BUMP, a generic tool for covariance modelling

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Basic facts



- Background error covariance (aka B matrix) is a key aspect of variational DA systems.
- In the practical implementation, the **B** matrix itself is not required, only its effect on a state vector.
- B must be symmetric and positive, so we generally build its square-root U: B = UU^T.
- Usual covariance models are:
 - static **B**: a sequence of parametrized operators
 - ensemble-based **B**: a localized sample covariance matrix
 - hybrid B: a linear combination of previous models
- All covariance models require a smoother to spread the innovation information. In most implementations, smoothers are grid-specific (e.g. spectral transform, recursive filters).



BUMP library



- BUMP: "Background error on Unstructured Mesh Package"
- It is designed to work on any grid (gaussian, cubed-sphere, unstructured, limited-area, ocean).
- It can diagnose parameters for all the usual covariance models.
- It implements a generic smoother, NICAS ("Normalized Interpolated Convolution from an Adaptive Subgrid").
- The code is written in Fortran 90, slightly above 20.000 lines.
- It is part of the SABER repository ("System-Agnostic Background Error Representation"), which will include other covariance modelling libraries in the future.
- It is fully interfaced with OOPS, for both diagnostic and application parts.

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Static **B** basics



- The static **B** is a robust and well-conditioned model, based on a sequence of parametrized operators.
- The parameters can be defined using ensemble data over a long period, giving a climatological estimate.
- They can also be estimated over a shorter sliding window, and updated at every cycle.
- The most common static **B** model is:

$$\mathsf{B}^{s} = \mathsf{K}_{\rho} \Sigma \mathsf{C} \Sigma^{\mathrm{T}} \mathsf{K}_{\rho}^{\mathrm{T}} \tag{1}$$

where

- C is a correlation matrix
- Σ is a diagonal matrix of standard deviations
- K_p is a multivariate balance operator

Static ${\bf B}$ with ${\sf BUMP}$



BUMP can be used for all these operators:

- The correlation length-scales of **C** are estimated globally or locally, and used to set up the NICAS smoother, which is exactly normalized $(C_{ii} = 1)$.
- The standard-deviations in Σ are estimated locally and potentially filtered, to remove the sampling noise (objective filtering of Ménétrier *et al.*, 2015a,b).
- A vertical balance operator computing regressions between variables can be diagnosed and applied with BUMP (still under development), as part of a more complex K_p.

In the OOPS framework, the static B components can come from BUMP or from your own model, and be combined as you wish.

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Static B

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Sample covariance

An ensemble of N forecasts $\{\mathbf{x}_{p}^{b}\}$ is used to estimate the sample covariance matrix $\widetilde{\mathbf{B}}$:

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$$\widetilde{\mathbf{B}} = \frac{1}{N-1} \sum_{p=1}^{N} \delta \mathbf{x}_{p}^{b} \delta \mathbf{x}_{p}^{b\mathrm{T}}$$
(2)

where $\delta \mathbf{x}_{p}^{b}$ is the pth ensemble perturbation:

$$\delta \mathbf{x}_{p}^{b} = \mathbf{x}_{p}^{b} - \langle \mathbf{x}^{b} \rangle$$
 and $\langle \mathbf{x}^{b} \rangle = \frac{1}{N} \sum_{p=1}^{N} \mathbf{x}_{p}^{b}$ (3)

Asymptotic sample covariance: $\mathbf{B} = \lim_{N \to \infty} \widetilde{\mathbf{B}}$

Since the ensemble size $N < \infty$, \widetilde{B} is affected by sampling noise: $\widetilde{B}^e = \widetilde{B} - B$ (4)



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Sample covariance





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Sample covariance

Sampling noise strongly depends on the ensemble size:



We don't have oil, but we have ideas!

Localized covariance



Sampling noise on \widetilde{B} can be damped via a Schur product (element-by-element) with a localization matrix L:

$$\widehat{\mathbf{B}} = \mathbf{L} \circ \widetilde{\mathbf{B}} \quad \Leftrightarrow \quad \widehat{B}_{ij} = L_{ij} \widetilde{B}_{ij} \tag{5}$$

In practice, L damps the long-distance correlations that are small and more affected by sampling noise (hence the "localization").



Localization: what is the optimal length-scale?

The localization length-scale is critical to remove the sampling noise while keeping the relevant covariance signal:

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Localization: what is the optimal length-scale?

The localization length-scale is critical to remove the sampling noise while keeping the relevant covariance signal:

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Start reducing the sampling noise ...

Localization: what is the optimal length-scale?



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Less and less sampling noise ...

Localization: what is the optimal length-scale?

The localization length-scale is critical to remove the sampling noise while keeping the relevant covariance signal:

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Good ! Almost no sampling noise anymore...

Localization: what is the optimal length-scale?



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Well, we are loosing some signal now...

Localization: what is the optimal length-scale?

The localization length-scale is critical to remove the sampling noise while keeping the relevant covariance signal:

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Hey, stop loosing signal !

Localization: what is the optimal length-scale?



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Localized and hybridized covariance

Deficiencies of the localized covariance matrix $\widehat{\mathbf{B}}$ can be corrected via a hybridization with a static covariance matrix:

 $\widehat{\mathbf{B}}^{h} = \beta^{e2} \ \widehat{\mathbf{B}} + \beta^{s2} \mathbf{B}^{s} \quad \Leftrightarrow \quad \widehat{B}^{h}_{ij} = \beta^{e2} \widehat{B}_{ij} + \beta^{s2} B^{s}_{ij} \tag{6}$

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For a homogeneous \mathbf{B}^{s} :



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Hybridization: what are the optimal coefficients

$$\widehat{\mathbf{B}}^{h} = \beta^{e2} \ \widehat{\mathbf{B}} + \beta^{s2} \mathbf{B}^{s} \quad \Leftrightarrow \quad \widehat{B}^{h}_{ij} = \beta^{e2} \widehat{B}_{ij} + \beta^{s2} B^{s}_{ij}$$



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How to optimize localization and hybridization?



Existing methods are empirical and costly (e.g. OSSE, brute-force optimization). We need a new method that:

- uses only ensemble members,
- is affordable for high-dimensional systems,
- can be generic enough to be run with all kinds of grids.

Principle :



Localization + hybridization = linear filtering of \widetilde{B}

How to optimize localization and hybridization?

Asymptotic sample covariance: $\mathbf{B} = \lim_{N \to \infty} \widetilde{\mathbf{B}}$ Residual noise (after localization/hybridization): $\widehat{\mathbf{B}}^h - \mathbf{B}$ Objectives:

• Express $\beta^{e^2} \mathbf{L}$ and β^{s^2} minimizing the error $\mathbb{E} \left[\|\widehat{\mathbf{B}}^h - \mathbf{B}\|^2 \right]$.

 \rightarrow Linear filtering theory.

Some statistics involve the asymptotic sample covariance.

• Express statistics on asymptotic quantities (unknown) with expected sample quantities (knowable).

ightarrow Centered moments sampling theory (non-Gaussian case).



Sampling noise properties



Homogeneous variance / length-scale



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Sampling noise properties





Sampling noise amplitude related to the asymptotic variance
Sampling noise properties



Homogeneous variance / heterogeneous length-scale



Sampling noise length-scale related to the asymptotic length-scale

Ensemble/hybrid B Introduction Static **B** The NICAS smoother BUMP usage How to optimize localization and hybridization? TIRIT Optimal localization alone (without hybridization): $L'_{ij} = \frac{\mathbb{E}\left[B_{ij}^2\right]}{\mathbb{E}\left[\widetilde{B}_{i}^2\right]}$ $=\frac{(N-1)^2}{N(N-3)}+\frac{N-1}{N(N-2)(N-3)}\frac{\mathbb{E}\left[\widetilde{B}_{ii}\widetilde{B}_{jj}\right]}{\mathbb{E}\left[\widetilde{B}_{ij}^2\right]}-\frac{N}{(N-2)(N-3)}\frac{\mathbb{E}\left[\widetilde{\Xi}_{ijij}\right]}{\mathbb{E}\left[\widetilde{B}_{ij}^2\right]}$ where Ξ is the sample fourth-order centered moment. $\boldsymbol{\beta^{s2}} = \frac{\sum_{ij} \left(1 - \boldsymbol{L}'_{ij}\right) \mathbb{E}\left[\widetilde{\boldsymbol{B}}_{ij}\right] \boldsymbol{B}_{ij}^{s}}{\sum_{ij} \frac{\operatorname{Var}\left[\widetilde{\boldsymbol{B}}_{ij}\right]}{\mathbb{E}\left[\widetilde{\boldsymbol{B}}_{ij}^{2}\right]} \boldsymbol{B}_{ij}^{s2}} \quad \text{and} \quad \boldsymbol{\beta^{e2}} \boldsymbol{L}_{ij} = \boldsymbol{L}'_{ij} - \frac{\mathbb{E}\left[\widetilde{\boldsymbol{B}}_{ij}\right]}{\mathbb{E}\left[\widetilde{\boldsymbol{B}}_{ij}^{2}\right]} \boldsymbol{\beta^{s2}} \boldsymbol{B}_{ij}^{s}$



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Practical application







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Correlation (black) et localization (colors) for various ensemble sizes

Localization length-scale increases as the ensemble size increases (less sampling noise to remove)



Ensemble size sensitivity



Ensemble and static coefficients as a function of the ensemble size

Less weight on the static covariance as the ensemble size increases (less deficiencies to correct).

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Summary



- The sample covariance is affected by sampling noise.
- This sampling noise decreases if the ensemble size increases.
- Using a huge ensemble is too costly for operational applications.
- Localization and hybridization can be used to filter out the sampling noise.
- The asymptotic sample covariance is the filtering target.
- We combine the linear filtering theory and the centered moments sampling theory.
- This leads to practicable formulas for optimal localization and hybridization weights.
- We compute robust estimates using ergodicity assumptions.
- These statistics can be computed globally, or locally.
- Thus, we get global, or local estimates of the optimal localization and hybridization weights.

And in BUMP?



- This method, HDIAG, is fully implemented in BUMP.
- Only the ensemble is needed for the localization.
- For the hybridization diagnostic, a randomization of the static covariance is required.
- Diagnostics can be computed globally, locally, using masks, taking boundaries into account, etc.

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Correlation diagnosed and fitted by BUMP, as a function of horizontal separation (km) and vertical separation (hPa)

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Localization diagnosed and fitted by BUMP, as a function of horizontal separation (km) and vertical separation (hPa)

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Explicit convolution



Main goal: designing a generic method to apply a normalized convolution operator on any grid type.

Standard methods:

- Spectral/wavelet transforms \rightarrow regular grid required
- Recursive filters
- Explicit/implicit diffusion

- \rightarrow regular grid required + normalization issue
- \rightarrow potentially high cost + normalization issue

Advantages of an explicit convolution C :

- Work on any grid type
- Exact normalization $(C_{ii} = 1)$

Drawback: the computational cost scales as $O(n^2)$, where n is the size of the model grid...

Explicit convolution



 $\mathbf{C} \approx \mathbf{S} \mathbf{C}^{s} \mathbf{S}^{\mathrm{T}}$

(7)

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where

- S is an interpolation from the subgrid to the model grid
- \mathbf{C}^{s} is a convolution matrix on the subgrid

If $n^s \ll n$, then the total cost scales as O(n) (interpolation cost).

Issues with this approach:

- If the subgrid density is too coarse compared to the convolution length-scale, the convolution is distorded.
- Normalization breaks down because of the interpolation: even if C^s is normalized, SC^sS^T is not.

Convolution on a subgrid



Convolution function on model grid



Model grid (blue) Large convolution length-scale

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Convolution on a subgrid

Subsampling: 1 point over 3



Model grid (blue) and subgrid (red) Large convolution length-scale

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Convolution on a subgrid

Subsampling: 1 point over 6



Model grid (blue) and subgrid (red) Large convolution length-scale 

Convolution on a subgrid

Subsampling: 1 point over 12



Model grid (blue) and subgrid (red) Large convolution length-scale

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Convolution on a subgrid





Model grid (blue) Small convolution length-scale

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Convolution on a subgrid

Subsampling: 1 point over 3



Model grid (blue) and subgrid (red) Small convolution length-scale



Convolution on a subgrid

Subsampling: 1 point over 6



Model grid (blue) and subgrid (red) Small convolution length-scale Introduction Static B Ensemble/hybrid B OCCONCOLOR OF BUMP usage



Convolution on a subgrid

Subsampling: 1 point over 12



Model grid (blue) and subgrid (red) Small convolution length-scale



Explicit convolution

The **NICAS** method (Normalized Interpolated Convolution from an Adaptive Subgrid) is given by:

$$\widetilde{\mathbf{C}} = \mathbf{NSC}^{s}\mathbf{S}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}$$
(8)

where

- N is a diagonal normalization matrix.
- The subgrid is locally adapted to the convolution length-scale.

Several questions:

- What subgrid?
- What convolution function?
- What parallelization method?



Length-scale and subgrid density



Homogeneous convolution length-scale \rightarrow homogenous subgrid:



A fast trial-and-error algorithm using a K-D tree ensures that the horizontal subsampling is well distributed.



Length-scale and subgrid density



Heterogenous convolution length-scale \rightarrow heterogenous subgrid:



A fast trial-and-error algorithm using a K-D tree ensures that the horizontal subsampling is well distributed.

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Convolution function

Gaspari and Cohn (1999) function, global support radius r

ightarrow homogeneous normalized distance $d'_{ij} = rac{d_{ij}}{r}$



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Convolution function

Gaspari and Cohn (1999) function, global support radius r

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Convolution function

Gaspari and Cohn (1999) function, local support radius r

ightarrow heterogeneous normalized distance $d'_{ij} = rac{d_{ij}}{\sqrt{(r_i^2 + r_j^2)/2}}$



Homogeneous or heterogenous support radius







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Homogeneous or heterogenous support radius






Sharp convolution support radius gradients

Ensemble/hybrid B

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Gaspari and Cohn (1999) function, local support radius r

The NICAS smoother

ightarrow heterogeneous normalized distance $d'_{ij} = rac{d_{ij}}{\sqrt{(r_i^2 + r_j^2)/2}}$





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Sharp convolution support radius gradients

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Gaspari and Cohn (1999) function, local support radius r

ightarrow heterogeneous normalized distance $\widetilde{d}'_{ij} = \sum_{k=i}^{j-1} d'_{k,k+1}$ (network)

The NICAS smoother





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Convolution functions with complex boundaries





^{0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0}

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Implicit diffusion (left) and NICAS (right) on the ORCA grid.

^{0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0}



Subgrid resolution



The subgrid resolution ρ is defined as the number of points required to describe half the Gaspari and Cohn (1999) function.



 $\rho = 8$ (2827 points)



Subgrid resolution



The subgrid resolution ρ is defined as the number of points required to describe half the Gaspari and Cohn (1999) function.



 $\rho = 6$ (1590 points)



Subgrid resolution



The subgrid resolution ρ is defined as the number of points required to describe half the Gaspari and Cohn (1999) function.



 $\rho = 4$ (706 points)

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Subgrid resolution

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 $\rho = 8 (2827 \text{ points})$

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Subgrid resolution

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Subgrid resolution

The subgrid resolution ρ is defined as the number of points required to describe half the Gaspari and Cohn (1999) function.



 $\rho = 4$ (706 points)

Square-root formulation

Static **B**

Introduction

• Basic NICAS method:

$$\widetilde{\mathbf{C}} = \mathbf{NSC}^{s} \mathbf{S}^{\mathrm{T}} \mathbf{N}^{\mathrm{T}}$$
(9)

• If C^s is built as $U^s U^{s\mathrm{T}}$, then the square-root of \widetilde{C} is given by: $\widetilde{U} = NSU^s \tag{10}$

which can be useful for square-root preconditioning in ${\rm EnVar}$ minimizations.

• Using the formulation:

$$\widetilde{\mathbf{C}} = \mathbf{N}\mathbf{S}\mathbf{U}^{s}\mathbf{U}^{s\mathrm{T}}\mathbf{S}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}$$
(11)

also ensures that $\widetilde{\textbf{C}}$ is positive-semidefinite.

 In practice, the Gaspari and Cohn (1999) function is actually used in the square-root U^s.



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MPI communications

Running **NICAS** with several MPI tasks:

- Communications are always performed on the subgrid, never on the model grid.
- Only **local** communications between halos are required, no global communications.
- NICAS can be applied with 1, 2 or 3 communication steps:

$$\widetilde{\mathbf{C}} = \mathbf{N}\mathbf{S} \boxtimes \mathbf{U}^{s} \mathbf{U}^{s^{\mathrm{T}}} \mathbf{S}^{\mathrm{T}} \mathbf{N}^{\mathrm{T}}$$
(12)

$$\widetilde{\mathbf{C}} = \mathbf{N}\mathbf{S} \boxtimes \mathbf{U}^{s}\mathbf{U}^{sT} \boxtimes \mathbf{S}^{T}\mathbf{N}^{T}$$
(13)

$$\widetilde{\mathbf{C}} = \mathbf{N}\mathbf{S} \boxtimes \mathbf{U}^{s} \boxtimes \mathbf{U}^{sT} \boxtimes \mathbf{S}^{T}\mathbf{N}^{T}$$
(14)

More communication steps \Rightarrow smaller halos.

Hybrid parallization with OpenMP is used to improve efficiency.

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BUMP usage



- BUMP usage in OOPS
 - BUMP is fully interfaced with OOPS.
 - The BUMP parameters are set from the YAML file.
 - Default parameters and short descriptions can be found in bump/type_nam.F90
 - Documentation can be found on GitHub page: https://github.com/JCSDA/saber
 - Support using the GitHub page or my email: benjamin.menetrier@irit.fr
 - To get started, some examples of BUMP usage for a static B and for an ensemble/hybrid B.

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Static B with BUMP: example 1



NICAS smoother (for correlation) with a prescribed support radius

oump:	
datadir: bump	<pre># Bump—specific directory</pre>
default seed: 1	# Default random seed
forced_radii: 1	# Forced length—scale
method: cor	# Static correlation
mpicom: 2	<pre># NICAS communication steps</pre>
new_nicas: 1	# New NICAS smoother
ntry: 10	# Subsampling quality
prefix: your_experiment	# BUMP files base
resol: 8.0	# Subsampling resolution
rh: 1000.0e3	# Horizontal support radius
rv: 1000.0	# Vertical support radius
<pre>strategy: specific univariate</pre>	# Multivariate strategy

Important keys you might change:

- The horizontal support radius (in m): rh
- The vertical support radius (in your vertical unit): rv
- The subsampling resolution: resol

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Important keys you might change:

- The diagnostic horizontal bin size (in m): dc
- The diagnostic subsampling size: nc1
- The number of diagnostic bins: nc3

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Static B with BUMP: example 2

Correlation radius estimation with HDIAG



Important keys you might change:

- The diagnostic horizontal bin size (in m): dc
- The diagnostic subsampling size: nc1
- The number of diagnostic bins: nc3

Introduction Static B Ensemble/hybrid B The NICAS smoother BUMP usage 00000000 Static B with BUMP: example 3 **ÍRIT** Use HDIAG diagnostic in NICAS, 1 step bump: datadir:bump # Bump-specific directory dc: 100.0e3 # Diagnostic bins size default seed: 1 # Default random seed method: cor # Static correlation mpicom: 2 # NICAS communication steps # Diagnostic subsampling size nc1: 500 nc3: 20 # Number of diagnostic bins ne: 50 # Ensemble size new hdiag: 1 # New HDIAG diagnostic new nicas: 1 # New NICAS smoother n | 0r | 11# Number of diagnostic levels ntry: 10 # Subsampling quality prefix: your experiment # BUMP files base resol: 8 0 # Subsampling resolution strategy: specific univariate # Multivariate strategy

In the same run:

- Run HDIAG to estimate correlation radius
- Use it to set up the NICAS smoother

Introduction Static B Ensemble/hybrid B The NICAS smoother BUMP usage 00000000 Static B with BUMP: example 4 Use HDIAG diagnostic in NICAS, 2 steps bump: datadir: bump # Bump-specific directory default seed: 1 # Default random seed load cmat: 1 # Load radius data from HDIAG method: cor # Static correlation mpicom: 2 # NICAS communication steps new nicas: 1 # New NICAS smoother ntry: 10 # Subsampling quality prefix: your experiment # BUMP files base resol: 8 0 # Subsampling resolution strategy: specific univariate # Multivariate strategy

In the two runs:

- First run: estimate correlation radius with HDIAG (example 2)
- Second run: load HDIAG data (load_cmat: 1) to set up the NICAS smoother (this example)

Warning: the prefix key must be the same!

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Ensemble/hybrid B with BUMP



All the previous examples can be reused for the localization of an ensemble B, with only two keys to update:

- Method for localization: method: loc
- Multivariate strategy: strategy: common Other multivariate strategies are available in BUMP.

For the hybrid B the method is set at: method: hyb-rnd and a randomized pseudo-ensemble must be provided.

Full YAML files examples are provided with the QG model.

Other advanced BUMP features (anisotropic correlations, 4D localization, etc.) can also be activated from the YAML file.

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