BUMP, a generic tool for background error covariance modeling

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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).

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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, around 25.000 lines.
- It is part of the SABER repository ("System-Agnostic Background Error Representation"), which will include other covariance modeling libraries in the future.
- It is fully interfaced with OOPS, for both diagnostic and application parts.

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BUMP credo: subsampling



High-resolution grids are great for models dynamics, but very costly and not really useful for background error covariance modeling.

In general, the size of the background error structures that we can represent is significantly larger than the model grid cell size.

The credo of BUMP is:

You shall cleverly subsample the model grids. You shall perform costly operations on the subsampled mesh. You shall interpolate your final results on the model grid.

-The BUMP book



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Static ${\boldsymbol{\mathsf{B}}}$ 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:

$$\mathsf{B}^{s} = \mathsf{K}_{p} \boldsymbol{\Sigma} \mathsf{C} \boldsymbol{\Sigma}^{\mathrm{T}} \mathsf{K}_{p}^{\mathrm{T}}$$

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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Sample covariance



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

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

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 $\langle \mathbf{x}^{b} \rangle = \frac{1}{N} \sum_{p=1}^{N} \mathbf{x}_{p}^{b}$

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: $\widetilde{B}^e=\widetilde{B}-B$





















































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 $L\colon$

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

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



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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:



No impact

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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:



Start reducing the sampling noise ...

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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:



Less and less sampling noise...

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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:



Good ! Almost no sampling noise anymore...

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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:



Well, we are loosing some signal now...

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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:



Hey, stop loosing 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:



Localized and hybridized covariance



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

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

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



Hybridization: what are the optimal weights

Localization + hybridation:

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



Hybridization: what are the optimal weights

Localization + hybridation:

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Hybridization: what are the optimal weights

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Hybridization: what are the optimal weights

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Hybridization: what are the optimal weights

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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


Sampling noise properties



Heterogeneous variance / homogeneous length-scale



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

Introduction Static B Ensemble/hybrid B The NICAS smoother BUMP usage าเรา How to optimize localization and hybridization? 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. $\boldsymbol{\beta^{s2}} = \frac{\sum_{ij} \left(1 - \boldsymbol{L}'_{ij}\right) \mathbb{E}\left[\widetilde{\boldsymbol{B}}_{ij}\right] \boldsymbol{B}_{ij}^{s}}{\sum_{ij} \frac{\operatorname{Var}\left[\widetilde{\boldsymbol{B}}_{ij}\right]}{\mathbb{E}\left[\widetilde{\boldsymbol{B}}_{ij}^{2}\right]} \boldsymbol{B}_{ij}^{s2}} \quad \text{and} \quad \boldsymbol{\beta^{e2}} \boldsymbol{L}_{ij} = \boldsymbol{L}'_{ij} - \frac{\mathbb{E}\left[\widetilde{\boldsymbol{B}}_{ij}\right]}{\mathbb{E}\left[\widetilde{\boldsymbol{B}}_{ij}^{2}\right]} \boldsymbol{\beta^{s2}} \boldsymbol{B}_{ij}^{s}$



Full model grid (FV3 cubed-sphere grid - C180)

TRI

Homogenous and isotropic sampling



Homogenous subsampling for origin points

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Homogenous and isotropic sampling



Homogenous and isotropic sampling





Homogenous and isotropic sampling





Homogenous and isotropic sampling





Homogenous and isotropic sampling





Homogenous and isotropic sampling





Ergodicity assumption



For each couple of points, BUMP uses the ensemble to estimate:

- the sample variances \widetilde{B}_{ii} and \widetilde{B}_{ji}
- the sample covariance \widetilde{B}_{ii}
- the sample fourth-order centered moment $\widetilde{\Xi}_{ijij}$

Local averaging



Local averaging centers (red points)

Ergodicity assumption



For each couple of points, BUMP uses the ensemble to estimate:

- the sample variances \widetilde{B}_{ii} and \widetilde{B}_{ji}
- the sample covariance \widetilde{B}_{ii}
- the sample fourth-order centered moment $\widetilde{\Xi}_{iii}$

With the spatial and angular ergodicity assumption, these values are averaged locally for each distance class, to get estimations of the following expectations:

$$\mathbb{E} \Big[\widetilde{B}_{ij} \widetilde{B}_{jj} \Big]$$
 , $\mathbb{E} \Big[\widetilde{B}_{ij}^2 \Big]$ and $\mathbb{E} \Big[\widetilde{\Xi}_{ijij} \Big]$

These quantities are useful to compute the localization function and hybridization weights with the previous formulas.

Local averaging



For a given local averaging center:



Local averaging



For a given local averaging center:



Local averaging



For a given local averaging center:



Local averaging



For a given local averaging center:



Local averaging



For a given local averaging center:



Local averaging



For a given local averaging center:



Local averaging



For a given local averaging center:



Local averaging



For a given local averaging center:







Fit with a Gaspari-Cohn (1999) function



Localization length-scale (support radius actually, km)

Support radius interpolation





Localization support radius (km) at local averaging centers

Support radius interpolation





Localization support radius (km) interpolated on the model grid

HDIAG process



- 1. Define a homogeneous subsampling of the model grid (origin points).
- 2. For each origin point, find distant points for a series of distance classes.
- 3. For each local averaging center (a subset of origin points):
 - Average diagnostic values over a given radius.
 - Compute the localization and hybridization weights using the Ménétrier et al. (2015) formula.
 - Fit the raw localization function with a parametrized function (e.g. Gaspari-Cohn, 1999) to get the localization support radius.
- 4. Interpolate the localization support radius and hybridization weights over the model grid.



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

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



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Ensemble size sensitivity



Ensemble and static weights as a function of the ensemble size

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

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.

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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



To limit the computational cost, we approximate C on a subgrid (subset of n^s points of the model grid):

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

where

- $\bullet~{\bf S}$ 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

Convolution on a subgrid



Subsampling: 1 point over 3



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

Convolution on a subgrid



Convolution function on model grid



Model grid (blue) Small convolution length-scale

Convolution on a subgrid



Subsampling: 1 point over 3



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



Subsampling: 1 point over 6



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

Convolution on a subgrid



Subsampling: 1 point over 12



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

Explicit convolution



 $\widetilde{\boldsymbol{\mathsf{C}}} = \boldsymbol{\mathsf{NSC}}^{s}\boldsymbol{\mathsf{S}}^{\mathrm{T}}\boldsymbol{\mathsf{N}}^{\mathrm{T}}$

where

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

To illustrate how NICAS works:

- Example of adaptive subgrid.
- Steps of a Dirac test: apply $\widetilde{\mathsf{C}}$ to a vector $\boldsymbol{\delta}^k$ where

$$\delta_i^k = \begin{cases} 1 & \text{if } i = k \\ 0 & \text{if } i \neq k \end{cases}$$

Adaptive subgrid



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Localization support radius (km) interpolated on the model grid

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Adaptive subgrid



Adaptive support radius-based subgrid

NICAS steps



Initial vector:



NICAS steps



Adjoint normalization:

 $N^{T}\delta^{k}$

NICAS steps



Adjoint interpolation:

 $S^{T}N^{T}\delta^{k}$

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NICAS steps





NICAS steps





Interpolation: $SC^{s}S^{T}N^{T}\delta^{k}$

NICAS steps





Normalization: NSC^sS^TN^T δ^{k}

Result of the Dirac test





Localization support radius (km)

Result of the Dirac test





Application of NICAS on Dirac functions

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A scalar parameter controls the subgrid resolution. Simple trade-off between cost and accuracy.

Complex boundaries





Application of masked anisotropic NICAS on Dirac functions

Complex boundaries



0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0



0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

On the ORCA1 grid of NEMOVAR: implicit diffusion (top) and NICAS (bottom, 50x faster)



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Square-root formulation

• Basic NICAS method:

$$\widetilde{\mathsf{C}} = \mathsf{NSC}^s \mathsf{S}^{\mathrm{T}} \mathsf{N}^{\mathrm{T}}$$

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

which can be useful for square-root preconditioning in variational methods.

• Using the formulation:

 $\widetilde{\boldsymbol{\mathsf{C}}} = \boldsymbol{\mathsf{NSU}}^{s}\boldsymbol{\mathsf{U}}^{s\mathrm{T}}\boldsymbol{\mathsf{S}}^{\mathrm{T}}\boldsymbol{\mathsf{N}}^{\mathrm{T}}$

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

• A good approximation of the Gaspari and Cohn (1999) function square-root can be obtained by multiplying the function length-scale by an empirical scalar factor.



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:

$$\begin{split} \widetilde{\mathbf{C}} &= \mathbf{N} \mathbf{S} \ \boxtimes \ \mathbf{U}^{s} \mathbf{U}^{s\mathrm{T}} \mathbf{S}^{\mathrm{T}} \mathbf{N}^{\mathrm{T}} \\ \widetilde{\mathbf{C}} &= \mathbf{N} \mathbf{S} \ \boxtimes \ \mathbf{U}^{s} \mathbf{U}^{s\mathrm{T}} \ \boxtimes \ \mathbf{S}^{\mathrm{T}} \mathbf{N}^{\mathrm{T}} \\ \widetilde{\mathbf{C}} &= \mathbf{N} \mathbf{S} \ \boxtimes \ \mathbf{U}^{s} \ \boxtimes \ \mathbf{U}^{s\mathrm{T}} \ \boxtimes \ \mathbf{S}^{\mathrm{T}} \mathbf{N}^{\mathrm{T}} \end{split}$$

More communication steps \Rightarrow smaller halos.

• Hybrid parallelization with OpenMP is used to improve efficiency.

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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.

Static B with BUMP: example 1



NICAS smoother (for correlation) with a prescribed support radius

oump:			
	datadir: bump	#	Bump-specific directory
	forced radii: 1	#	Forced length-scale
	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	#	NICAS Subgrid resolution
	rh: 1000.0e3	#	Horizontal support radius
	rv: 1000.0	#	Vertical support radius
	strategy: specific univariate	#	Multivariate strategy

Important keys you might change:

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

The NICAS smoother BUMP usage Introduction Static B Ensemble/hybrid B 00000000 Static B with BUMP: example 2 Correlation radius estimation with HDIAG bump: datadir:bump # Bump-specific directory dc: 100.0e3 # Diagnostic bins size method cor # Static correlation nc1: 500 # Diagnostic subsampling size nc3: 20 # Number of diagnostic bins ne: 50 # Ensemble size new hdiag: 1 # New HDIAG diagnostic n | 0 r | 11# Number of diagnostic levels ntrv: 10 # Subsampling quality prefix: your experiment # BUMP files base strategy: specific univariate # Multivariate strategy

Important keys you might change:

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

The NICAS smoother BUMP usage Introduction Static B Ensemble/hybrid B 00000000 Static B with BUMP: example 3 Use HDIAG diagnostic in NICAS, 1 step bump: datadir:bump # Bump-specific directory dc: 100.0e3 # Diagnostic bins size # Static correlation method cor mpicom: 2 # NICAS communication steps nc1: 500 # Diagnostic subsampling size nc3 20 # Number of diagnostic bins ne: 50 # Ensemble size # New HDIAG diagnostic new hdiag: 1 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 # NICAS subgrid resolution strategy: specific univariate # Multivariate strategy

In the same run:

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



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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