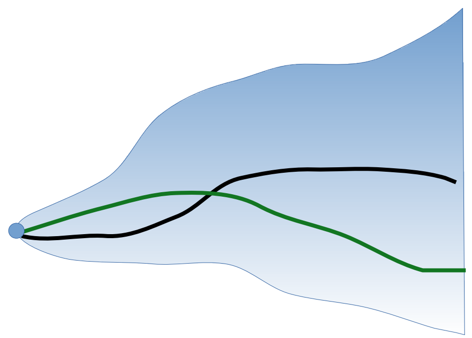
$$\mathrm{DSS}_{n,i}(\tau) = \frac{1}{2}\log(2\pi) + \frac{1}{2}\log\,\sigma^2_{n,i}(\tau) + \frac{1}{2}\frac{M-3}{M-1}\left(\bar{y}_{n,i}(\tau) - x_{n,i}(\tau)\right)^2 / \sigma^2_{n,i}(\tau),$$

Logarithmic penalty for the ensemble spread

Mean squared error of reduced centered variable

where $\sigma^2_{n,i}$ is an estimator of the ith variable ensemble variance:

$$\sigma^2_{n,i}(\tau) = \frac{1}{M-1}\sum_{m=1}^{M} |y_{m,n,i}(\tau) - \bar{y}_{n,i}(\tau)|^2.$$



This score can then be averaged over the N realizations:

$$\mathrm{DSS}_i(\tau) = \frac{1}{N}\sum_{n=1}^{N} \mathrm{DSS}_{n,i}(\tau).$$

The lower the DSS score, the more reliable the ensemble forecasts are for this particular variable.

Leutbecher (2019)

How to get a reliable ensemble?

- Postprocessing
- Try to construct directly such an ensemble from the start

  → **Initial conditions projection methods**

(e.g. singular vectors for the ECMWF ensemble predictions)

Buizza & Palmer (1995).

Technical prerequisite

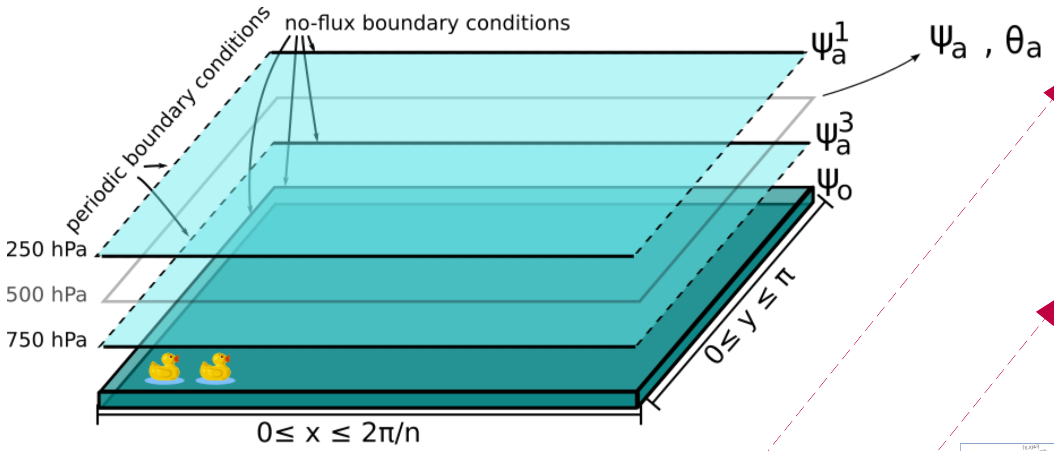
How to initialize ensemble consistently to obtain **reliable** results?

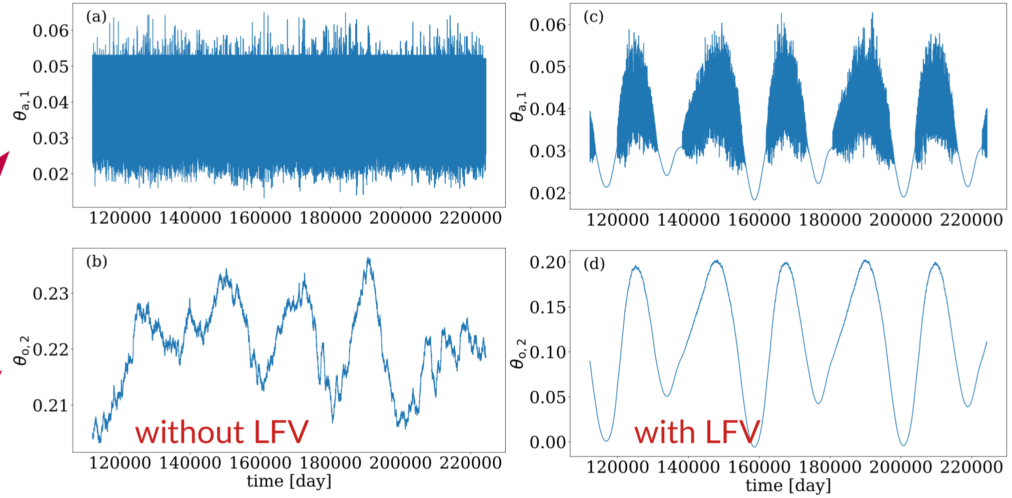
In the present work, we study the projections of the initial conditions on mainly:

- **Lyapunov vectors**
  - **→ Local stability vectors (Covariant or obtained through orthogonalization)**
- **Empirical Orthogonal Functions (EOF)**
  - **→ Related to the covariance matrix of the fields**
  - **→ Global mode "explaining" the variance**
- **Dynamical Mode Decomposition (DMD) and its adjoint modes**
  - **→ Global modes related to Linear Inverse Models (LIM)**
  - **→ Also related to the Koopman (KM) and Perron-Frobenius (PF) operators of the system at hand** (Tu et al., 2014)
  - **→ Related to the propagation of probability densities in the system**
  - **→ Data-driven, easy to compute, can be computed from analysis**

How to get a reliable ensemble for S2S forecasts?

MAOOAM - QG atmosphere coupled to a shallow-water ocean



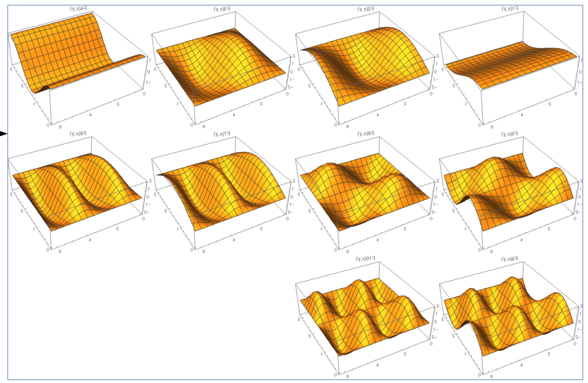


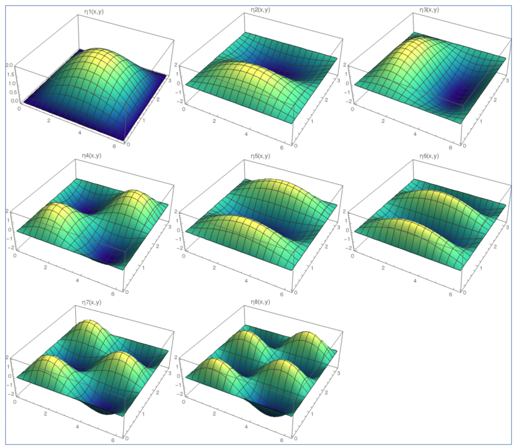
Atm. streamfunction $\psi_a(x,y) = \sum_{i=1}^{n_a} \psi_{a,i} F_i(x,y)$

Atm. temperature $\theta_a(x,y) = \sum_{i=1}^{n_a} \theta_{a,i} F_i(x,y)$

Oc. streamfunction $\psi_o(x,y) = \sum_{i=1}^{n_o} \psi_{o,i} \phi_i(x,y)$

Oc. temperature $\theta_o(x,y) = \sum_{i=1}^{n_o} \theta_{o,i} \phi_i(x,y)$





Experiments design

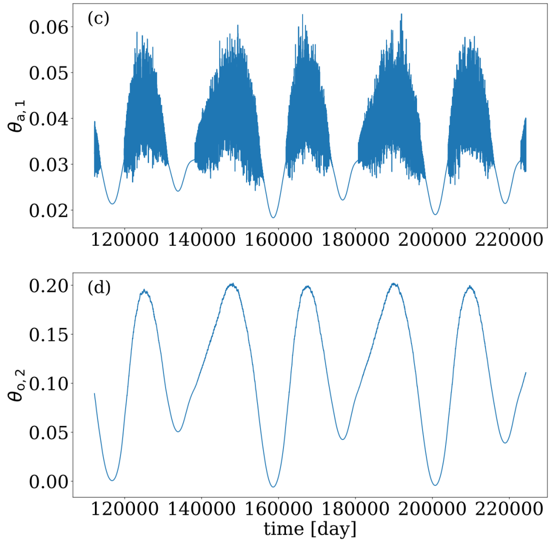
N ensemble forecasts along a reference trajectory:

Control run IC: $\boldsymbol{x}_n^{\text{ctrl}}(0) = \boldsymbol{x}_n(0) + \boldsymbol{\delta x}_0^{\text{ctrl}}$ n = 1,…,N

Perfect ensemble IC: $\boldsymbol{y}_{m,n}(0) = \boldsymbol{x}_n^{\text{ctrl}}(0) + \boldsymbol{\delta x}_0^m \quad , \quad m = 1, \ldots, M-1$

$\boldsymbol{\delta x}_0^M = 0$

Same distribution U[-ε/2,ε/2]



<u>Experiments</u>
Projection onto subspaces spanned by selected vectors:

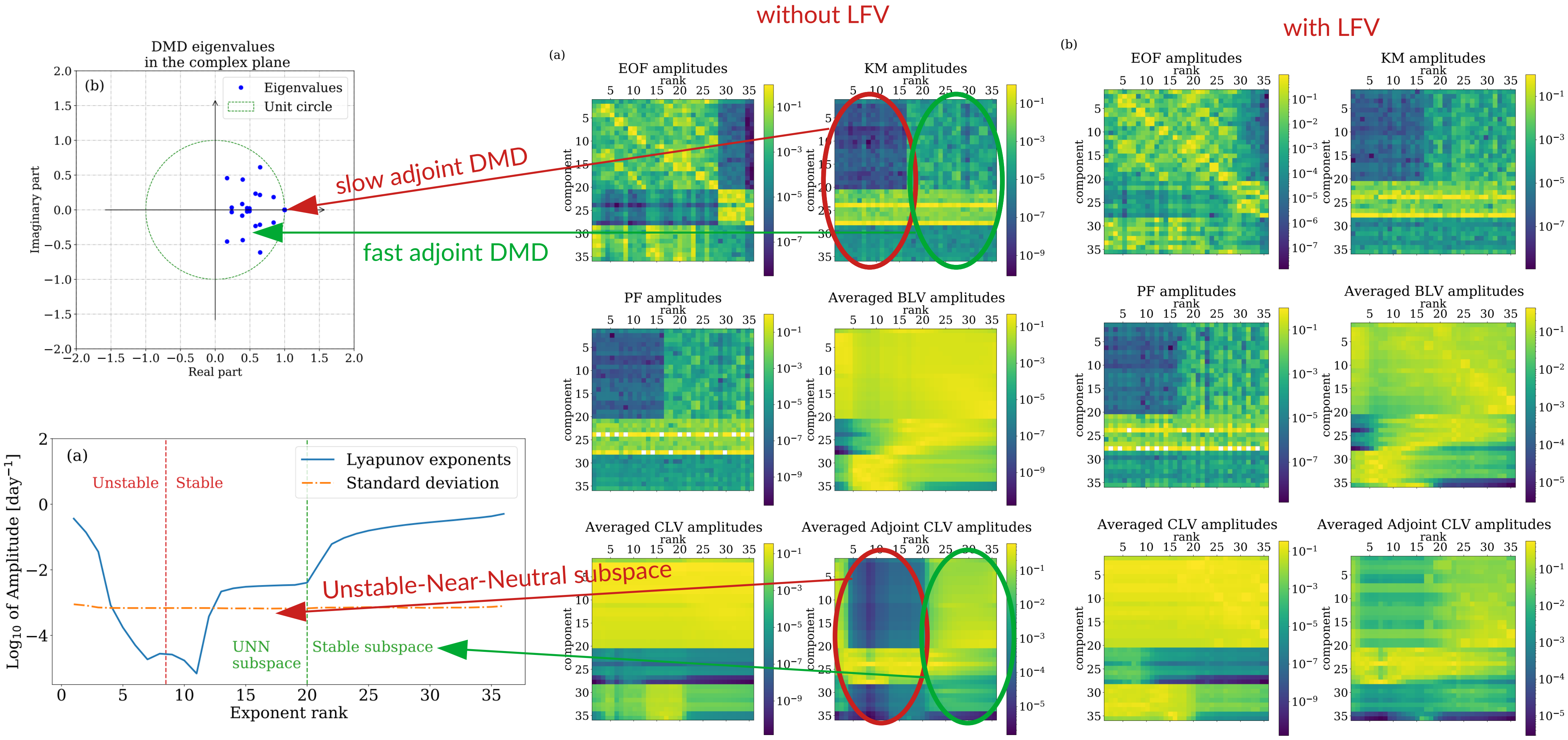
Projector: $\Pi = B(B^* B)^{-1} B^*$ where B is the column matrix of the selected vectors

Projected perturbations: $\boldsymbol{\delta x}'^m_0 = \Pi\, \boldsymbol{\delta x}_0^m$

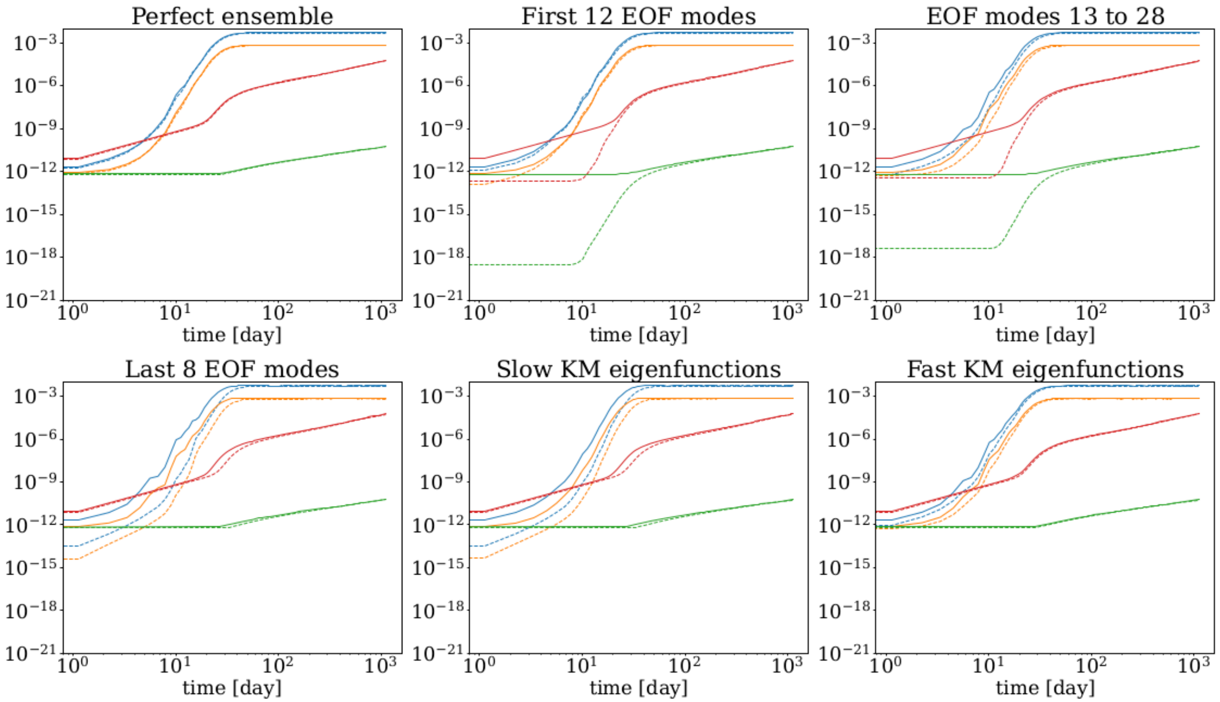
New ensembles: $\boldsymbol{y}'_{m,n}(0) = \boldsymbol{x}_n^{\text{ctrl}}(0) + \boldsymbol{\delta x}'^m_0 \quad , \quad m = 1, \ldots, M$

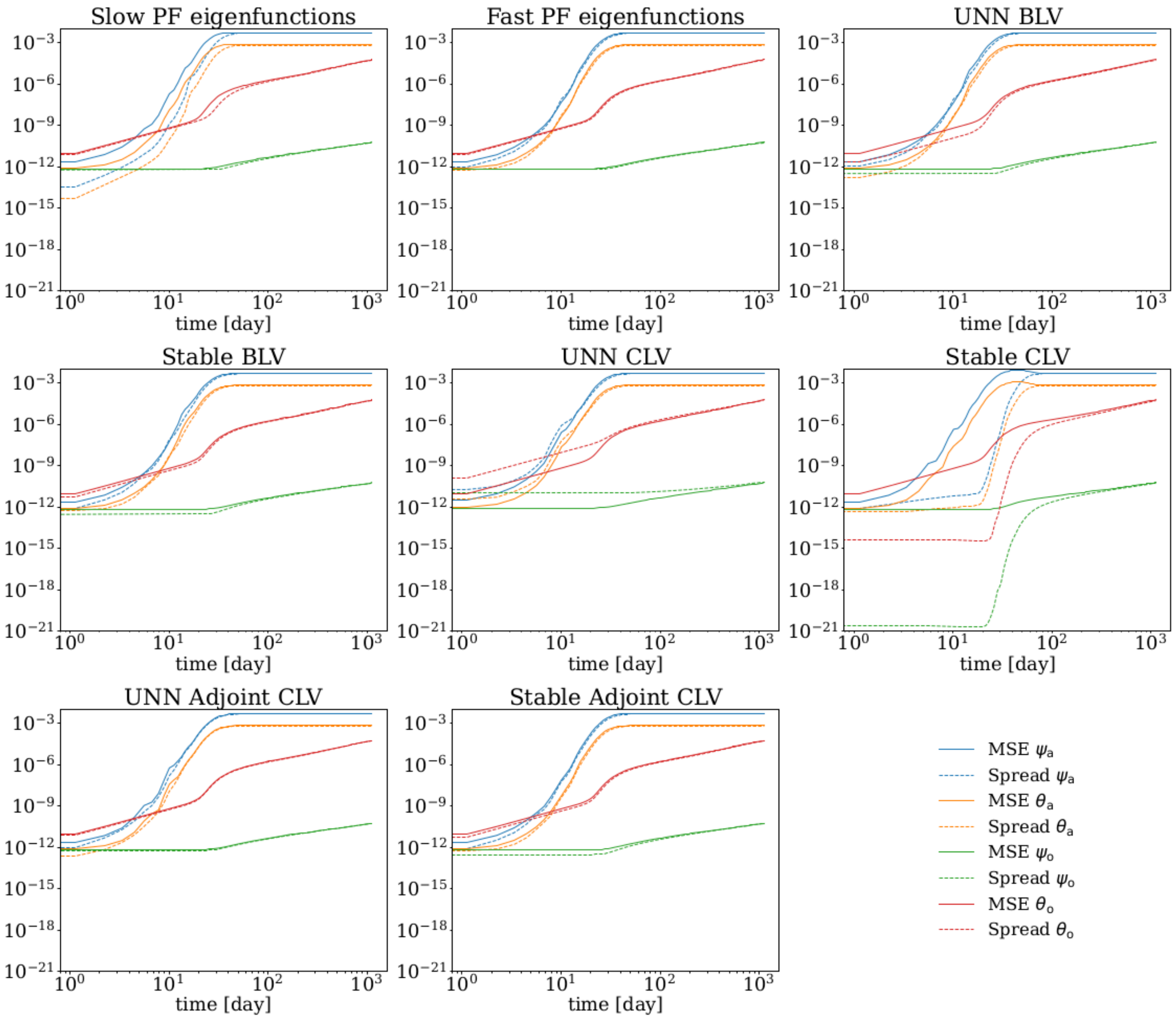
<u>Goal:</u>
→ Obtain forecasts as reliable as the ones provided by the perfect ensembles.

Selected bases: analysis of the reference trajectory



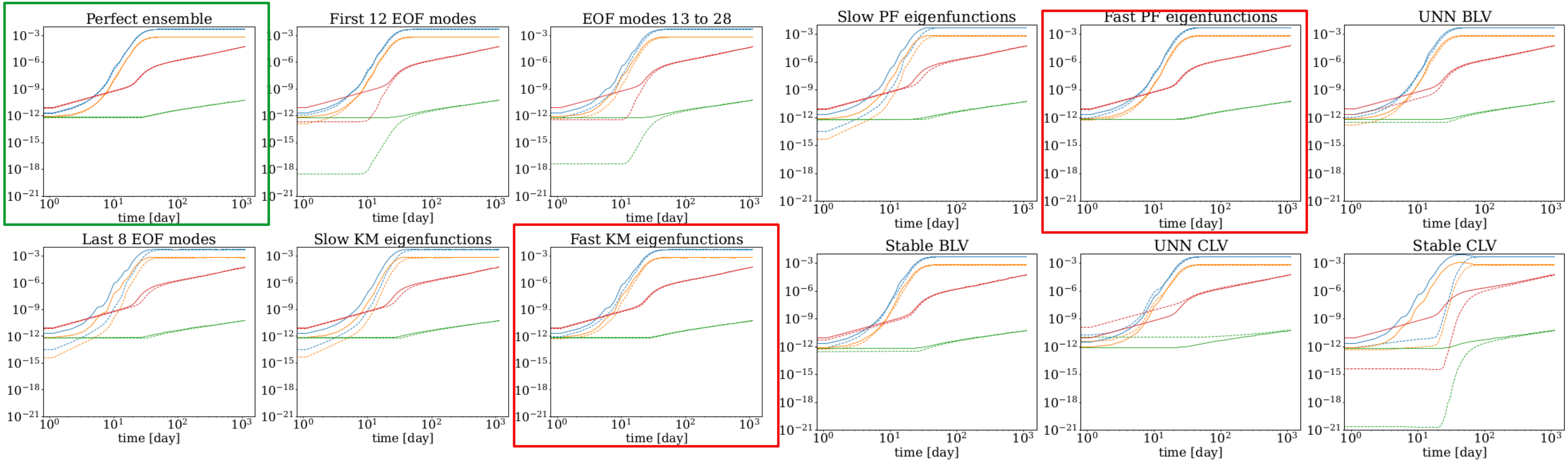
Results (MSE)

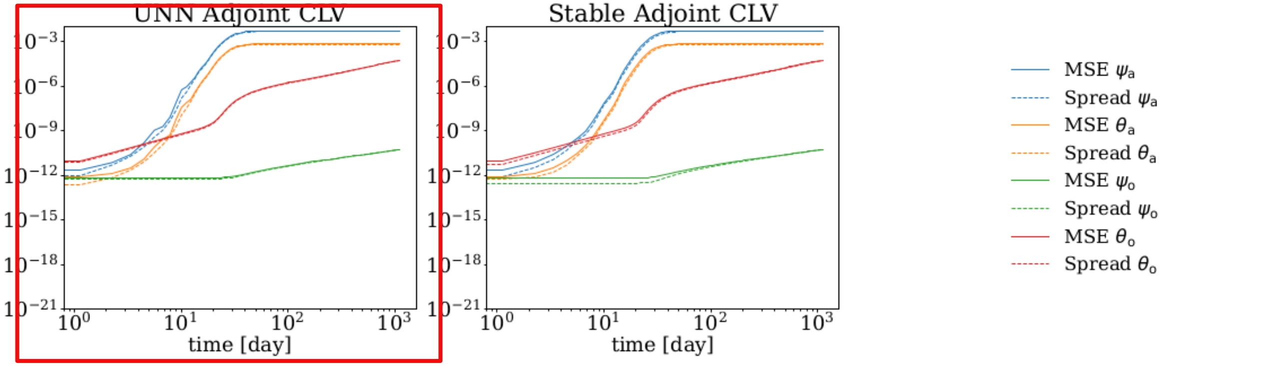




MSE ~ Spread^2 → Reliable ensemble

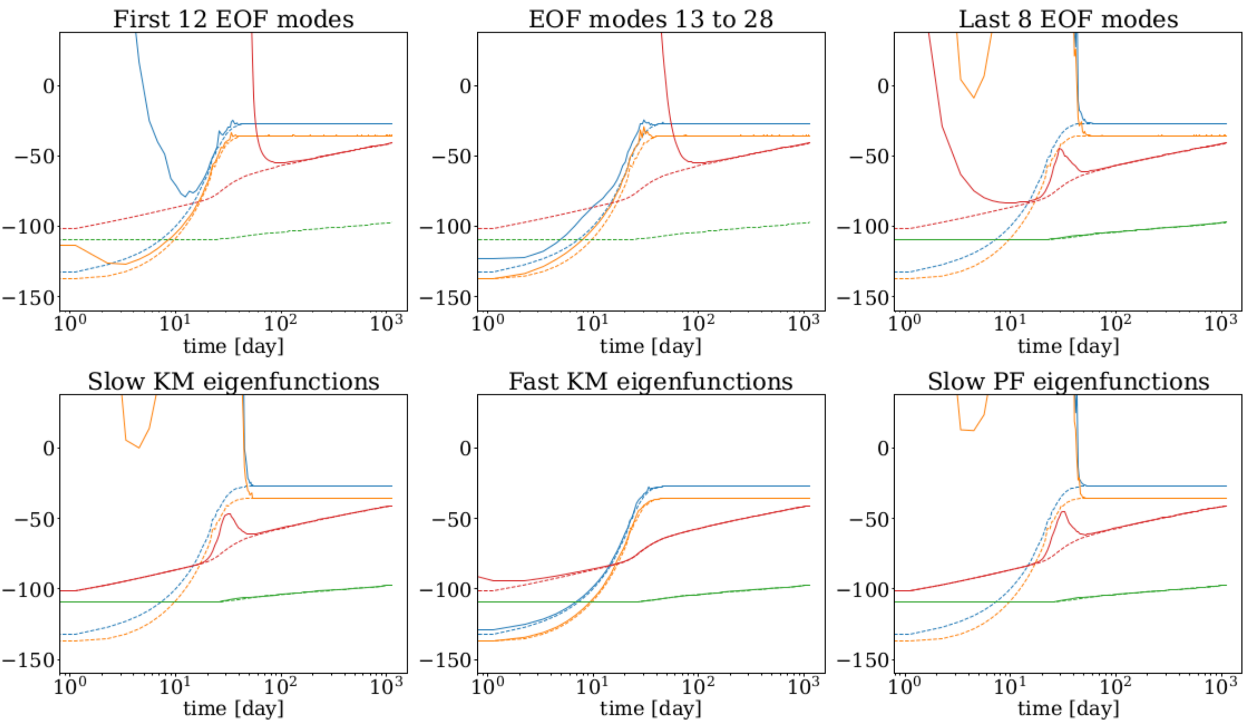
Results (MSE)

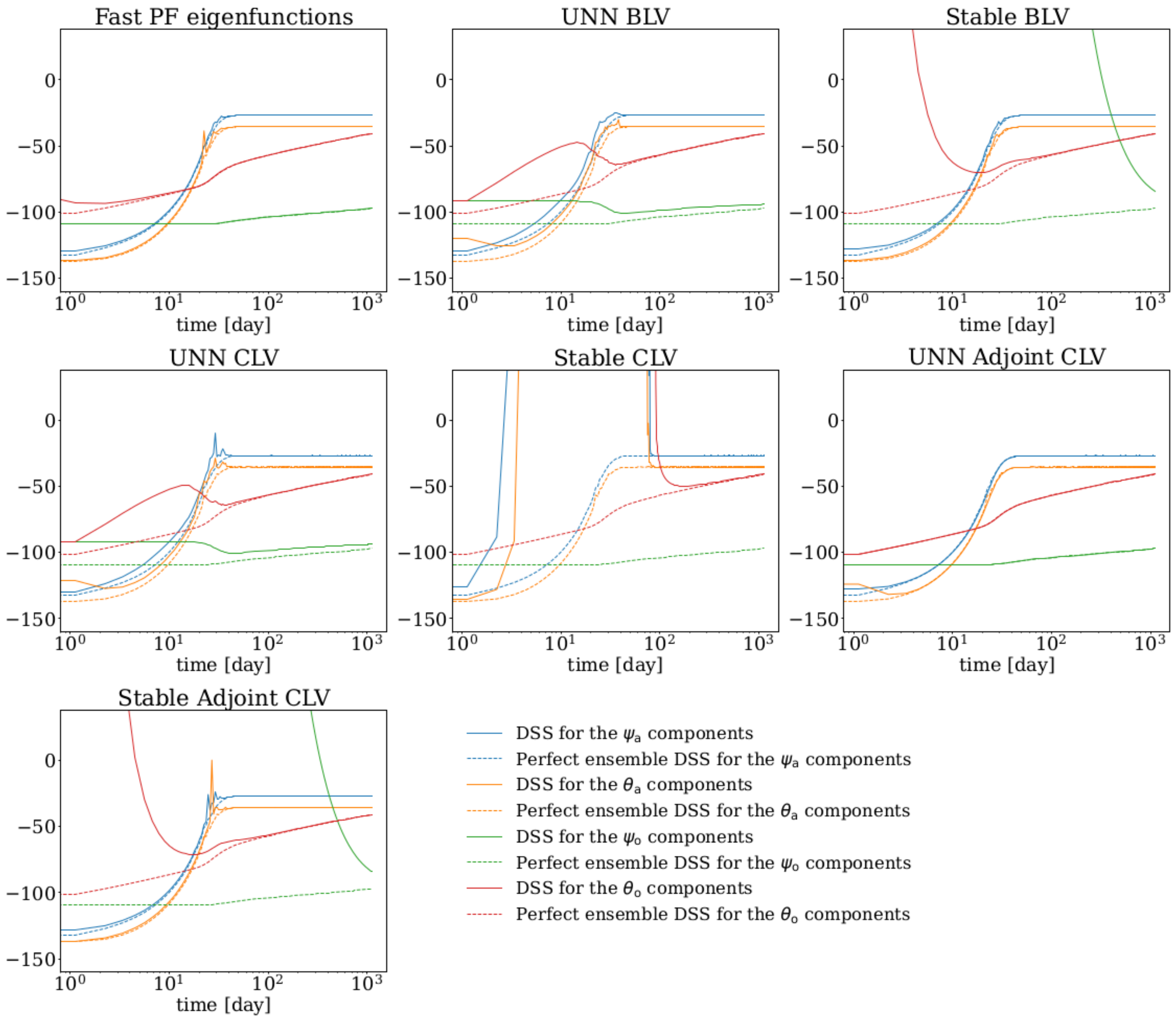




MSE ~ Spread^2 → Reliable ensemble

Results (DSS)

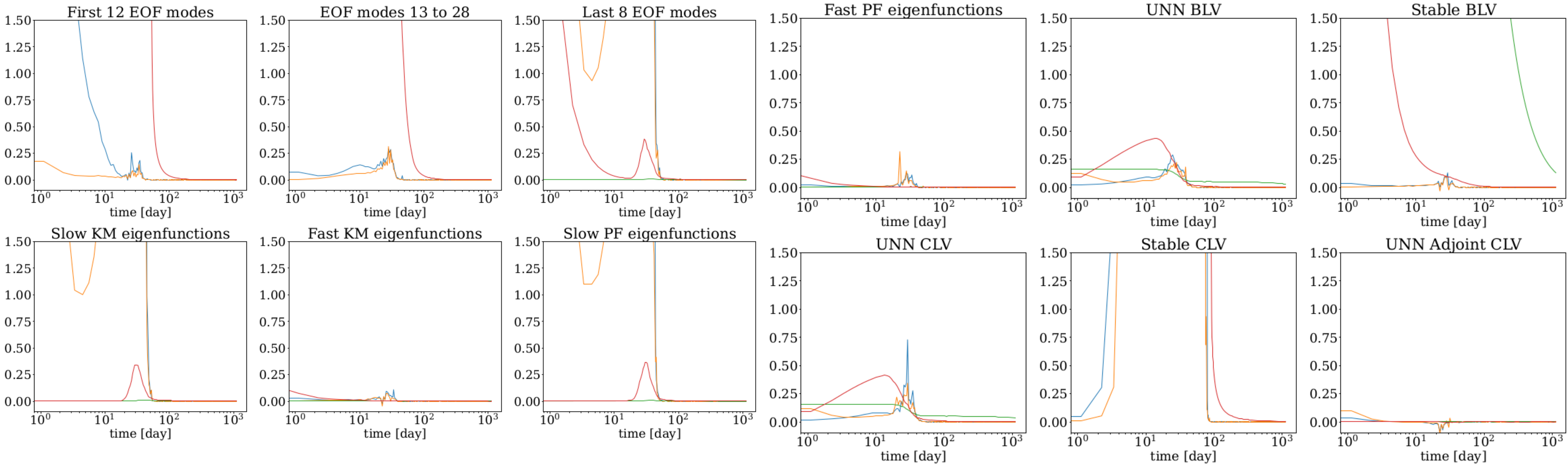


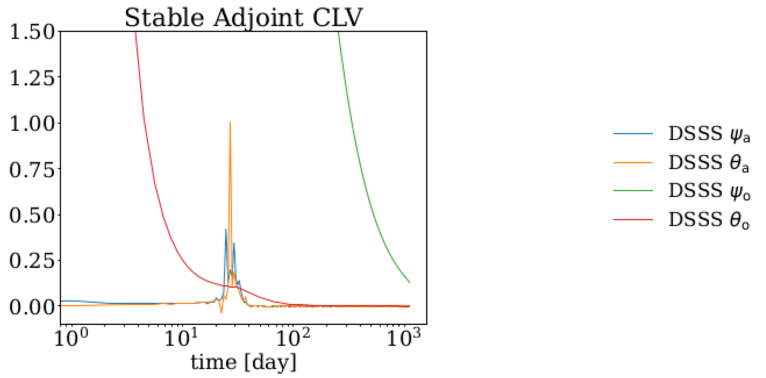


Aggregated DSS over ψ_a , θ_a , ψ_o and θ_o:

- The lower the DSS the better
- Dotted lines: DSS of the perfect ensemble random ICs
- Solid lines: DSS of the projected ICs

Results (DSSS)



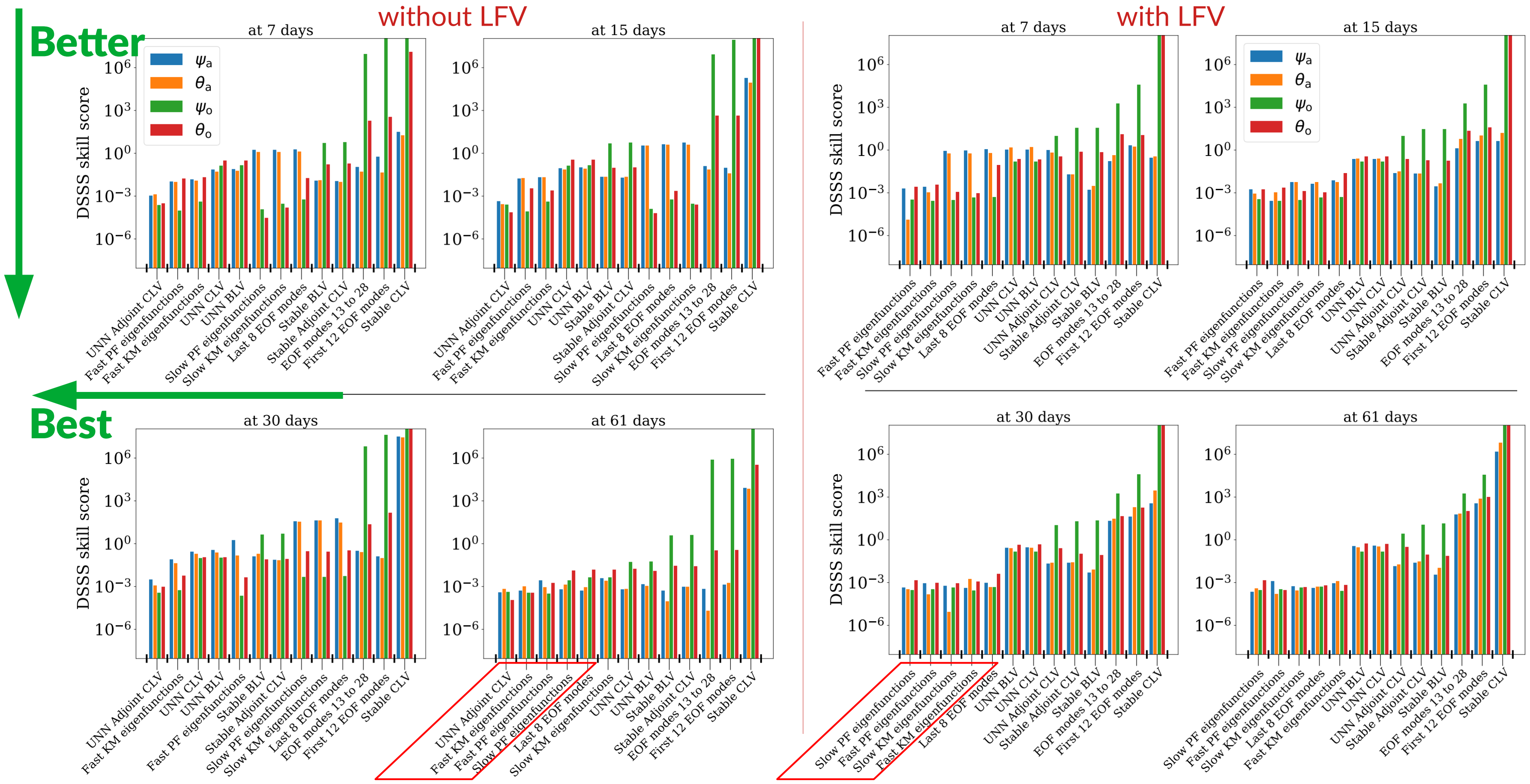


Skill score:

$DSSS = 1 – DSS_{method} / DSS_{perfect}$

The smaller the better ! 0 = perfect ensemble

Results: DSSS skill scores at different lead times



DMD based method

DSSS:
Skill score based on the Dawid-Sebastiani score. Worth 0 if same reliability as the perfect ensemble.

Dawid & Sebastiani (1999)

Leutbecher (2019)

Skill score:

$$DSSS = 1 - DSS_{method} / DSS_{perfect}$$

Conclusion

Key message:

- Approximated KM and PF eigenfunctions obtained using DMD provide reliable ensemble forecasts, and are "easy" to compute.
- Competitive at the S2S timescale with local Lyapunov vectors
- Results seem to not depend on the regime (with or withour LFV)

Forthcoming developments:

- Many, but most notably, replication of the study with a higher-dimensional system, with a non-trivial dimensionality reduction to make DMD tractable.
- Ultimately, development of the approach in a realistic S2S framework.
- Can it be used to initialize ensembles in the ocean alone with forcing from the atmosphere? (project starting soon with A. Aydogdu (CMCC))

Takeaway message

To initialize ensemble forecast for S2S:

- ensembles of initial conditions can be constructed in relevant subspaces constructed with *measures* of the system valid at these timescales (through global DMD modes)

Reference

Jonathan Demaeyer, Stephen G. Penny, Stéphane Vannitsem. Identifying efficient ensemble perturbations for initializing subseasonal-to-seasonal prediction. JAMES, 2022, doi: 10.1029/2021MS002828

THANK YOU

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Lyapunov vectors (BLVs & CLVs)

Considering a dynamical system $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})$ and the evolution of perturbations in its tangent space:

$$\dot{\boldsymbol{\delta x}}(\tau) = \left.\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right|_{\boldsymbol{x}(\tau)} \boldsymbol{\delta x}(\tau)$$

given by $\boldsymbol{\delta x}(t) = \mathsf{M}(t, t_0)\, \boldsymbol{\delta x}_0 \quad , \quad \boldsymbol{\delta x}_0 = \boldsymbol{\delta x}(t_0)$

where M is the propagator (of the perturbations).

- The Backward Lyapunov Vectors (BLVs) are the eigenvectors of

$$\left(\mathsf{M}(t, t_0)\mathsf{M}(t, t_0)^{\mathsf{T}}\right)^{1/(2(t-t_0))}$$ in the limit $t_0 \to \infty$

➡ Can be interpreted as an orthonormal basis defining volumes covariant with the dynamics. Is related to the singular vector, i.e. the eigenvectors of the matrix above with finite t and t_0.

- The Covariant Lyapunov Vectors (CLVs) are such that: $\mathsf{M}(t, t_0)\, \boldsymbol{\varphi}_i(t_0) = \Lambda_i(t, t_0)\, \boldsymbol{\varphi}_i(t)$
- The adjoint CLVs $\tilde{\boldsymbol{\varphi}}_i$ are adjoint (biorthonormal) to the CLVs: $\tilde{\boldsymbol{\varphi}}_i^{\mathsf{T}}\, \boldsymbol{\varphi}_j = \delta_{i,j}$

➡ Both can be interpreted as directions covariant with the dynamics.

Dynamical Modes Decomposition (DMD)

- Considering 2 collections of states of a dynamical system X=[$\mathbf{x}_0$ ... $\mathbf{x}_{K-1}$] and Y=[$\mathbf{x}_1$ ... $\mathbf{x}_K$], then one define

$$\mathrm{M}^{\mathrm{DMD}} = \mathrm{Y}\,\mathrm{X}^{+}$$ where X^{+} is the pseudoinvere

as the DMD decomposition of the observable **g**(**x**)=**x** the system. Related to Linear Inverse Modeling

Penland (1989)

- The left eigenvectors $\mathbf{w}_i$ of M^{DMD} provides approximation of the system's Koopman operator eigenfunctions and are called *adjoint* DMD modes. (Tu et al., 2014)

- The Koopman K operator is an ∞-dimensional linear operator propagating the observable of the system. For an observable *g* :

$$\mathcal{K}^{\tau}\, g(\boldsymbol{x}) = g\left(\boldsymbol{\Phi}^{\tau}(\boldsymbol{x})\right)$$ where ϕ is the flow of the system $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})$

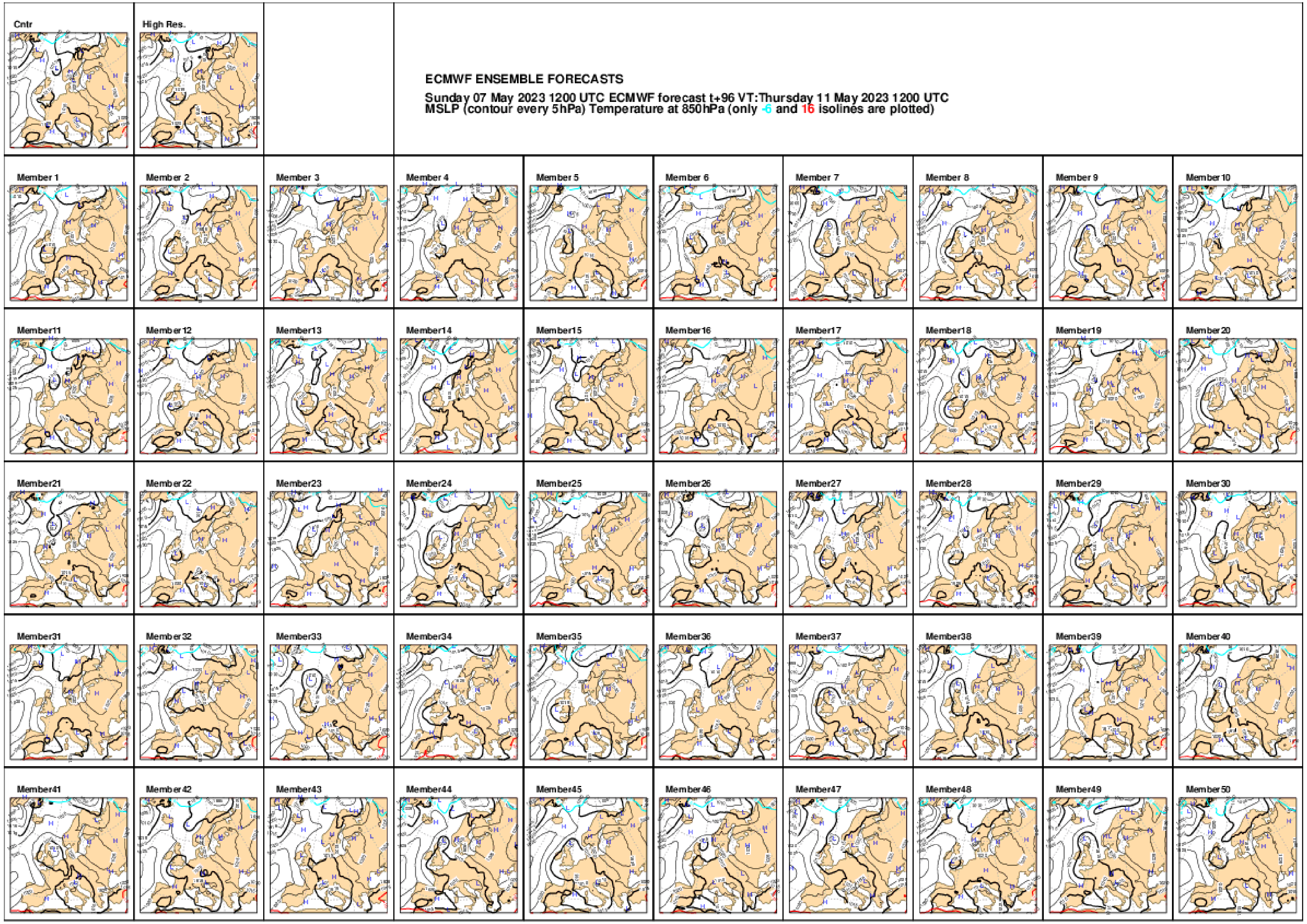
- The action of the Koopman operator can then be approximated with the DMD as

$$\sum_{i=1}^{P} \boldsymbol{c}_i^{\mathrm{DMD}}\, \lambda_i^{\mathrm{DMD}}\, \boldsymbol{w}_i^{*} \quad \boldsymbol{x}$$ ⇒ where the $\mathbf{c}_i^{DMD}$ are modes depending on the observable *g*

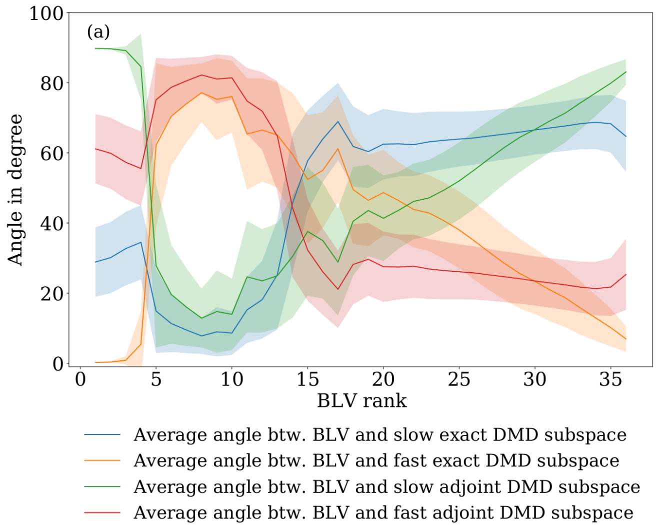
The $\mathbf{w}_i$ define approximate invariant manifolds for the Koopman operator

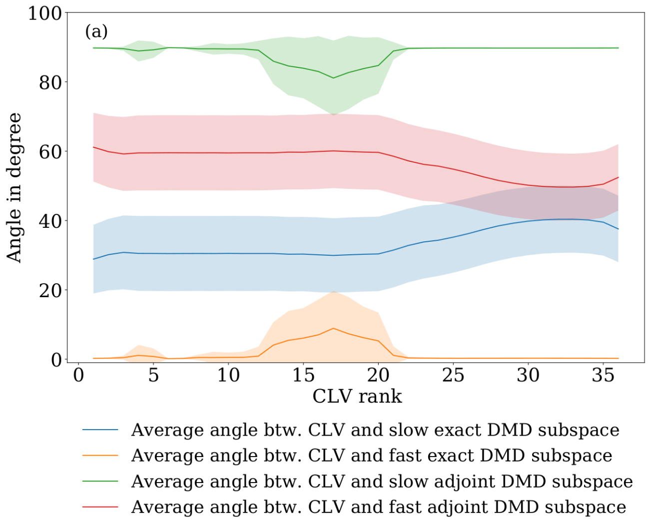
Same decomposition exists for the Perron-Frobenius (PF) operator propagating the probability distributions in the system.

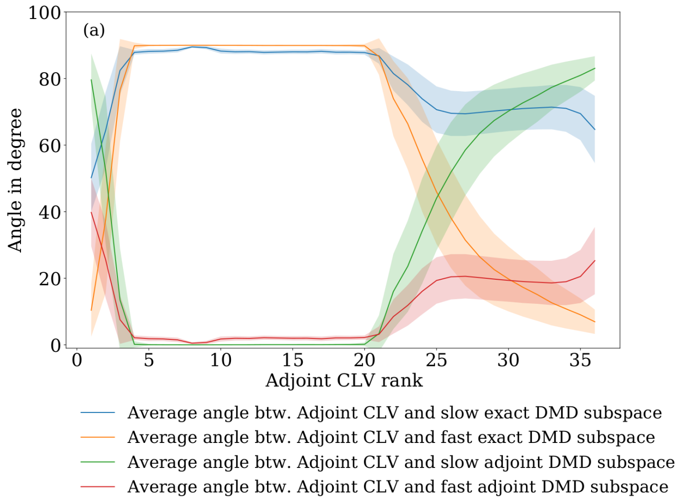
Ensemble (probabilistic) forecasting



Backup: Correspondence between bases







Fast BLVs close to adjoint DMDs (KM eigenfunctions) → Explains good results obtained with fast BLVs in Vannitsem & Duan (2020)

CLVs related to DMDs (KM modes)

Adjoint CLVs related to adjoint DMDs (KM eigenfunctions)