EUROPEAN CENTRE FOR RESEARCH AND ADVANCED TRAINING IN SCIENTIFIC COMPUTING

A scale-dependent hybrid background-error covariance matrix for global ocean DA *

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Accounting for spatial scale dependency in variational DA

- Minimize separate cost functions for “large” and “small” scale information (Li et al. 2015)
  - How to separate scales is not obvious; complicates the problem of specifying **R**
- Multiple scale **B** model (Met Office; Mirouze et al. 2016) (1)
  - Block-diagonal (uncorrelated) with respect to the separated scales
- Use a hierarchy of nested grids (Srinivasan et al. 2022)
  - **B** length-scale controlled by the grid resolution
- Scale-dependent localization (SDL) of an ensemble covariance matrix (Buehner & Shlyaeva 2015) (2)
  - Requires an ensemble; expensive

Here we describe an approach that extends (1) and uses features of (2)

Scale-dependent ensemble perturbations

- In NEMOVAR, we use an ensemble to define the error covariances of **transformed** (assumed approximately uncorrelated) background variables.
- We first remove the balanced component from the ensemble perturbation matrix:

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

- Next, use a sequence of filters $\mathbf{F}_i$ (here, diffusion) with different length scales D_i , where $D_i > D_{i-1}$, to construct an augmented set of perturbations (from **small scale** to **large scale**):

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

Scale-dependent ensemble perturbations

- Rearrange the filtered perturbations into overlapping ranges of scales from **large** (small i) to **small** (large i):

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

- The original perturbation is recovered from the telescoping sum

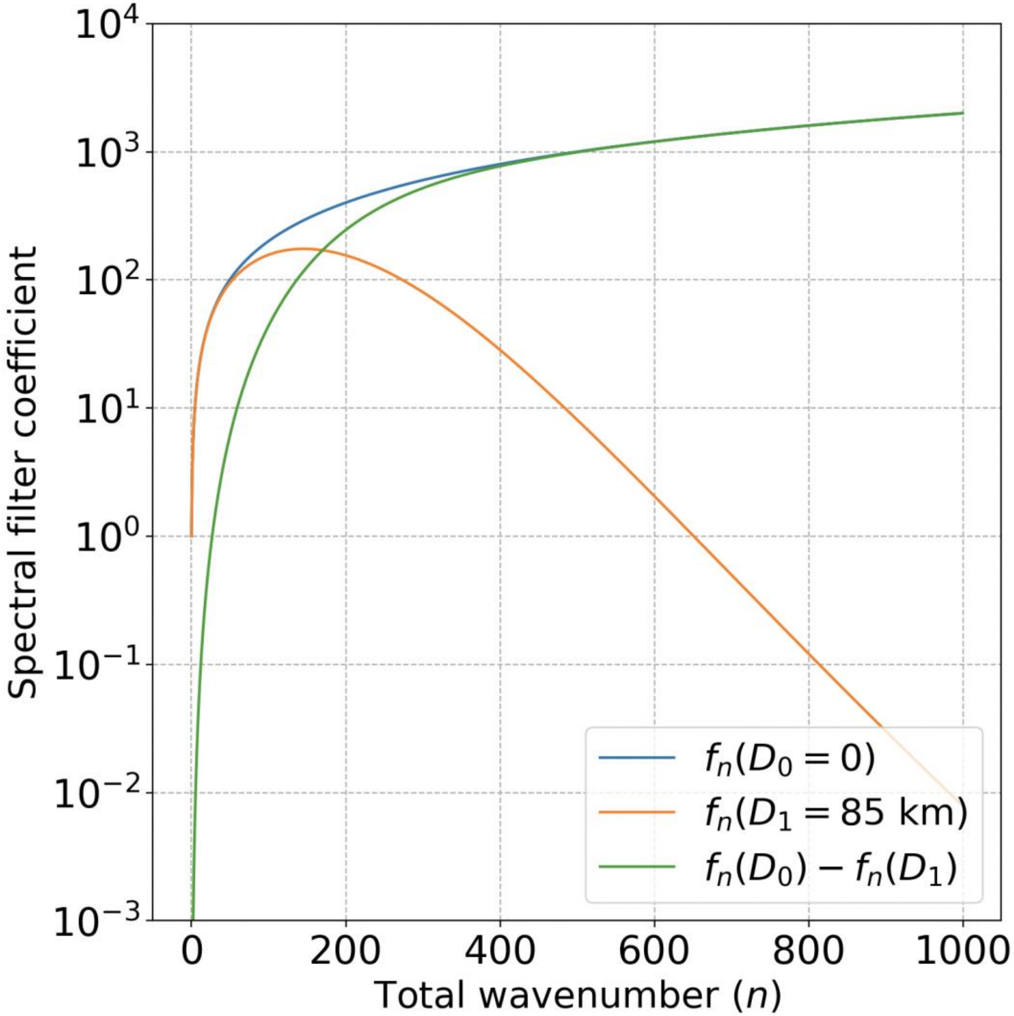
$$\widehat{\mathbf{X}} = \sum_{i=1}^{N_{\mathrm{s}}} \widehat{\mathbf{X}}_i$$

- 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 implicit diffusion filtering on the sphere

Example with two separated scales



Filtering kernel:

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

Spectral coefficients:

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

Filtering length-scale:

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

where $M = 10$ in the example

(Weaver and Mirouze 2013)

Scale-dependent covariance modelling

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

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

- Here, we define a scale-dependent covariance model (SDM) as

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

- $\mathbf{C}_{ij}$ must be symmetric, positive semi-definite. We define it as

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

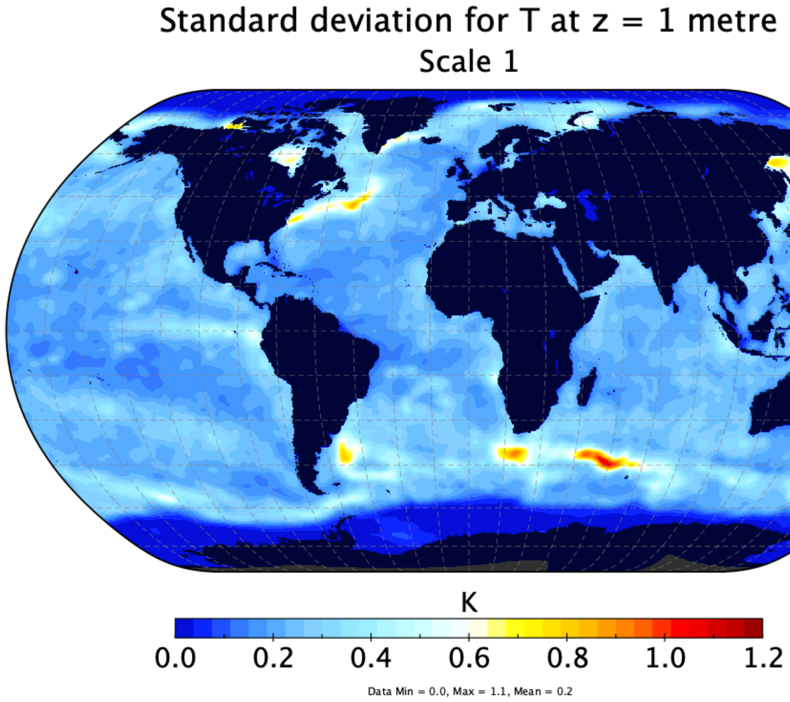
- We use the “square-root” of a diffusion operator to model the components:

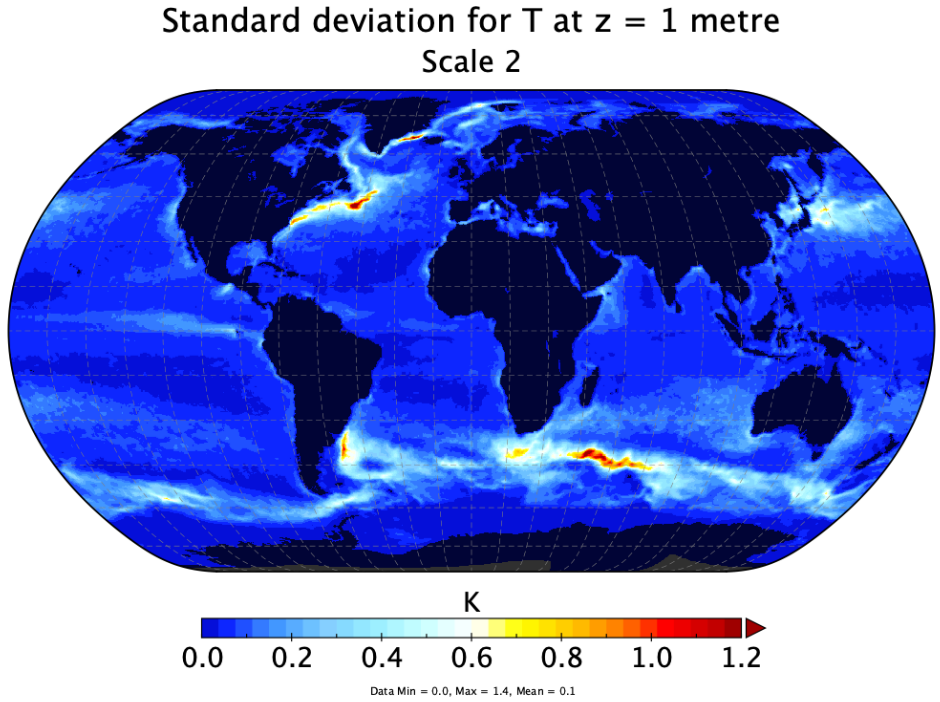
$$\mathbf{U}_i = \mathbf{\Gamma}_i \, \mathbf{V}_i \, \mathbf{W}^{-1/2} \quad \text{and} \quad \mathbf{U}_j^\mathrm{T} = \mathbf{W}^{-1/2} \, \mathbf{V}_j^\mathrm{T} \, \mathbf{\Gamma}_j$$

Scale-dependent variance estimation

- Climatological statistics from an 11-member ensemble from ECMWF pre-OCEAN6 configuration (ORCA025_Z75)
- Two ranges of scales where D_2 = 3 times the local horizontal resolution

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

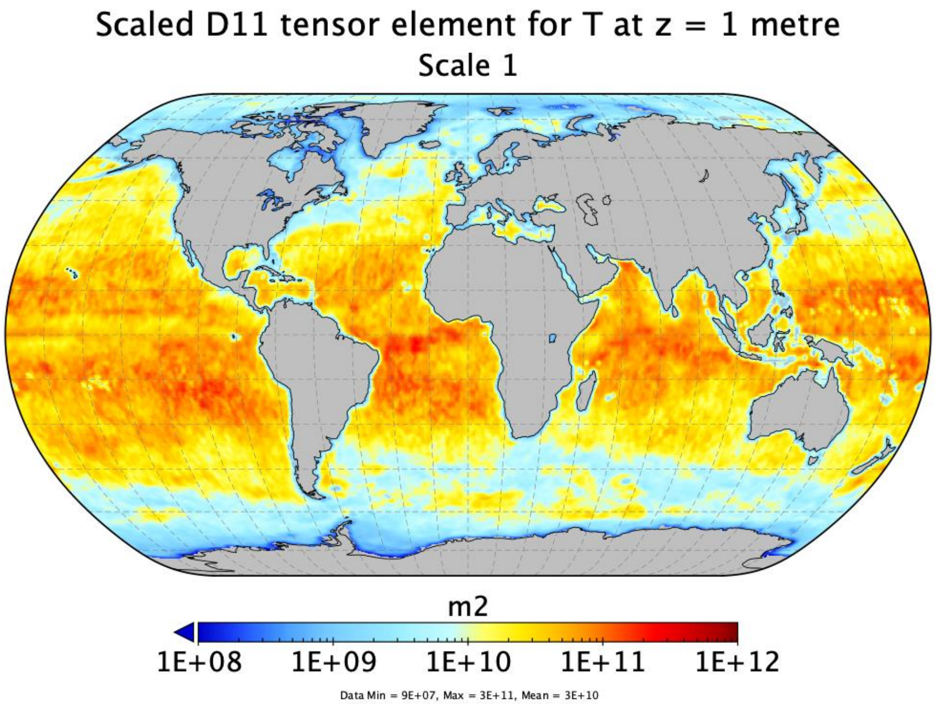




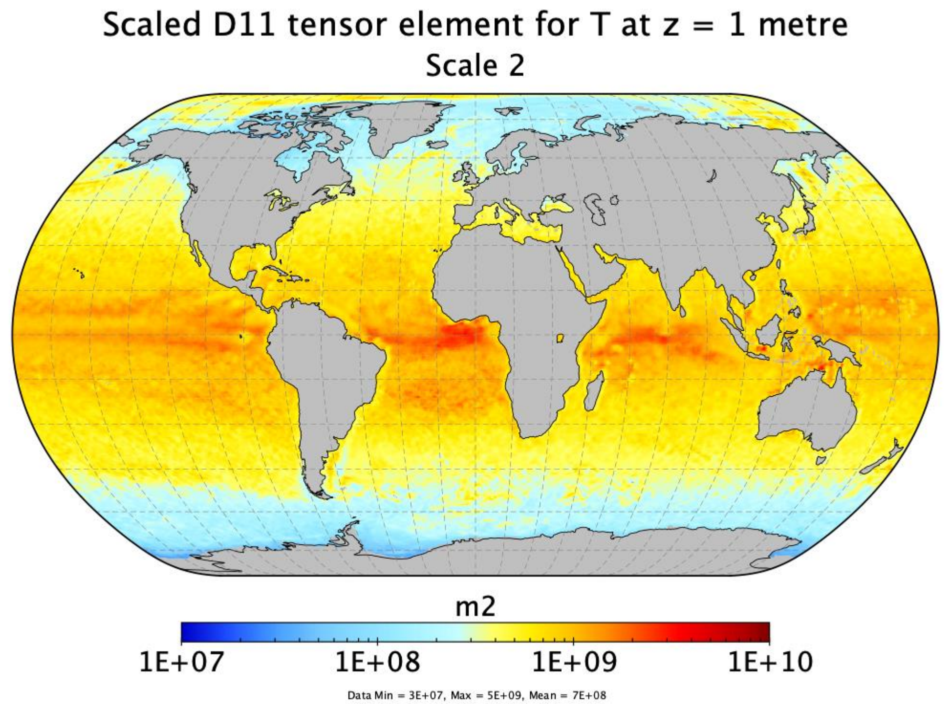
Scale-dependent correlation (diffusion) tensor estimation

- Directional length-scale tensor $\boldsymbol{D}(\mathbf{z})$ estimated from the inverse of the local ensemble gradient tensor (Weaver et al. 2021): $\boldsymbol{D}(\mathbf{z}) = \left(\widetilde{\boldsymbol{H}}(\mathbf{z})\right)^{-1}$ where

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



100 km 1000 km



10 km 100 km

Computational cost

- $\mathbf{B}_{\mathrm{SDM}}$ requires N_{s} applications of the diffusion operator.
- However, the computational cost does *not* scale with N_{s} !

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 with **1 scale** = **23**

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

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 **fine grid** = **43**

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

- So the cost with $N_{\mathrm{s}} = 2$ can be made comparable to the cost with $N_{\mathrm{s}} = 1$!

- First, we normalize $\mathbf{B}_{\text{SDM}}$ to isolate the total standard deviations:

$$\mathbf{B} = \mathbf{\Sigma} \underbrace{\mathbf{\Gamma} \mathbf{B}_{\text{SDM}} \mathbf{\Gamma}}_{\mathbf{C}_{\text{SDM}}} \mathbf{\Sigma}$$

- The normalization factors are $\{\mathbf{\Gamma}\}_{nn} = \left(\sqrt{\{\mathbf{B}_{\text{SDM}}\}_{nn}}\right)^{-1}$
- This 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.
  - When $i \neq j$ they are *not* equal to 1 and are *not* explicitly known. They can be estimated, however, by reworking the randomization algorithm.

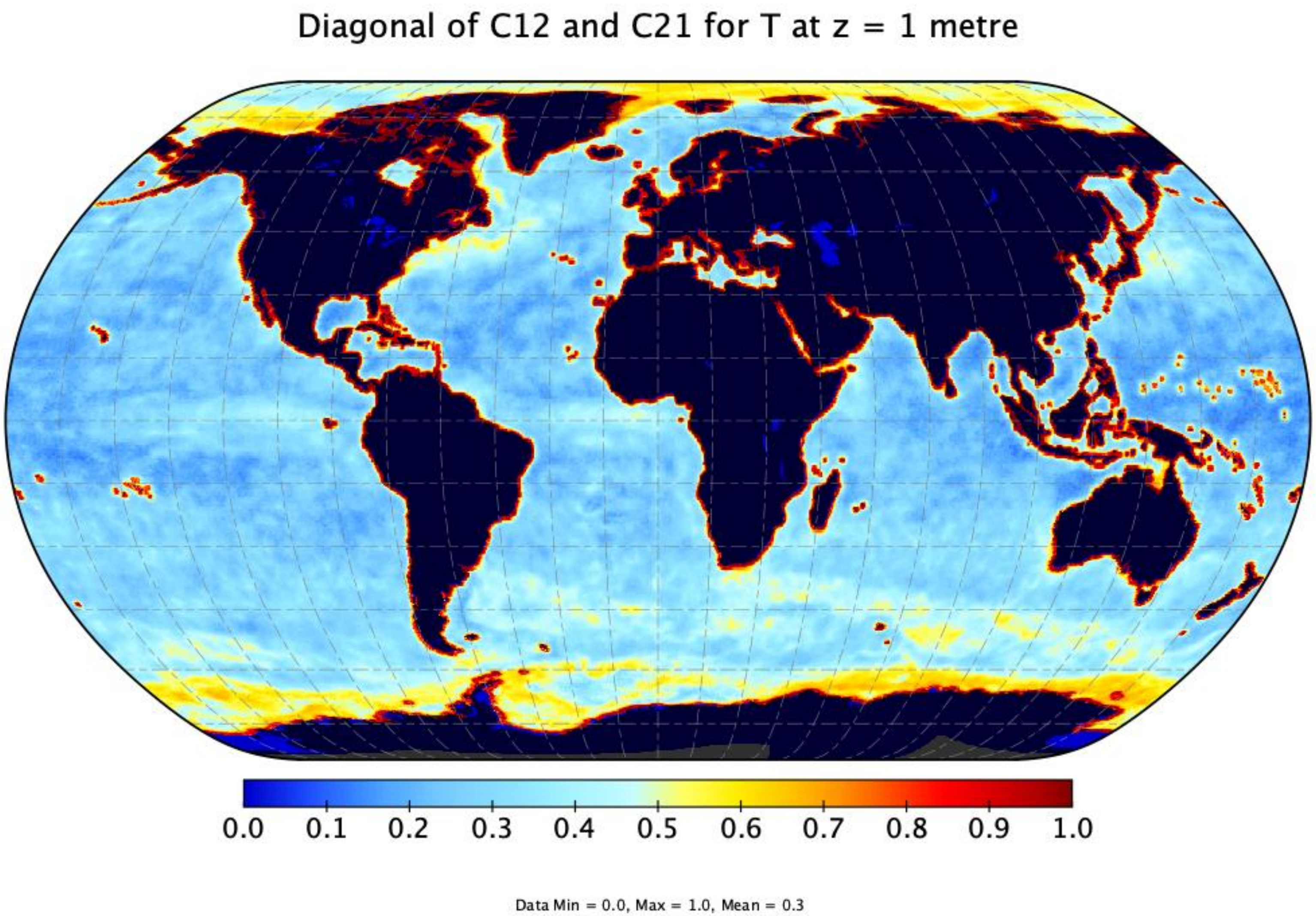
- **Hybrid scale-dependent** standard deviations:

$$\mathbf{\Sigma}_i = g\left(\mathbf{\Sigma}_i^{\text{flow}}, \mathbf{\Sigma}_i^{\text{clim}}\right)$$

- **Hybrid total** standard deviations:

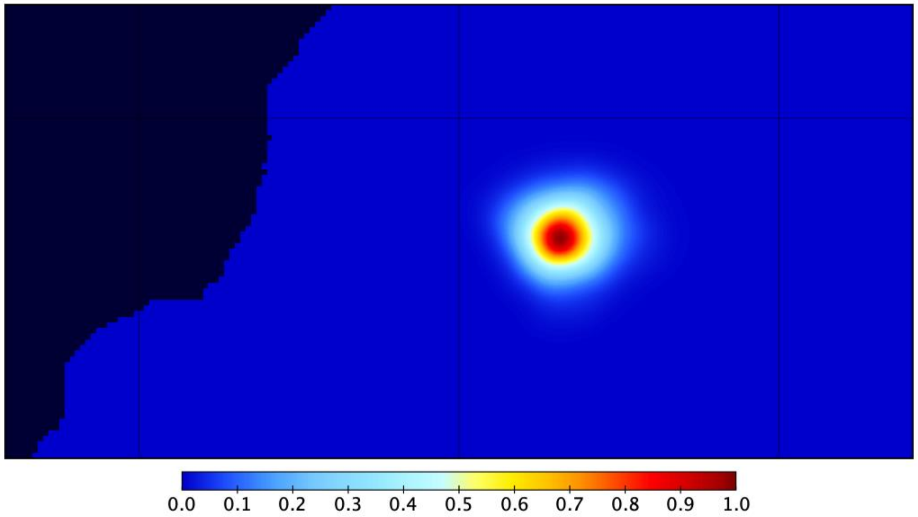
$$\mathbf{\Sigma} = h\left(\mathbf{\Sigma}^{\text{flow}}, \mathbf{\Sigma}^{\text{clim}}, \mathbf{\Sigma}^{\text{param}}\right)$$

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

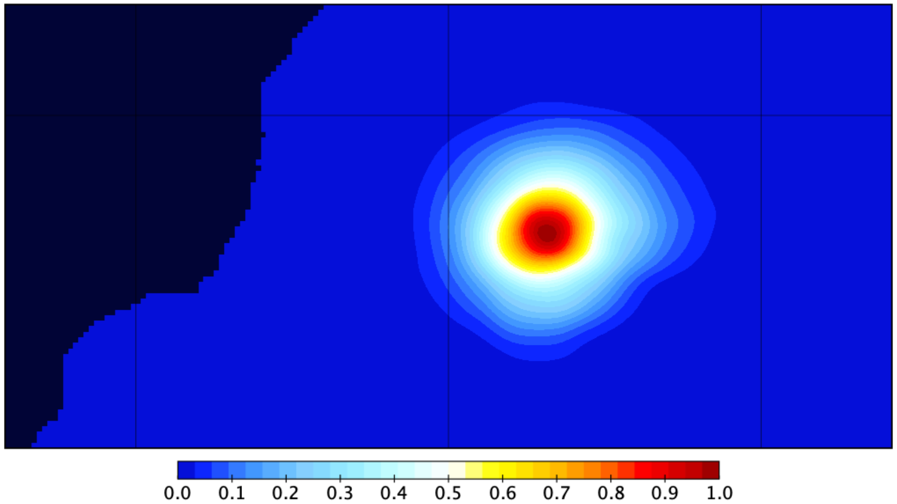


- Example of T-T correlations at 1 metre depth

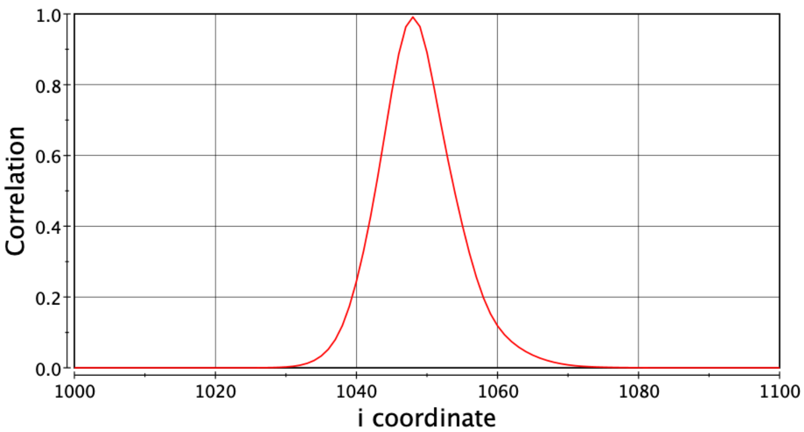
1 scale



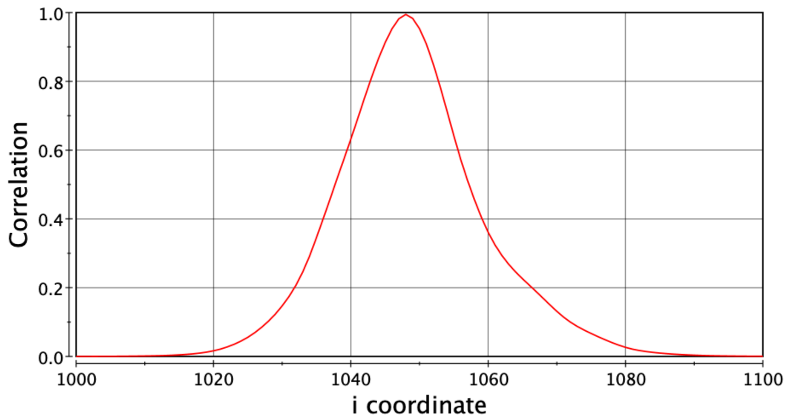
2 scales



1 scale

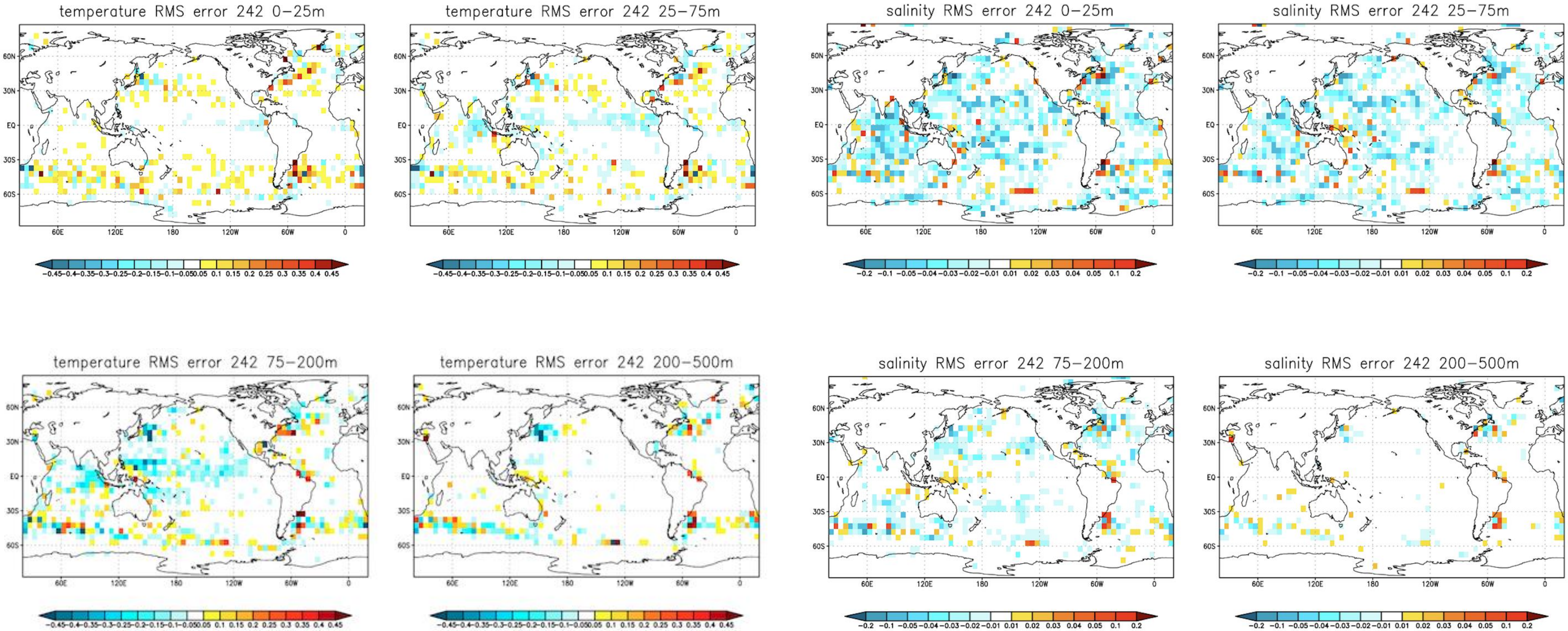


2 scales



Preliminary results from a data assimilation experiment

- RMS error **2 scales** minus RMS error **1 scale** (blue means improvement)
- Averaged results for the period 01/01/2010 – 01/01/2012



Summary and outlook

- Separate an ensemble into a range of scales and model the same-scale and cross-scale covariances using a diffusion operator.
  - The choice of scales depends on model resolution and the cost vs benefits of increasing N_s.

- We can use objective methods for estimating and for filtering the scale-dependent variances and correlation tensor.
  - Little modification is required to estimation methods developed for a single scale formulation.

- 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.

References

- Buehner, M. and A. Shlyaeva, 2015: Scale-dependent background-error covariance localisation, *Tellus*, **67**, 28027.
- Mirouze, I., Blockley, E. W., Lea, D. J., Martin, M. J. and M. J. Bell, 2016: A multiple length-scale correlation operator for oceand data assimilation. *Tellus A*, **68**, 29744.
- Srinivasan, A., Chin, T. M., Chassignet, E. P., Iskandarani, M. and N. Groves, 2022: A statistical interpolation code for ocean analysis and forecasting. Journal of Atmospheric and Oceanic Technology, 367-386.
- Weaver, A. T., Chrust, M., Ménétrier, B. and A. Piacentini, 2021: An evaluation of methods for normalizing diffusion-based covariance operators in variational data assimilation. *Quarterly Journal of the Royal Meteorological Society*, **147**, 289-320.
- Weaver, A. T. and I. Mirouze, 2013: On the diffusion equation and its application to isotropic and anisotropic correlation modelling in variational assimilation. *Quarterly Journal of the Royal Meteorological Society*, **139**, 242-260.