

# WP4: Added value of the SEEDS assimilation scheme

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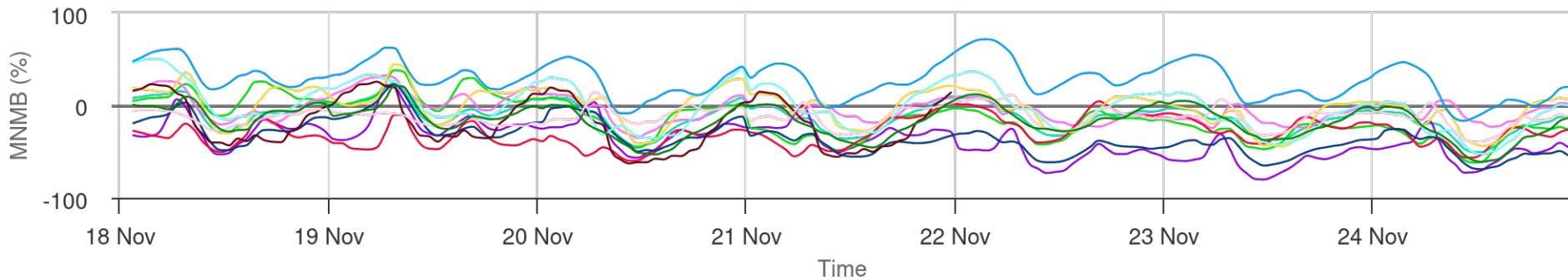
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Acknowledgments: B. Ménétrier (Met Norway)

# Motivation: air quality forecasts biases

## NO2 - ALL - 2023/11/18-2023/11/25

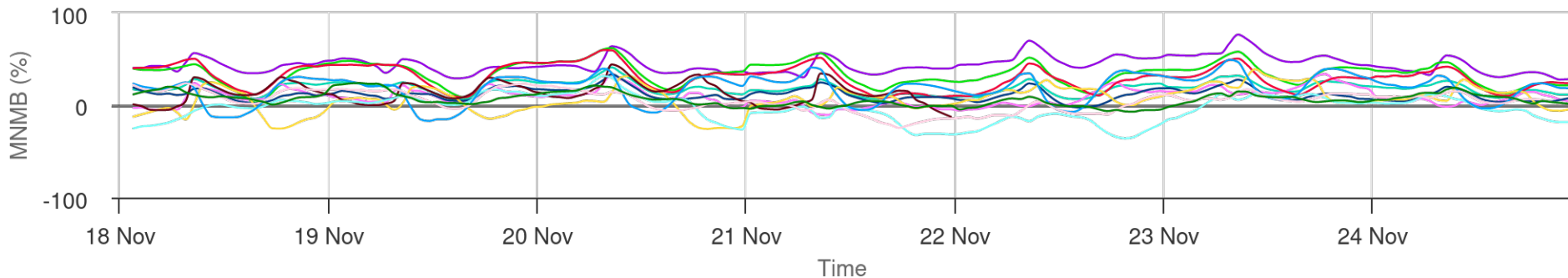
Obs - hourly data



ENSEMBLE CHIMERE DEHM EMEP EURAD GEMAQ LOTOS MATCH MINNI  
MOCAGE MONARCH SILAM

## O3 - ALL - 2023/11/18-2023/11/25

Obs - hourly data



ENSEMBLE CHIMERE DEHM EMEP EURAD GEMAQ LOTOS MATCH MINNI  
MOCAGE MONARCH SILAM

# Motivation: Near Real Time observations

AIRBASE\_O3 O3 Nobs N=948  
Avg: 22.7 Min: 1 Max: 24



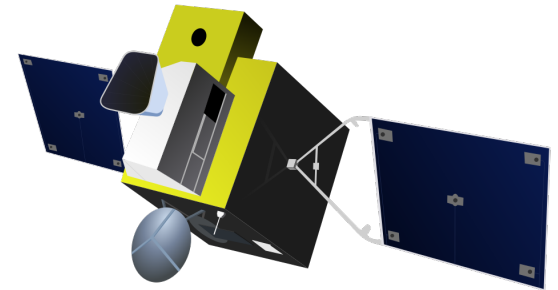
AIRBASE\_NO2 NO2 Nobs N=699  
Avg: 22.3 Min: 1 Max: 24



AIRBASE\_PM10 PM10 Nobs N=602  
Avg: 22.9 Min: 1 Max: 24



AIRBASE\_PM2.5 PM2.5 Nobs N=299  
Avg: 22.8 Min: 3 Max: 24



Sentinel-4: 8x8 km<sup>2</sup> hourly columns of NO<sub>2</sub>, O<sub>3</sub>, SO<sub>2</sub>, HCHO and aerosols



# Data Assimilation in CAMS models

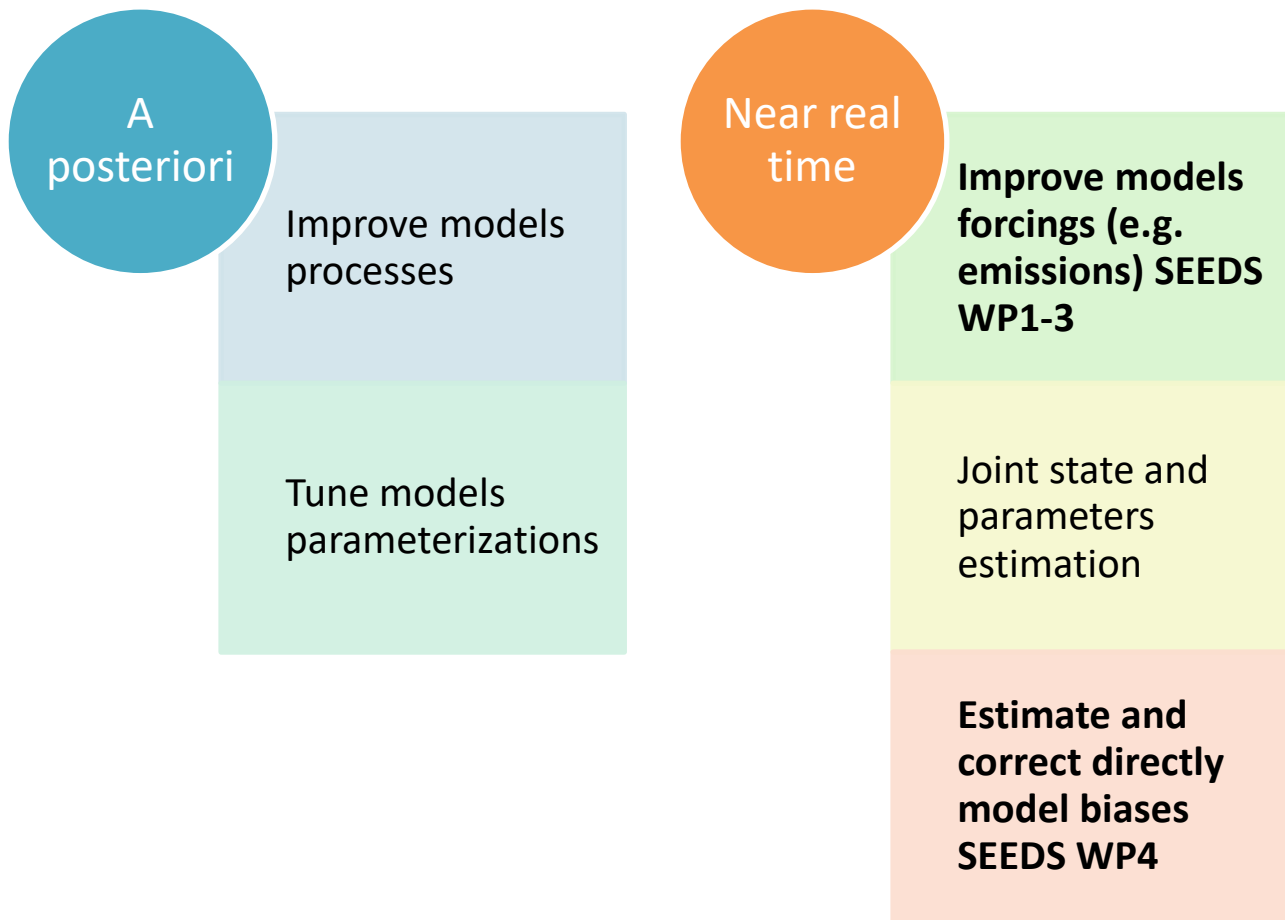
MODEL	ASSIMILATION ALGORITHM	ASSIMILATED OBSERVATIONS
CHIMERE	Kriging	O <sub>3</sub> , NO <sub>2</sub> , PM <sub>10</sub> , PM <sub>2.5</sub>
EMEP	3D-Var	O <sub>3</sub> , NO <sub>2</sub> , SO <sub>2</sub> , PM <sub>10</sub> + SAT NO <sub>2</sub>
EURAD-IM	3D-Var	O <sub>3</sub> , NO <sub>2</sub> , PM <sub>10</sub> , PM <sub>2.5</sub> + SATELLITE NO <sub>2</sub> , SO <sub>2</sub> , CO
LOTOS-EUROS	EnKF	O <sub>3</sub> , NO <sub>2</sub> , PM <sub>10</sub> , PM <sub>2.5</sub> + SAT NO <sub>2</sub>
MATCH	3D-Var	O <sub>3</sub> , NO <sub>2</sub> , SO <sub>2</sub> CO, PM <sub>10</sub> , PM <sub>2.5</sub>
MOCAGE	3D-Var	O <sub>3</sub> , NO <sub>2</sub> , PM <sub>10</sub> , PM <sub>2.5</sub>
SILAM	3D-Var	O <sub>3</sub> , NO <sub>2</sub> , SO <sub>2</sub> , CO, PM <sub>10</sub> , PM <sub>2.5</sub>
DEHM	Optimal Interpolation	O <sub>3</sub> , NO <sub>2</sub>
GEM-AQ	Optimal Interpolation	O <sub>3</sub> , NO <sub>2</sub> , SO <sub>2</sub> CO, PM <sub>10</sub> , PM <sub>2.5</sub>
MONARCH	LETKF	O <sub>3</sub> , NO <sub>2</sub> , SO <sub>2</sub> CO, PM <sub>10</sub> , PM <sub>2.5</sub>
MINNI	Optimal Interpolation	O <sub>3</sub> , NO <sub>2</sub> , SO <sub>2</sub> CO, PM <sub>10</sub> , PM <sub>2.5</sub>




# Motivation

Problem is: the impact of DA on forecasts is not very significant

Solutions:





# SEEDS WP4 objectives

Estimate and correct model biases in NRT ... with the help of air quality ensembles<sup>1</sup>:

1. Compute ensembles of forecasts based on perturbations of key forcing fields (e.g. emissions, deposition).
2. Assess the added value of an assimilation scheme that includes model error (4DEnVar) with respect to the sequential filters used in CAMS operations (use MOCAGE 3DVar as reference).
3. Provide an open-source assimilation code that can be adapted to other CAMS models equipped with ensemble forecasts, or to the CAMS ensemble itself.

<sup>1</sup>Emili et al. Accounting for model error in air quality forecasts: an application of 4DEnVar to the assimilation of atmospheric composition using QG-Chem 1.0, GMD, 2016

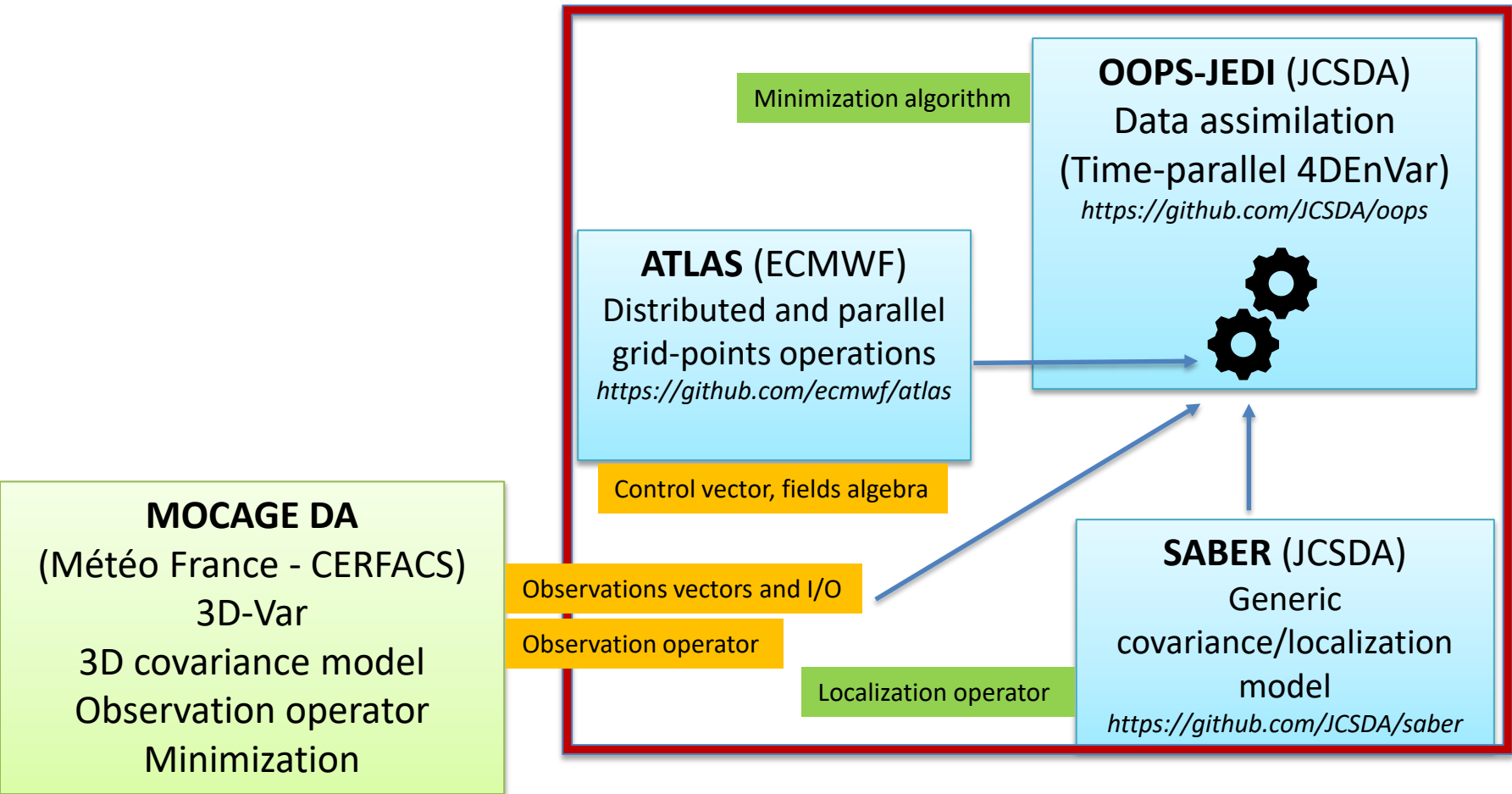




# Air Quality (AQ) Data Assimilation

## Task 4.2

<https://github.com/andreapiacentini/aq/releases/tag/v1.1.0>







# Ensembles of air quality forecasts

—————> *Time* —————>

Forecast (0-72h)



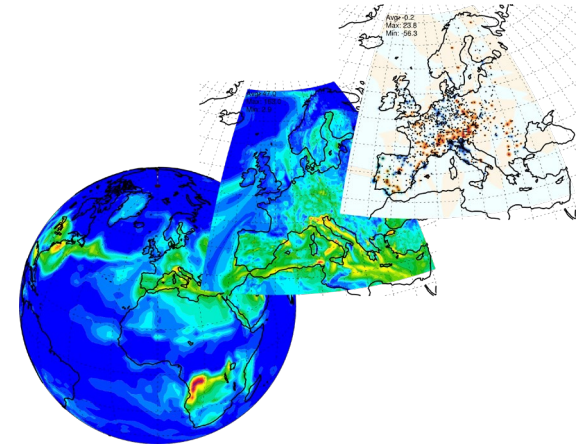
Perturbed forecast (0-24h)



# Ensembles perturbations

Use MOCAGE chemical transport model:

- RACM tropospheric chemistry
- 3DVar assimilation
- CAMS operational configuration (10 km)



Perturbed quantity	Perturbed Parameters	Species	Probability distribution
Emissions	Total flux	Emitted species	Lognormal ( $\mu=0, \sigma=0.4$ ) / multiplicative [0.45, 2.19]
Dry deposition	Dry deposition velocities	Deposited species	Lognormal ( $\mu=0, \sigma=0.5$ ) / multiplicative [0.37, 2.66]
Initial Condition	3D chemical state	All	Lognormal ( $\mu=0, \sigma=0.2$ ) / multiplicative [0.67, 1.48]
Vertical diffusion	Diffusion coefficient	All	Lognormal ( $\mu=0, \sigma=0.4$ ) / multiplicative [0.45, 2.19]

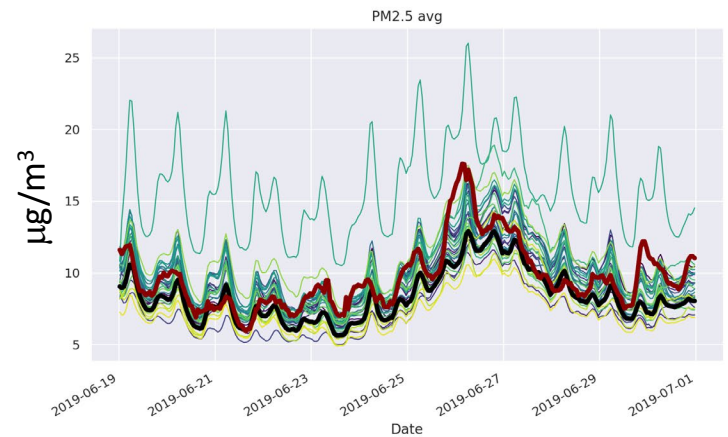
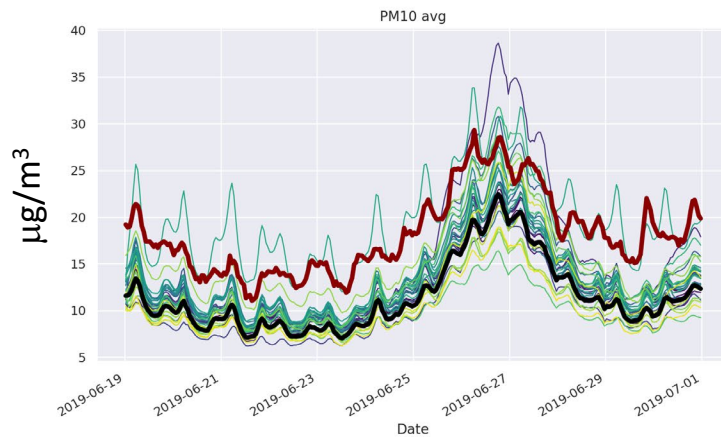
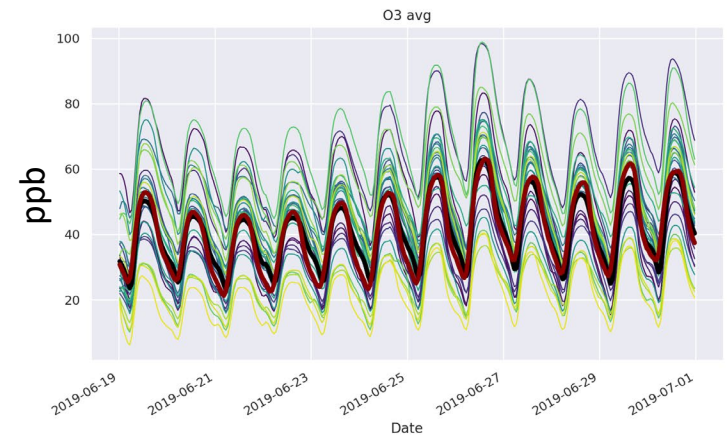
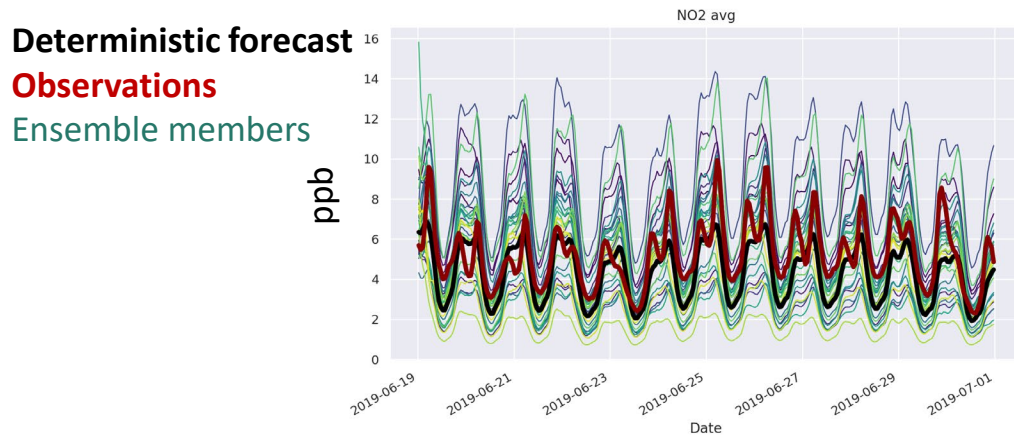
Table 1: Configuration used for the ensemble generation. The 95% confidence interval corresponding to the given lognormal distribution is reported in brackets in the 4th column.

Feedback from satellite emissions estimations WPs in SEEDS:

- ✓ NO<sub>x</sub> emissions perturbations reduced (->  $\sigma=0.2$  [0.67,1.48])
- ✓ Isoprene emissions perturbations increased (->  $\sigma=0.57$  [0.32,3.06])

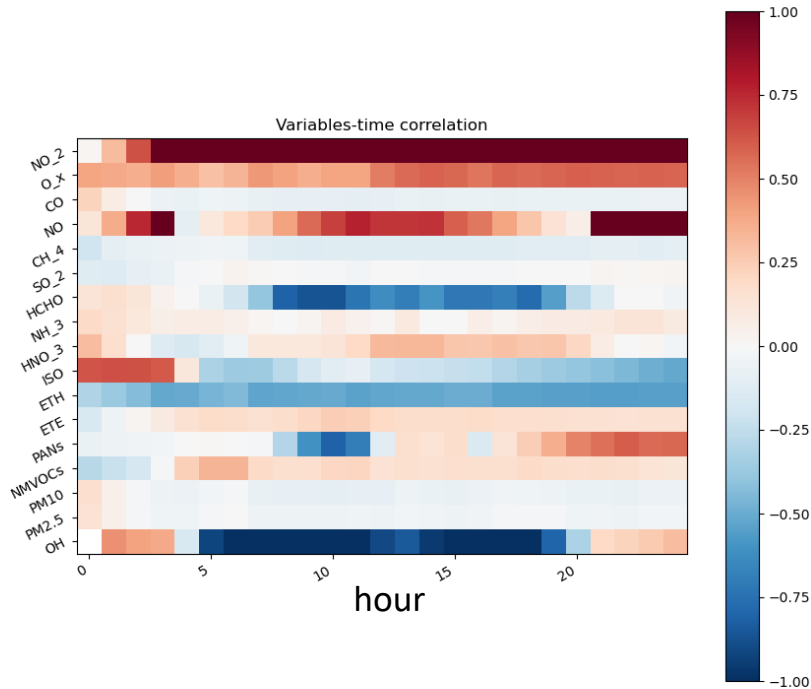
# Ensembles verification

Evaluation against CAMS surface observations (SEEDS D4.1): average over all EU sites



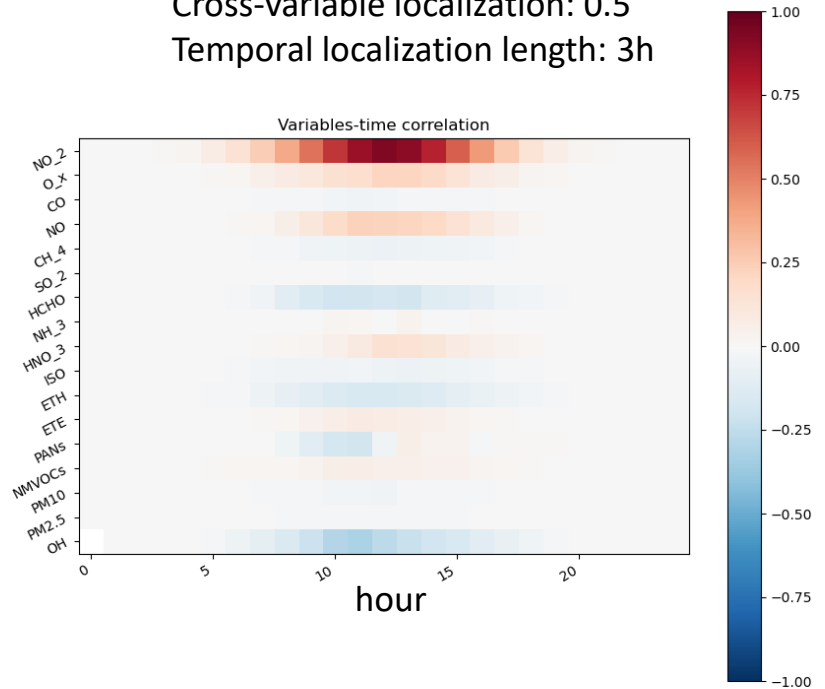
# 4D Covariance and localization

## Raw ensemble correlations



## Localized correlations

Cross-variable localization: 0.5  
Temporal localization length: 3h



# 4D assimilation

Time →

Surface observations of  
 $O_3$ ,  $NO_2$ ,  $PM_{10}$ ,  $PM_{2.5}$

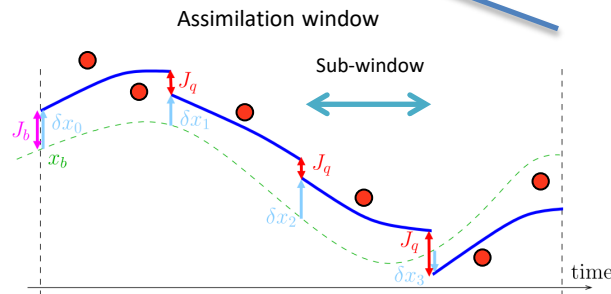
Forecast (0-72h)

4DEnVar  
(0-24h)

4D analysis (0-24h)

Perturbed forecast (0-24h)

AQ code



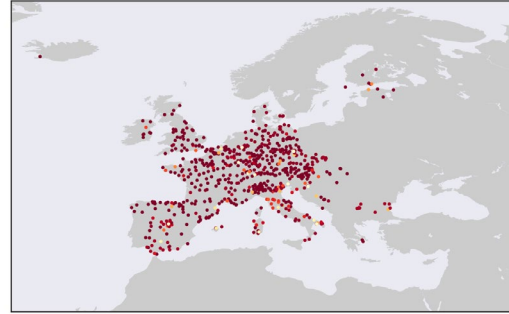


# Assimilated network

AIRBASE\_O3 O3 Nobs N=948  
Avg: 22.7 Min: 1 Max: 24



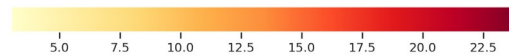
AIRBASE\_NO2 NO2 Nobs N=699  
Avg: 22.3 Min: 1 Max: 24



AIRBASE\_PM10 PM10 Nobs N=602  
Avg: 22.9 Min: 1 Max: 24



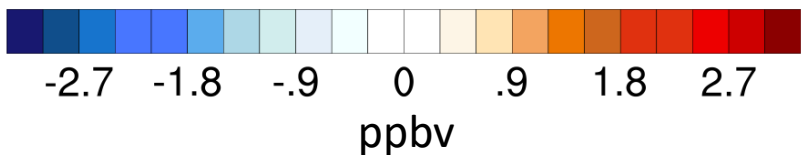
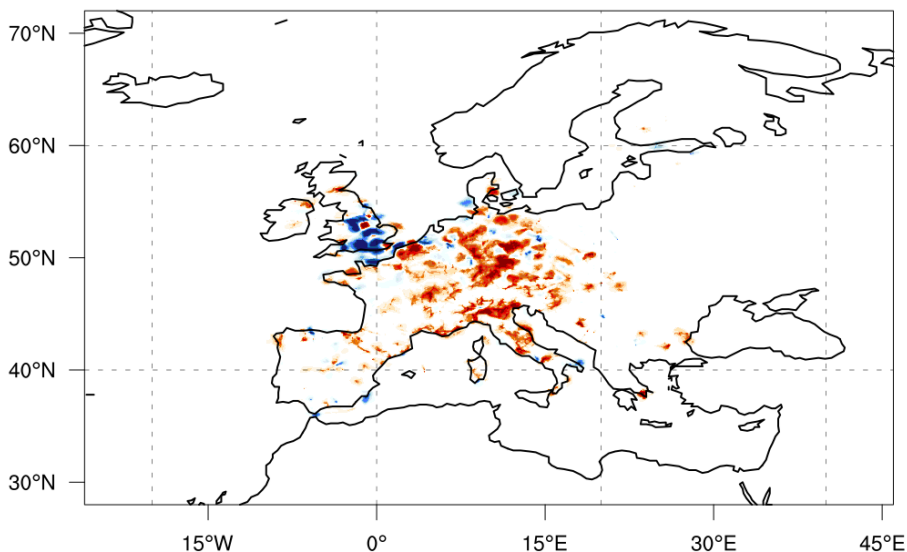
AIRBASE\_PM2.5 PM2.5 Nobs N=299  
Avg: 22.8 Min: 3 Max: 24



# Comparison with 3D-Var

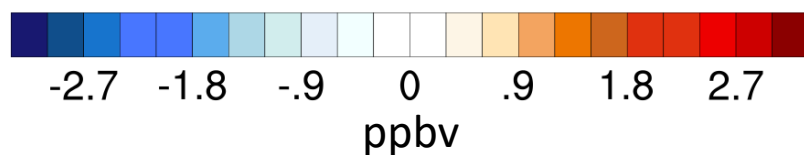
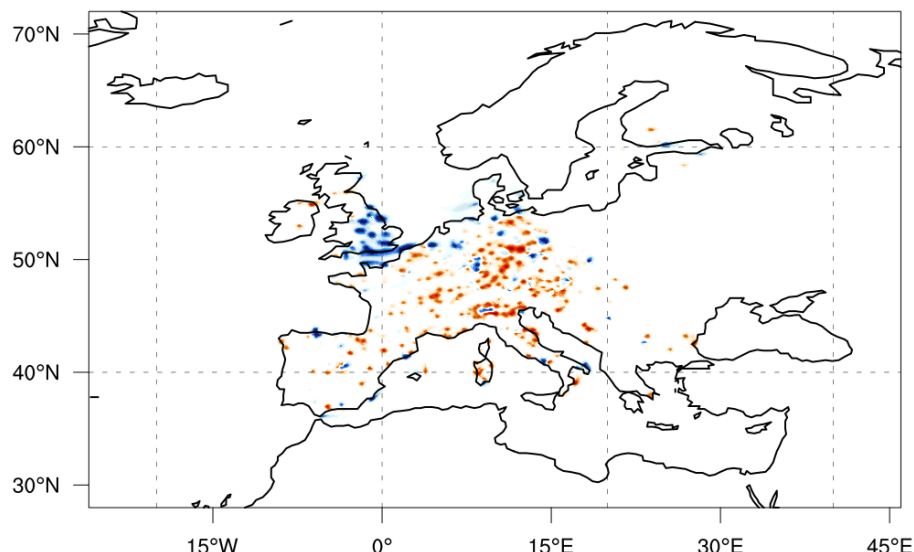
## 4DEnVar (Analysis-Forecast)

NO<sub>2</sub> Avg: 0.04 Max: 35.2 Min: -16.6



## 3D-Var (Analysis-Forecast)

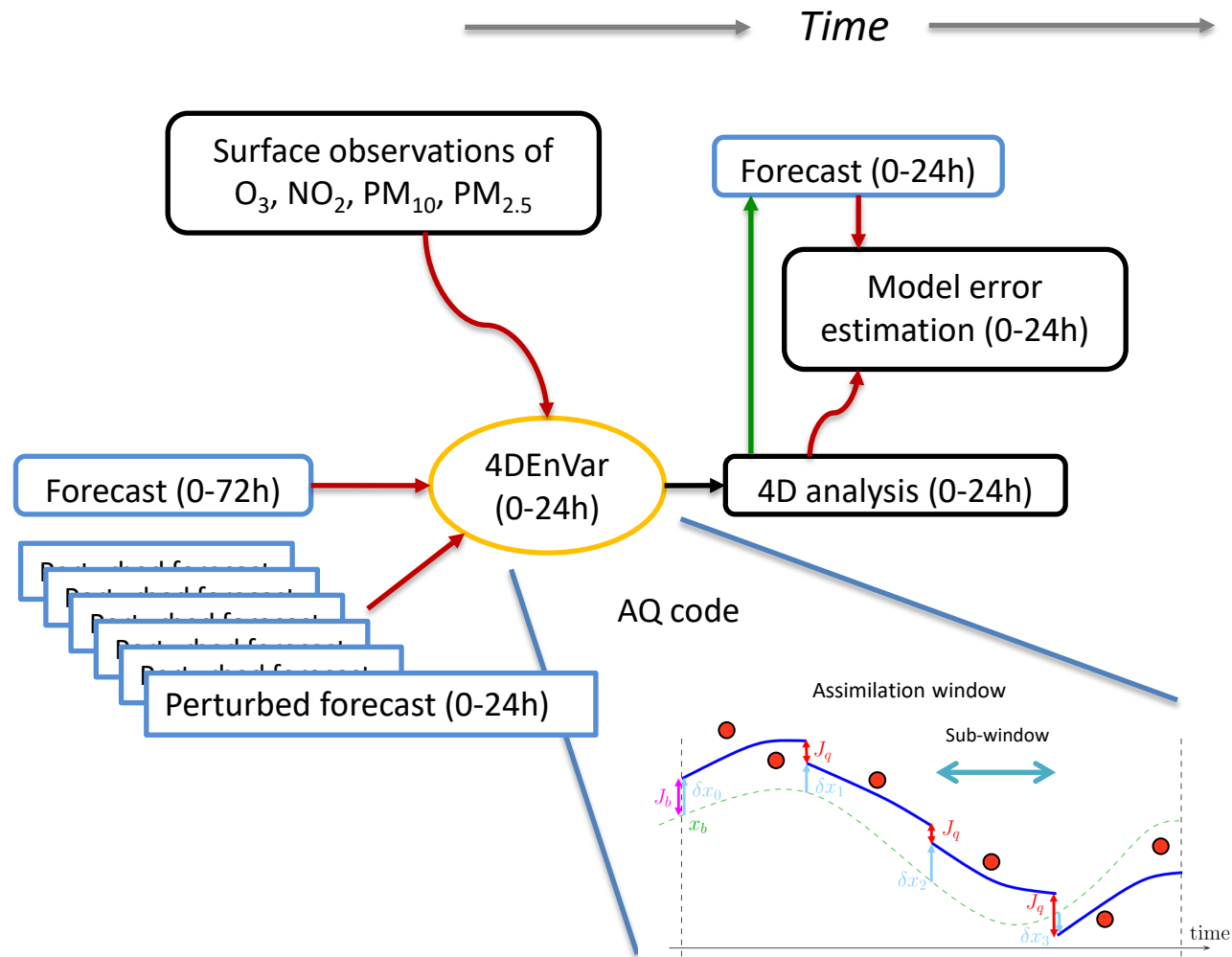
NO<sub>2</sub> Avg: 0.00 Max: 4.8 Min: -24.2



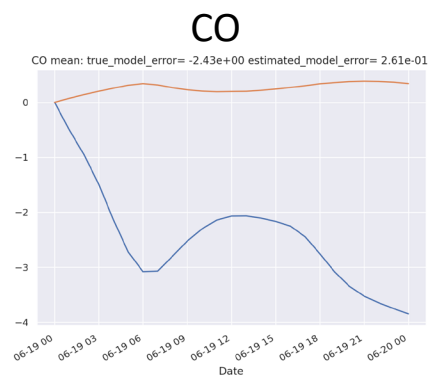
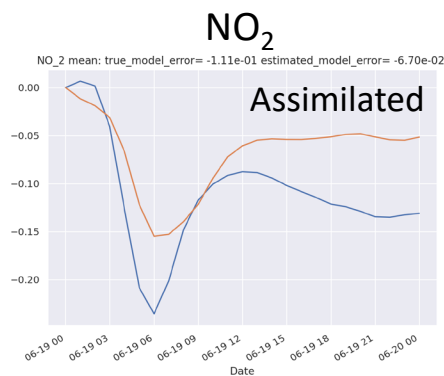
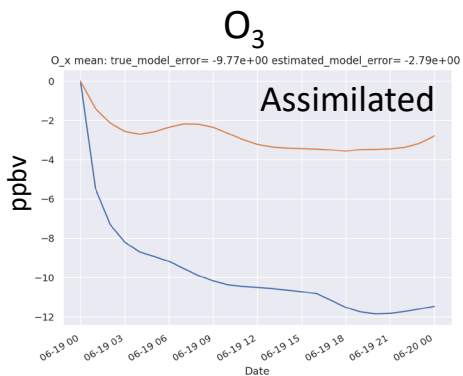
Note: 4DEnVar assimilates logarithms of concentrations, 3DVar absolute concentrations



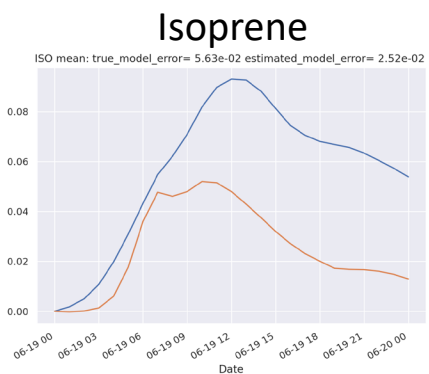
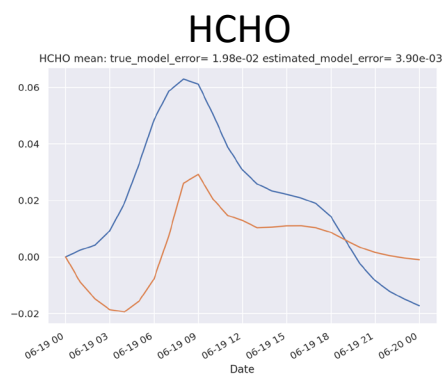
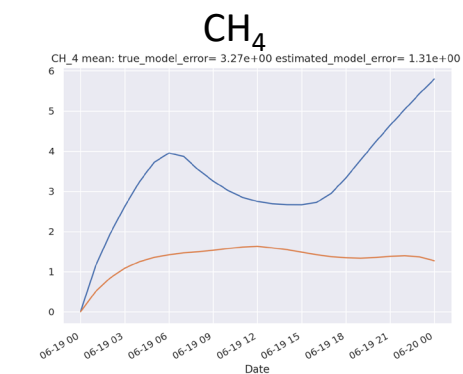
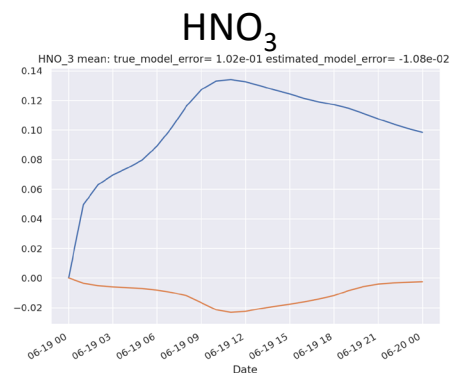
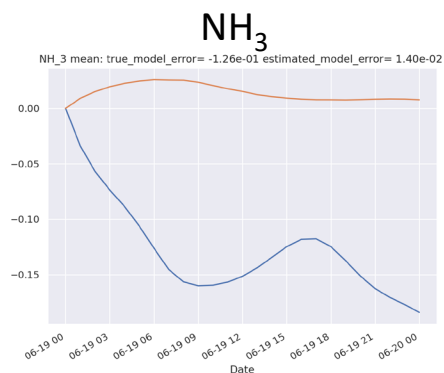
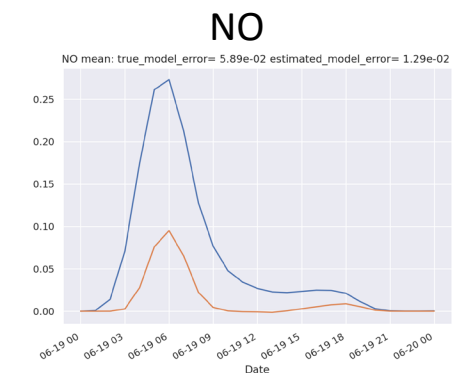
# Model error estimation



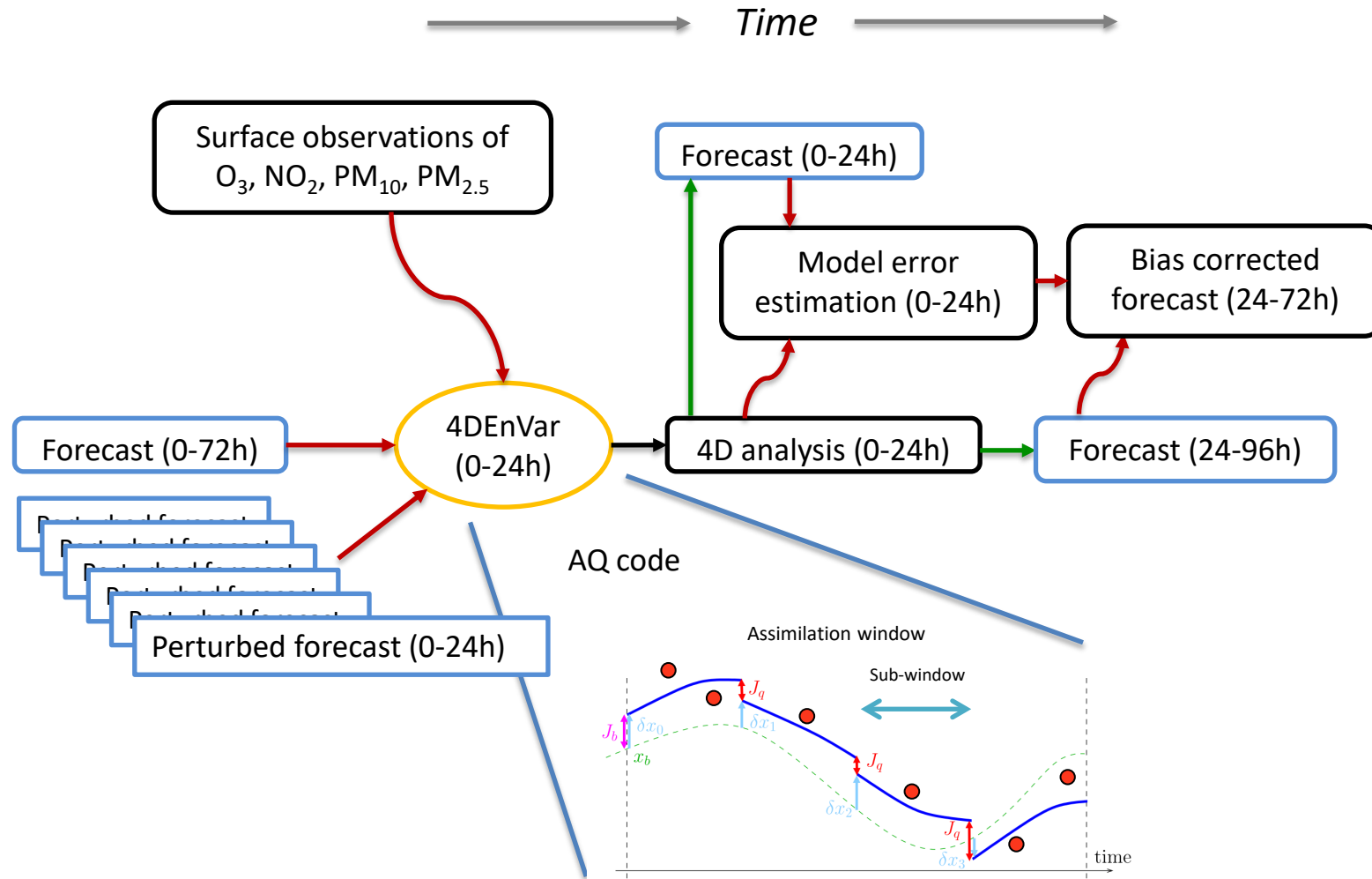
# Model error estimation: synthetic experiments



True model error  
Estimated model error  
(spatially averaged over  
continental surfaces)

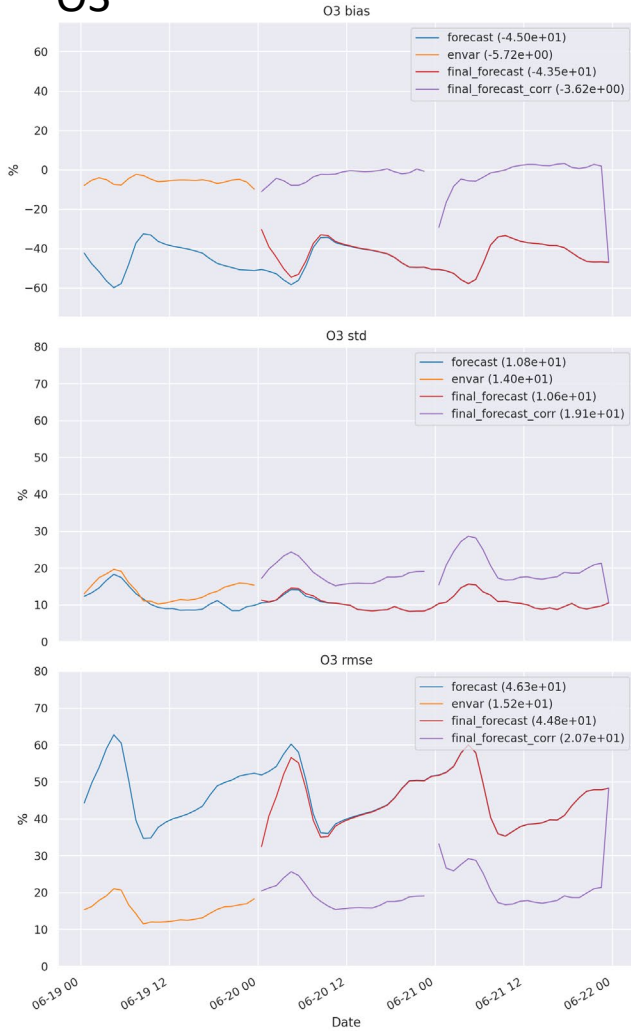


# Bias correction

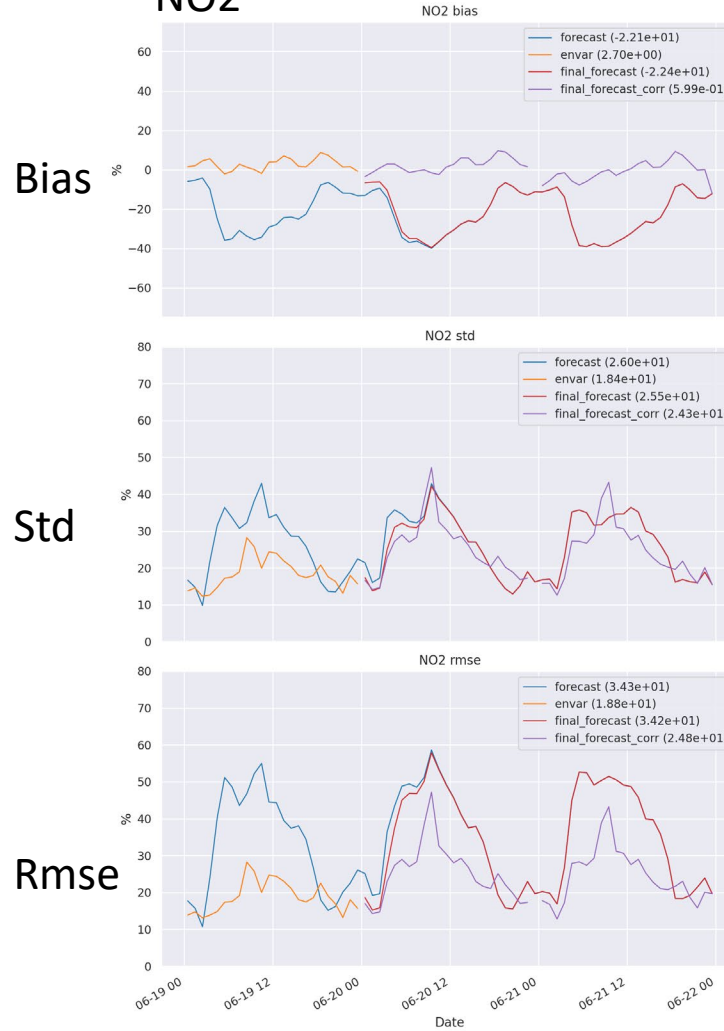


# Bias correction: synthetic experiments

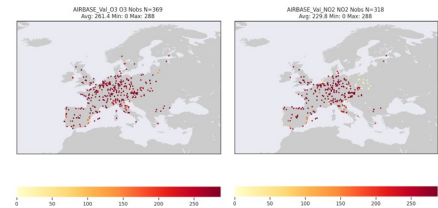
O3



NO2

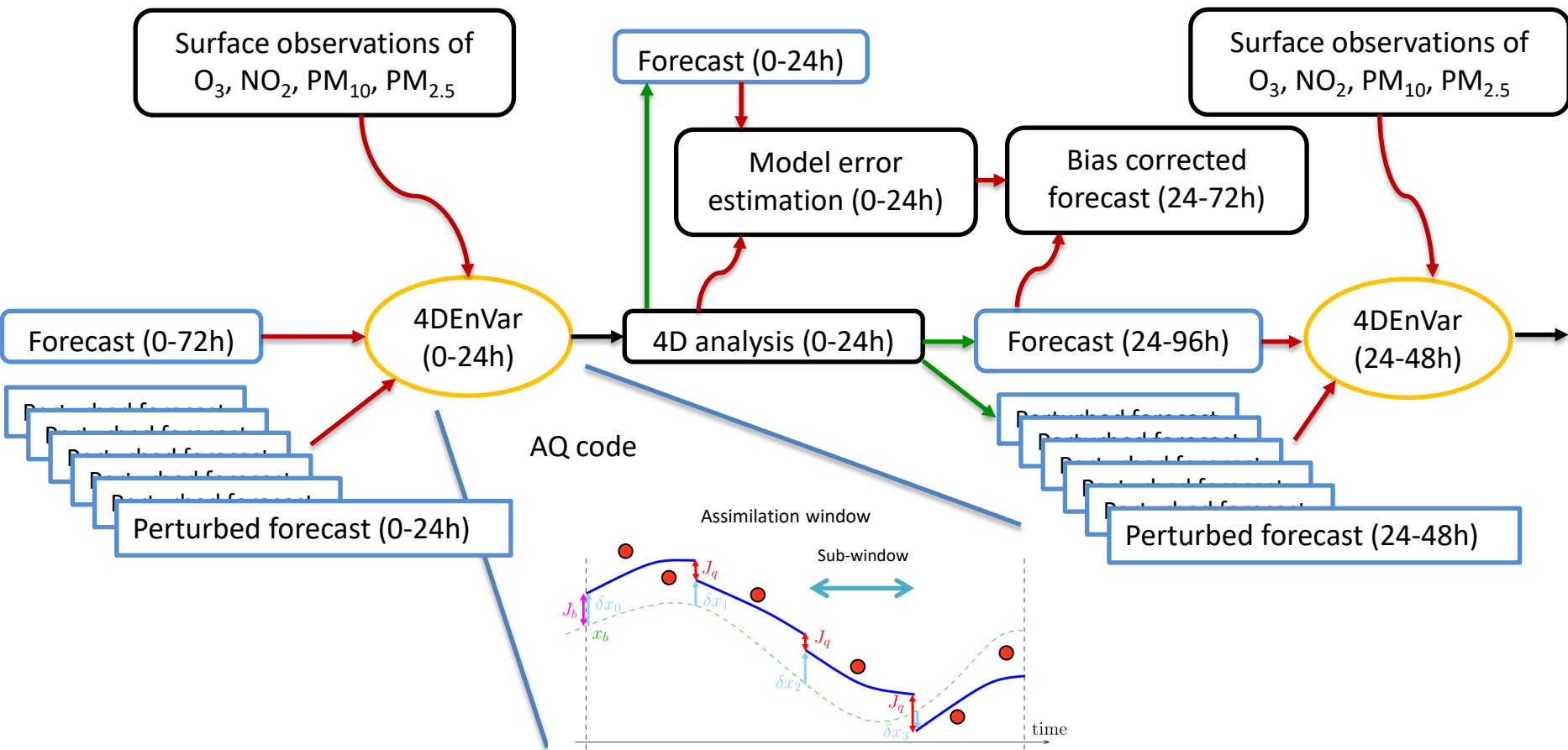


- Forecast (72h)
  - 4DEnVar analysis (24h)
  - Forecast initialized with the analysis (48h)
  - Bias corrected forecast (48h)
- (averaged over all validation stations)



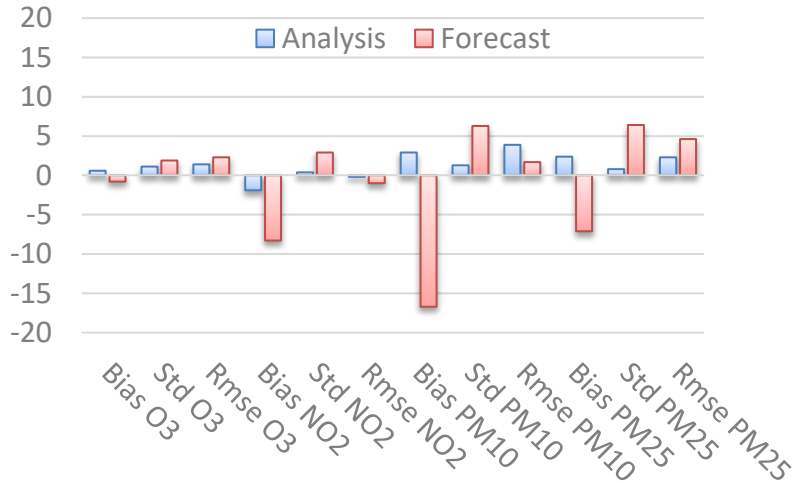
# Assimilation cycles with real observations

Time →



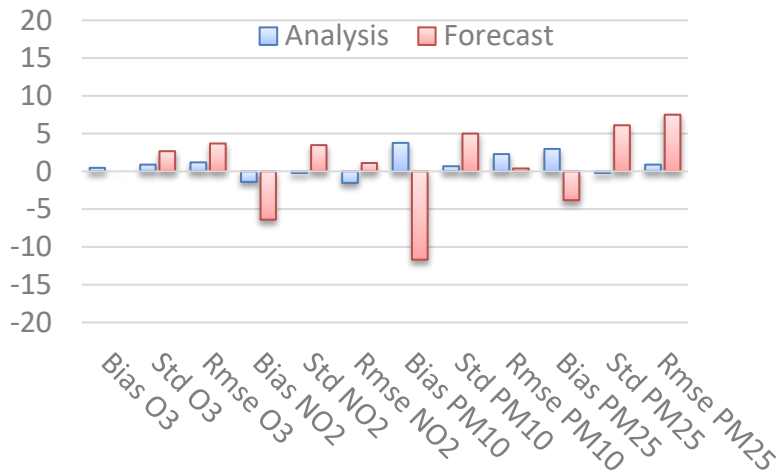
# Assimilation cycles: validation statistics

## Winter episode

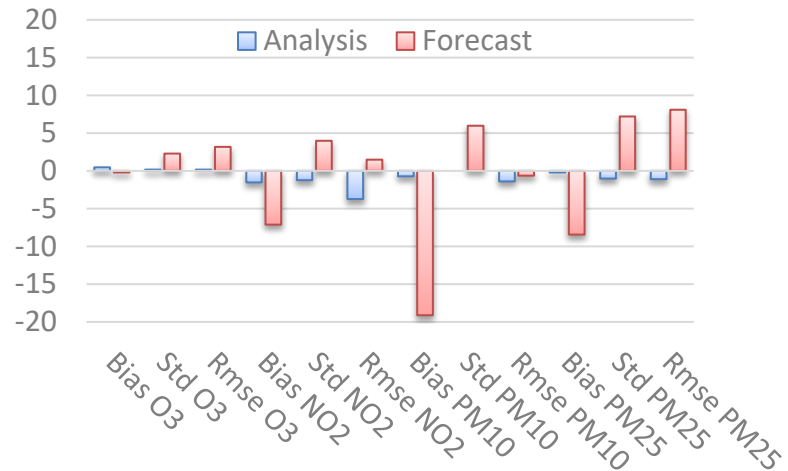


Median improvement of analysis and forecast skills (%) with respect to the operational 3DVar over all validation sites (negative values mean improvement)

## Summer episode



## Summer episode (larger localiz.)






# Conclusions and perspectives

- ✓ **Developed a model-agnostic 4DEnVar data assimilation code (AQ v1.1):**
  - Only inputs are forecast, ensemble members and observations
  - Handles a single analysis cycle with multiple time slots
  - Highly optimized (24 hours analysis in about 70 minutes on 200 CPU cores for 10km resolution CAMS domain, 30 ensemble members, 20 species and 7 vertical levels)
  - Open source and based on community libraries (JEDI, ATLAS)
  
- ✓ **Evaluated the DA and the bias correction strategy within a CAMS operational set-up:**
  - Used MOCAGE operational CAMS configuration
  - Developed the 4DEnVar workflow for MOCAGE
  - Synthetic and real observations experiments
  - See the D4.2-4.3 report for more details





# Conclusions and perspectives

- 4DEnVar algorithm shows promising results in a controlled environment (better than 3DVar)
  - Positive DA results with real observations but not game-changer wrt 3DVar
  - Forecast bias correction quite effective but at the cost of degraded standard deviation
- 
- Deeper evaluation of results for unobserved species
  - Lumping of coemitted species in ensemble perturbations
  - Towards more realistic ensembles that include uncertainties in the chemical scheme (CAM5 ensemble) and other key sources of error
  - Preparation for the assimilation of satellite data



[www.seedsproject.eu](http://www.seedsproject.eu) | [info@seedsproject.no](mailto:info@seedsproject.no)



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