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EUROPEAN CENTRE FOR RESEARCH AND ADVANCED TRAINING IN SCIENTIFIC COMPUTING

Scale-dependent background-error covariance modelling, with application to global ocean DA *

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Accounting for spatial scale dependency in **B** (in NEMOVAR*)

- Multiple (two) scale **B** model (Met Office; Mirouze et al. 2016)
  - Block-diagonal (uncorrelated) with respect to the separated scales.
  - Variances and length-scales are estimated by fitting a linear combination of Gaussian functions to samples of background error (Carneiro et al. 2021).
- Scale-dependent localization (SDL) (Buehner & Shlyaeva 2015)
  - Requires localizing an ensemble (sample) covariance matrix.
  - Cost increases with ensemble size and number of scales.
- Scale-dependent covariance model (SDM) (new)
  - Combines features of the Met Office **B** model and SDL.
  - Accounts for cross-covariances between different scales.
  - Inexpensive procedures for estimating scale-dependent **B** model parameters from ensembles.
  - Cheaper than SDL.
  - Hybridizes naturally with SDL.

* Collaborative ocean DA software development between CERFACS, ECMWF, INRIA and Met Office

Scale-dependent ensemble perturbations

- The ECMWF implementation of NEMOVAR for ORAS6/OCEAN6 defines (a single-scale) **B** from an Ensemble of Data Assimilations (EDA).
- The ensemble is used to define the error covariances of **transformed** (assumed approximately uncorrelated) background variables.
- The balanced component is removed from the ensemble perturbation matrix:

$$\widehat{\mathbf{X}} = \mathbf{K}_{\mathrm{b}}^{-1}\mathbf{X} = \frac{1}{\sqrt{N_{\mathrm{e}}-1}}\left(\hat{\boldsymbol{\epsilon}}_1' \quad \dots \quad \hat{\boldsymbol{\epsilon}}_{N_{\mathrm{e}}}' \right)$$

- For SDL and SDM, a sequence of diffusion-based filters $\mathbf{F}_i$ with different length scales D_i (with $D_i > D_{i-1}$) are used to construct an augmented set of perturbations *from* **small scale** (small i) *to* **large scale** (large i) :

$$\widehat{\mathbf{X}}_i^{\mathrm{F}} = \mathbf{F}_i \widehat{\mathbf{X}}, \qquad i = 1, \dots, N_{\mathrm{s}} \qquad \text{with} \qquad \mathbf{F}_1 = \mathbf{I}$$

Scale-dependent ensemble perturbations

- The filtered perturbations are rearranged into overlapping ranges of scales *from* **large** (small i) *to* **small** (large i):

$$\begin{aligned}\widehat{\mathbf{X}}_1 &= \widehat{\mathbf{X}}^{\mathrm{F}}_{N_\mathrm{s}} \\ \widehat{\mathbf{X}}_i &= \widehat{\mathbf{X}}^{\mathrm{F}}_{N_\mathrm{s}-i+1} - \widehat{\mathbf{X}}_{i-1}, \qquad i = 2, \ldots, N_\mathrm{s}\end{aligned}$$

- The original perturbation is recovered from the telescoping sum

$$\widehat{\mathbf{X}} = \sum_{i=1}^{N_\mathrm{s}} \widehat{\mathbf{X}}_i$$

- The sample error covariance matrix can be written as

$$\widetilde{\mathbf{B}} = \widehat{\mathbf{X}}\widehat{\mathbf{X}}^{\mathrm{T}} = \sum_{i=1}^{N_\mathrm{s}} \sum_{j=1}^{N_\mathrm{s}} \widehat{\mathbf{X}}_i \widehat{\mathbf{X}}_j^{\mathrm{T}}$$

Scale-dependent covariance modelling

- With scale-dependent localization (SDL), we define

$$\mathbf{B}_{\mathrm{SDL}} = \sum_{i=1}^{N_\mathrm{s}} \sum_{j=1}^{N_\mathrm{s}} \mathbf{L}_{ij} \circ \widehat{\mathbf{X}}_i \widehat{\mathbf{X}}_j^\mathrm{T} = \sum_{n=1}^{N_\mathrm{e}} \sum_{i=1}^{N_\mathrm{s}} \sum_{j=1}^{N_\mathrm{s}} \mathbf{\Lambda}_i^{(n)} \mathbf{L}_{ij} \mathbf{\Lambda}_j^{(n)}$$

- With the scale-dependent covariance model (SDM), we define

$$\mathbf{B}_{\mathrm{SDM}} = \sum_{i=1}^{N_\mathrm{s}} \sum_{j=1}^{N_\mathrm{s}} \mathbf{\Sigma}_i \, \mathbf{C}_{ij} \, \mathbf{\Sigma}_j$$

- $\mathbf{B}_{\mathrm{SDM}}$ must be symmetric, positive semi-definite. We *define*

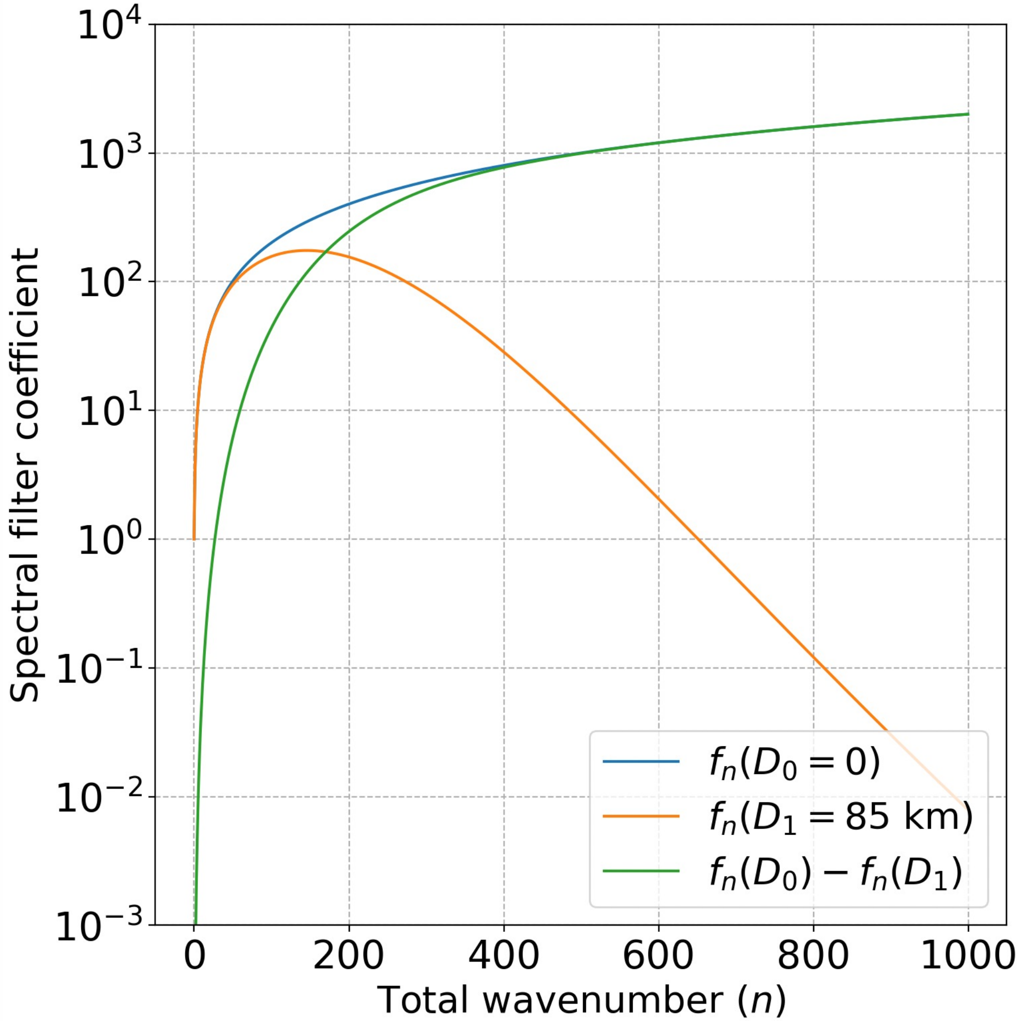
$$\mathbf{C}_{ij} = \mathbf{U}_i \mathbf{U}_j^\mathrm{T}$$

- We use the "square-root" of a diffusion operator to model the components:

$$\mathbf{U}_i = \mathbf{\Gamma}_i \, \mathbf{V}_i \, \mathbf{W}^{-1/2} \quad \text{and} \quad \mathbf{U}_j^\mathrm{T} = \mathbf{W}^{-1/2} \, \mathbf{V}_j^\mathrm{T} \, \mathbf{\Gamma}_j$$

Scale-dependent filtering on the sphere using an implicit diffusion operator

Example with two separated scales



Filtering kernel (Matérn like):

$$f(\theta) = \frac{1}{4\pi a^2} \sum_{n=0}^{\infty} f_n \, P_n(\cos\theta)$$

Spectral coefficients:

$$f_n = \sqrt{2n+1} \left(1 + \frac{L_i^2}{a^2} n(n+1)\right)^{-M}$$

Filtering length-scale
(Lindgren et al. 2011 definition):

$$D_i = L_i \sqrt{2M - 2}$$

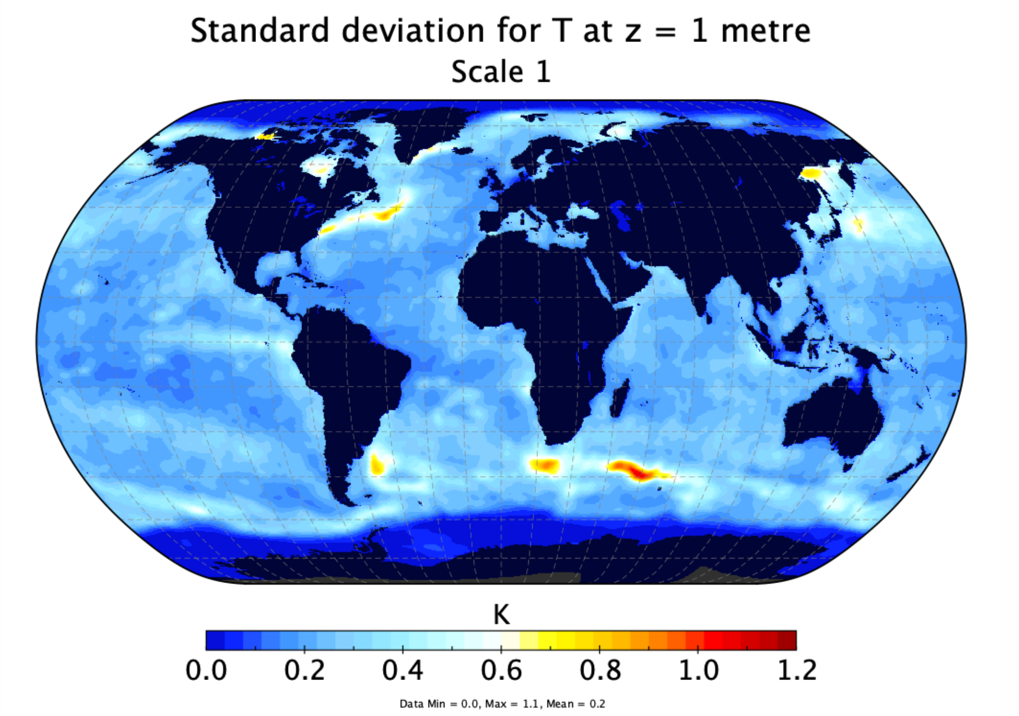
where $M = 10$ in the example

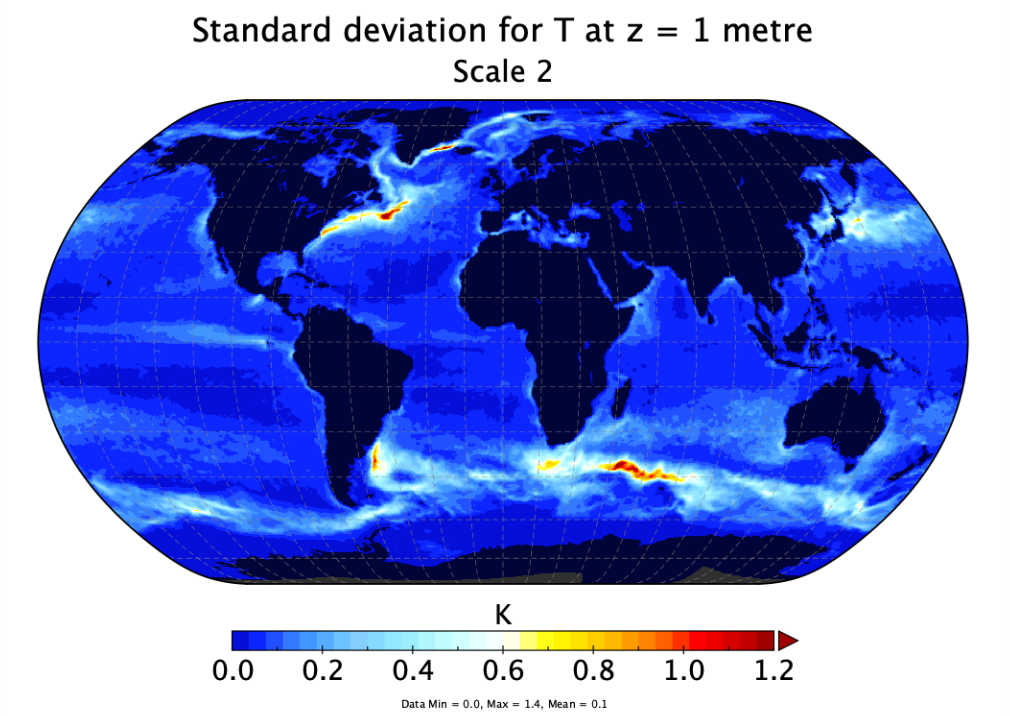
(Weaver and Mirouze 2013)

Scale-dependent variance estimation

- Climatological statistics from an 11-member ensemble from ECMWF pre-OCEAN6 config. (eORCA025), with spatial filtering (Ménétrier et al. 2015).
- Two ranges of scales where D_2 = 3 x local horizontal resolution (≈ 85 km)

$$\widehat{\mathbf{X}}_1 = \widehat{\mathbf{X}}_2^{\mathrm{F}} \quad \text{and} \quad \widehat{\mathbf{X}}_2 = \widehat{\mathbf{X}} - \widehat{\mathbf{X}}_1$$

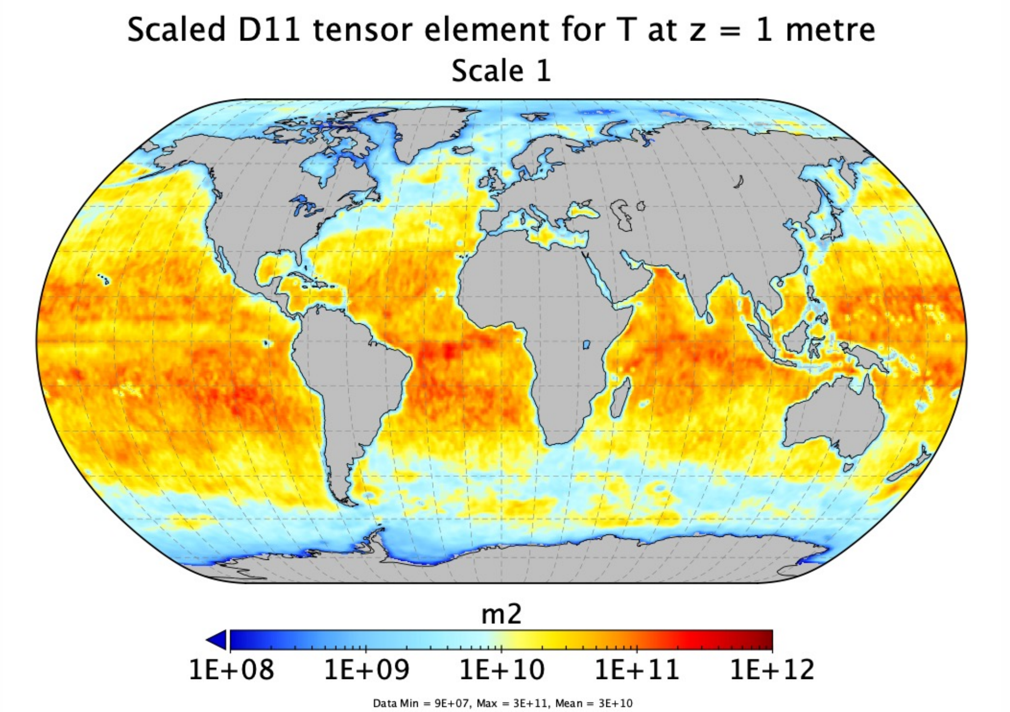




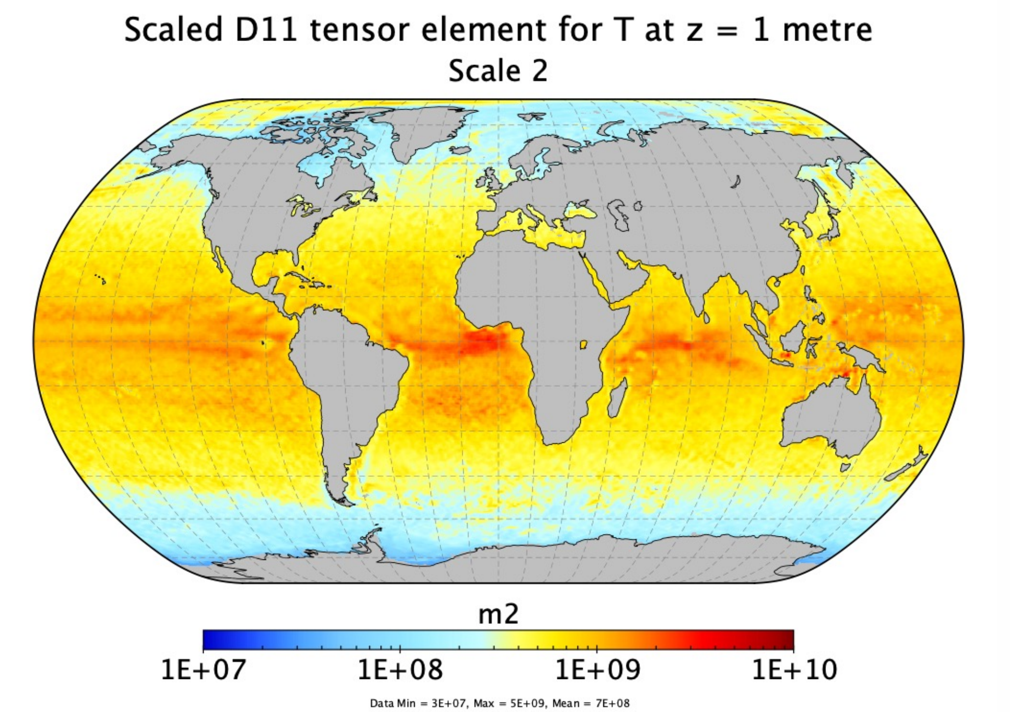
Scale-dependent correlation (diffusion) tensor estimation

- Directional length-scale tensor $\boldsymbol{D}(\mathbf{z})$ is estimated from the inverse of the local ensemble gradient tensor (Weaver et al. 2021), with spatial filtering (Michel et al. 2016):

$$\boldsymbol{D}(\mathbf{z}) = \left(\widetilde{\boldsymbol{H}}(\mathbf{z})\right)^{-1} \text{ where } \widetilde{\boldsymbol{H}}(\mathbf{z}) = \overline{\nabla\widetilde{\epsilon}(\mathbf{z})\left(\nabla\widetilde{\epsilon}(\mathbf{z})\right)^{\mathrm{T}}} \text{ and } \widetilde{\epsilon}(\mathbf{z}) = \epsilon(\mathbf{z})/\sigma(\mathbf{z})$$



100 km 1000 km



10 km 100 km

Computational cost

- $\mathbf{B}_{\mathrm{SDM}}$ requires N_{S} applications of the implicit diffusion operator, which we solve approximately using the Chebyshev Iteration (Weaver et al. 2016; 2018).

1) For the **small spatial scales**, the conditioning of the implicit diffusion matrix is improved since the length-scales are short.

   Ex: No. of Chebyshev solver iterations for the **small-scale term** with **2 scales** = **5**

   cf. No. of Chebyshev solver iterations with **1 scale** = **23**

2) For the **large spatial scales**, the diffusion operator can be applied on a coarse grid since the length-scales are long.

   Ex: No. of Cheby. solver iterations for the large-scale term on **coarse grid (=1/2 fine)** = **21**

   cf. No. of Cheby. solver iterations for the large-scale term on **fine grid** = **43**

- So the cost with N_{S} = 2 can be made comparable to the cost with N_{S} = 1 !

Normalization and hybrid variances

- Normalization is required to isolate the *total* standard deviations:

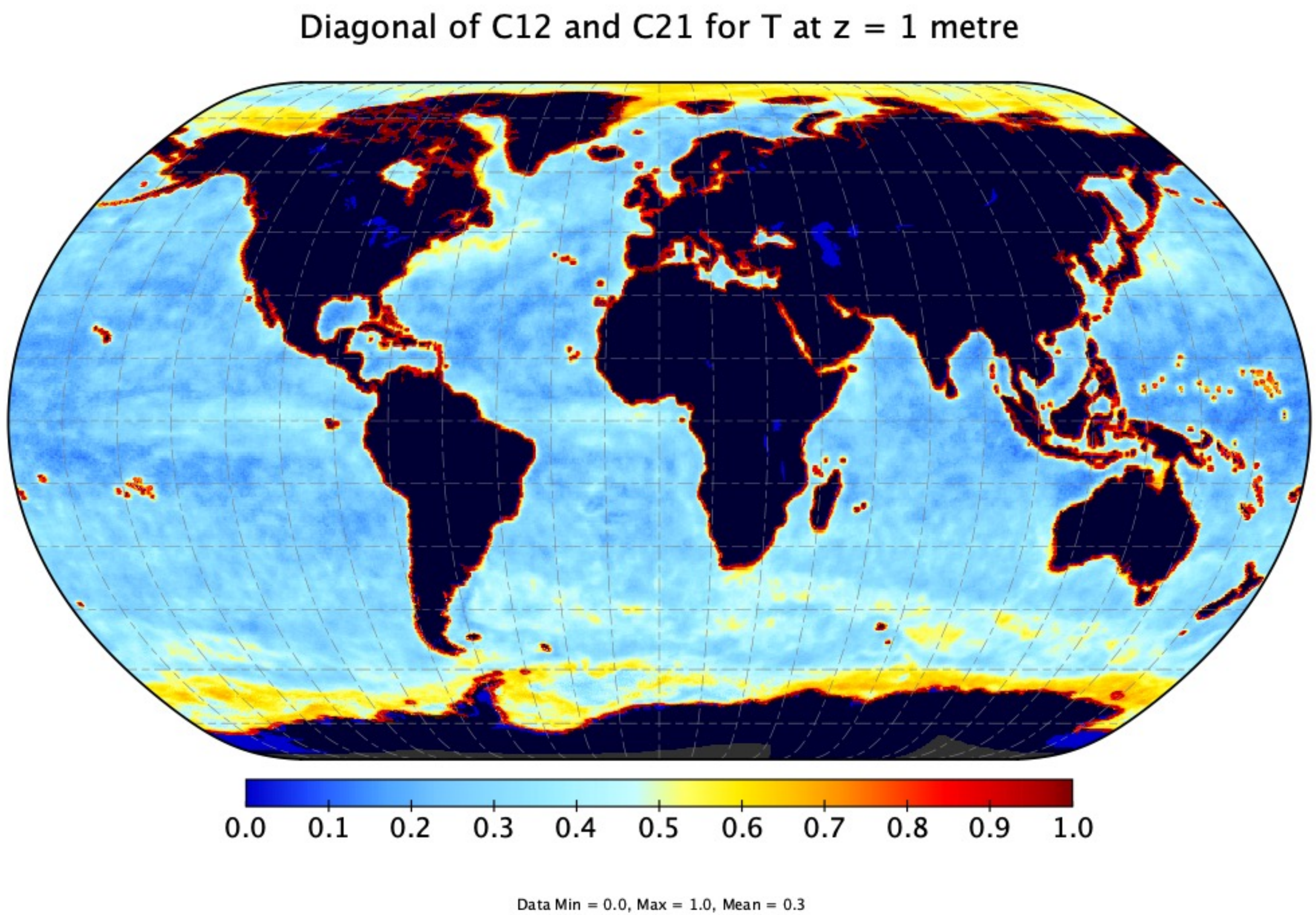
$$\mathbf{B} = \mathbf{\Sigma} \underbrace{\mathbf{\Gamma}\,\mathbf{B}_{\mathrm{SDM}}\,\mathbf{\Gamma}}_{\mathbf{C}_{\mathrm{SDM}}} \mathbf{\Sigma} \quad \text{where} \quad \mathbf{B}_{\mathrm{SDM}} = \sum_{i=1}^{N_s}\sum_{j=1}^{N_s} \mathbf{\Sigma}_i\,\mathbf{C}_{ij}\,\mathbf{\Sigma}_j$$

- The normalization factors are $\{\mathbf{\Gamma}\}_{nn} = \left(\sqrt{\{\mathbf{B}_{\mathrm{SDM}}\}_{nn}}\right)^{-1}$, which requires estimating the diagonal elements of $\mathbf{C}_{ij}$
  - When $i = j$, they are all equal to 1 if the diffusion operator is properly normalized, which can be done using a randomization algorithm.
  - When $i \neq j$, they are *not* equal to 1 and *not* explicitly known. They can be estimated, however, by reworking the randomization algorithm.

- **Hybrid scale-dependent** standard deviations: $\mathbf{\Sigma}_i = g\left(\mathbf{\Sigma}_i^{\mathrm{flow}}, \mathbf{\Sigma}_i^{\mathrm{clim}}\right)$

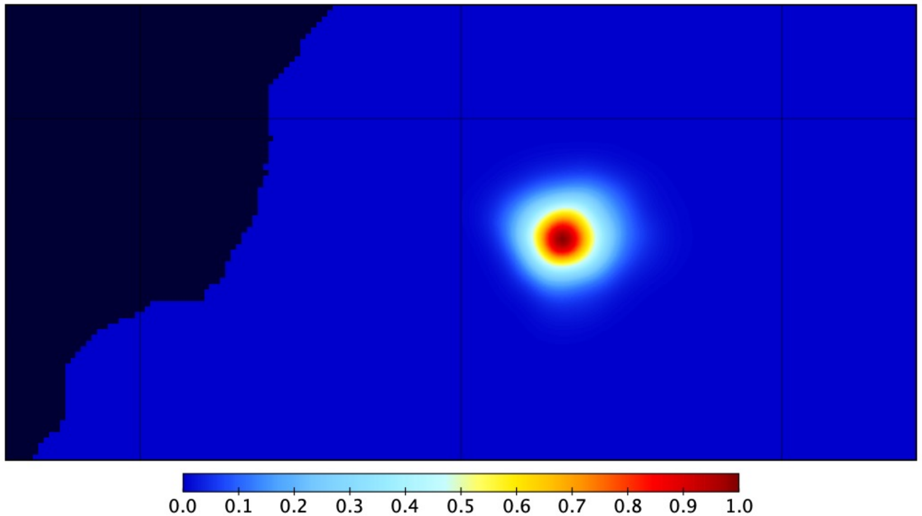
- **Hybrid total** standard deviations: $\mathbf{\Sigma} = h\left(\mathbf{\Sigma}^{\mathrm{flow}}, \mathbf{\Sigma}^{\mathrm{clim}}\right)$

Amplitude of the cross-scale covariance term $\mathbf{C}_{ij}$, $i \neq j$

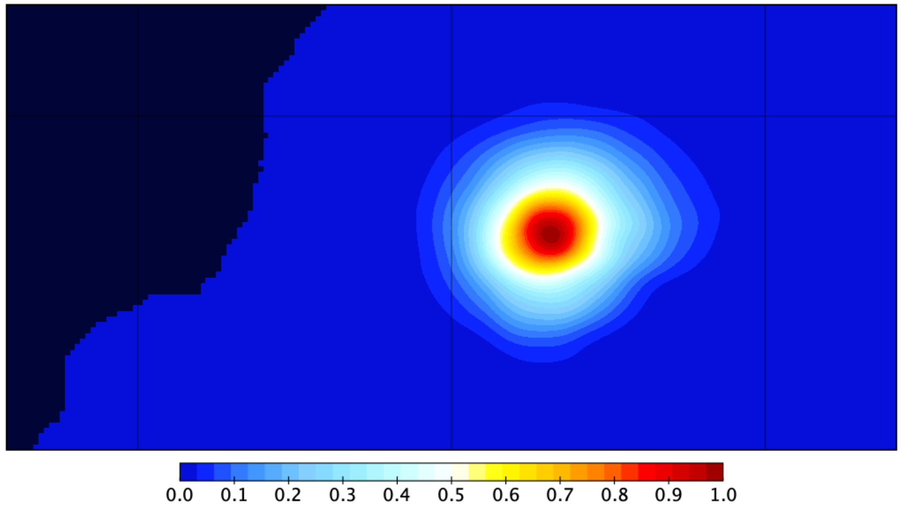


- Example of T-T correlations at 1 metre depth

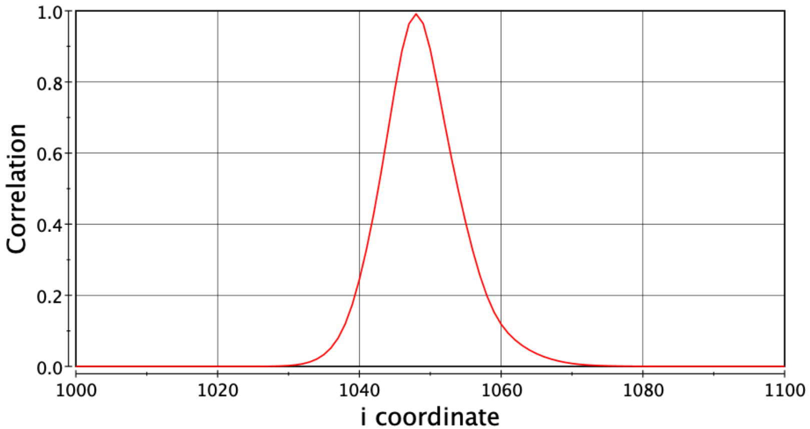
1 scale



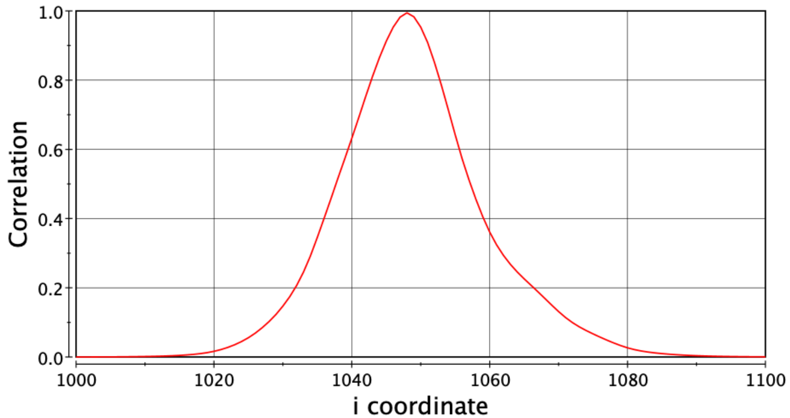
2 scales



1 scale

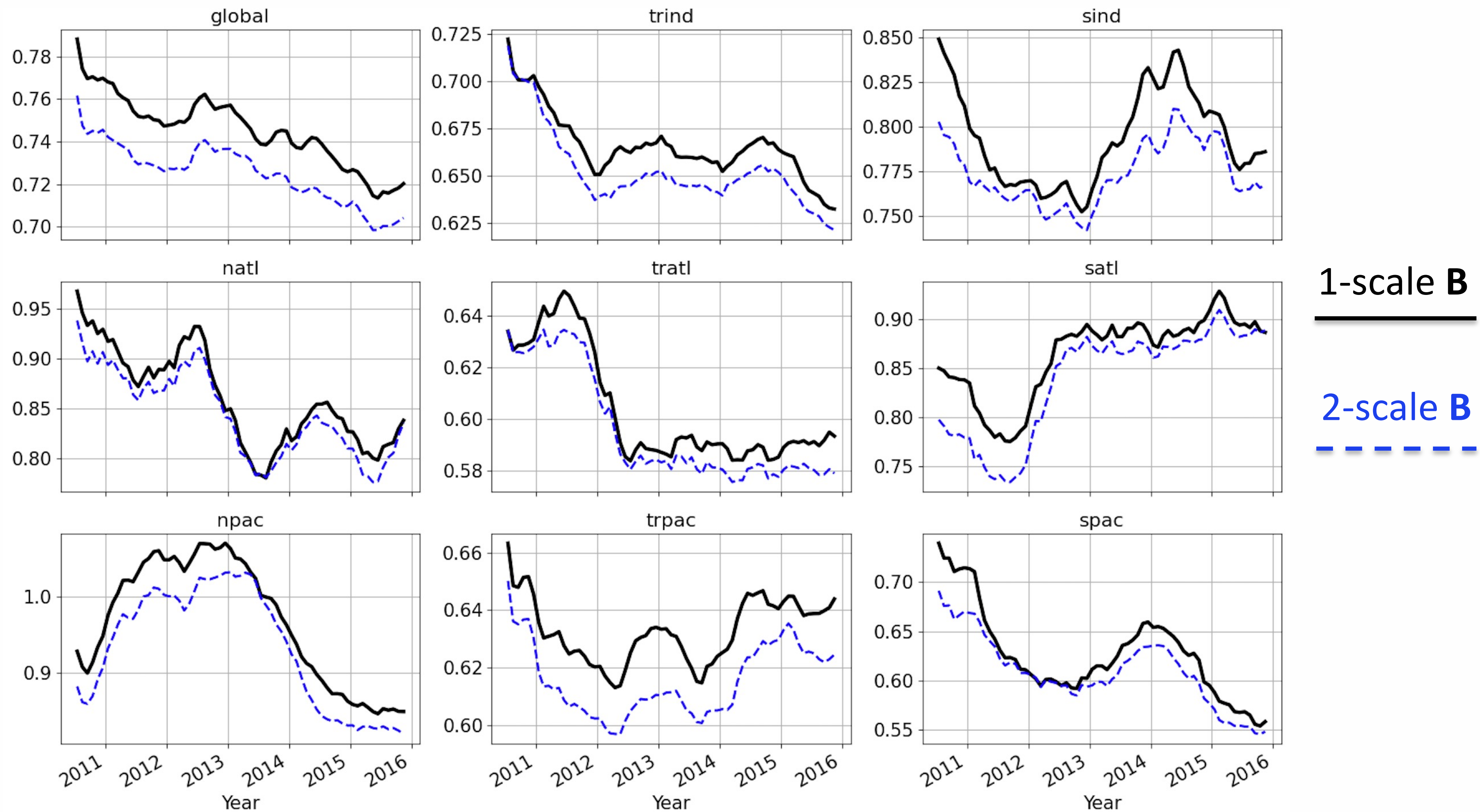


2 scales



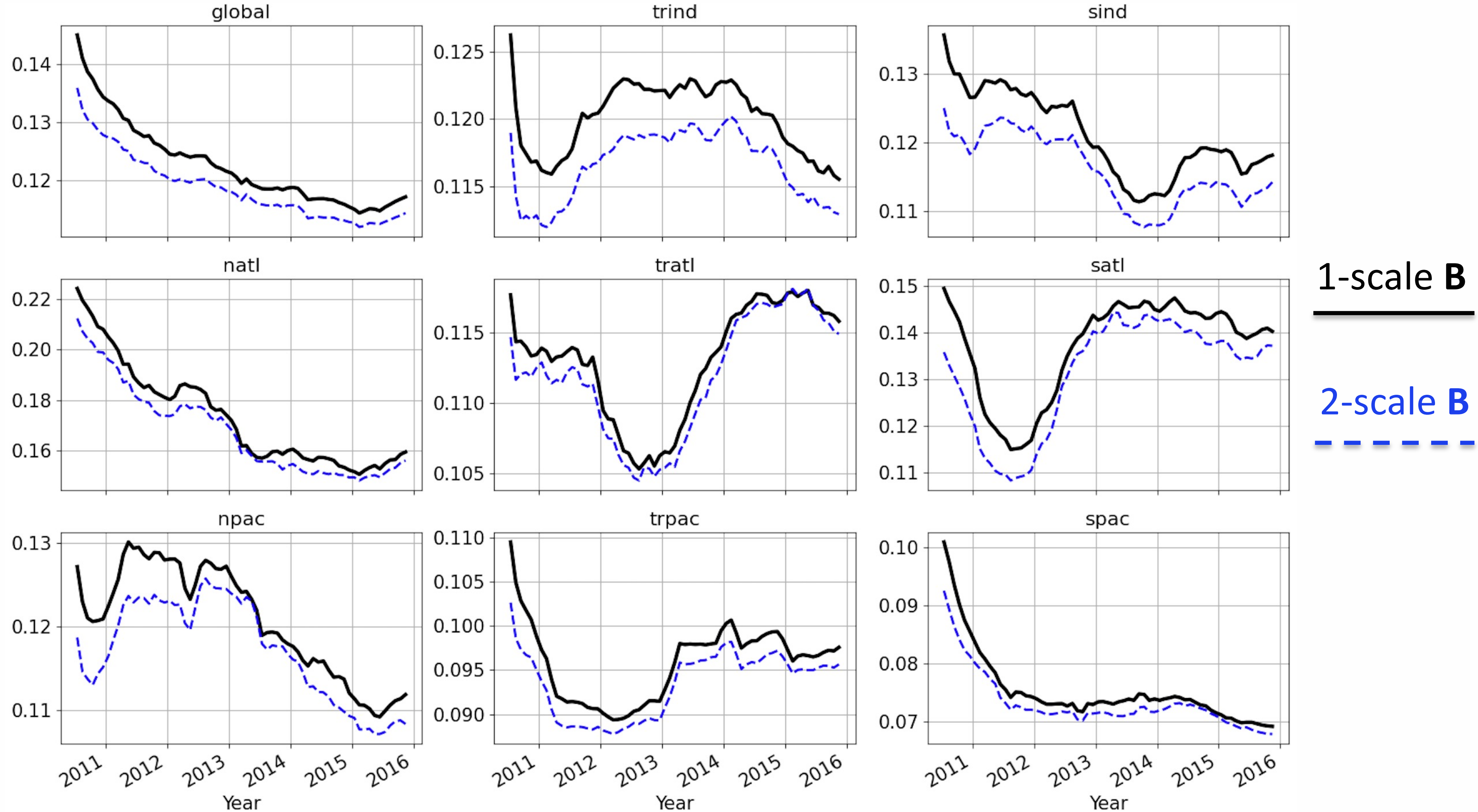
Cycled 3D-Var DA experiments using the ECMWF ORAS6 framework with a climatological **B**

- Time-series of the **temperature** RMS (obs – bkg) averaged over 0 – 1000 m



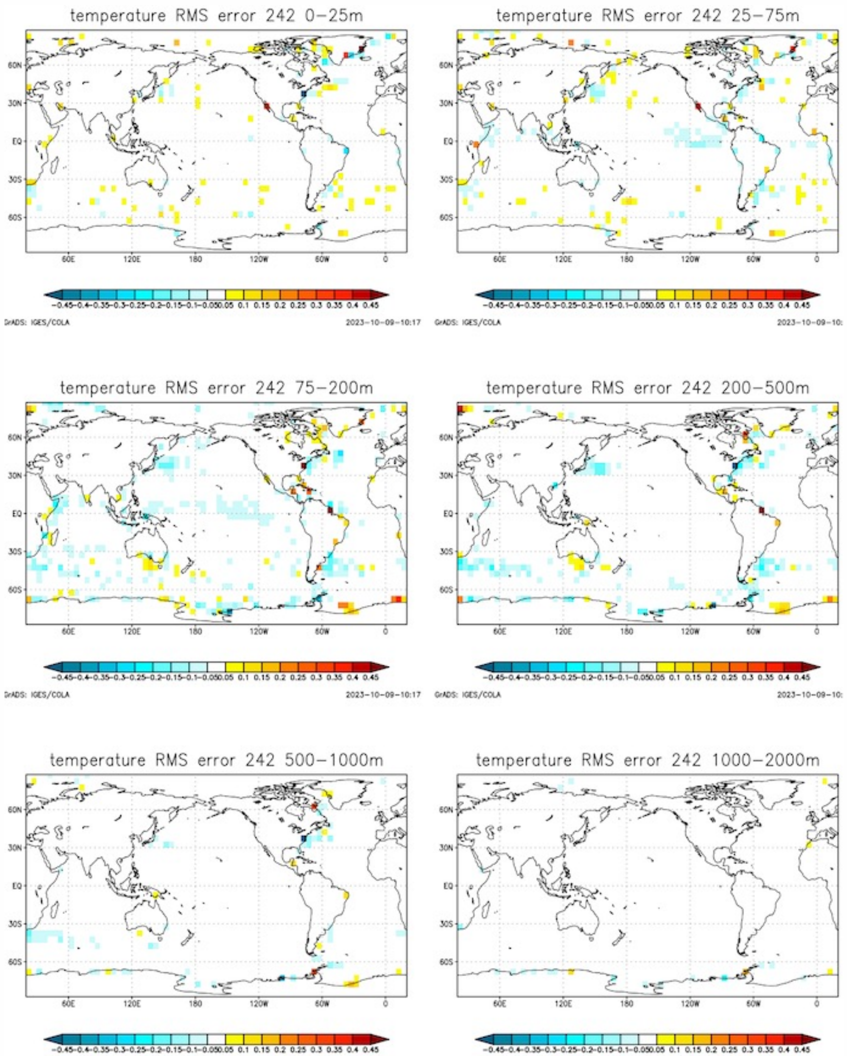
Cycled 3D-Var DA experiments using the ECMWF ORAS6 framework with a climatological **B**

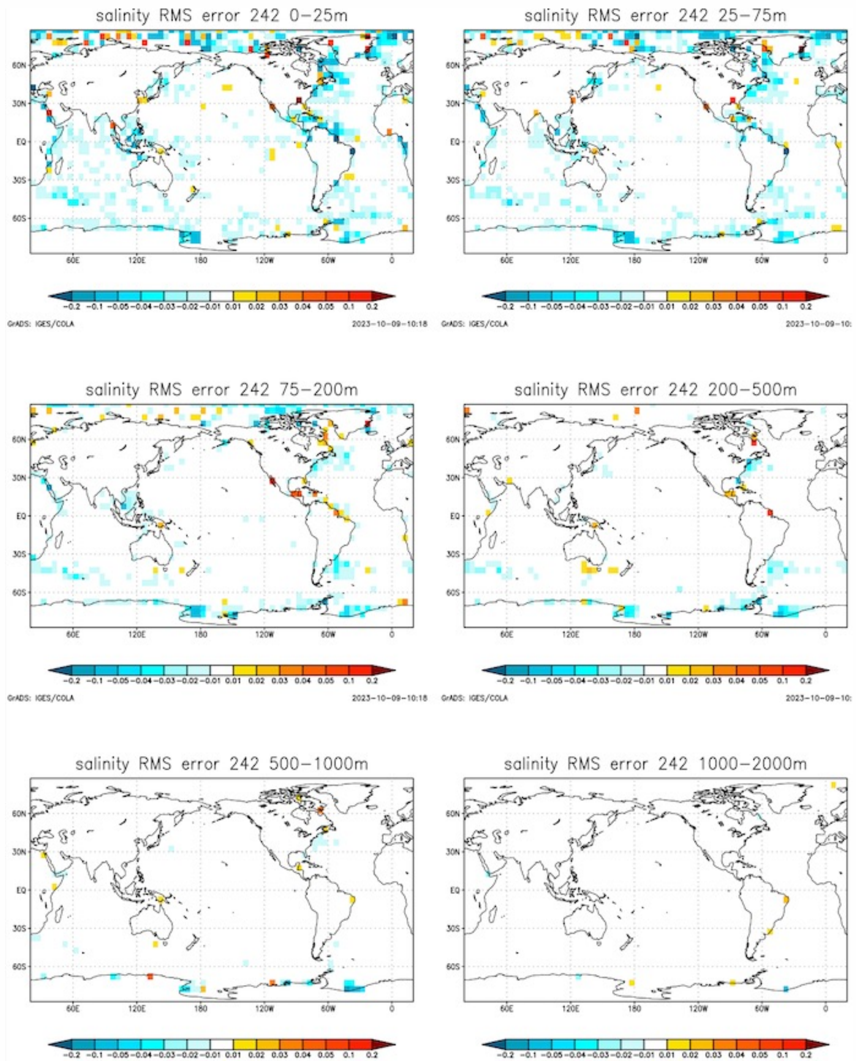
- Time-series of the **salinity** RMS (obs – bkg) averaged over 0 – 1000 m



Cycled 3D-Var DA experiments using the ECMWF ORAS6 framework with a climatological **B**

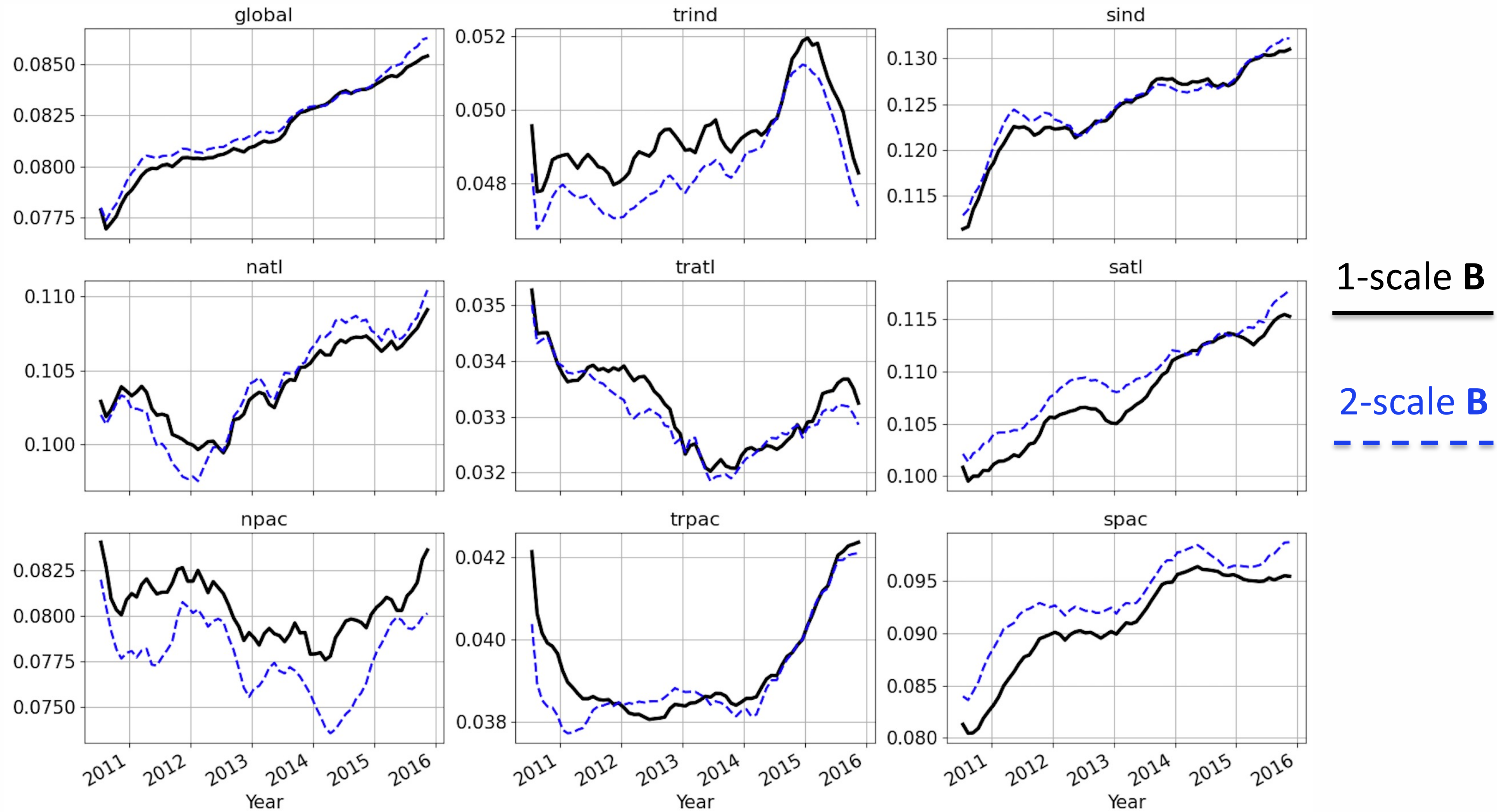
- RMS (obs – bkg) difference (2-scale **B** minus 1-scale **B**) for **temperature** & **salinity**





Cycled 3D-Var DA experiments using the ECMWF ORAS6 framework with a climatological **B**

- Time-series of the **sea surface height** SDV (obs – bkg)

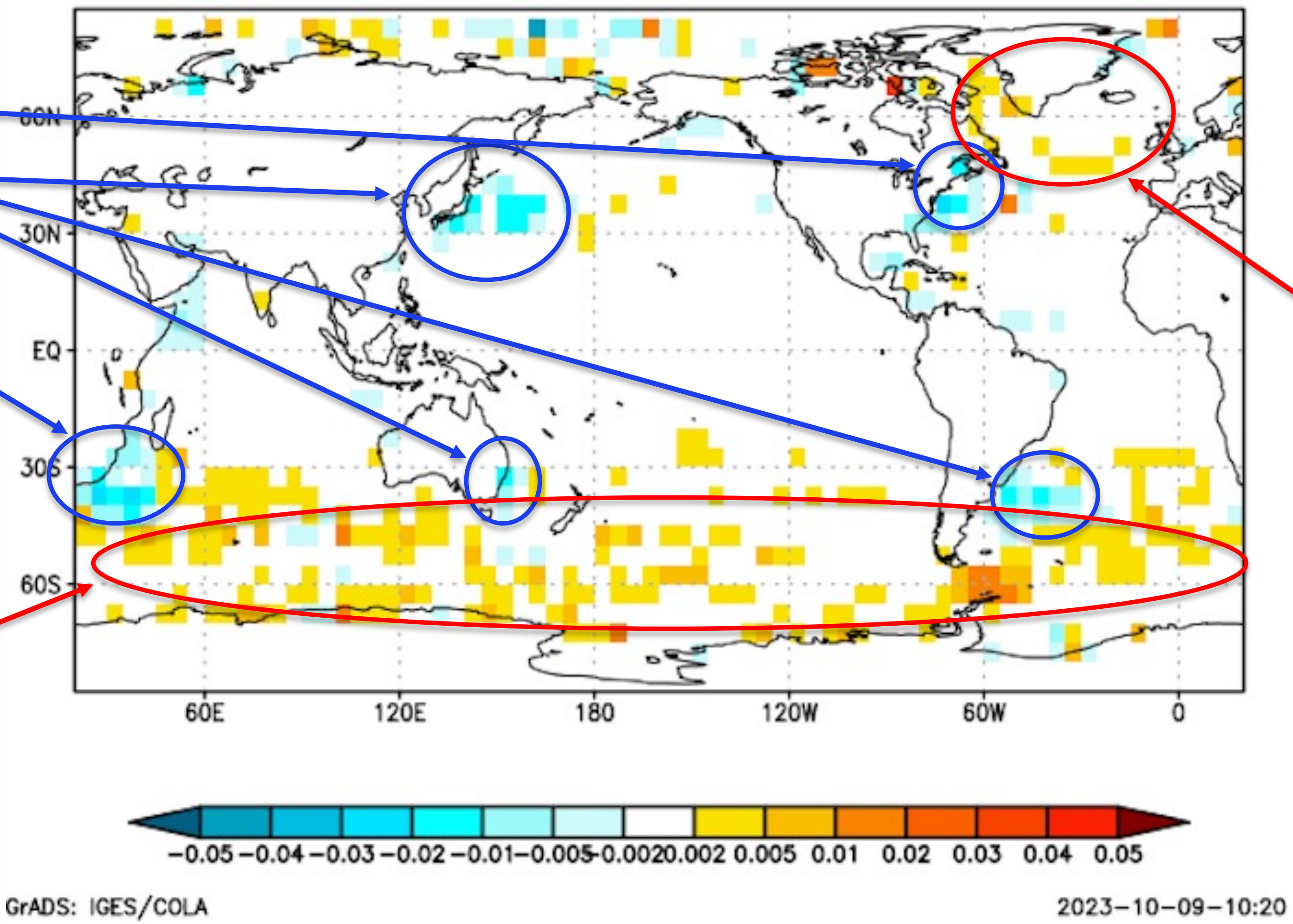


Cycled 3D-Var DA experiments using the ECMWF ORAS6 framework with a climatological **B**

- SDV (obs – bkg) difference (2-scale **B** minus 1-scale **B**) for **sea surface height**

Improvement
In boundary
current regions

Degradation



Degradation
in Circumpolar
Current

Summary and outlook

- SDM in NEMOVAR: separate an ensemble into a range of scales and model the same-scale and cross-scale covariances using a diffusion operator.
  - How many scales? Depends on model resolution and cost vs benefits of increasing N_s.
  - Vertical separation as well as horizontal separation?
- Objective and inexpensive methods can be used for estimating and filtering the scale-dependent **B** model parameters.
  - Little modification is required to estimation methods developed for a single scale formulation.
- First results with a climatological **B** are overall positive for temperature and salinity; mixed results for SSH (compared to one scale).
  - More diagnostics and understanding required.
- SDM (climatology) hybridizes naturally with SDL (flow-dependent).
  - Hybridization coefficients and localization length-scales can be estimated using BUMP (software developed by B. Ménétrier).
  - SDL and BUMP are already implemented in NEMOVAR.
  - Combining SDM, SDL and BUMP will be the subject of future work.

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