EUROPEAN CENTRE FOR RESEARCH AND ADVANCED TRAINING IN SCIENTIFIC COMPUTING

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

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CERFACS

DA-TT Technical Seminar, 14 March 2022

Outline

- Accounting for scale dependency
- Constructing scale-dependent ensemble perturbations
- Scale-dependent localization
- Scale-dependent modelled covariances
- Conclusions and ongoing work

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Accounting for scale dependency in DA

- Use correlation operators based on spectral/wavelet filters
  - Common in atmospheric DA systems; not convenient for ocean DA
- Minimize separate cost functions for “large” and “small” scale information (Li et al. 2015)
  - How to separate scales is not obvious in a realistic context; complicates the problem of specifying **R**
- Multiple scale **B** model (Met Office; Mirouze et al. 2016)
  - Block-diagonal (uncorrelated) with respect to the separated scales
- Scale-dependent localization (SDL) of an ensemble covariance matrix (Buehner & Shlyaeva 2015)
  - Requires an ensemble; expensive

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Scale-dependent ensemble perturbations

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

$$\widehat{\mathbf{X}} = \mathbf{K}_{\mathrm{b}}^{-1}\mathbf{X} = \frac{1}{\sqrt{N_{\mathrm{e}}-1}}\begin{pmatrix} \hat{\boldsymbol{\epsilon}}_1' & \dots & \hat{\boldsymbol{\epsilon}}_{N_{\mathrm{e}}}' \end{pmatrix}$$

- 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** to **large scale**):

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

Scale-dependent ensemble perturbations

- Rearrange the filtered perturbations (from **large scale** to **small scale**) such that their sum equals the original perturbations:

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

where $\mathbf{F}_{N_{\mathrm{s}}+1} = \mathbf{0}$ and $\sum_{i=1}^{N_{\mathrm{s}}} \widehat{\mathbf{X}}_i = \widehat{\mathbf{X}}$

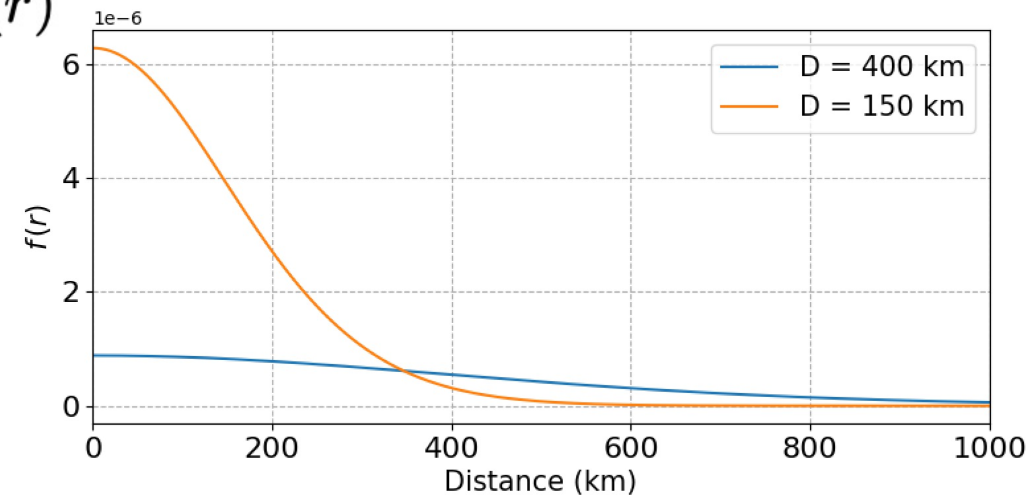
- The sample error covariance matrix for the control variables is

$$\widetilde{\mathbf{B}} = \widehat{\mathbf{X}}\,\widehat{\mathbf{X}}^{\mathrm{T}} = \begin{pmatrix} \mathbf{I} & \cdots & \mathbf{I} \end{pmatrix} \underbrace{\begin{pmatrix} \widehat{\mathbf{X}}_1 \\ \vdots \\ \widehat{\mathbf{X}}_{N_{\mathrm{s}}} \end{pmatrix} \begin{pmatrix} \widehat{\mathbf{X}}_1^{\mathrm{T}} & \cdots & \widehat{\mathbf{X}}_{N_{\mathrm{s}}}^{\mathrm{T}} \end{pmatrix}}_{\widetilde{\mathbf{B}}^{\mathrm{ss}}} \begin{pmatrix} \mathbf{I} \\ \vdots \\ \mathbf{I} \end{pmatrix}$$

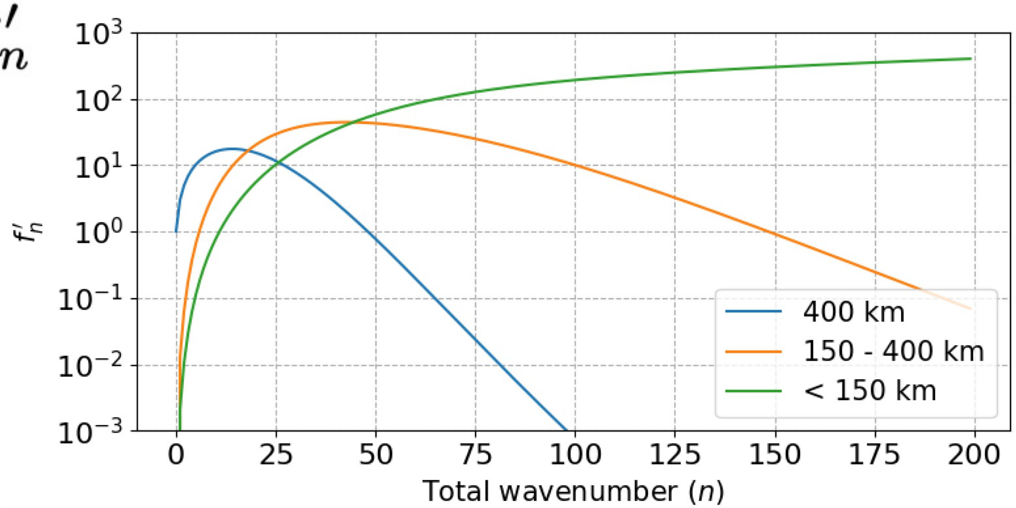
Scale-dependent implicit diffusion filtering

$M = 10$

$f(r)$



f'_n



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

$$r = a\sqrt{2(1-\cos\theta)}$$

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

$$L \approx D/\sqrt{2M-4}$$

$$f'_n = f_n(L_{i-1}) - f_n(L_i)$$

(Weaver & Courtier 2001; Weaver & Mirouze 2013)

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Scale-dependent localization (SDL)

- The idea behind SDL (Buehner & Shlyaeva 2015) is to localize (via a Schur product $\circ$) the scale-separated covariance matrix with scale-dependent localization blocks:

$$\mathbf{B}^{\mathrm{ss}} = \mathbf{L}^{\mathrm{ss}} \circ \widetilde{\mathbf{B}}^{\mathrm{ss}} \qquad \left(B^{\mathrm{ss}}_{kl} = L^{\mathrm{ss}}_{kl} \, \widetilde{B}^{\mathrm{ss}}_{kl} \right)$$

where

$$\mathbf{L}^{\mathrm{ss}} = \begin{pmatrix} \mathbf{L}_{11} & \cdots & \mathbf{L}_{1N_{\mathrm{s}}} \\ \vdots & \ddots & \vdots \\ \mathbf{L}_{N_{\mathrm{s}}1} & \cdots & \mathbf{L}_{N_{\mathrm{s}}N_{\mathrm{s}}} \end{pmatrix}$$

Scale-dependent localization (SDL)

- The localized covariance matrix in control variable space is

$$\mathbf{B}^{\mathrm{e}} = \begin{pmatrix} \mathbf{I} & \cdots & \mathbf{I} \end{pmatrix} \left(\mathbf{L}^{\mathrm{ss}} \circ \widetilde{\mathbf{B}}^{\mathrm{ss}} \right) \begin{pmatrix} \mathbf{I} \\ \vdots \\ \mathbf{I} \end{pmatrix} = \sum_{n=1}^{N_{\mathrm{e}}} \sum_{i=1}^{N_{\mathrm{s}}} \sum_{j=1}^{N_{\mathrm{s}}} \mathbf{\Lambda}_{ni} \, \mathbf{L}_{ij} \, \mathbf{\Lambda}_{nj}$$

where

$$\mathbf{\Lambda}_{ni} = \frac{1}{\sqrt{N_{\mathrm{e}} - 1}} \operatorname{diag}\left(\widehat{\boldsymbol{\epsilon}}'_{ni} \right)$$

- Buehner & Shlyaeva (2015) *define* the localization blocks as

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

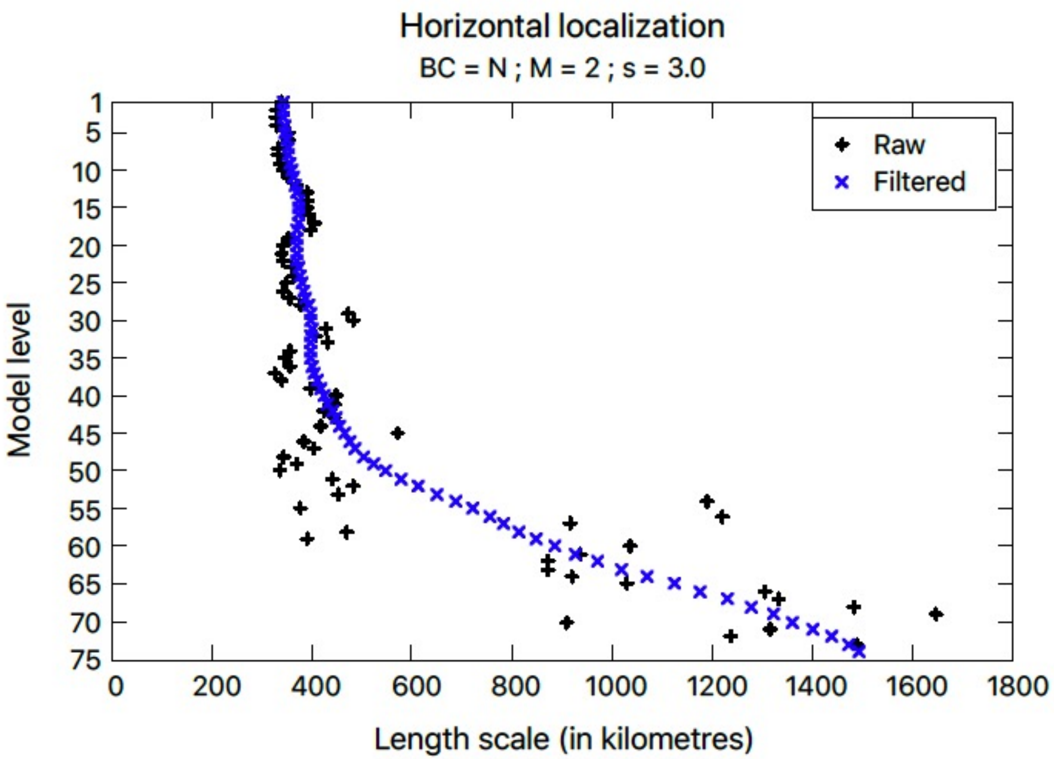
Defining the SDL blocks

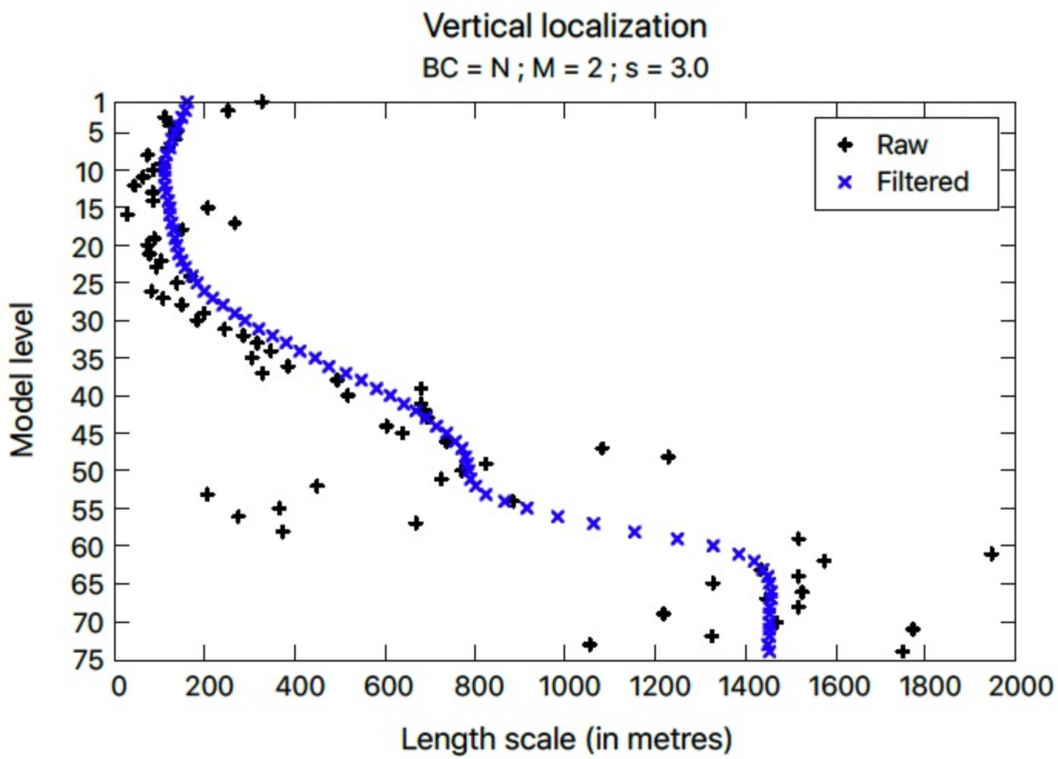
$$\mathbf{L}^{\mathrm{ss}} = \begin{pmatrix} \mathbf{U}_1 \\ \vdots \\ \mathbf{U}_{N_\mathrm{s}} \end{pmatrix} \begin{pmatrix} \mathbf{U}_1^\mathrm{T} & \cdots & \mathbf{U}_{N_\mathrm{s}}^\mathrm{T} \end{pmatrix}$$

- In NEMOVAR, we use an implicit diffusion operator to define $\mathbf{U}_i$
- We use an approximate implicit diffusion solver based on the Chebyshev iteration.
- For localization, we perform diffusion on a **coarse grid** since localization length scales are typically large.
- These two algorithmic features are crucial for making SDL affordable.
- We use BUMP (B. Ménétrier; imported from JEDI) to estimate the SDL length scales.

BUMP-estimated localization length scales

- Example from a 15-member ensemble for ORCA1_Z75 (ECMWF).
- No scale separation considered here.
- A vertical diffusion filter is applied to the raw estimates.





Variance filtering and/or hybridization

- Factor out the standard deviation matrix so that the variances can be filtered and/or hybridized separately:

$$\mathbf{B}^{\mathrm{e}} = \boldsymbol{\Sigma} \begin{pmatrix} \mathbf{I} & \cdots & \mathbf{I} \end{pmatrix} \left(\mathbf{L}^{\mathrm{ss}} \circ (\widetilde{\boldsymbol{\Sigma}}^{\mathrm{ss}})^{-1} \widetilde{\mathbf{B}}^{\mathrm{ss}} (\widetilde{\boldsymbol{\Sigma}}^{\mathrm{ss}})^{-1} \right) \begin{pmatrix} \mathbf{I} \\ \vdots \\ \mathbf{I} \end{pmatrix} \boldsymbol{\Sigma}$$

where $\widetilde{\boldsymbol{\Sigma}}^{\mathrm{ss}} = \mathrm{diag}(\widetilde{\boldsymbol{\Sigma}}, \dots, \widetilde{\boldsymbol{\Sigma}})$

$\widetilde{\boldsymbol{\Sigma}}$ contains **sample** ***total*** standard deviations

$\boldsymbol{\Sigma}$ contains **filtered** and/or **hybridized** ***total*** std deviations

- This is equivalent to the original formulation when $\boldsymbol{\Sigma} = \widetilde{\boldsymbol{\Sigma}}$

Variance preservation

- SDL does not preserve the total variance so an additional normalization matrix $\boldsymbol{\Gamma}^{\mathrm{e}}$ is required:

$$\mathbf{B}^{\mathrm{e}} = \underbrace{\boldsymbol{\Sigma}\,\boldsymbol{\Gamma}^{\mathrm{e}} \begin{pmatrix} \mathbf{I} & \cdots & \mathbf{I} \end{pmatrix} \left(\mathbf{L}^{\mathrm{ss}} \circ (\widetilde{\boldsymbol{\Sigma}}^{\mathrm{ss}})^{-1}\, \widetilde{\mathbf{B}}^{\mathrm{ss}}\, (\widetilde{\boldsymbol{\Sigma}}^{\mathrm{ss}})^{-1}\right) \begin{pmatrix} \mathbf{I} \\ \vdots \\ \mathbf{I} \end{pmatrix} \boldsymbol{\Gamma}^{\mathrm{e}}}_{\mathbf{C}^{\mathrm{e}}} \boldsymbol{\Sigma}$$

- $\mathbf{C}^{\mathrm{e}}$ should be a correlation matrix (1s on the diagonal).

- Computing this extra normalization is tricky!

Variance-preserving normalization

- To estimate the normalization factors we require an estimate of the diagonal of the blocks

$$\mathbf{U}_i \mathbf{U}_j^{\mathrm{T}}$$

- We can estimate the diagonal of the cross-scale blocks ($i \neq j$) simultaneously with the diagonal of the same-scale blocks

$$\mathbf{U}_i \mathbf{U}_i^{\mathrm{T}}$$

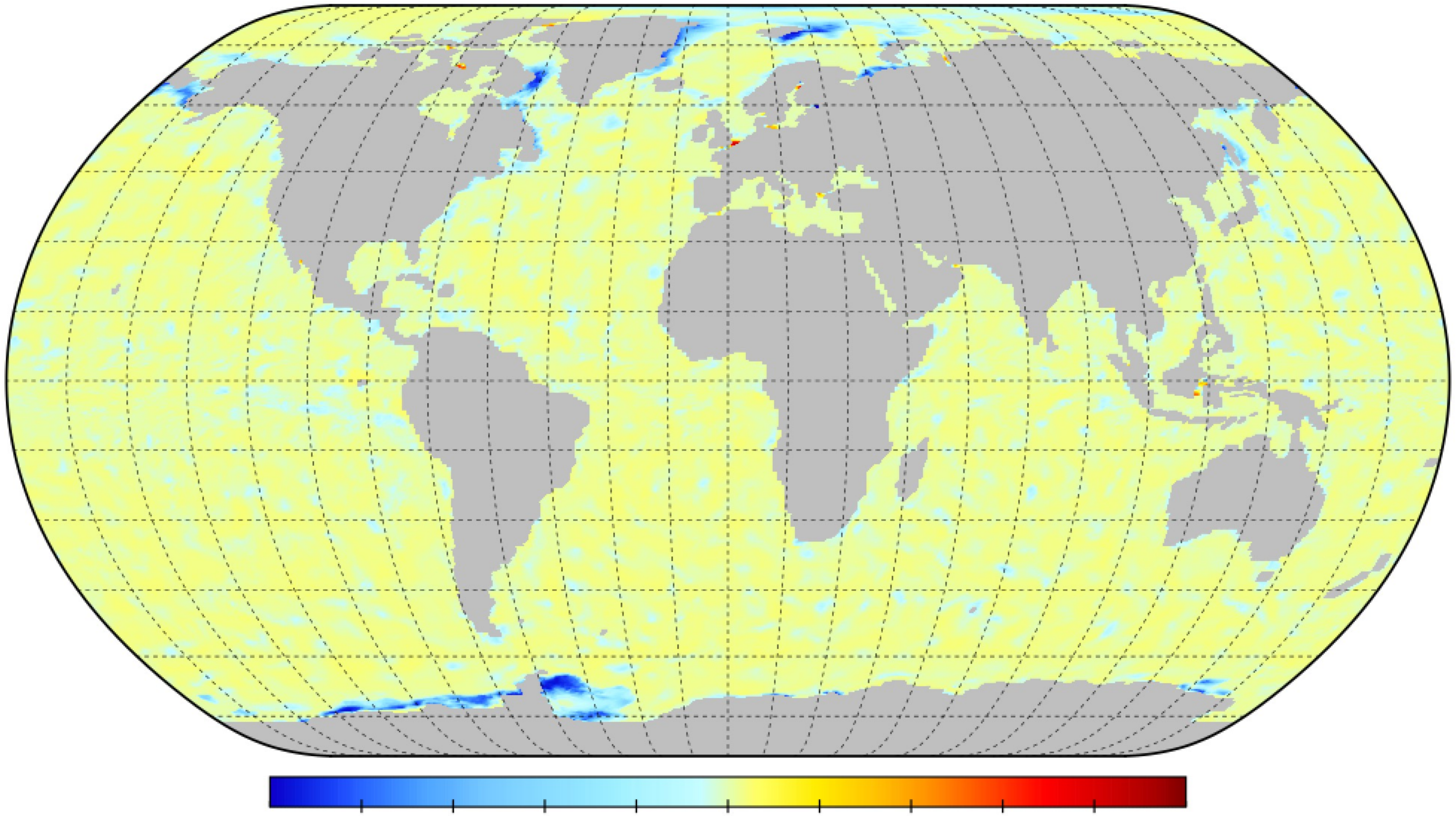
using a randomization (Monte Carlo) algorithm applied to

$$\left(\mathbf{U}_i + \mathbf{U}_j\right)\left(\mathbf{U}_i + \mathbf{U}_j\right)^{\mathrm{T}}$$

Is this extra normalization important?

Example with ensembles separated into 2 spectral bands:
< 220 km and > 220 km

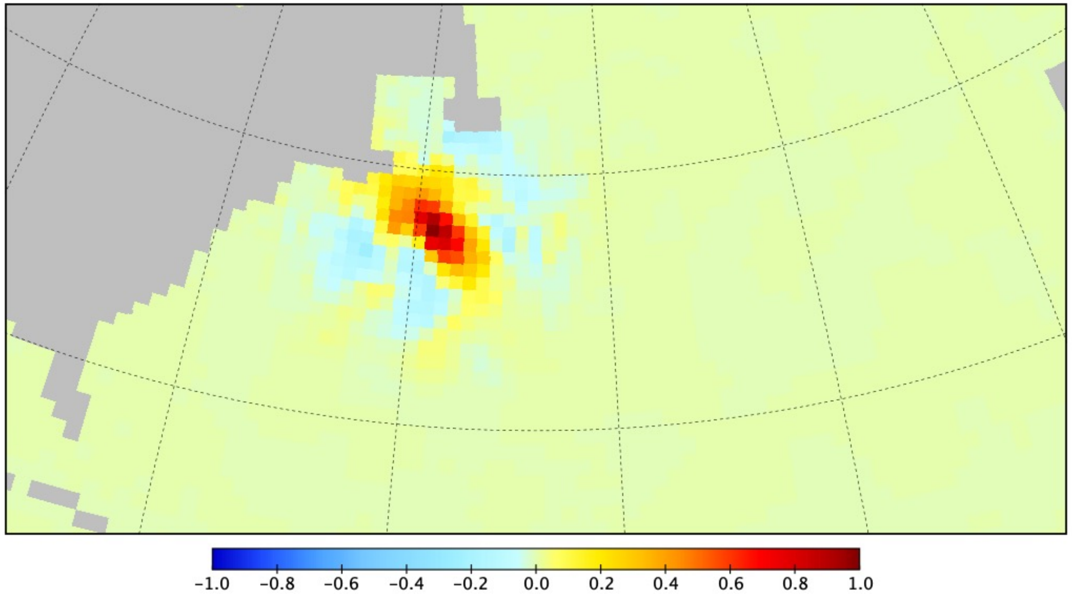
Temperature level 1 variance correction factor

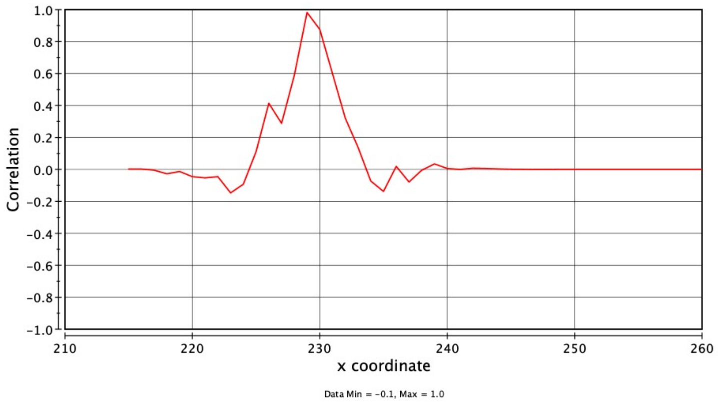


Scale-dependent localized correlations

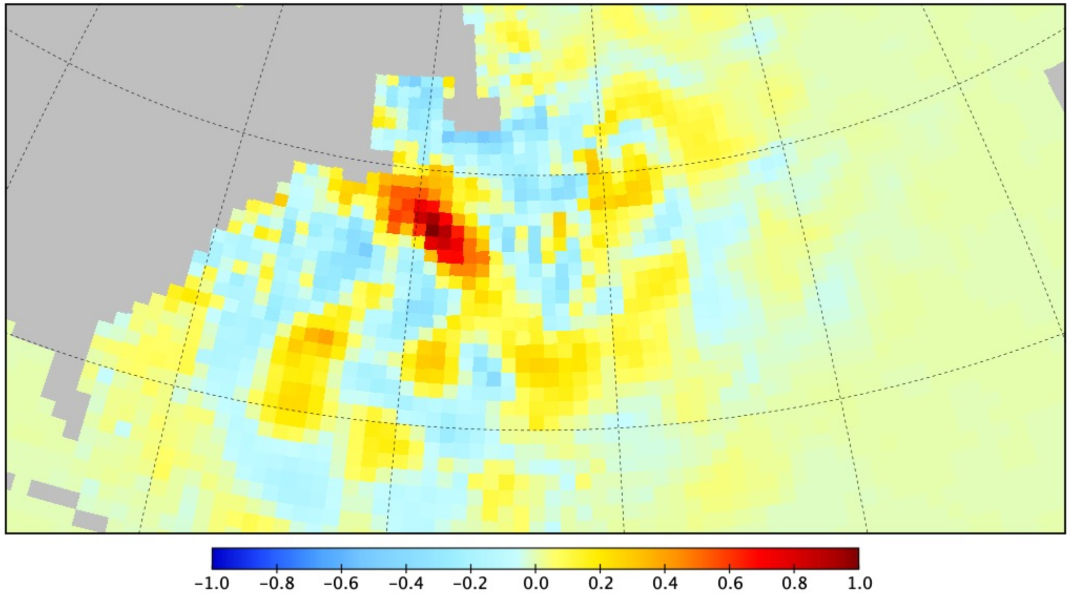
T-T correlations in level 1 in Gulf Stream region

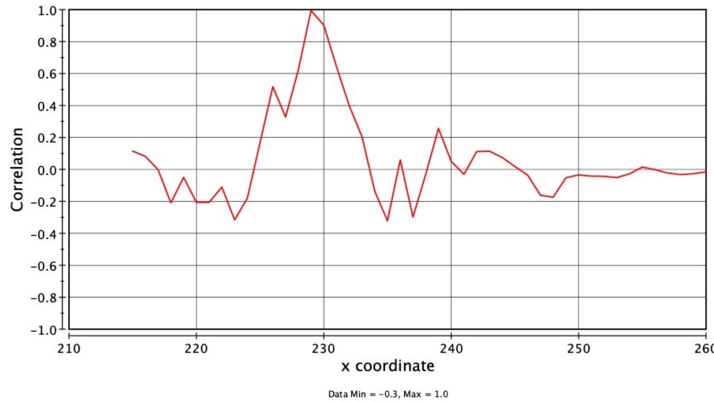
One scale





Two scales





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Scale-dependent modelled (SDM) covariances

- We can borrow ideas from SDL to define a corresponding scale-dependent **modelled** covariance matrix:

$$\mathbf{B}^{\mathrm{m}} = \underbrace{\boldsymbol{\Sigma}\,\boldsymbol{\Gamma}^{\mathrm{m}} \begin{pmatrix} \mathbf{I} & \cdots & \mathbf{I} \end{pmatrix} \begin{pmatrix} \boldsymbol{\Sigma}_1 & & \\ & \ddots & \\ & & \boldsymbol{\Sigma}_{N_\mathrm{s}} \end{pmatrix} \mathbf{C}^{\mathrm{ss}} \begin{pmatrix} \boldsymbol{\Sigma}_1 & & \\ & \ddots & \\ & & \boldsymbol{\Sigma}_{N_\mathrm{s}} \end{pmatrix} \begin{pmatrix} \mathbf{I} \\ \vdots \\ \mathbf{I} \end{pmatrix} \boldsymbol{\Gamma}^{\mathrm{m}}}_{\mathbf{C}^{\mathrm{m}}}\,\boldsymbol{\Sigma}$$

1. SDL-like formulation: $$\mathbf{C}^{\mathrm{ss}} = \begin{pmatrix} \mathbf{V}_1 \\ \vdots \\ \mathbf{V}_{N_\mathrm{s}} \end{pmatrix} \begin{pmatrix} \mathbf{V}_1^{\mathrm{T}} & \cdots & \mathbf{V}_{N_\mathrm{s}}^{\mathrm{T}} \end{pmatrix}$$

2. Met Office formulation: $$\mathbf{C}^{\mathrm{ss}} = \begin{pmatrix} \mathbf{V}_1 & & \\ & \ddots & \\ & & \mathbf{V}_{N_\mathrm{s}} \end{pmatrix} \begin{pmatrix} \mathbf{V}_1^{\mathrm{T}} & & \\ & \ddots & \\ & & \mathbf{V}_{N_\mathrm{s}}^{\mathrm{T}} \end{pmatrix}$$

Some remarks

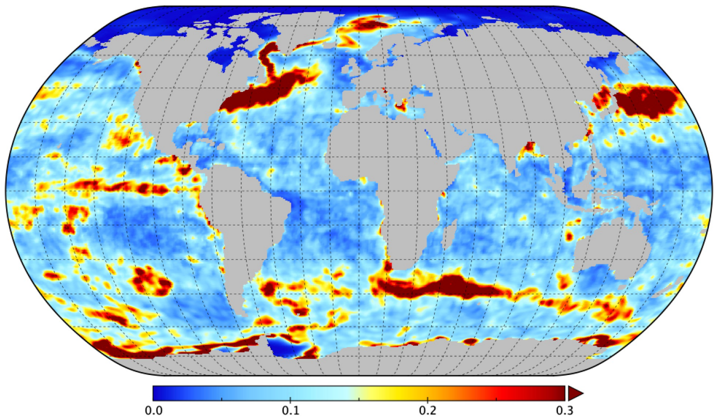
- As in SDL, an extra normalization matrix $\mathbf{\Gamma}^{\mathrm{m}}$ is required to ensure that the standard deviations actually used are those in $\mathbf{\Sigma}$.
- We can use the ensemble-gradient method (already available in NEMOVAR) to compute the correlation tensor for the **scale-separated** perturbations.
- The **scale-separated** ensemble variances and correlation tensor elements can be filtered using a diffusion operator with an optimally determined length scale (Ménétrier et al. 2015).
- The scale-dependent (filtered) variances provide objective estimates of the relative weighting factors for the different scale-dependent correlation matrices.

Scale-dependent standard deviations

Example with ensembles separated into 3 spectral bands:

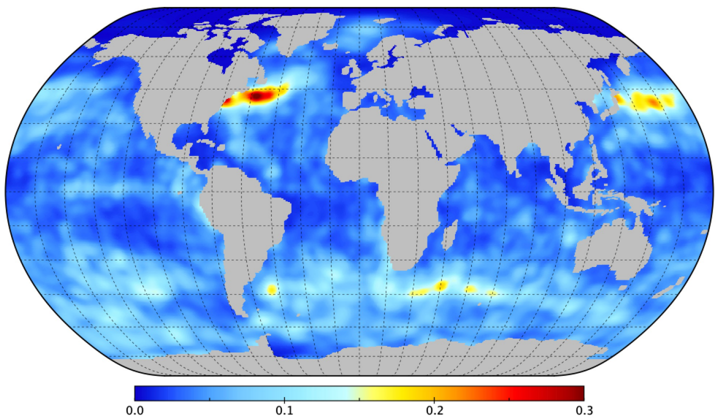
< 190 km; 190 km – 380 km; > 380 km

Estimated scale-dependent temperature standard deviations



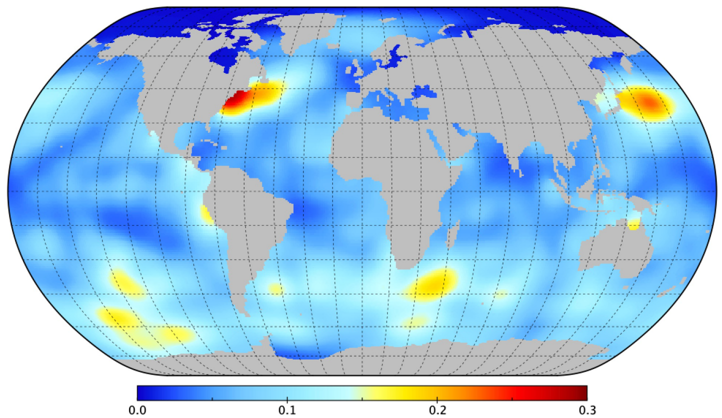
0.3 K

Max = 2.4 K



0.3 K

Max = 0.3 K



0.3 K

Max = 0.2 K

Scale-dependent length-scales

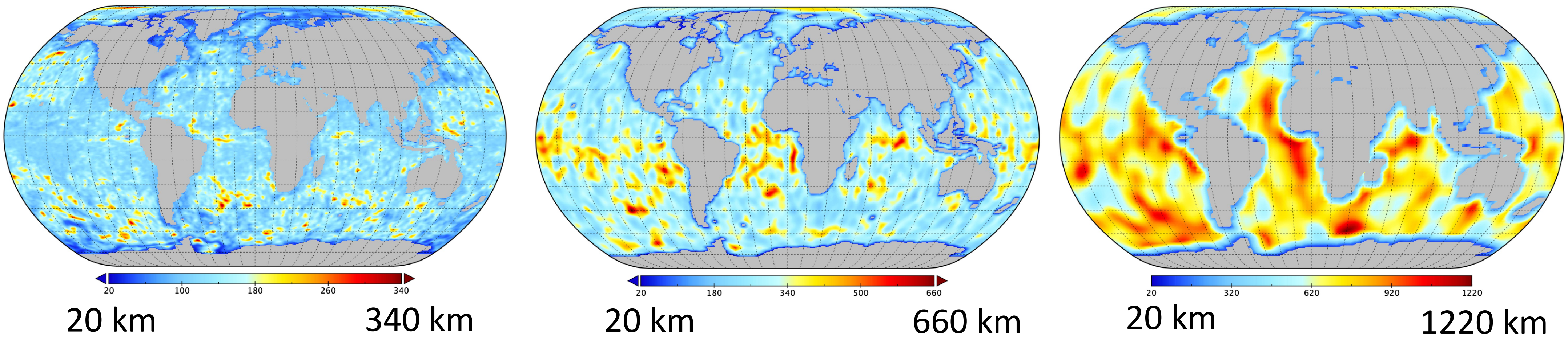
Example with ensembles separated into 3 spectral bands:

< 190 km; 190 km – 380 km; > 380 km

Correlation length scales are estimated from the inverse of

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

Estimated scale-dependent zonal length scales



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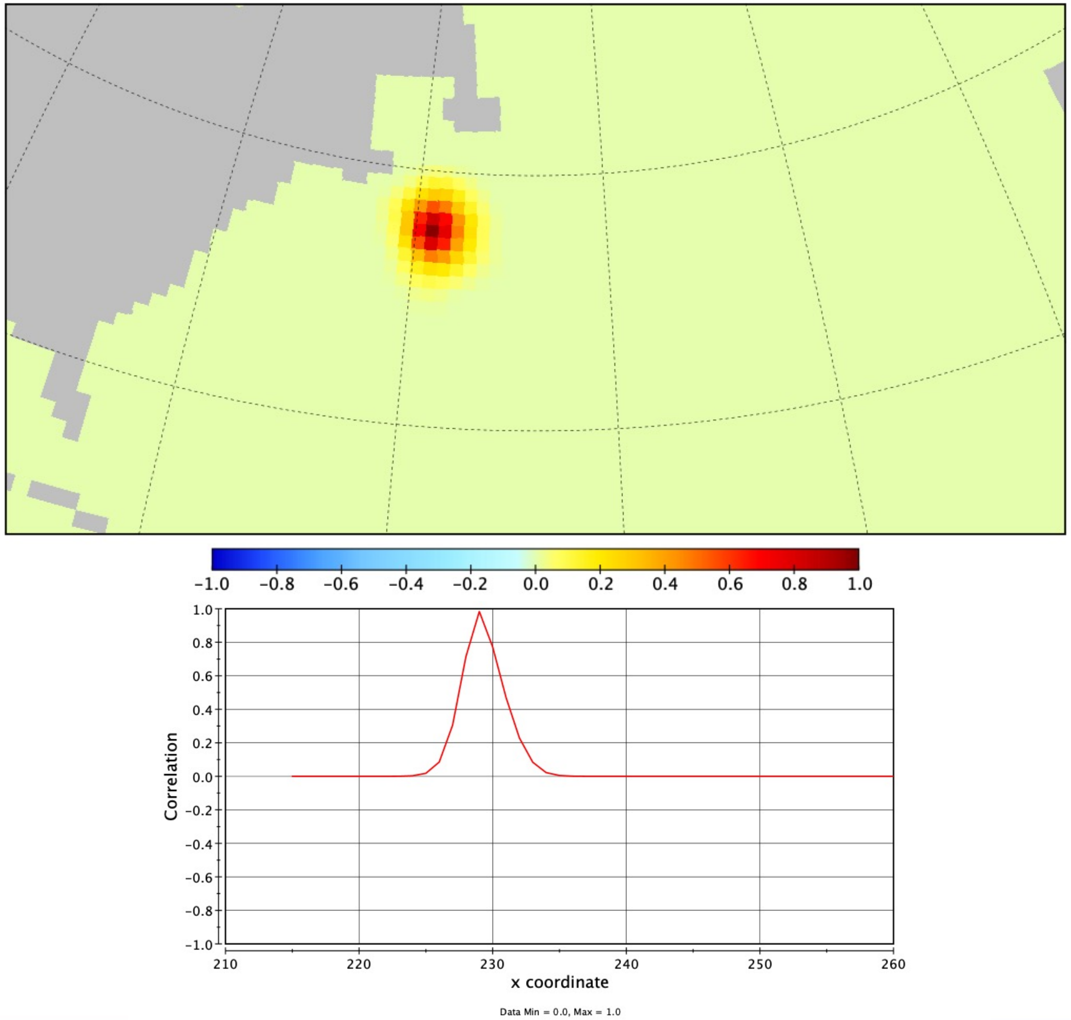
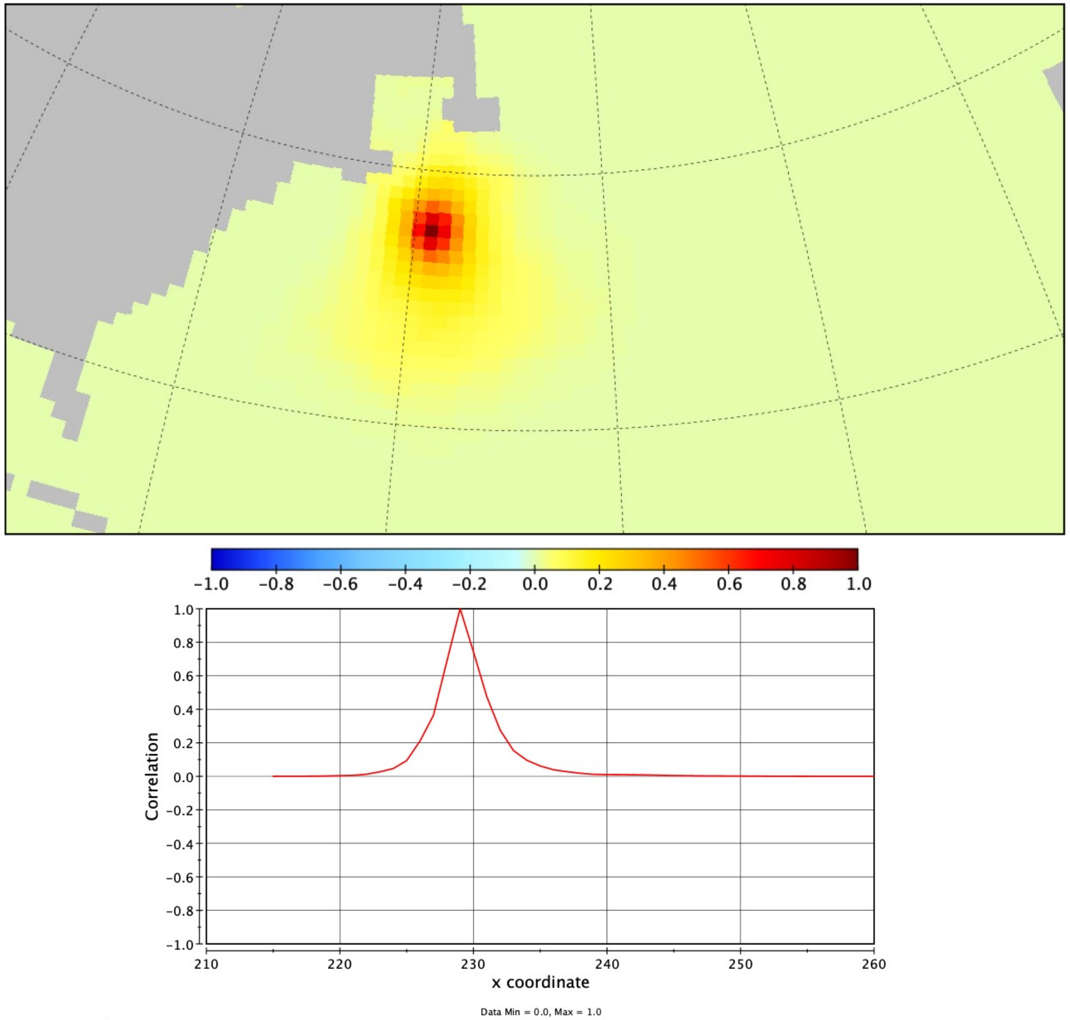
One scale



Three scales



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Conclusions and ongoing work

- Two methods (SDL and SDM) have been proposed for estimating and representing scale-dependent background error covariances.
- Both methods require an ensemble and can represent flow-dependent covariances.
- The SDL and SDM **B** matrices can be linearly combined to form a hybrid **B** (Lea et al. 2022):

$$\mathbf{B} = \beta_{\mathrm{m}}^2 \mathbf{B}_{\mathrm{c}}^{\mathrm{m}} + \beta_{\mathrm{e}}^2 \mathbf{B}^{\mathrm{e}}$$

  - SDL for the flow-dependent component $\mathbf{B}^{\mathrm{e}}$
  - SDM with climatological parameter estimates for $\mathbf{B}_{\mathrm{c}}^{\mathrm{m}}$
  - Hybridization weights β_{m}^2 and β_{e}^2 can be estimated using BUMP.
- All methods (SDL, SDM, hybrid) have been implemented in NEMOVAR
  - Experimentation is required to determine cost benefits.
  - This work is planned in collaboration with ECMWF (upcoming C3S contract).

Thanks for listening