Linear Stochastic Emulators of the Ocean Circulation based on Balanced Truncation: A Caution, perhaps, for Machine Learning?

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Linear Inverse Models (LIMs)

- LIMs are approximations of very large dynamical systems of greatly reduced dimension derived from large data sets.
- When there is a clear separation of the time-scales the data can be well represented by a Markov model (aka auto-regressive model):

$$\boldsymbol{x}(t+1) = \boldsymbol{\mathcal{A}}\boldsymbol{x}(t) + \boldsymbol{\mathcal{B}}\boldsymbol{\xi}(t)$$

$$\boldsymbol{y}(t+1) = \boldsymbol{\mathcal{C}}\boldsymbol{x}(t+1)$$

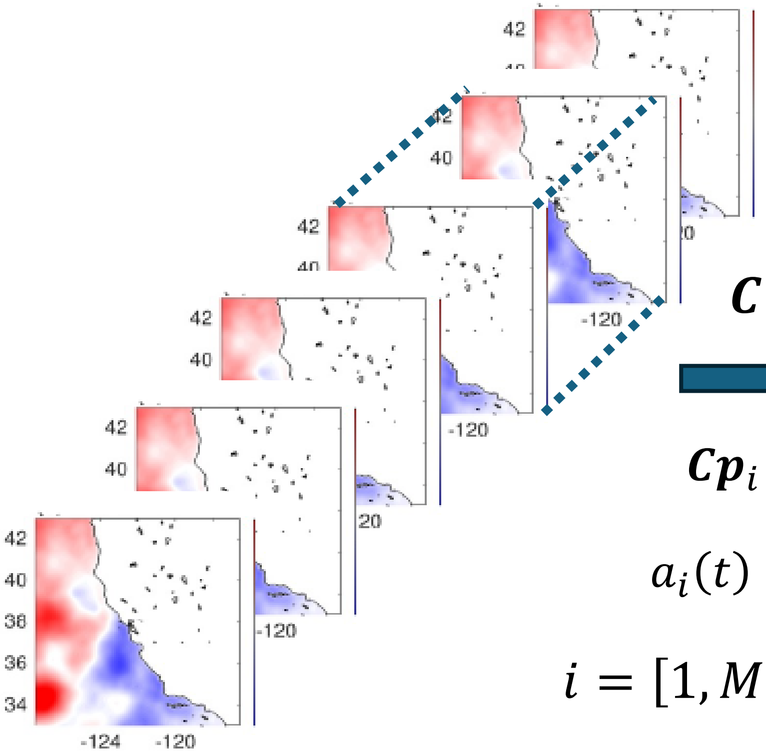
(Formally written as a 1st-order process but can be extended to higher order by augmenting with time derivatives, Neumaier & Schneider(2001))

$\boldsymbol{\mathcal{A}}$ = the transition matrix; $\boldsymbol{\xi}(t)$ = stochastic forcing, usually white in *time*, with spatial covariance given by $\boldsymbol{\mathcal{B}}\boldsymbol{\mathcal{B}}^T$; $\boldsymbol{y}$ = the output described by $\boldsymbol{\mathcal{C}}$

- For white noise forcing in time, $\boldsymbol{\mathcal{A}} = E\{\boldsymbol{x}(t+1)\boldsymbol{x}^T(t)\}/E\{\boldsymbol{x}(t)\boldsymbol{x}^T(t)\}$ (i.e. the ratio of the lag-1 to the lag-0 autocovariance of $\boldsymbol{x}$).
- $\boldsymbol{\mathcal{A}}$ has a high dimension → construct a reduced rank approx^n $\widetilde{\boldsymbol{\mathcal{A}}}$ using EOFs of $E\{\boldsymbol{x}(t)\boldsymbol{x}^T(t)\}$.
- LIMs have enjoyed considerable popularity in the geosciences.
- The typical approach of using only the EOFs though may be fundamentally flawed.
- In many ways linear inverse models are the prototype of machine learning, so there may be some valuable lessons here for more advanced machine learning approaches.

LIM Dimension Reduction based on EOFs

N individual realizations of $\boldsymbol{x}$



$$\boldsymbol{C} = E\{\boldsymbol{x}\boldsymbol{x}^T\}$$

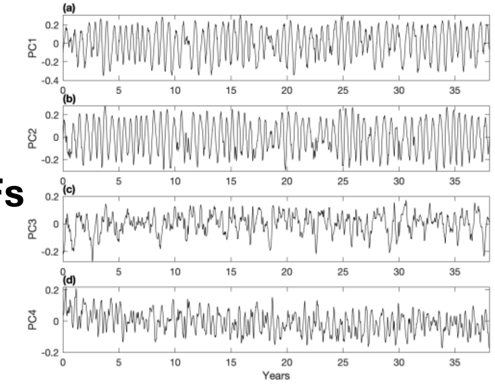
EOFs

$$\boldsymbol{C}\boldsymbol{p}_i = \lambda_i \boldsymbol{p}_i$$

$$a_i(t) = \boldsymbol{p}_i^T \boldsymbol{x}(t)$$

$$i = [1, M], M \ll N$$

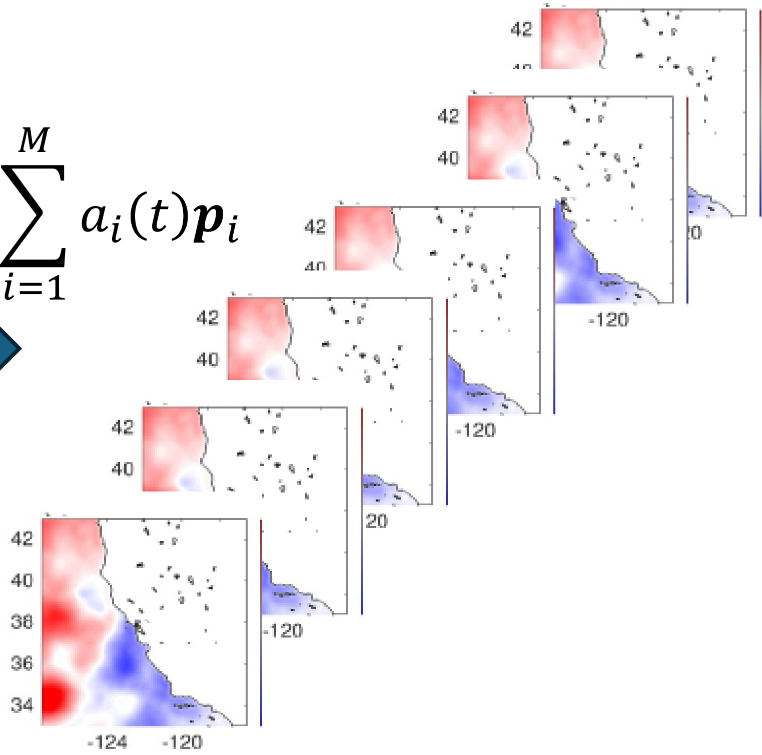
Principal component time series $a_i(t)$



$$\boldsymbol{a}(t+1) = \widetilde{\boldsymbol{\mathcal{A}}}\boldsymbol{a}(t) + \widetilde{\boldsymbol{\mathcal{B}}}\boldsymbol{\xi}(t)$$

$$\widetilde{\boldsymbol{y}}(t+1) = \widetilde{\boldsymbol{\mathcal{C}}}\boldsymbol{a}(t+1)$$

$$\boldsymbol{x}(t) = \sum_{i=1}^{M} a_i(t)\boldsymbol{p}_i$$



"Encoder" ***"Latent space"*** ***"Decoder"***

For most (if not all!) geophysical flows the transition matrix $\mathcal{A}$ is <u>non-normal</u>.
In this case the EOFs do tell the whole story.
The leading EOFs capture the variance but not the <u>cause</u> of the variance.

Normal vs Non-Normal Systems

Normal System

- $\mathcal{A}\mathcal{A}^T = \mathcal{A}^T\mathcal{A}$
- $\mathcal{A}$ has orthogonal eigenvectors
- $\mathcal{A}$ and $\mathcal{A}^T$ have identical eigenvectors

Non-normal System

- $\mathcal{A}\mathcal{A}^T \neq \mathcal{A}^T\mathcal{A}$
- $\mathcal{A}$ has non-orthogonal eigenvectors
- $\mathcal{A}$ and $\mathcal{A}^T$ have different eigenvectors

Why is this important?
Non-normal systems can support perturbations that can undergo rapid transient growth and sustain elevated levels of stochastically-induced variance compared to normal systems.

What makes $\mathcal{A}$ non-normal?
Any mathematical operator that breaks the symmetry of $\mathcal{A}$ will render it non-normal.

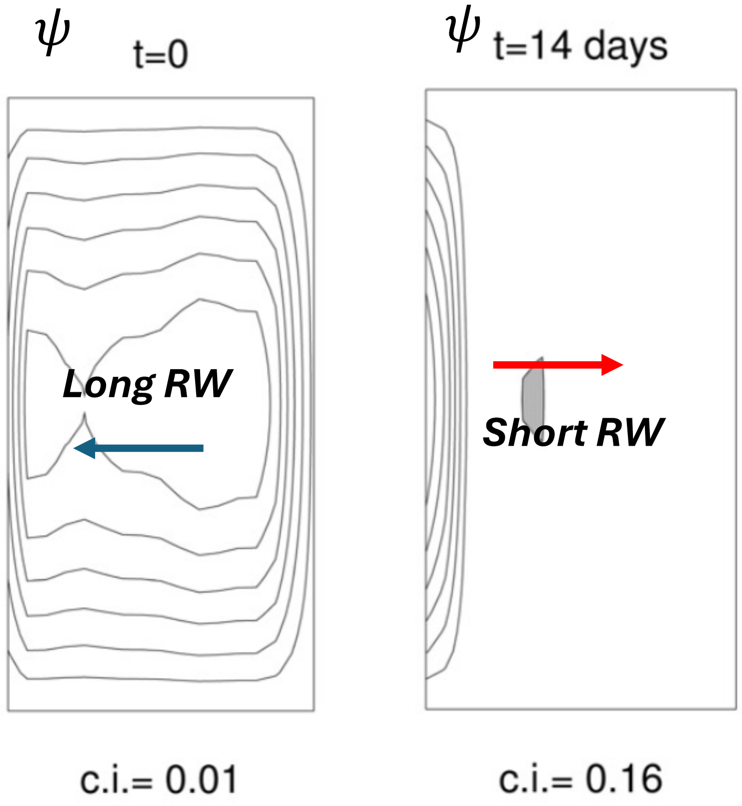
Some familiar physical causes of non-normality are:

- The β-effect (rotation and stretching)
- Strain and shear

Examples

The β-effect

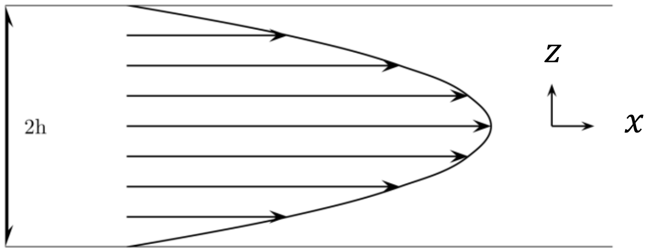
The linear barotropic vorticity eqn



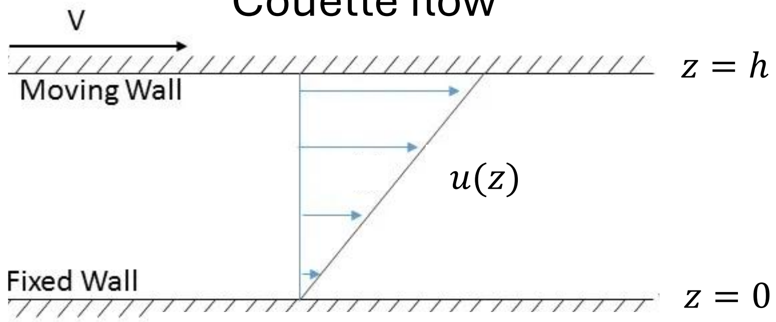
Perturbation growth accompanied by an increase in *enstrophy*

Shearing and Straining Flows

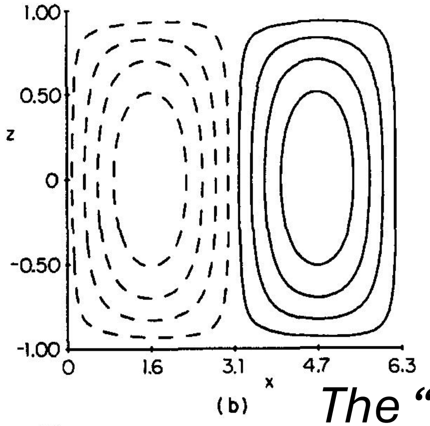
Poiseuille flow



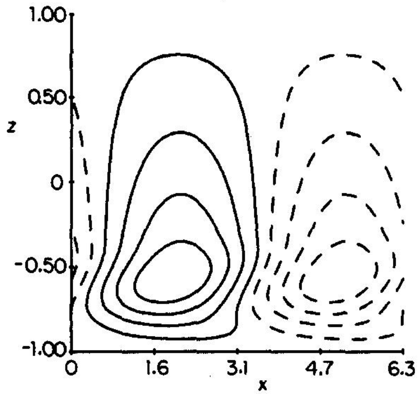
Couette flow



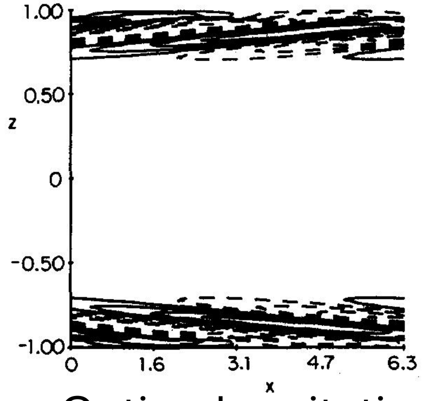
Most unstable mode



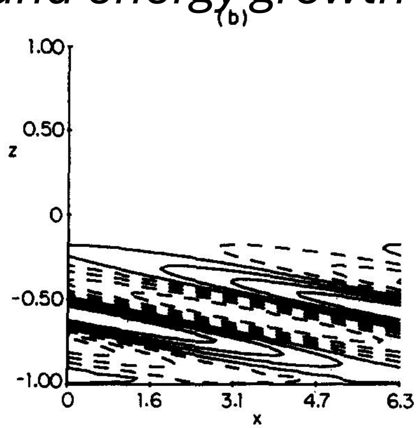
Most unstable mode



The "lift-up effect" and energy growth



Optimal excitation



Optimal excitation

Farrell (1988)

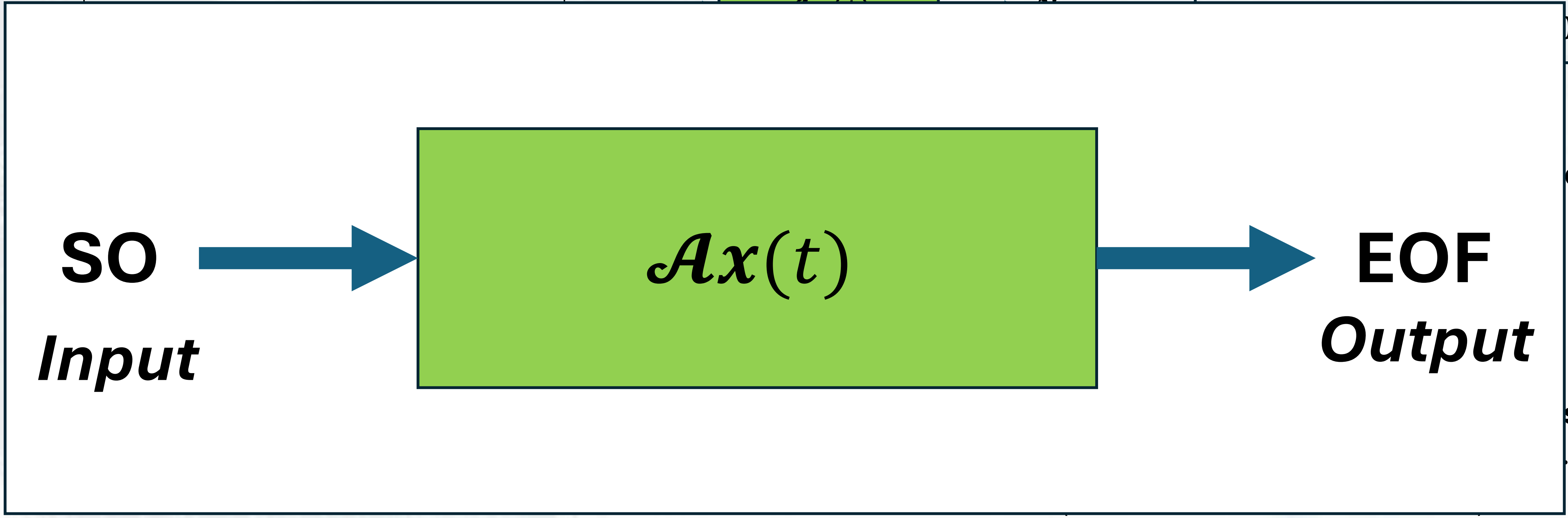
Stochastically Forced Systems & Balanced Truncation

The variance of a stochastically forced system can be quantified in terms of the ***output*** (EOFs) or in terms of the ***input*** (Stochastic Optimals).

$$\boldsymbol{x}(t+1) = \mathcal{A}\boldsymbol{x}(t) + \mathcal{B}\xi(t)$$

$\mathcal{B}\xi(t)$

$$\boldsymbol{P} - \mathcal{A}\boldsymbol{P}\mathcal{A}^T - \mathcal{B}\mathcal{B}^T = \boldsymbol{0}$$



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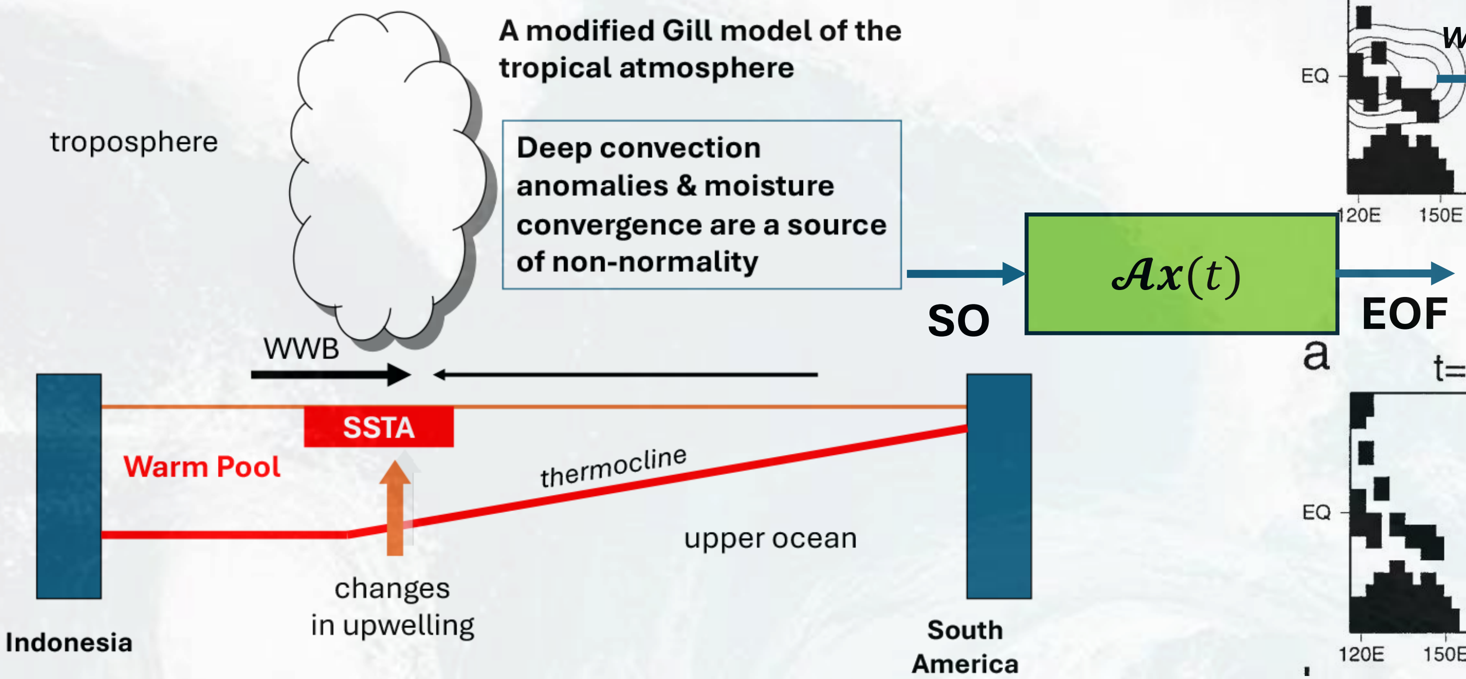
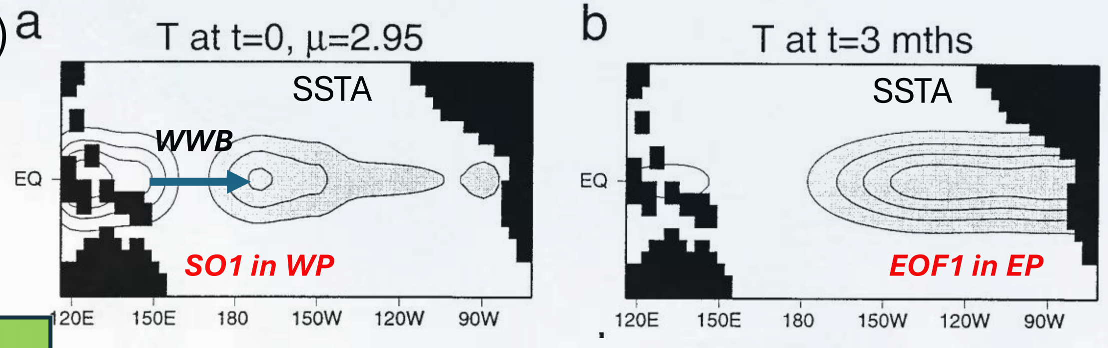
In highly non-normal systems, the most impactful stochastic optimals align with the least important EOFs meaning that dimension reduction based on EOFs alone will jettison the source of the leading variance! ***Balanced truncation is dimension reduction based on retaining the leading EOFs and SOs in the form of the Hankel Singular vectors.***

When things go wrong – an example

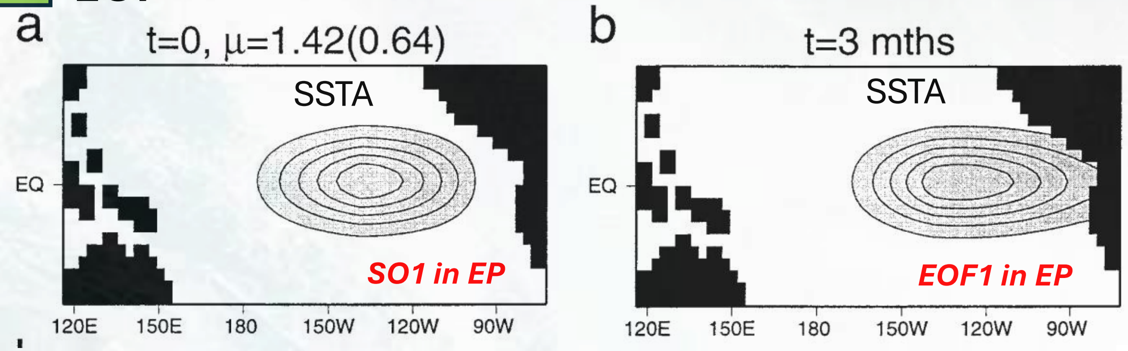
Optimal SST excitation for El Nino

An intermediate coupled model model of ENSO (Kleeman, 1991)





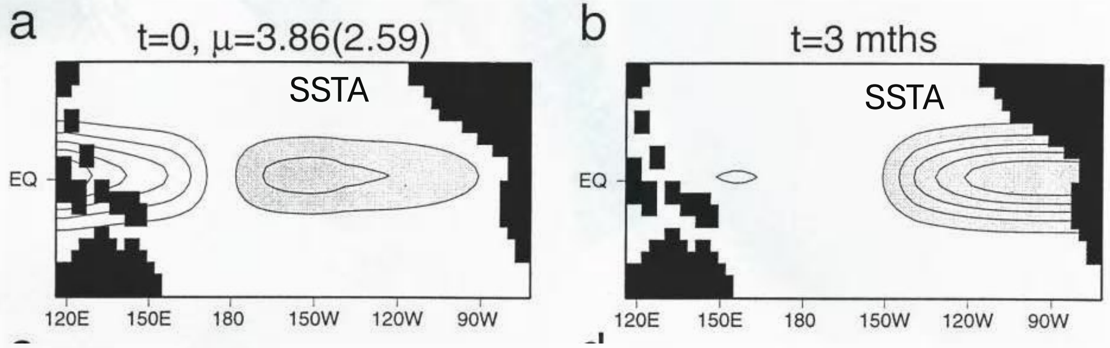
Direct from dynamical model



Traditional linear inverse model

A reduced gravity model of the tropical Pacific

Moore and Kleeman (1999, 2001)



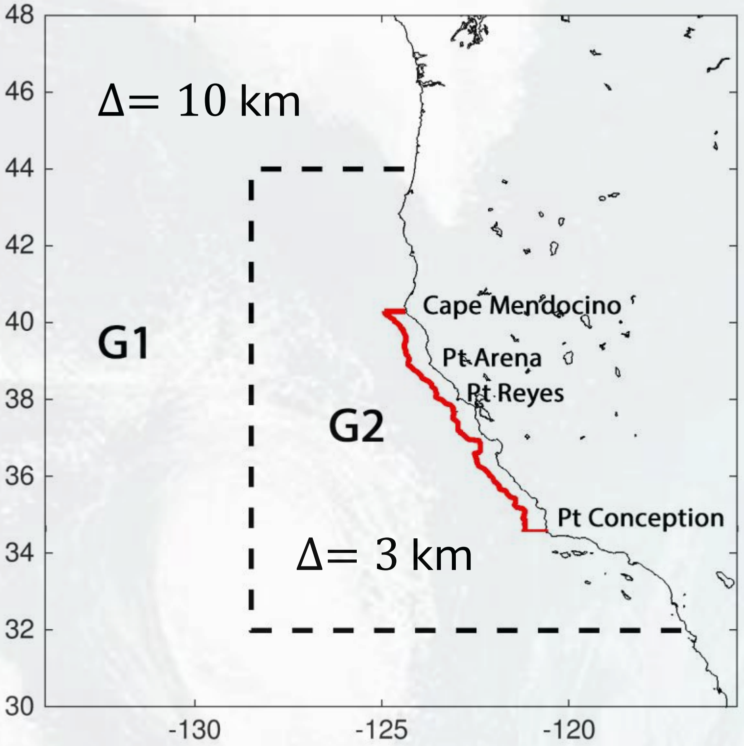
Corrected linear inverse model

All of the models generate realistic ENSO variability but one for the wrong reason! The importance of WWB and MJO as ENSO precursors is now well established from observations (McPhaden, 1999)

The California Current System

A Linear Stochastic Emulator of the California Current System

Motivation: Construct a computationally efficient emulator for generating large ensembles to provide a baseline for extreme events of upwelling, high pH and low oxygen – duration of forward model simulations is limited.



- ROMS, 3km resolution, 42 σ-levels (G2)
- Forced by ERA + CCMP winds, 1988-2010
- G2 open boundaries from a 4D-Var ocean reanalysis (G1) with 10km resolution.
- Limited time period – "extend" using a LIM.

Moore et al (2023)

Stochastic model:

$$\boldsymbol{x}(t+1) = \boldsymbol{\mathcal{A}}\boldsymbol{x}(t) + \boldsymbol{\mathcal{B}}\boldsymbol{\xi}(t)$$

$$\boldsymbol{y}(t+1) = \boldsymbol{\mathcal{C}}\boldsymbol{x}(t+1)$$

- $\boldsymbol{x}$ is 3D scaled fields of monthly mean T, S, u, v, and η
- Dimension $\sim 8 \times 10^6$
- Expand $\boldsymbol{x}$ in terms of multivariate 3D EOFs.

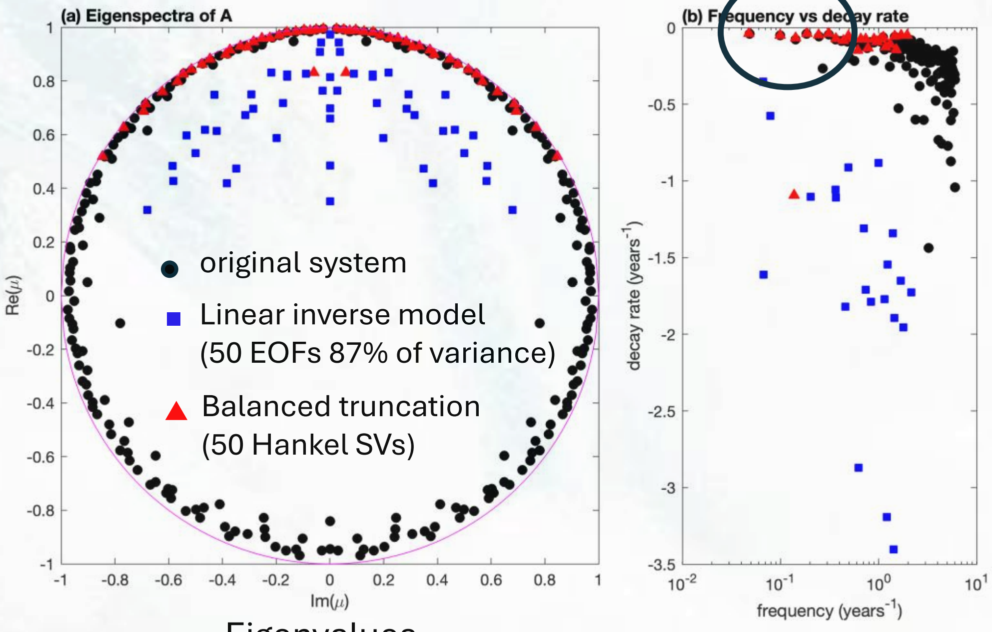
Principal Oscillation Patterns

$$\boldsymbol{\mathcal{A}}\boldsymbol{\phi}_i = \mu_i \boldsymbol{\phi}_i$$ Hasselmann (1988)

$\boldsymbol{\phi}_i$ = *Principal Oscillation Patterns (POPs)*

(empirical approximation of the dynamical modes)

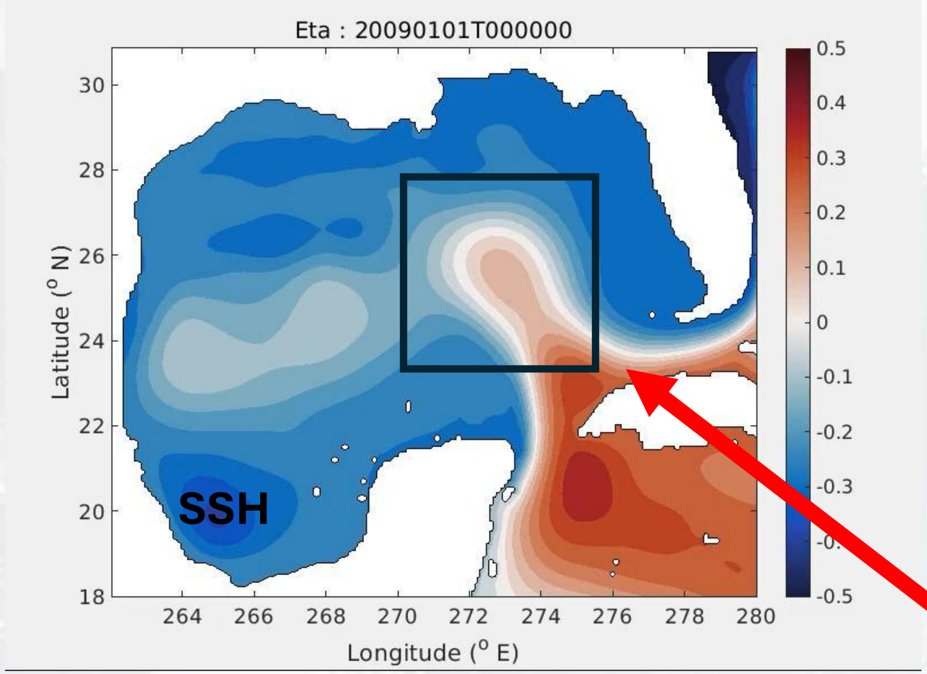
Leading POPs: PDO, NPGO, ENSO



Eigenvalues

A Linear Stochastic Emulator of the Intra-Americas Sea

Motivation: To gain insight into the dynamics of Loop Current Eddy shedding and predictability.



Stochastic model:

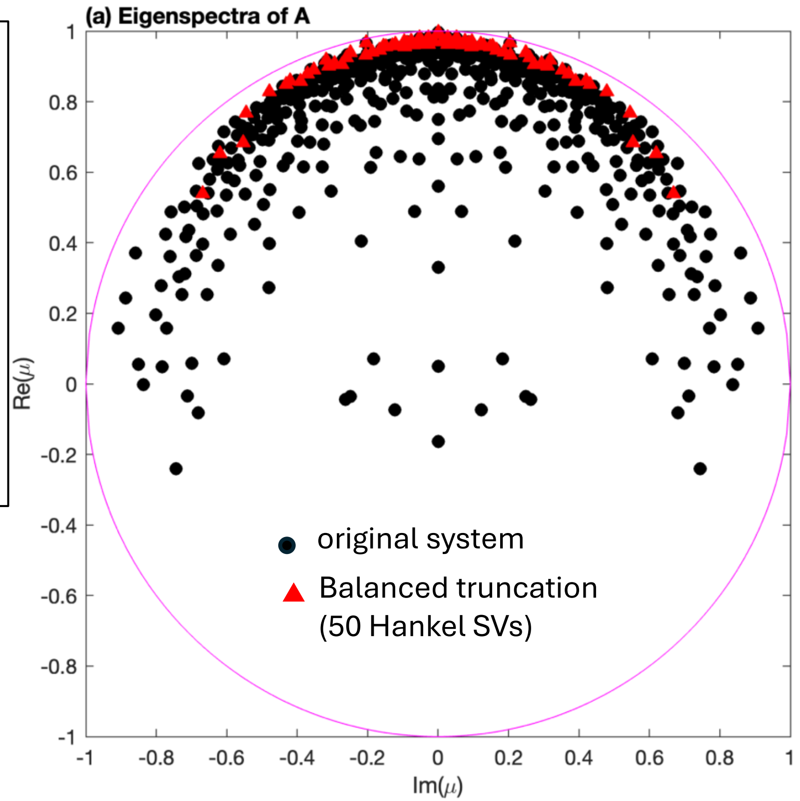
$$x(t+1) = \mathcal{A}x(t) + \mathcal{B}\xi(t)$$

$$y(t+1) = \mathcal{C}x(t+1)$$

x is 3D scaled fields of 7-day average ρ.

Dimension $\sim 4 \times 10^6$

The leading EOFs capture eddy shedding but not the precursors



POP eigenvalues

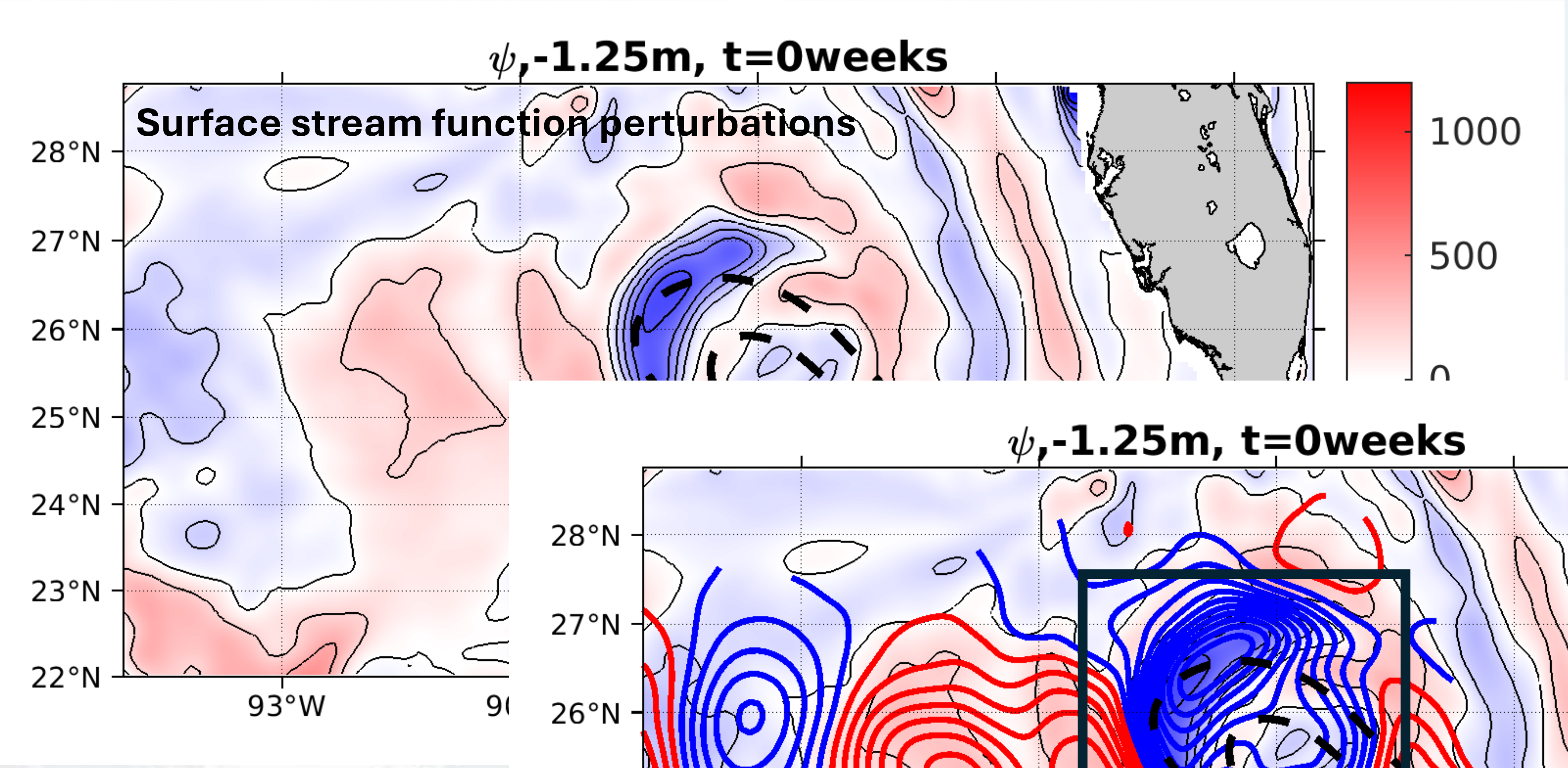
- MITgcm, ~0.1° resolution, 80 z-levels
- Forced by annual seasonal cycle for 40 yrs
- Annual mean open boundaries from GLORYS

- 3D EOFs for 7-day mean anomalies of ρ.
- System dimension is $\sim 4 \times 10^6$.

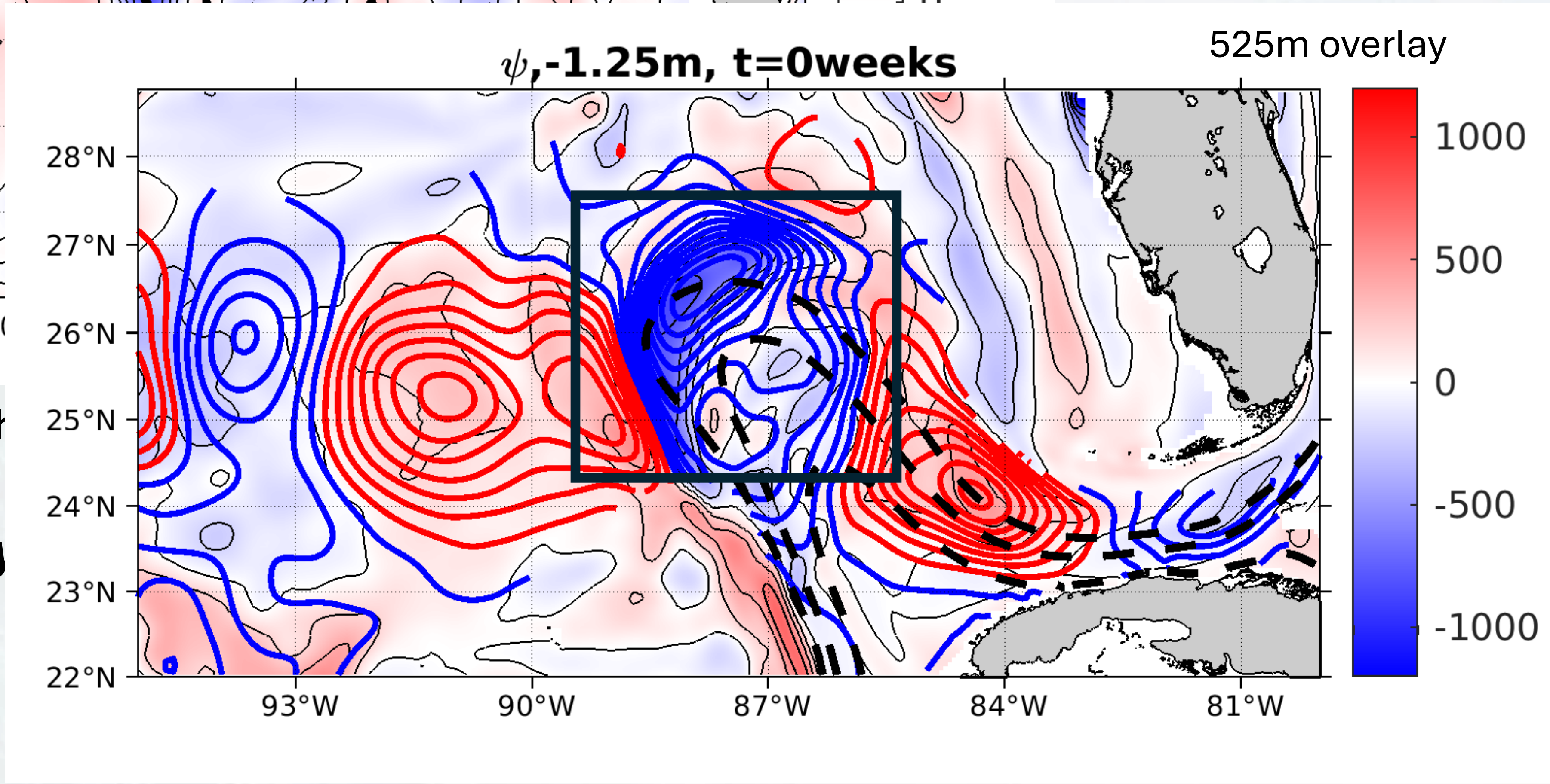
$$\mathcal{A}\boldsymbol{\phi}_i = \mu_i \boldsymbol{\phi}_i$$

$\boldsymbol{\phi}_i$ = *Principal Oscillation Patterns (POPs)*

(empirical approximation of the dynamical modes)



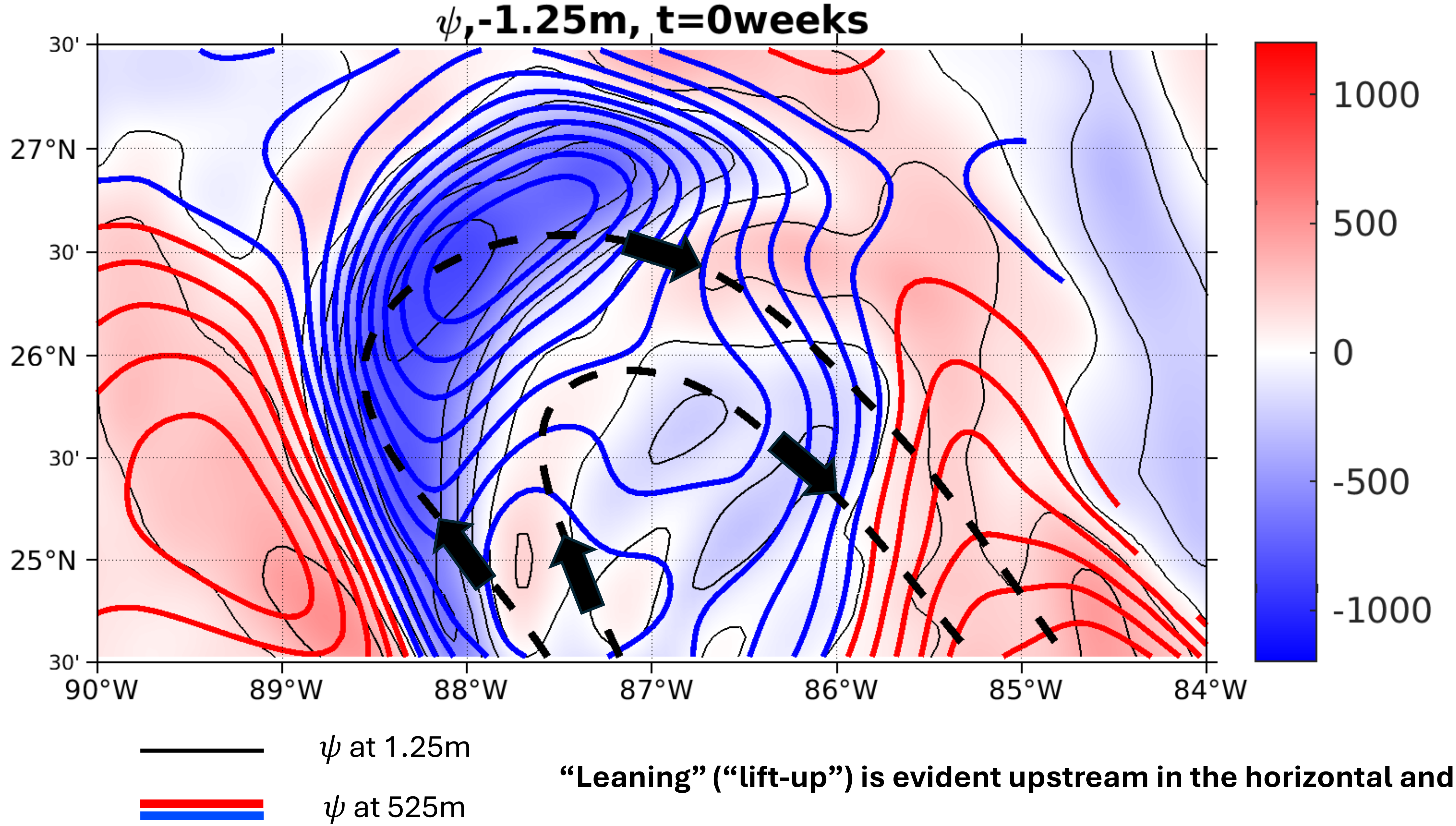
Mean Loop Current stream function



A perturbation with

Precursors of eddy

Precursors of eddy shedding – the stochastic optimals



"Leaning" ("lift-up") is evident upstream in the horizontal and vertical

Summary and Reflections

- The theory of linear dynamical systems reveals, in a very transparent way, the potential dangers of dimension reduction (”latent space”) if we don’t respect the underlying dynamics of the system under consideration.
- EOFs provide only half of the story – they inform you where the variance occurs, but not about what is generating it.
- If you are only interested in capturing the majority of the variance of the system, then the leading EOFs are all you need, but you may not faithfully reproduce the dynamics of the circulation.
- ML approaches that rely on EOFs for dimension reduction may suffer from the same shortcomings as LIMs.
- It is possible that other approaches to the latent space may suffer from the same shortcomings.
- An appeal: Let’s not let our zeal for trying something new and exciting make us lose sight of the fundamental dynamics that underpin the system!
- Otherwise, we may end up “throwing away the baby with the bath water…”