August 13, 2026

MPAS-JEDI 3D/4DEnVar

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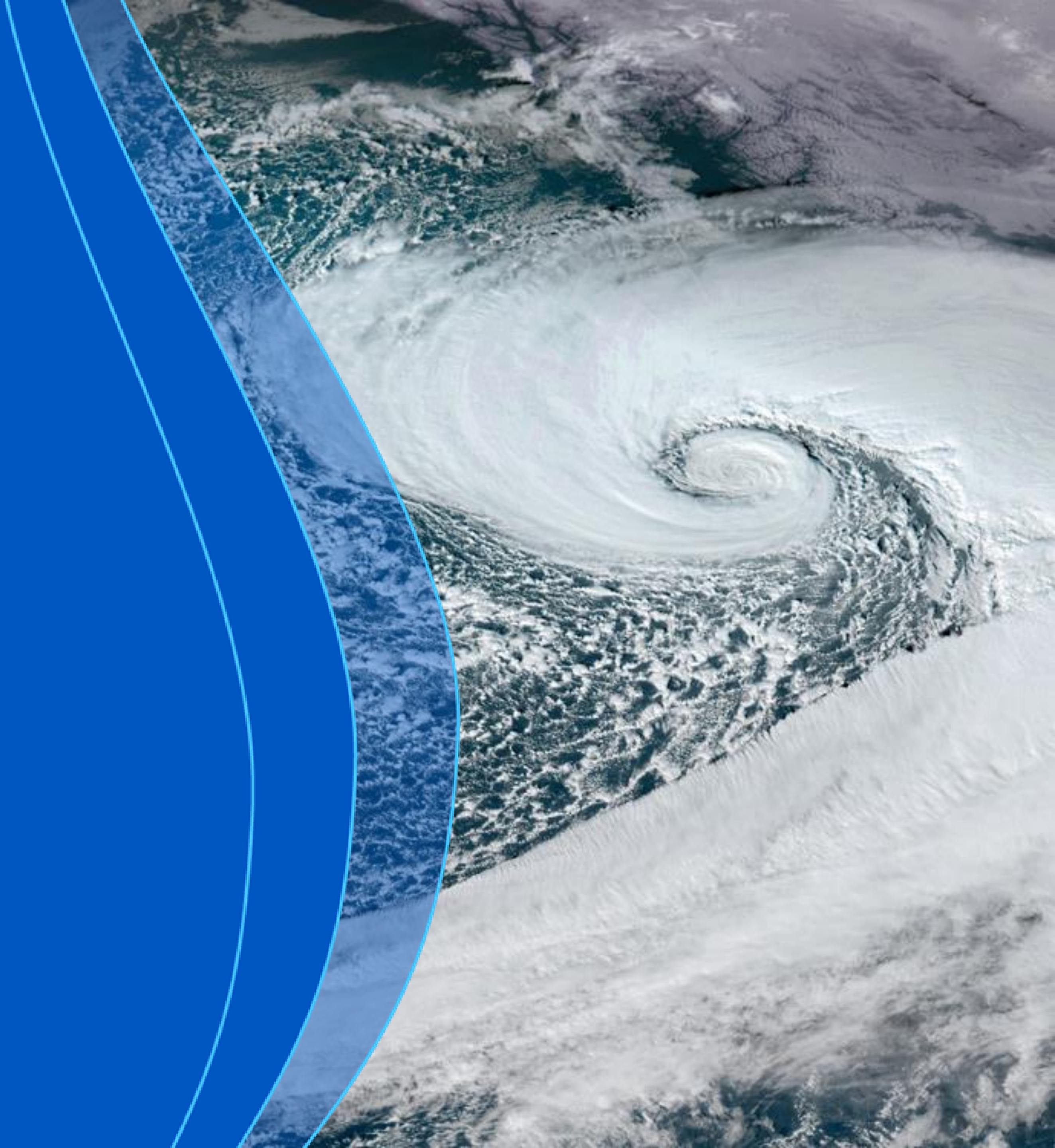


Overview

1. **Variational Cost Function**
2. Ensemble Error Covariance Matrix
3. Overview of 3DEnVar
4. Setting up a .yaml file for 3DEnVar
5. Overview of 4DEnVar
6. Setting up a .yaml file for 4DEnVar

The Problem to solve

We want to find the **analysis state** (x) that minimizing a cost function with an optimal fit to the background and observations.

$$\boldsymbol{J}(x) = \boxed{\frac{1}{2}(x - x_b)^T \boldsymbol{B}^{-1}(x - x_b)} + \boxed{\frac{1}{2}(h(x) - y)^T \boldsymbol{R}^{-1}(h(x) - y)}$$

Distance to background

Distance to observations

$\boldsymbol{B}$: background error covariance matrix

$\boldsymbol{R}$: observation error covariance matrix

Incremental Cost Function in JEDI

Original-form:

$$J(x) = \frac{1}{2}(x - x_b)^T \boldsymbol{B}^{-1}(x - x_b) + \frac{1}{2}(h(x) - y)^T \boldsymbol{R}^{-1}(h(x) - y)$$

Incremental-form:

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

$\boldsymbol{\delta x = x - x_g}$ $\quad \delta x_g = x_b - x_g$ $\quad \boldsymbol{d = y - h(x_g)}$

The minimization deals with increments to a known reference state

- Cost function minimizes δx=x− x_g instead of the full state (x)
- Start from $x_g = x_b$ and $\delta x_g = 0$
- **After minimization->** $x_a = x_g + \delta x$

About dual-resolution

- Analysis increment and ensemble can be at a lower resolution than the background and analysis

$$J(\delta x) = \frac{1}{2}\left(\delta x - \delta x_g\right)^T \boldsymbol{B}^{-1}\left(\delta x - \delta x_g\right) + \frac{1}{2}(\boldsymbol{H}\delta x - d)^T \boldsymbol{R}^{-1}(\boldsymbol{H}\delta x - d)$$

$$\boldsymbol{\delta x = x - x_g} \qquad \delta x_g = x_b - x_g \qquad \boldsymbol{d = y - h(x_g)}$$

- Hofx : based on the high-resolution nonlinear background state
- inner-loop minimization : low-resolution
- After converge, the low-res analysis increment is interpolated up to high resolution, and added to the high-res background state, to obtain the final analysis.

Practical session 4.3: dual-resolution 3DEnVar test case at 120km-240km

Appropriately assign B and R is critical

We want to find the analysis state (x) that minimizing a cost function with **an optimal fit** to the background and observations.

Distance to background **Distance to observations**

$$J(\delta x) = \boxed{\frac{1}{2}(\delta x - \delta x_g)^T B^{-1} (\delta x - \delta x_g)} + \boxed{\frac{1}{2}(H\delta x - d)^T R^{-1} (H\delta x - d)}$$

The weighting between the two components is determined by B (background error) and R (observation error).

- A larger B means background is less accurate -> x will get closer to observation
- A larger R means observation is less accurate -> x will get closer to background

Two types of background error covariance (B)

$$J(\delta x) = \frac{1}{2}\left(\delta x - \delta x_g\right)^T B^{-1}\left(\delta x - \delta x_g\right) + \frac{1}{2}(H\delta x - d)^T R^{-1}(H\delta x - d$$

1. **Static B**

   -> from statistic (e.g. a month of model forecasts), does not vary with time

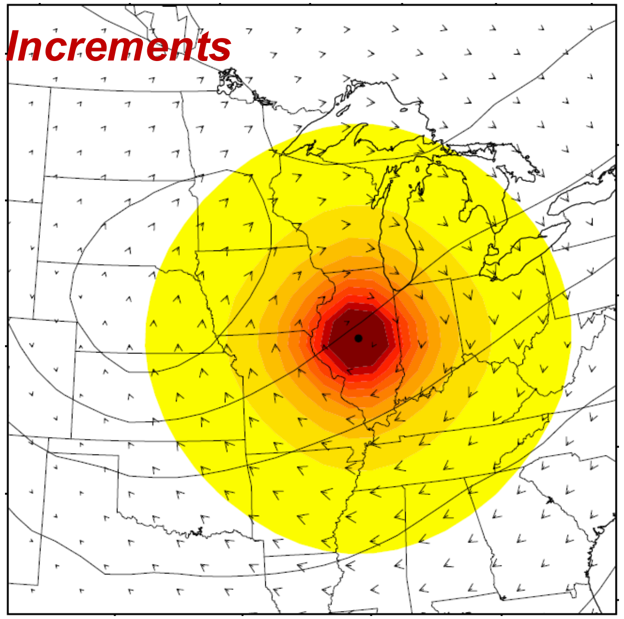
2. **Ensemble B**

   -> flow-dependent, reflect the background error in different time

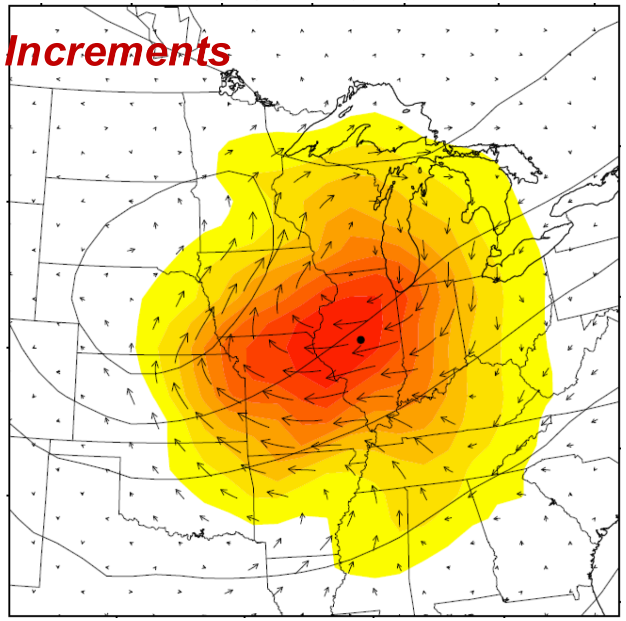
Example to show the B effect (Single observation tests)

Assimilate a single Temperature observation

Static B

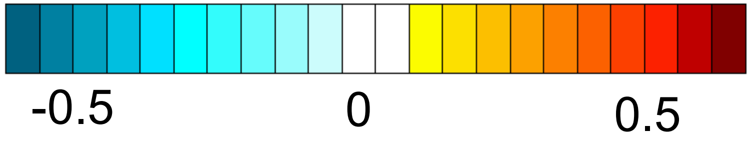


Ensemble B



Ensemble $\boldsymbol{B}$:

- Errors of the day are sampled
- flow-dependent update



Increments of temperature (shaded) and horizontal winds (vector)

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Derive B matrix from an ensemble of forecasts

ensemble size

State variable of ensemble mean

$$\boldsymbol{B_e} = \frac{1}{n-1}\sum_{i=1}^{\boldsymbol{n}}(\boldsymbol{x_i} - \boldsymbol{\bar{x}})(x_i - \bar{x})^T$$

State variable of each ensemble member

$$\boldsymbol{B_e} = \frac{1}{n-1}\sum_{i=1}^{\boldsymbol{n}}(\delta x_{\boldsymbol{i}})(\delta x_{\boldsymbol{i}})^T$$

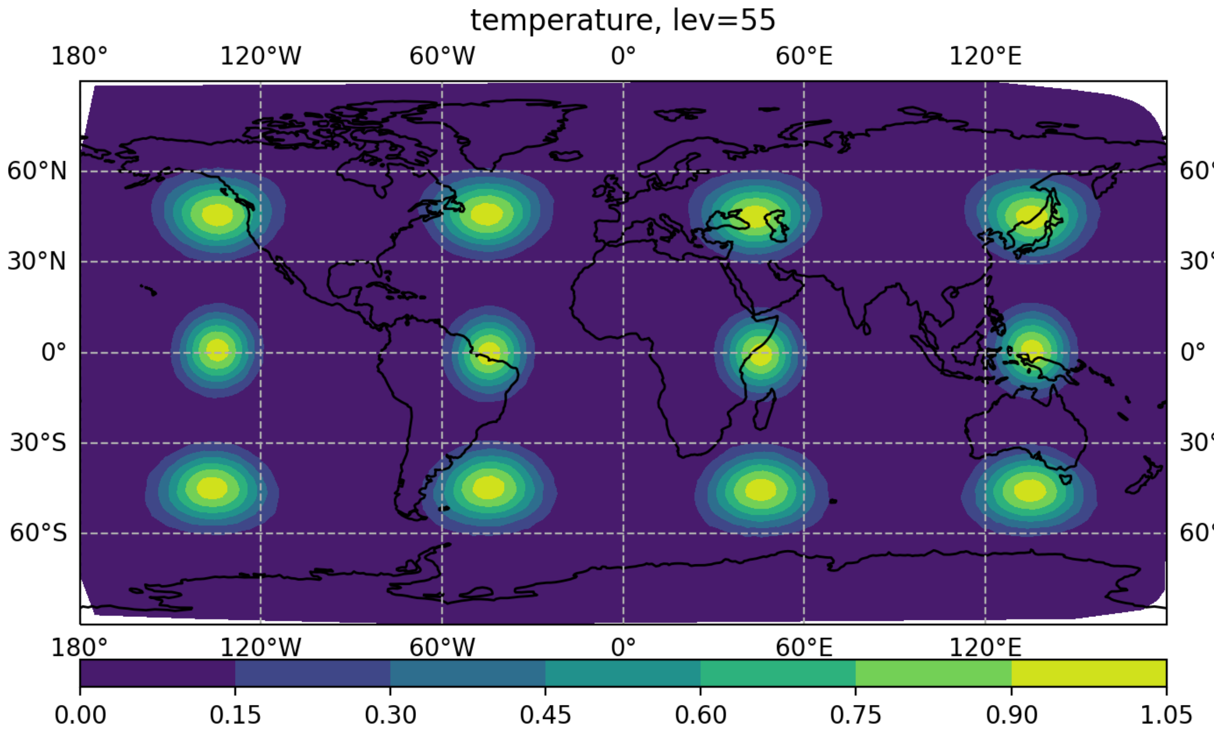
ensemble perturbation

- Sample covariance matrix
- The ensemble mean provides an estimation of the truth
- The perturbations from the mean estimate the uncertainty, which is used to model background-error covariance matrix.
- Ensemble spread is the standard deviation from ensemble mean.

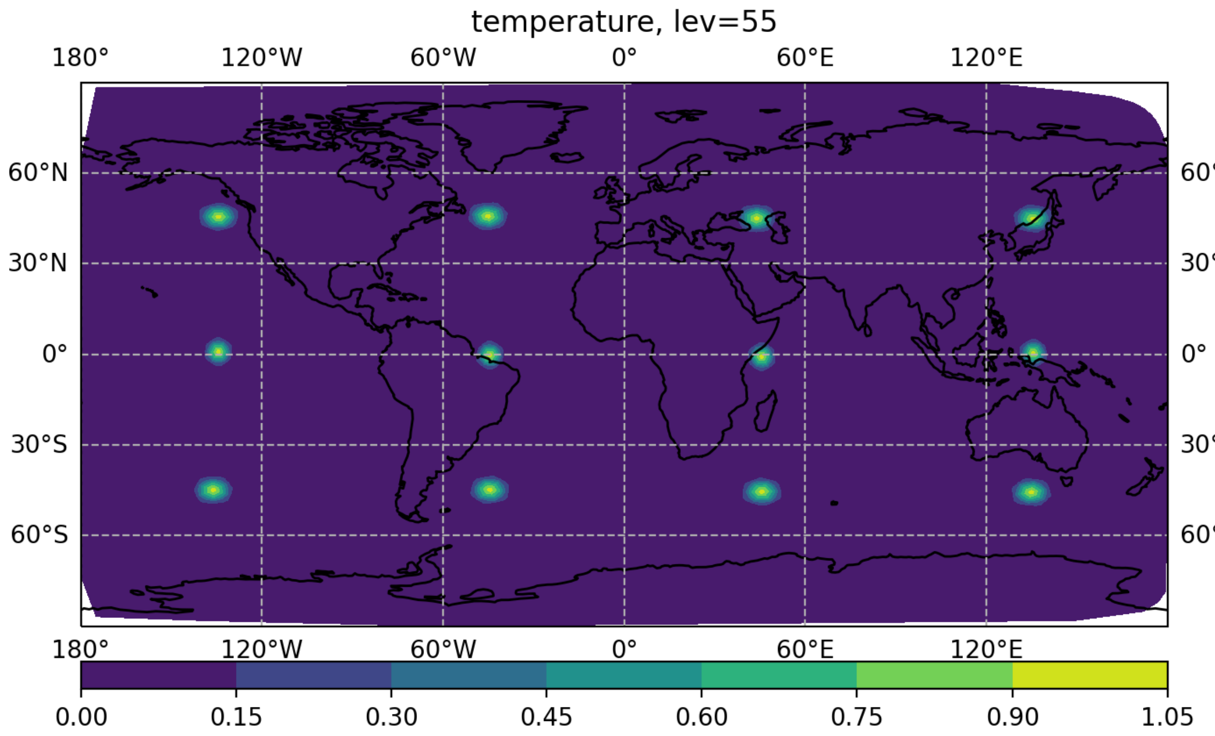
Localization of ensemble B matix: $B = L \circ B_e$

L is a correlation matrix, to reduce spurious correlation due to limited ensemble size

larger localization scales



Smaller localization scale



Influence a a small area

EnVar uses a pure ensemble B to updates a deterministic forecast

In hybrid methods, B can be a weighted sum of static B ($\boldsymbol{B_s}$) and ensemble B ($\boldsymbol{B_e}$).

$$\boldsymbol{B} = \beta_s \boldsymbol{B_s} + \beta_e \boldsymbol{B_e}$$

$$\underbrace{\beta_s}_{=0} + \underbrace{\beta_e}_{=1} = 1$$

pure ensemble B

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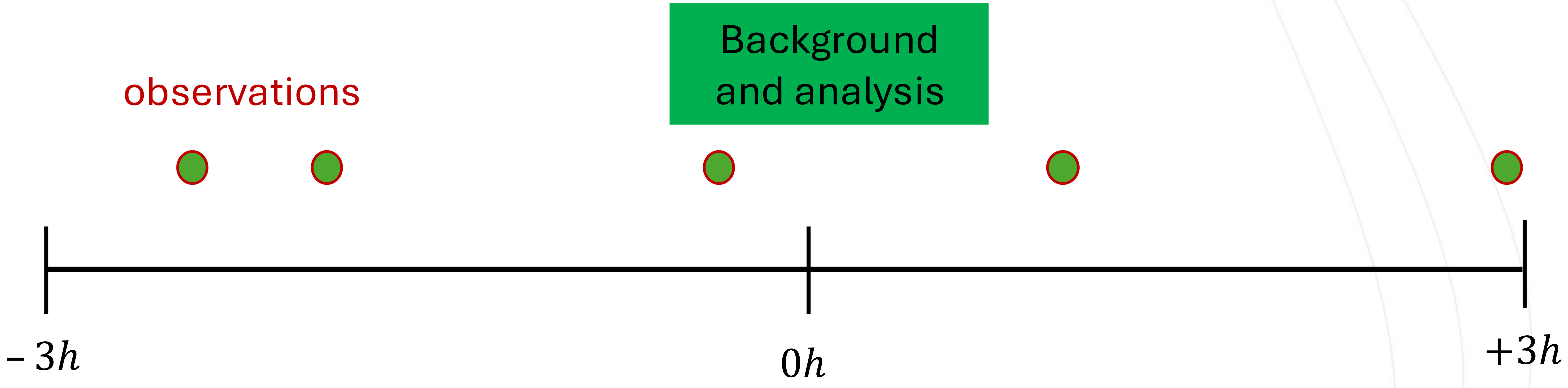
3DEnVar using a 6h assimilation window



- All observations in 3DEnVar are assumed to be valid at the same time as the background.
- Innovation $(\boldsymbol{Hx} - \boldsymbol{y_o})$ is calculated relative to background at that single time

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Configure the analysis time for 3DEnvar

```
_member config: &memberConfig
  date: &analysisdate '2018-04-15T00:00:00Z'
  state variables: &incvars
  - air_temperature
  - water_vapor_mixing_ratio_wrt_moist_air
  - eastward_wind
  - northward_wind
  - air_pressure_at_surface
  stream name: ensemble
cost function:
  cost type: 3D-Var
  time window:
    begin: '2018-04-14T21:00:00Z'
    length: PT6H
  geometry:
    nml_file: "./Data/480km/namelist.atmosphere_2018041500"
    streams_file: "./Data/480km/streams.atmosphere"
    deallocate non-da fields: true
  analysis variables: *incvars
  background:
    state variables: [air_temperature, water_vapor_mixing_ratio_wrt_moist_air...]
    filename: "./Data/480km/bg/restart.2018-04-15_00.00.00.nc"
    date: *analysisdate
```

analysis time (center of window)

~test/testinput/3denvar_bumploc.yaml

Start of assimilation window

length of assimilation window

background at analysis time

Configure the ensemble B

```yaml
background error:
  covariance model: ensemble
  localization:
    localization method: SABER
    saber central block:
      saber block name: BUMP_NICAS
      active variables: *incvars
      read:
        io:
          files prefix: Data/bump/mpas_parametersbump_loc
        drivers:
          multivariate strategy: duplicated
          read local nicas: true
  members:
  - filename: Data/480km/bg/ensemble/mem01/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig
  - filename: Data/480km/bg/ensemble/mem02/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig
  - filename: Data/480km/bg/ensemble/mem03/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig
  - filename: Data/480km/bg/ensemble/mem04/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig
  - filename: Data/480km/bg/ensemble/mem05/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig
```

set ensemble B for 3DEnVar

Specifying members used to compute ensemble B

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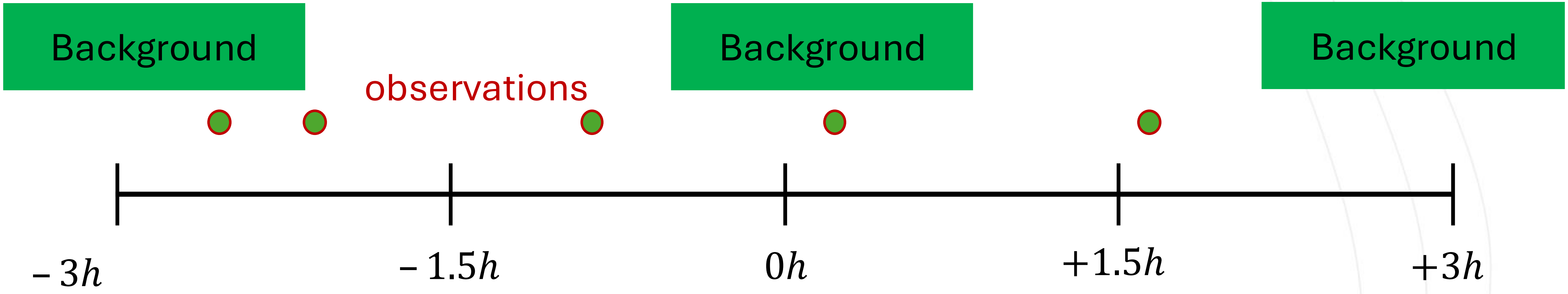
4DEnVar



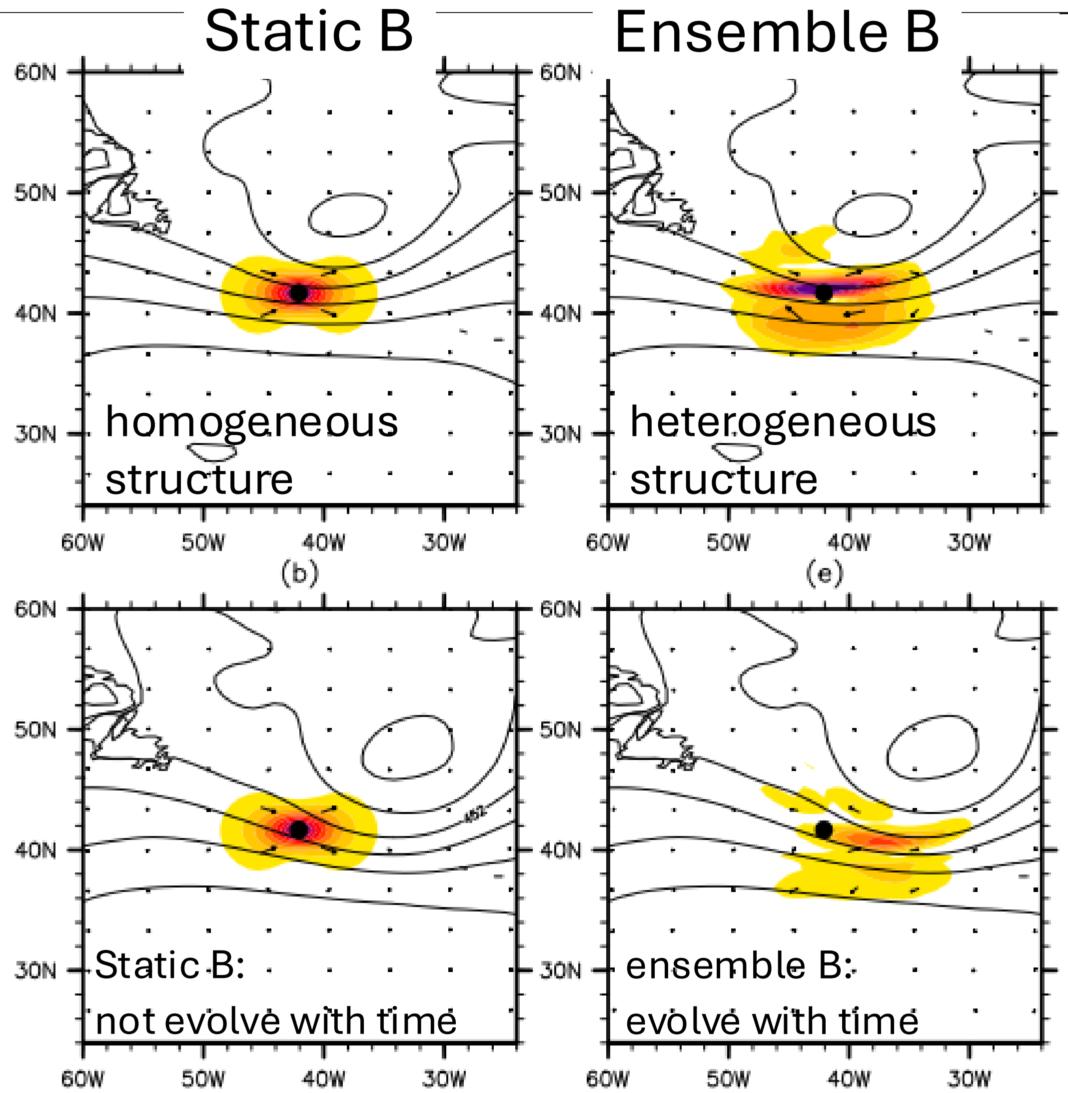
- All observations in 4DEnVar are binned within a smaller subwindow and innovations ($\boldsymbol{Hx} - \boldsymbol{y}_o$) are calculated relative to background valid at that time.
- Ensemble needed at the center of each subwindow ($\boldsymbol{K}$ ensemble required).

The 4D ensemble $\boldsymbol{B}$ is used to propagate the innovation

Analysis increment

Start of window

end of window



Lorenc et al. (2015)

increments have moved downstream by the end of the assimilation window

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6. **Setting up a .yaml file for 4DEnVar**

Configure the analysis times for 4DEnvar

```yaml
- _member config 1: &memberConfig1
    date: &date1 '2018-04-14T21:00:00Z'
    state variables: &incvars
    - air_temperature
    - water_vapor_mixing_ratio_wrt_moist_air
    - eastward_wind
    - northward_wind
    - air_pressure_at_surface
    stream name: ensemble
  _member config 2: &memberConfig2
    <<: *memberConfig1
    date: &date2 '2018-04-15T00:00:00Z'
  _member config 3: &memberConfig3
    <<: *memberConfig1
    date: &date3 '2018-04-15T03:00:00Z'
  cost function:
    cost type: 4D-Ens-Var
    time window:
      begin: '2018-04-14T21:00:00Z'
      length: PT6H
    subwindow: PT3H
```

subwindow1

subwindow2

subwindow3

test/testinput/4denvar_bumploc.yaml

Background needed for each subwindow

```
background:
  states:
  - state variables: &stvars
    filename: "./Data/480km/bg/restart.2018-04-14_21.00.00.nc"
    date: *date1
  - state variables: *stvars
    filename: "./Data/480km/bg/restart.2018-04-15_00.00.00.nc"
    date: *date2
  - state variables: *stvars
    filename: "./Data/480km/bg/restart.2018-04-15_03.00.00.nc"
    date: *date3
```

[air_temperature, water_vapor_mixing_ratio_wrt_moist_air, eastward_wind, northward_wind, air_pressure_at_surface, air_potential_temperature, dry_air_density, u, water_vapor_mixing_ratio_wrt_dry_air, air_pressure, landmask, seaice_fraction, snowc …]

bg (subwindow 1)

bg (subwindow 2)

bg (subwindow 3)

Configure the ensemble B

```yaml
background error:
  covariance model: ensemble
  localization:
    localization method: SABER
    saber central block:
      saber block name: BUMP_NICAS
      active variables: *incvars
      read:
        io:
          files prefix: Data/bump/mpas_parametersbump_loc
        drivers:
          multivariate strategy: duplicated
          read local nicas: true
```

set ensemble B for 4DEnVar

Ensemble files needed for each subwindow

```yaml
members:
- states:
  - filename: Data/480km/bg/ensemble/mem01/x1.2562.init.2018-04-14_21.00.00.nc
    <<: *memberConfig1
  - filename: Data/480km/bg/ensemble/mem01/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig2
  - filename: Data/480km/bg/ensemble/mem01/x1.2562.init.2018-04-15_03.00.00.nc
    <<: *memberConfig3
- states:
  - filename: Data/480km/bg/ensemble/mem02/x1.2562.init.2018-04-14_21.00.00.nc
    <<: *memberConfig1
  - filename: Data/480km/bg/ensemble/mem02/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig2
  - filename: Data/480km/bg/ensemble/mem02/x1.2562.init.2018-04-15_03.00.00.nc
    <<: *memberConfig3
- states:
  - filename: Data/480km/bg/ensemble/mem03/x1.2562.init.2018-04-14_21.00.00.nc
    <<: *memberConfig1
  - filename: Data/480km/bg/ensemble/mem03/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig2
  - filename: Data/480km/bg/ensemble/mem03/x1.2562.init.2018-04-15_03.00.00.nc
    <<: *memberConfig3
- states:
  - filename: Data/480km/bg/ensemble/mem04/x1.2562.init.2018-04-14_21.00.00.nc
    <<: *memberConfig1
  - filename: Data/480km/bg/ensemble/mem04/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig2
  - filename: Data/480km/bg/ensemble/mem04/x1.2562.init.2018-04-15_03.00.00.nc
    <<: *memberConfig3
- states:
  - filename: Data/480km/bg/ensemble/mem05/x1.2562.init.2018-04-14_21.00.00.nc
    <<: *memberConfig1
  - filename: Data/480km/bg/ensemble/mem05/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig2
  - filename: Data/480km/bg/ensemble/mem05/x1.2562.init.2018-04-15_03.00.00.nc
    <<: *memberConfig3
```

A simpler way to configure ensemble input

```yaml
members from template:
  template:
    states:
    - state variables: *incvars
      date: 2018-04-14T21:00:00Z
      filename: ../ensemble/2018041418/%iMember%/mpasout.2018-04-14_21.00.00.nc
    - state variables: *incvars
      date: 2018-04-15T00:00:00Z
      filename: ../ensemble/2018041418/%iMember%/mpasout.2018-04-15_00.00.00.nc
    - state variables: *incvars
      date: 2018-04-15T03:00:00Z
      filename: ../ensemble/2018041418/%iMember%/mpasout.2018-04-15_03.00.00.nc
  pattern: %iMember%
  start: 1
  zero padding: 2
  nmembers: 20
```

See 4denvar.yaml in practical session 4.4

Nodes/Cores setting

3DEnVar

```
#PBS -l select=1:ncpus=64:mpiprocs=64:mem=235GB
```

4DEnVar with 3 sub-windows

```
#PBS -l select=3:ncpus=64:mpiprocs=64:mem=235GB
```

References

- Liu, Z., and Coauthors, 2022: Data assimilation for the Model for Prediction Across Scales - Atmosphere with the Joint Effort for Data assimilation Integration (JEDI-MPAS 1.0.0): EnVar implementation and evaluation. *Geosci. Model Dev.*, **15**, 7859–7878, https://doi.org/10.5194/gmd-15-7859-2022.

- Lorenc, A. C., N. E. Bowler, A. M. Clayton, S. R. Pring, and D. Fairbairn, 2015: Comparison of hybrid-4DEnVar and hybrid-4DVar data assimilation methods for global NWP. *Mon. Weather Rev.*, **143**, 212–229, https://doi.org/10.1175/MWR-D-14-00195.1.

- Nystrom, R. G., Snyder, C., Liu, Z., Jung, B. J., Ban, J., & Banos, I. H. (2025). A hybrid four-dimensional variational data assimilation system for the Model for Prediction Across Scales (MPAS-atmosphere): Leveraging the Joint Effort for Data assimilation Integration (JEDI). *Journal of Advances in Modeling Earth Systems*, 17, e2025MS005183. https://doi.org/10.1029/2025MS005183