Stochastic array design with the sangoma_arm tool

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A simple problem

$\mathbf{x}$ augmented state vector $(n,1)$ over time interval of interest

(let me insist on the fact that this is an augmented state vector – everything that will be shown in this talk includes time as well as space in the definition of observations and prior state estimate)

$\mathbf{y}^o$ observations $(p,1)$ verifying $\mathbf{y}^o = H(\mathbf{x}^t) + \varepsilon$, with:

$H(\ )$ observation operator (not necessarily linear, but use linearized approximation)

$\varepsilon \in N(0, \mathbf{R})$

Q: how can we characterize the performance of an observational array $(H, \mathbf{R})$?

Assume we have a prior state estimate of $\mathbf{x}$ and associated error statistics (if not, any observational array will bring valuable information proportionately to its cost):

$\mathbf{x}^f = \mathbf{x}^t + \eta$, with:

$\eta \in N(0, \mathbf{P}^f)$

A qualitative/intuitive criterion of array performance

Incremental information brought in by the array (on top of prior):

Innovation vector $\mathbf{d} \equiv \mathbf{y}^o - \mathbf{y}^g = \mathbf{y}^o - H\left(\mathbf{x}^f\right) \approx \varepsilon - \mathbf{H}\eta$

The 2nd-order statistics of innovation can be used to characterize that incremental information:

$$\left\langle \mathbf{d}\mathbf{d}^T \right\rangle = \mathbf{R} + \mathbf{H}\mathbf{P}^f\mathbf{H}^T$$

Qualitative/intuitive criterion of array performance:

- $\mathbf{R}$ "dominates"

  → most of the discrepancies are attributable to observational error

  → observations are not very useful

- $\mathbf{H}\mathbf{P}^f\mathbf{H}^T$ "dominates"

  → most of the discrepancies are attributable to prior state errors

  → observations can be used to identify and correct prior state errors

Towards a formal criterion of array performance

Two paths (among others) to formalize the intuitive order relationship…

Bennett's "array modes" (e.g. Bennett et al., 1997): these are orthonormal rotation vectors $\boldsymbol{\beta}$ obtained by diagonalizing the representer matrix:

$$\mathbf{HP}^f\mathbf{H}^T = \boldsymbol{\beta}\boldsymbol{\lambda}\boldsymbol{\beta}^T$$

$\boldsymbol{\beta}$: observable degrees of freedom of the physical system for that configuration
$\boldsymbol{\lambda}$: spectrum of RM, to be compared to the diagonal of $\mathbf{R}$ (obs. noise floor)

Le Hénaff & De Mey (Le Hénaff et al., 2009): in the general case of non-homogeneous, non-diagonal $\mathbf{R}$, and observational samples scattered in time, space, and across variables, use spectrum $\boldsymbol{\sigma}$ and array modes $\boldsymbol{\mu}$ of the scaled representer matrix $\boldsymbol{\chi}$:

$$\boldsymbol{\chi} = \mathbf{R}^{-1/2}\mathbf{HP}^f\mathbf{H}^T\mathbf{R}^{-1/2} = \boldsymbol{\mu}\boldsymbol{\sigma}\boldsymbol{\mu}^T$$

$\boldsymbol{\mu}$: spectrum of SRM, to be compared to the diagonal of $\mathbf{I}$ (obs. noise floor)

Representer Matrix Spectrum (RM Spectrum) method

Le Hénaff, De Mey and Marsaleix, *Ocean Dynamics*, 2009:

Scaled Representer Matrix: $\boldsymbol{\chi} = \mathbf{R}^{-1/2}\mathbf{H}\mathbf{P}^{f}\mathbf{H}^{T}\mathbf{R}^{-1/2} = \boldsymbol{\mu}\boldsymbol{\sigma}\boldsymbol{\mu}^{T}$ (RMS1)

- $\boldsymbol{\mu}$: "*array modes*"
- $\boldsymbol{\sigma}$: spectrum of SRM, to be compared to the diagonal of $\mathbf{I}$ (obs. noise floor)

From (RMS1) and the orthogonality of array modes:

$$\boldsymbol{\mu}^{T}\boldsymbol{\chi}\boldsymbol{\mu} = \boldsymbol{\mu}^{T}\mathbf{R}^{-1/2}\mathbf{H}\mathbf{P}^{f}\mathbf{H}^{T}\mathbf{R}^{-1/2}\boldsymbol{\mu} = \boldsymbol{\sigma} \qquad \text{(RMS2)}$$

- $\boldsymbol{\sigma}$ appears as a rotated scaled representer matrix in the new basis defined by $\boldsymbol{\mu}^{T}$
- $\boldsymbol{\rho}_{\mu} = \mathbf{P}^{f}\mathbf{H}^{T}\mathbf{R}^{-1/2}\boldsymbol{\mu}$ can be seen as a matrix of representers for the array modes = "*modal representers*"

Stochastic implementation of RM analysis (1/2) (ArM, De Mey, 2010)

Assume we have a way of generating *m* prior error samples e.g. from forecast Ensemble anomalies, or stochastic modelling.

Matrix of samples (centered): $\mathbf{A}^f$

We get stochastic estimates:

- $\hat{\mathbf{P}}^f = \frac{1}{m-1}\mathbf{A}^f\mathbf{A}^{fT}$ (ARM1)
- $\hat{\chi} = \frac{1}{m-1}(\mathbf{R}^{-1/2}\mathbf{H}\mathbf{A}^f)(\mathbf{R}^{-1/2}\mathbf{H}\mathbf{A}^f)^T = \mathbf{S}\mathbf{S}^T$ (ARM2)

using $\mathbf{S} = \frac{1}{\sqrt{m-1}}\mathbf{R}^{-1/2}\mathbf{H}\mathbf{A}^f$ = scaled Ensemble observation anomalies (e.g. Sakov et al., *Ocean Dynamics*, 2009)

Stochastic implementation of RM analysis (2/2) (ArM, De Mey, 2010)

From (ARM2), the ev problem in the RM Spectrum method is now a sv problem in ArM.

We now have the following stochastic estimates:

- $\hat{\boldsymbol{\sigma}}$ = RM spectrum estimate = squares of the singular values of **S**
- $\hat{\boldsymbol{\mu}}$ = Array Mode estimates = singular vectors of **S**
- $\hat{\boldsymbol{\rho}}_{\mu} = \dfrac{1}{\sqrt{m-1}} \mathbf{A}\mathbf{S}^T \hat{\boldsymbol{\mu}}$ = Modal representer estimates

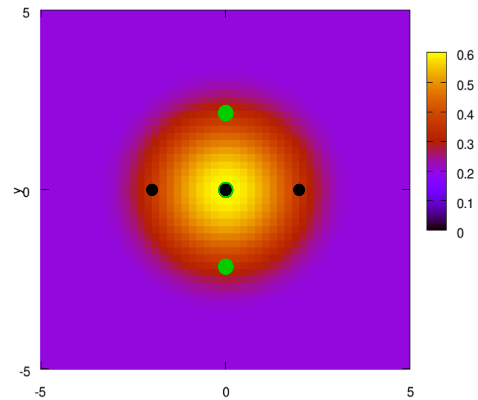
In practice there is no limitation in the choice of observation operator.

- It can operate in space, time, and across variables.
- In practice we calculate $\mathbf{HA}^f$ as $H(\mathbf{A}^f)$ when calculating **S** (e.g. Ensemble members made to generate their own observation proxies).

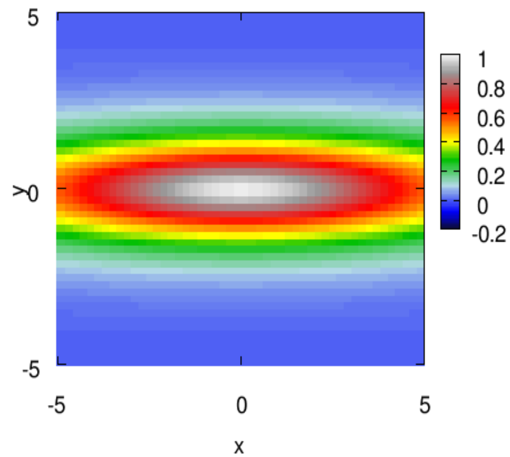
```fortran
SUBROUTINE sangoma_arm( &
  nstate, nens, nobs, ndof, Af, Df, R, arm_spect, arm, arm_rep, status &
  ) BIND( C, name="sangoma_arm_" )

! PURPOSE
! Calculate array modes and associated quantities

! INPUT
! nstate                state size
! nens                  Ensemble size
! nobs                  number of observations
! ndof                  =MIN(nens,nobs) number of d.o.f.s of problem
! Af                    forecast ensemble anomalies, defined as Af(nstate,nens)
! Df                    same as Af in data space, defined as Df(nobs,nens)
!                       note: df can be directly generated by the model, or
!                       linearly calculated as H*Af, H(nobs,nstate) = obs.op.
! R                     observation error covariance matrix, def as R(nobs,nobs)

! OUTPUT
! arm_spect             array mode spectrum, defined as arm_spect(ndof)
! arm                   array modes, defined as arm(nobs,ndof)
! arm_rep               modal representers, defined as arm_rep(nstate,ndof)
! status                status flag (0=success)

! NOTES
! 1. The actual precision of REAL is to be provided by the compiler.  Only
!    KIND=8 will work with the current version (promotion of REAL to DOUBLE
!    PRECISION) because of the use of Dxxxxx BLAS/LAPACK calls.  This can
!    be changed in a later version.
! 2. State space and data space are n-dimensional + (optionally) time.
!    - Each state-space sample and data-space sample can contain
!      information from several instants if desired.
!    - Modal representers can span space *and* time.
```

A simple 2D, univariate example (1/3)

Prior state error variance



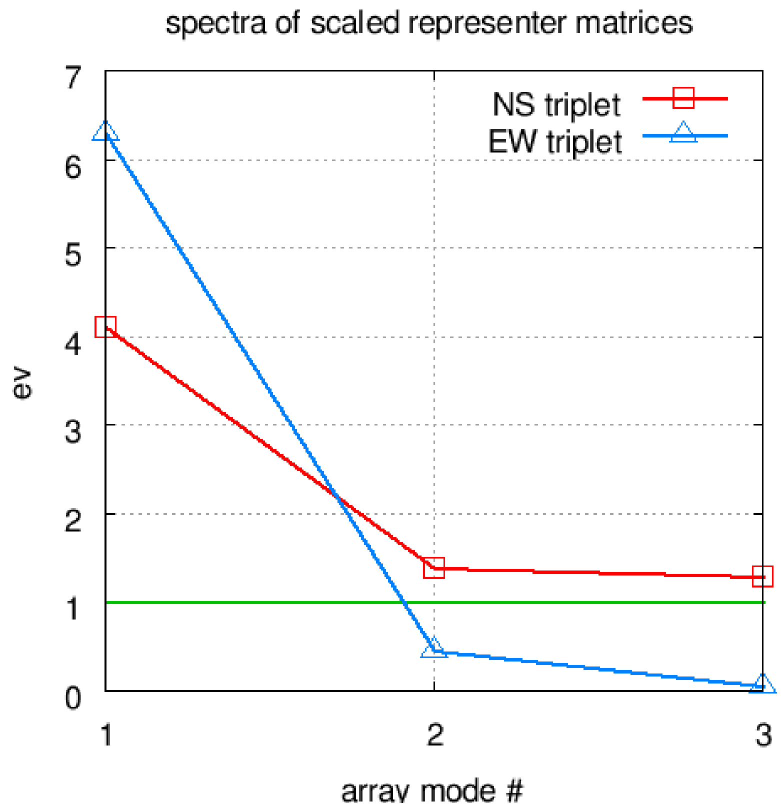
Prior state error correlation



A simple 2D, univariate example (2/3)

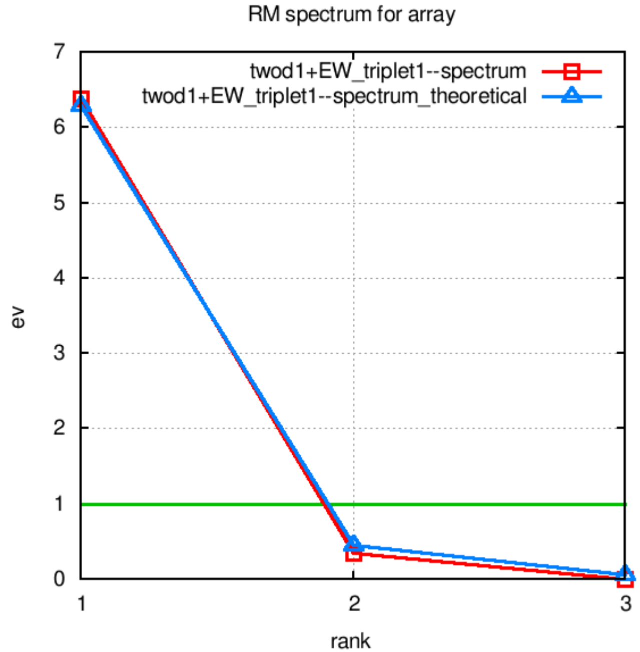
Two observational strategies:

- N-S triplet detects more d.o.f.s (3) amidst observational noise
- E-W triplet more redundant (1 d.o.f.)



A simple 2D, univariate example (3/3)

- 20 random samples with $\mathbf{P}^f$ statistics (Gaussian generator)

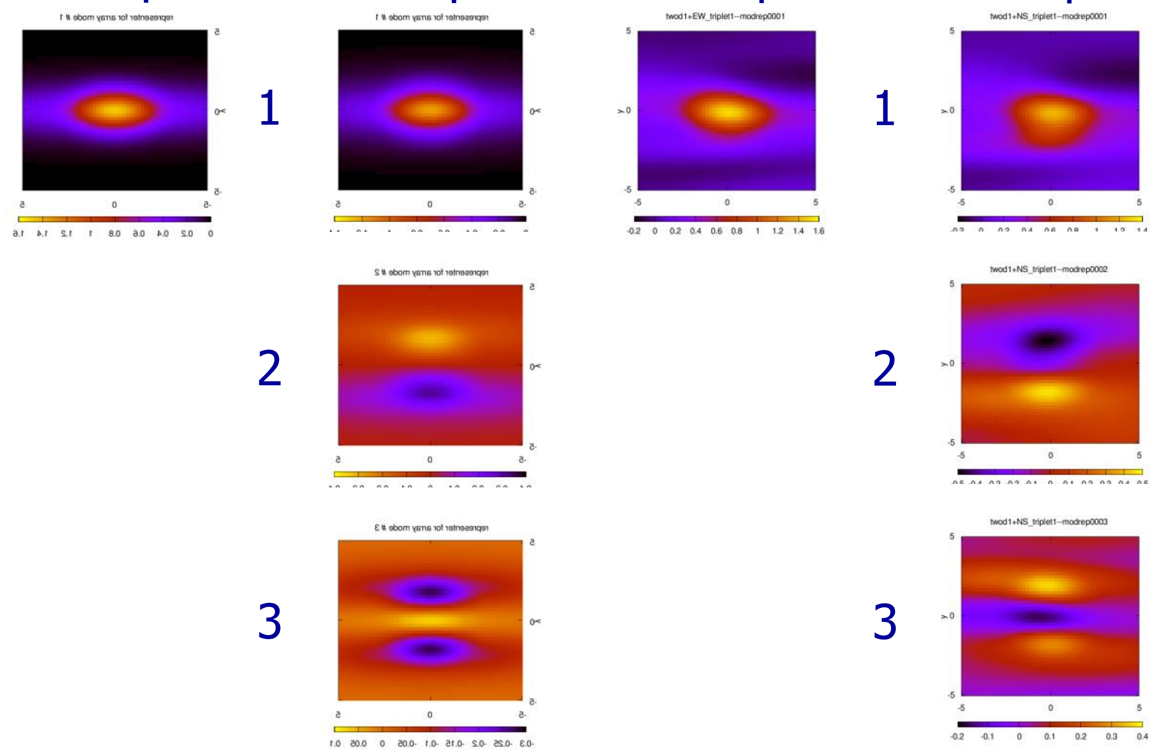


EW triplet
Theoretical vs.
sangoma_arm
RM spectrum estimates

Detectable modal representers

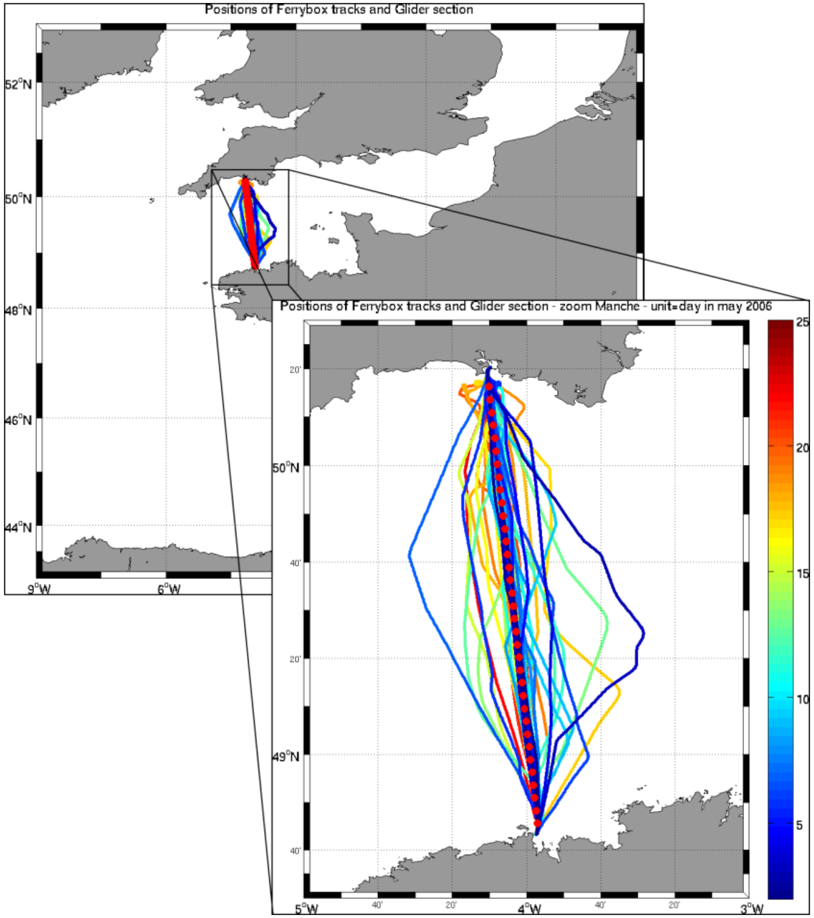
(Theor.) RM Spectrum | sangoma_arm

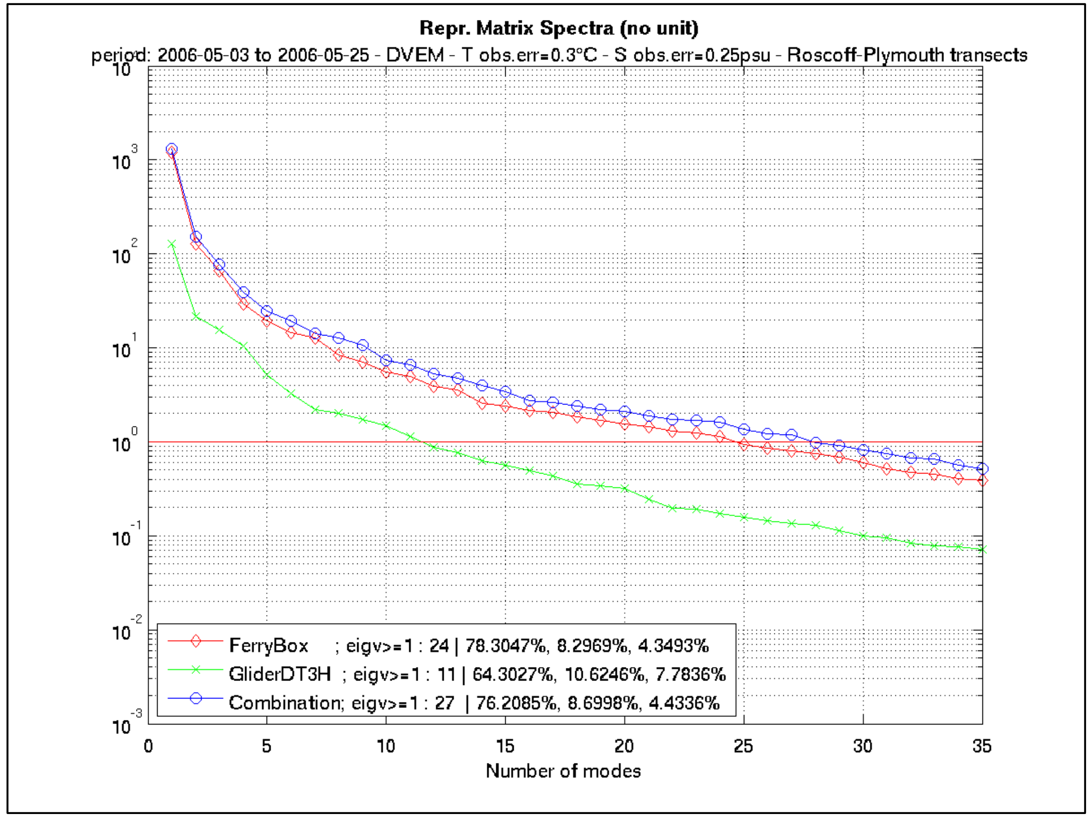
EW triplet | NS triplet | EW triplet | NS triplet



(Color scales not exactly the same – signs not important – only shapes are to be trusted)

Roscoff-Plymouth Ferrybox vs. Glider, [sangoma_]arm analysis





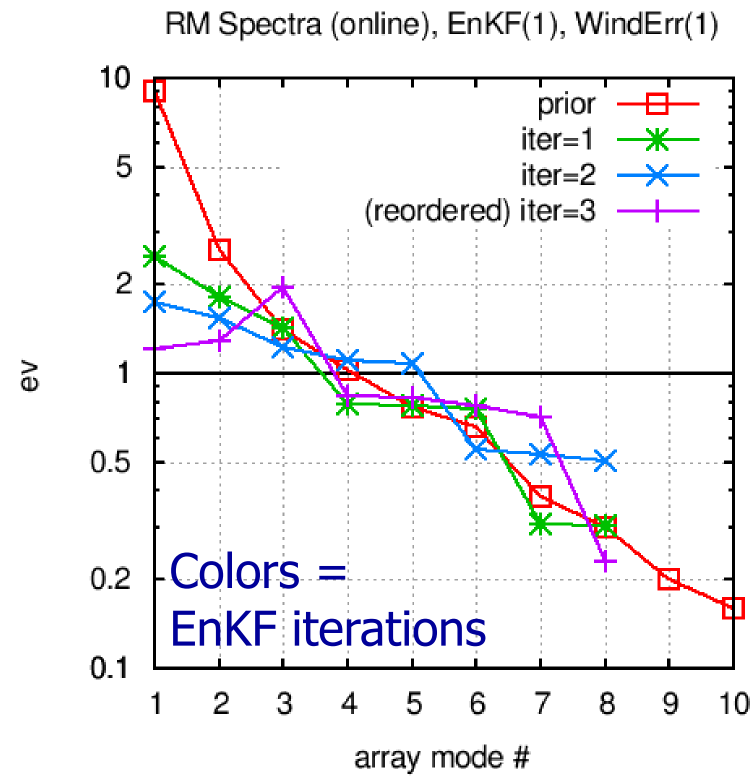
- Higher repeat cycle of ferrybox critical here, despite being surface only, because of HF model errors (linked to tidal front displacements)

Ifremer

Charria (Ifremer), Lamouroux (Noveltis), De Mey (LEGOS)

Online [sangoma_]arm diagnostic analysis with 4-D local EnKF

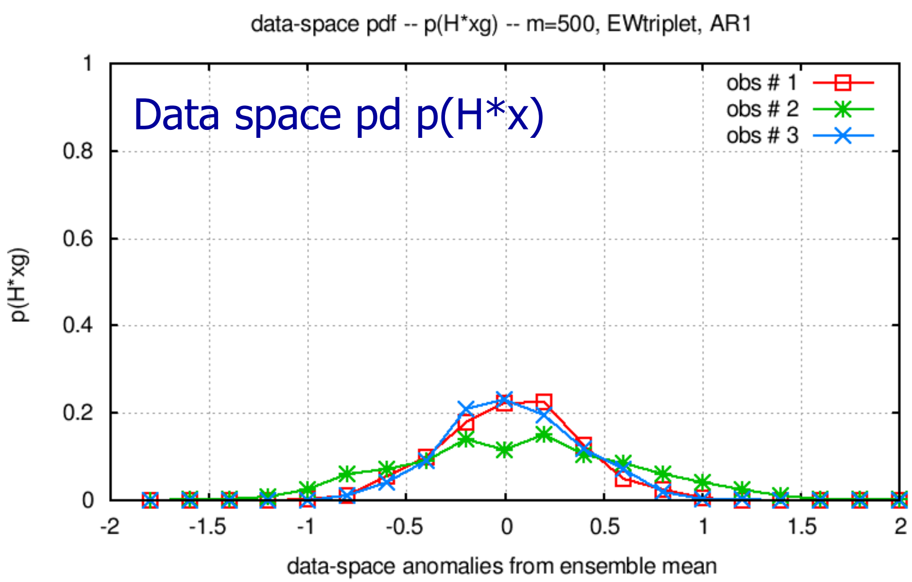
- Assimilate simulated <u>SWOT</u> wide-swath altimeter on 10-day orbit for 2 months in summer 2004 in Bay of Biscay
- Carry out ArM analysis <u>online</u> at each 10-day assim cycle (invariant $\mathbf{H}$)
- Localized EnKF (BELUGA)
- Rank is approximately conserved through assimilation
- Spectra whiten in detectable range
  - Array info is being extracted
  - Mostly large-scale and mesoscale error processes constrained
  - No eigenvalue decrease for high-frequency shelf processes → need for sustained observations of such processes

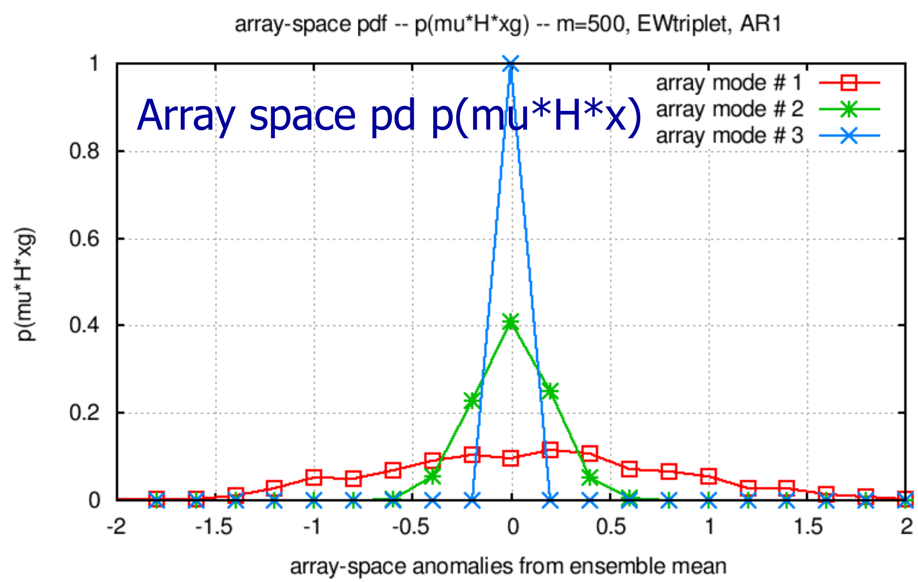


Detectable range
(4 eigenvalues)

Can array modes help Ensemble consistency analyses?

- Problem: check whether model forecast *pdf* (from Ensemble) and observations (innovation *pdf*) are consistent with each other
- Low-order array-space forecast pd's have broadest base (by design)
  - Hierarchize ensemble consistency checks from easiest to hardest to pass
  - Perhaps use some form of Brier score
- Sangoma_arm_CA tool in preparation





EW triplet, AR1 process, 500 members