3DVar, B modeling, hybrid-EnVar

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What problem a minimization algorithm solves?

Cost function in incremental form:

$$J(\delta\boldsymbol{x}) = \frac{1}{2}(\delta\boldsymbol{x} - \delta\boldsymbol{x}_{\mathrm{g}})^{\mathrm{T}}\mathbf{B}^{-1}(\delta\boldsymbol{x} - \delta\boldsymbol{x}_{\mathrm{g}}) + \frac{1}{2}(\mathbf{H}\delta\boldsymbol{x} - \boldsymbol{d})^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{H}\delta\boldsymbol{x} - \boldsymbol{d})$$

Gradient of cost function:

$$\nabla_{\delta\boldsymbol{x}} J(\delta\boldsymbol{x}) = \mathbf{B}^{-1}(\delta\boldsymbol{x} - \delta\boldsymbol{x}_{\mathrm{g}}) + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{H}\delta\boldsymbol{x} - \boldsymbol{d}) = 0$$

Analytical solution of analysis increment:

$$(\mathbf{B}^{-1} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H})\delta\boldsymbol{x}_{a} = \mathbf{B}^{-1}\delta\boldsymbol{x}_{\mathrm{g}} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\boldsymbol{d}$$

↓

$$\mathbf{A}\delta\boldsymbol{x}_{a} = \boldsymbol{b}$$

Final linear algebra system to solve iteratively through minimization algorithms available in OOPS

No need for computing B^{-1} in each iteration!

Instead, in each iteration of a minimization algorithm, we compute

$$\mathbf{B}\boldsymbol{r}_k \qquad \boldsymbol{r}_k = \boldsymbol{b} - \mathbf{A}\delta\boldsymbol{x}_k$$

Further reading for minimization algorithms in OOPS

https://jointcenterforsatellitedataassimilation-jedi-docs.readthedocs-hosted.com/en/latest/inside/jedi-components/oops/algorithmic_details/solvers.html

Analytical solution of analysis increment:

$$(\mathbf{B}^{-1} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H})\delta\boldsymbol{x}_a = \mathbf{B}^{-1}\delta\boldsymbol{x}_g + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\boldsymbol{d}$$

↓

$$\mathbf{A}\delta\boldsymbol{x}_a = \boldsymbol{b}$$

Final linear algebra system to solve iteratively through minimization algorithms available in OOPS

How B is modeled in MPAS-JEDI's 3DVar?

$$B = K_1 K_2 \Sigma C \Sigma^T K_2^T K_1^T$$

- B is decomposed as a sequence of operators (or linear variable changes) (**K_1 , K_2 Σ, and C)** and their adjoint operators **(K_1^T**, **K_2^T**)
- Reason for doing this is that, mathematically, B matrix is a very large-dimension matrix, we can not store the full matrix in memory. We have to apply these operators in local grid points.

$B = K_1 K_2 \Sigma C \Sigma^T K_2^T K_1^T$

- K_1 is a linear variable change from stream function ($\delta\psi$) and velocity potential ($\delta\chi$) to zonal (δu) and meridional (δv) winds. This is similar to GSI or WRFDA.

$$\begin{bmatrix} \delta u \\ \delta v \end{bmatrix} = \begin{bmatrix} -\partial_y & -\partial_x \\ \partial_x & -\partial_y \end{bmatrix} \begin{bmatrix} \delta\psi \\ \delta\chi \end{bmatrix}$$

- K_1^T is a corresponding adjoint operator.

$B = K_1 K_2 \Sigma C \Sigma^T K_2^T K_1^T$

- K_2 applies the linear variable change from 'unbalanced' variables to full variables. This is also similar to GSI or WRFDA

$$\begin{bmatrix} \delta\psi \\ \delta\chi \\ \delta T \\ \delta Q \\ \delta p_s \end{bmatrix} = \begin{bmatrix} \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \boldsymbol{L} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \boldsymbol{M} & \mathbf{0} & \boldsymbol{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{I} & \mathbf{0} \\ \boldsymbol{N} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{I} \end{bmatrix} \begin{bmatrix} \delta\psi \\ \delta\chi_u \\ \delta T_u \\ \delta Q \\ \delta p_{s,u} \end{bmatrix}$$

- $\delta\chi = \delta\chi_b + \delta\chi_u = \boldsymbol{L}\delta\psi + \delta\chi_u$
- $\delta T = \delta T_b + \delta T_u = \boldsymbol{M}\delta\psi + \delta T_u$
- $\delta p_s = \delta p_{s,b} + \delta p_{s,u} = \boldsymbol{N}\delta\psi + \delta\chi_u$

  - $\delta\psi$ is a predictor for the balanced part of $\delta\chi$, δT , and δp_s.
  - Full matrix for **M** & **N**, diagonal matrix for **L**

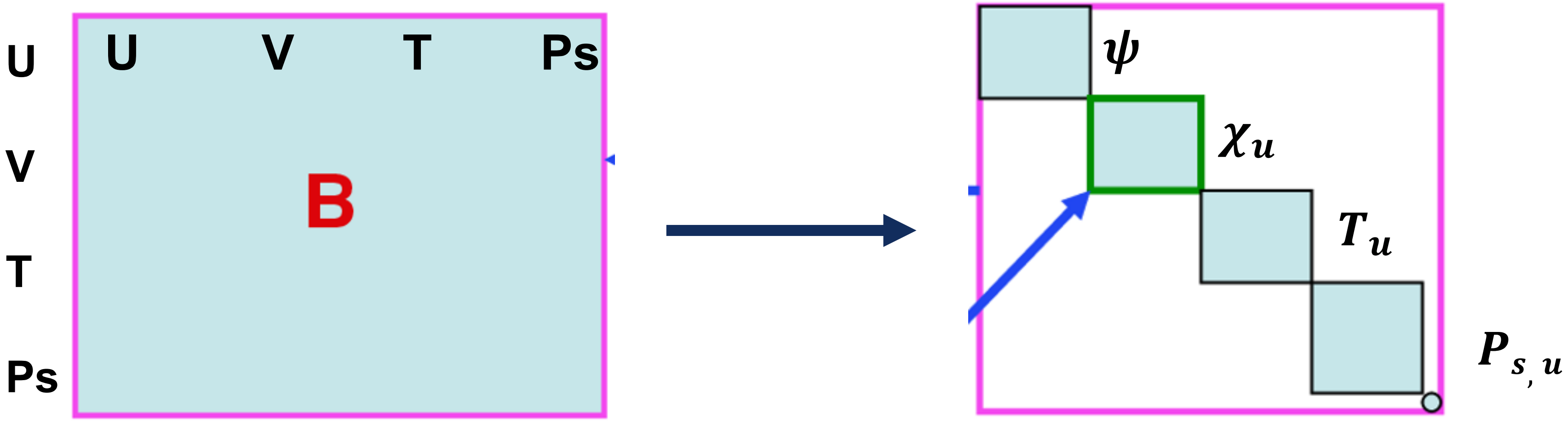
- K_2^T is a corresponding adjoint operator.

$B = K_1 K_2 \Sigma C \Sigma^T K_2^T K_1^T$

- $\Sigma C \Sigma^T$ represents the spatial covariance for $\{\delta\psi, \delta\chi_u, \delta T_u, \delta Q, \delta p_{s,u}\}$. These variables are assumed to have not cross-variable correlations.

- $\Sigma = \Sigma^T$ is a diagonal matrix with error standard deviation

- C is a block diagonal matrix. Each block represents the spatial correlation for $\{\delta\psi, \delta\chi_u, \delta T_u, \delta Q, \delta p_{s,u}\}$



$\mathbf{B = K_1 K_2 \Sigma C \Sigma^T K_2^T K_1^T}$

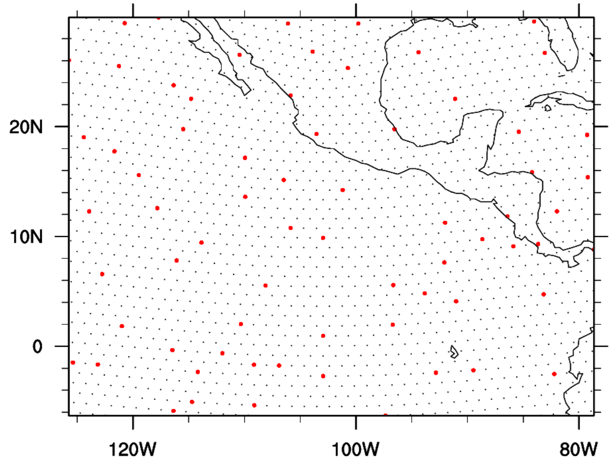
- Even with a single variable, the dimension for spatial correlation is still large.
- SABER/BUMP-NICAS applies the spatial correlation at a coarse grid ($\mathbf{C^s}$).

$$\mathbf{C} = \mathbf{N S C^s S^T N^T}$$

$\mathbf{C} \rightarrow \mathbb{R}^{m \times m}$, $\mathbf{C^s} \rightarrow \mathbb{R}^{m_s \times m_s}$ with $m_s \ll m$

$\mathbf{N}$: diagonal matrix for normalization
(to ensure the diagonal component of C equals "1")

$\mathbf{S} = \mathbf{S^v S^h}$: Interpolation from coarse grid to full grid



Matrix $\mathbf{C^S}$ are pre-computed and stored in files according to statistics for correlation length-scales of each variable

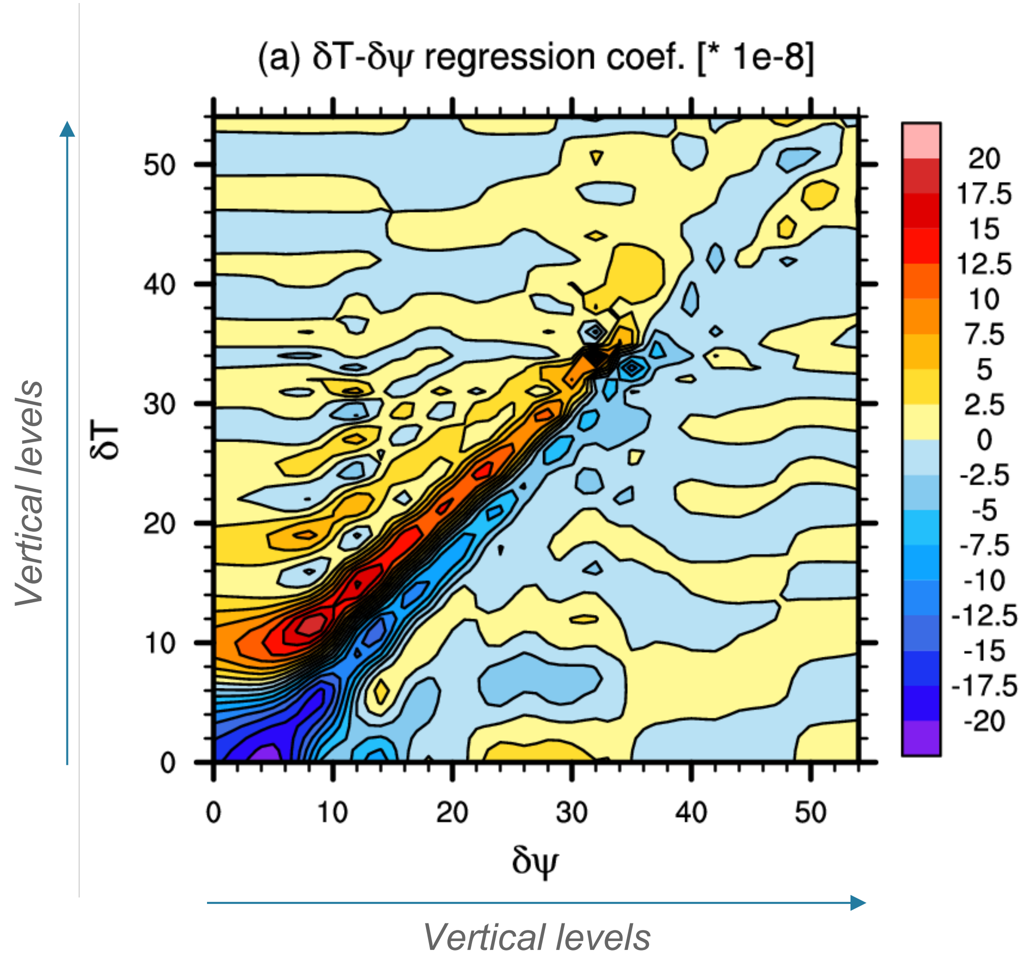
How B (K_1, K_2, Σ, C^S) is estimated?

- Through the so-called 'NMC' method, which uses forecast difference pairs to do statistics, e.g., B provided in the tutorial practice is generated with
  - 366 pairs (over 3 months) of GFS 48 hour and 24 hour forecast differences at MPAS 60 km mesh.
- Additional tunings are applied to the estimated B.
  - Reducing the error STD for all variables by a factor of 1/3
  - Reducing the diagnosed horizontal lengths for $\delta\psi$ and $\delta\chi_u$ by a factor of 1/2

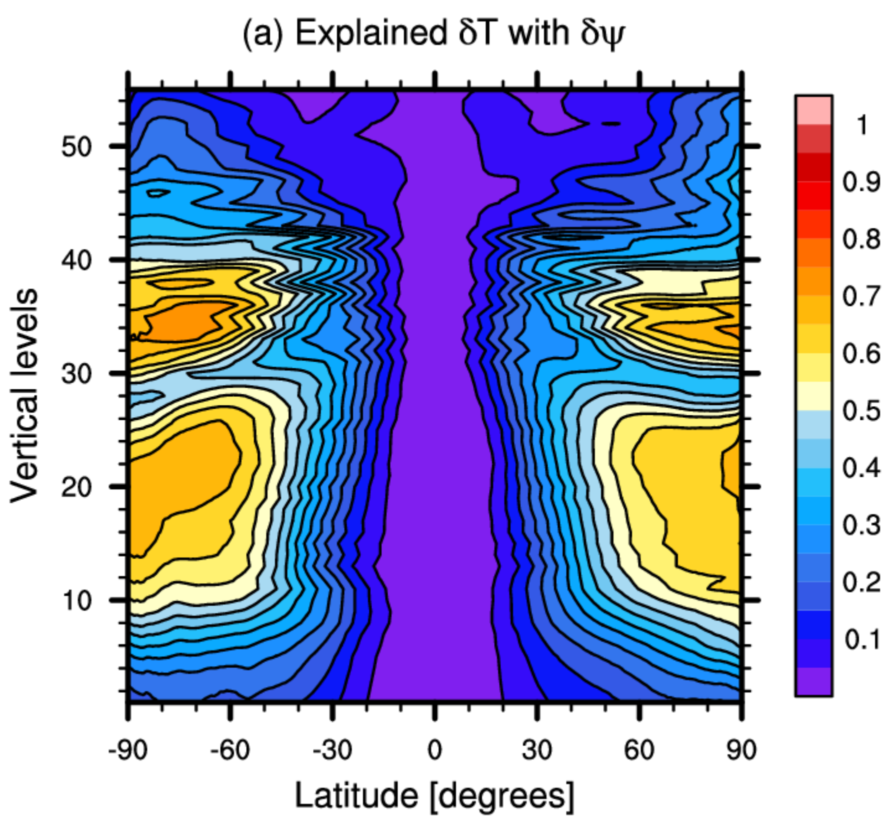
NOT ready to support B estimation tool

(Jung et al., 2023 under review)

Estimated *M* at 34.8° N latitude

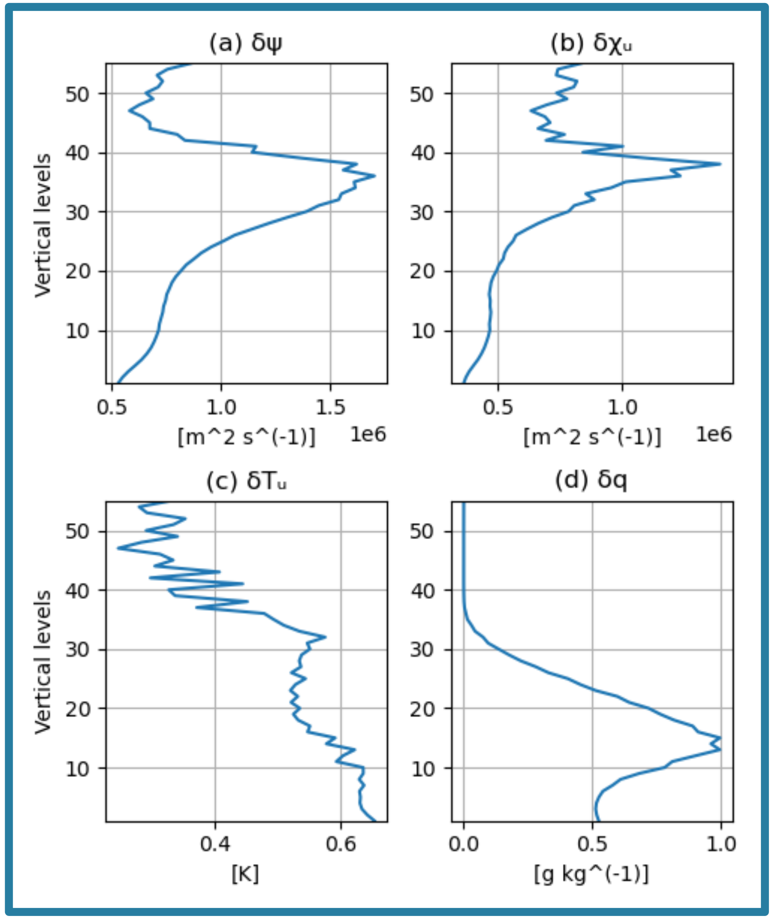


Ratio of balanced variance to total variance

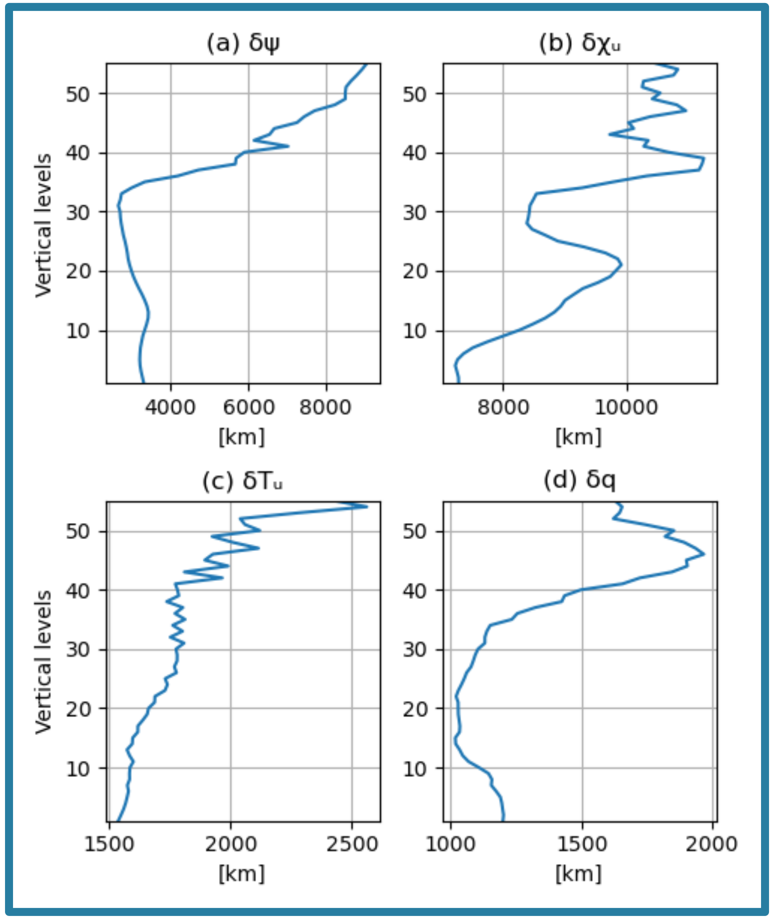


$$\frac{\langle \delta T_b, \delta T \rangle}{\langle \delta T, \delta T \rangle}$$

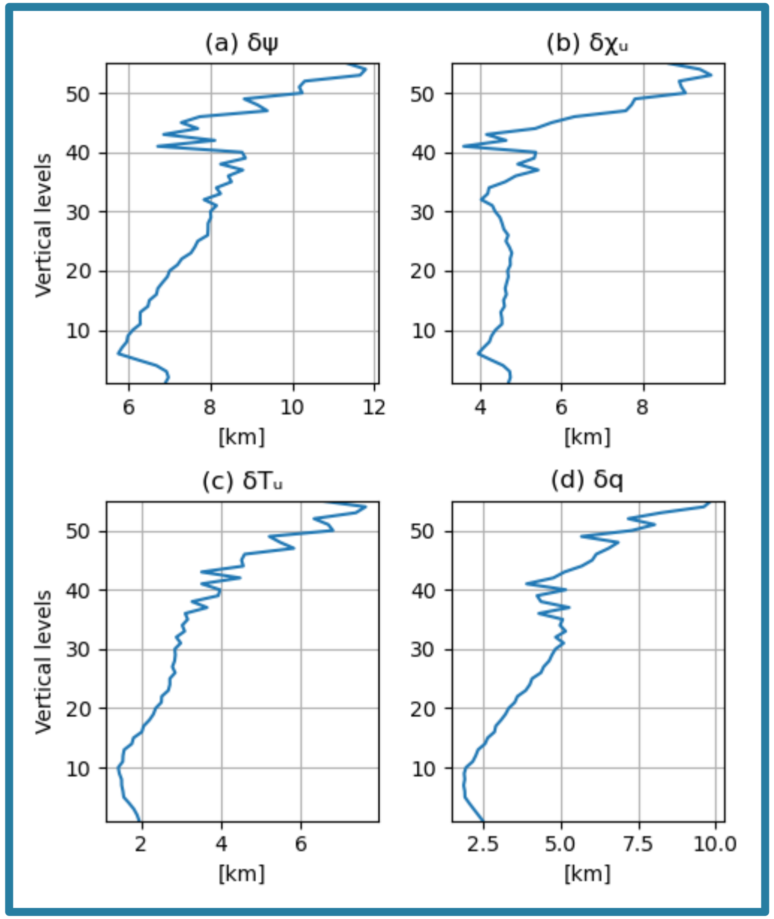
Estimated Σ



Estimated Horizontal correlation length-scale



Estimated vertical Correlation length-scales

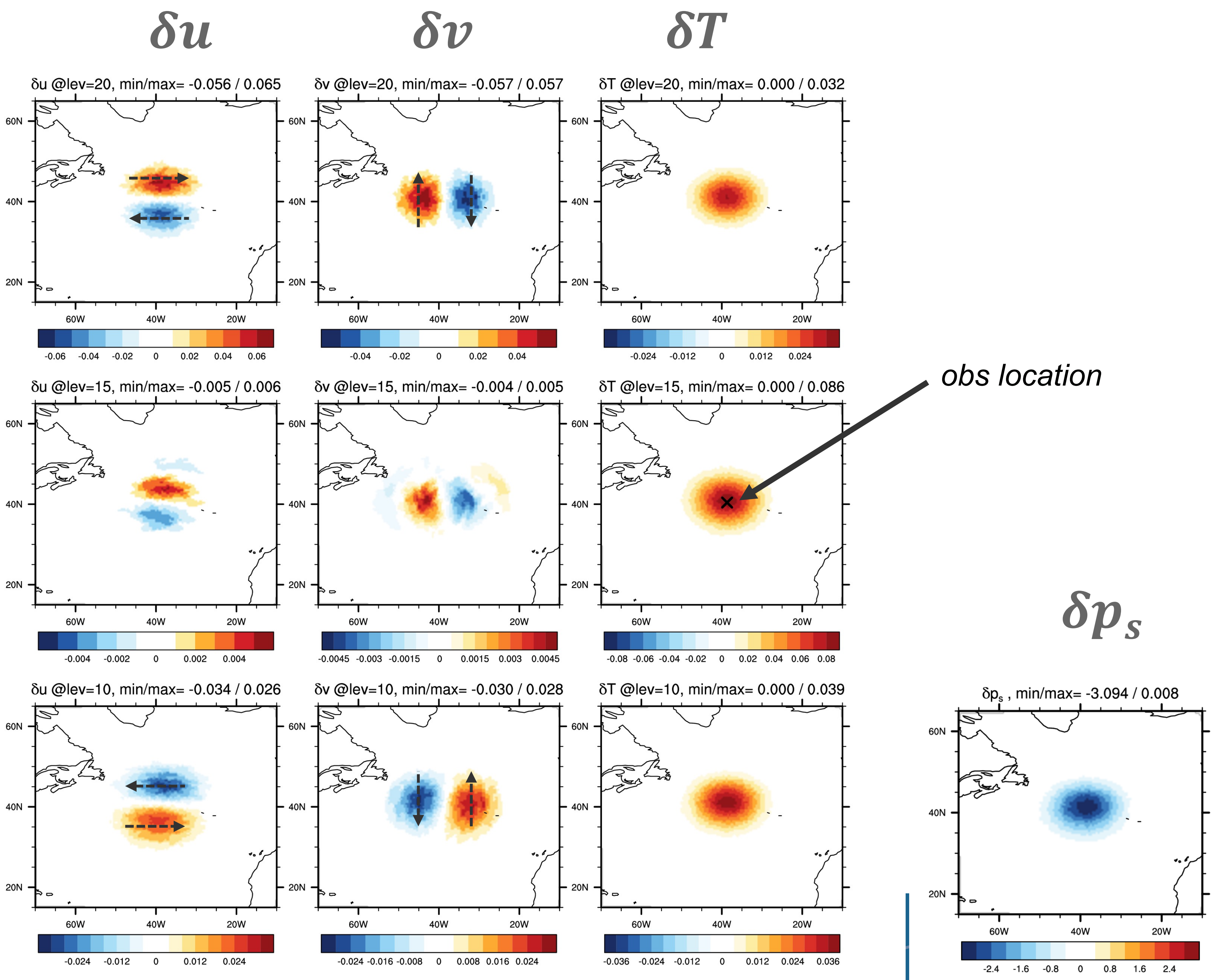


Single T obs test

Model level = 20

Model level = 15

Model level = 10



Previous slides present ‘multivariate’ B, MPAS-JEDI can easily do ‘univariate’ B, in that case:

$$B=\Sigma C \Sigma^T$$

- i.e., no cross-variable correlation between analysis variables (U, V, T, Q, Ps)

YAML configuration for 3DVar (1/6)

```
cost function:
  cost type: 3D-Var
  window begin: 2018-04-14T21:00:00Z
  window length: PT6H
  analysis variables: &incvars
[spechum,surface_pressure,temperature,uReconstructMeridional,uReconstructZonal]
  background:
    state variables:
[spechum,surface_pressure,temperature,uReconstructMeridional,uReconstructZonal,theta,rho,u,qv,pressure,landmask,xice,snowc,skintemp,ivgtyp,isltyp,snowh,vegfra,u10,v10,lai,smois,tslb,pressure_p]
    filename: ./bg.2018-04-15_00.00.00.nc
    date: &analysisDate 2018-04-15T00:00:00Z
```

YAML configuration for 3DVar (2/6)

$$B = K_1 K_2 \Sigma C \Sigma^T K_2^T K_1^T$$

```
cost function:
  ...
  background error:
    covariance model: SABER
    saber central block:
C       saber block name: BUMP_NICAS
        ... more config ...
    saber outer blocks:
Σ     - saber block name: StdDev
        ... more config ...
K2    - saber block name: BUMP_VerticalBalance
        ... more config ...
K1  linear variable change:
        linear variable change name: Control2Analysis
        ... more config ...
```

YAML configuration for 3DVar (3/6)

$$B=K_1K_2\Sigma C\Sigma^TK_2^TK_1^T$$

```
  background error:
    covariance model: SABER
    saber central block:
      saber block name: BUMP_NICAS
      active variables: &ctlvars
[stream_function,velocity_potential,temperature,spechum,surface_pressure]
      read:
        io:
          data directory: ./BUMP_files/bump_nicas
          files prefix: bumpcov_nicas
        drivers:
          multivariate strategy: univariate
          read local nicas: true
```

YAML configuration for 3DVar (4/6)

$$B = K_1 K_2 \Sigma C \Sigma^T K_2^T K_1^T$$

```
background error:
  covariance model: SABER
  saber central block:
    saber block name: BUMP_NICAS
    ... more config ...
  saber outer blocks:
  - saber block name: StdDev
    read:
      model file:
        filename: ./BUMP_files/stddev/mpas.stddev_0p33.2018-04-15_00.00.00.nc
        date: *analysisDate
        stream name: control
```

YAML configuration for 3DVar (5/6)

$$B = K_1 K_2 \Sigma C \Sigma^T K_2^T K_1^T$$


```yaml
- saber block name: BUMP_VerticalBalance
  read:
    io:
      data directory: ./BUMP_files/bump_vertical_balance
      files prefix: bumpcov_vbal
    drivers:
      read local sampling: true
      read vertical balance: true
    vertical balance:
      vbal:
      - balanced variable: velocity_potential
        unbalanced variable: stream_function
        diagonal regression: true
      - balanced variable: temperature
        unbalanced variable: stream_function
      - balanced variable: surface_pressure
        unbalanced variable: stream_function
```

YAML configuration for 3DVar (6/6)

$$B=K_1K_2\Sigma C\Sigma^TK_2^TK_1^T$$

```
background error:
  covariance model: SABER
  saber central block:
    saber block name: BUMP_NICAS
    ... more config ...
  saber outer blocks:
  - saber block name: StdDev
    ... more config ...
  - saber block name: BUMP_VerticalBalance
    ... more config ...
  linear variable change:
    linear variable change name: Control2Analysis
    input variables: *ctlvars
    output variables: *incvars
```

YAML configuration for Hybrid-3DEnVar (1/2)

- 3DVar setting

```
background error:
  covariance model: SABER
  ... more config ...
```

- 3DEnVar setting

```
background error:
  covariance model: ensemble
  ... more config ...
```

- We can configure the hybrid covariance as a linear combination of two Bs !

$$\mathbf{B}_{\mathbf{hybrid}} = \alpha \mathbf{B}_{\mathbf{static}} + \beta \mathbf{B}_{\mathbf{ensemble}}$$

(Hamill and Snyder, 2000)

YAML configuration for Hybrid-3DEnVar (2/2)

- We can configure the hybrid covariance as a linear combination of two Bs !

```
background error:
    covariance model: hybrid
    components:
    - weight:
        value: 0.5
      covariance:
        covariance model: SABER
        ... more config ...
    - weight:
        value: 0.5
      covariance:
        covariance model: ensemble
        ... more config ...
```

$$\mathbf{B}_{\text{hybrid}} = \alpha \mathbf{B}_{\text{static}} + \beta \mathbf{B}_{\text{ensemble}}$$

2-stream I/O (1/3)

- To reduce disk space usage, we use “mpasout” file instead of “restart” file for MPAS-JEDI’s background and analysis file.

- Also “static” fields in a separate file and “mpasout” file excludes “static” fields.

- So MPAS-JEDI will need to read in two streams (two files)
  - “**static**” stream: mesh info, sfc input variables (landmask, shdmin, albedo12m, etc) and parameters for gravity wave drag over orography.
  - “**da_state**” stream (i.e., ‘mpasout’ file): fields needed for DA purposes (either analysis variables or fixed input needed for CRTM or other obs operators).

2-stream I/O (2/3)

- For cold start forecast, both “static” and “input” stream file should be set to the “init.nc” file, generated by MPAS *init_atmosphere* executable.
  - In “namelist.atmosphere”

```
&restart
    config_do_DAcycling = false
/
```

static.nc is a link to an init.nc file, time information will NOT be used
init.nc file will be actual initial condition file

- For forecast step of cycling exp, “input” stream should point the file generated from “da_state” stream. Usually we keep using “init.nc” for “static” stream
  - In “namelist.atmosphere”

```
&restart
    config_do_DAcycling = true
/
```

static.nc is a link to an init.nc file, time information will NOT be used
mpasout.nc file will be actual initial condition file

This is NOT a clean implementation. A clean implementation will be in a future official MPAS-A model release.

2-stream I/O (3/3)

- For DA step of cycling exp, setting will be
  - In “namelist.atmosphere”

```
&restart
    config_do_DAcycling = true
/
&assimilation
    config_jedi_da = true
/
```

static.nc is a link to an init.nc file, time information will NOT be used
mpasout.nc type file will be background and analysis file

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