10th International Symposium on Data Assimilation
Kobe, Japan
October 21-25, 2024

ARIANET
A SUEZ company

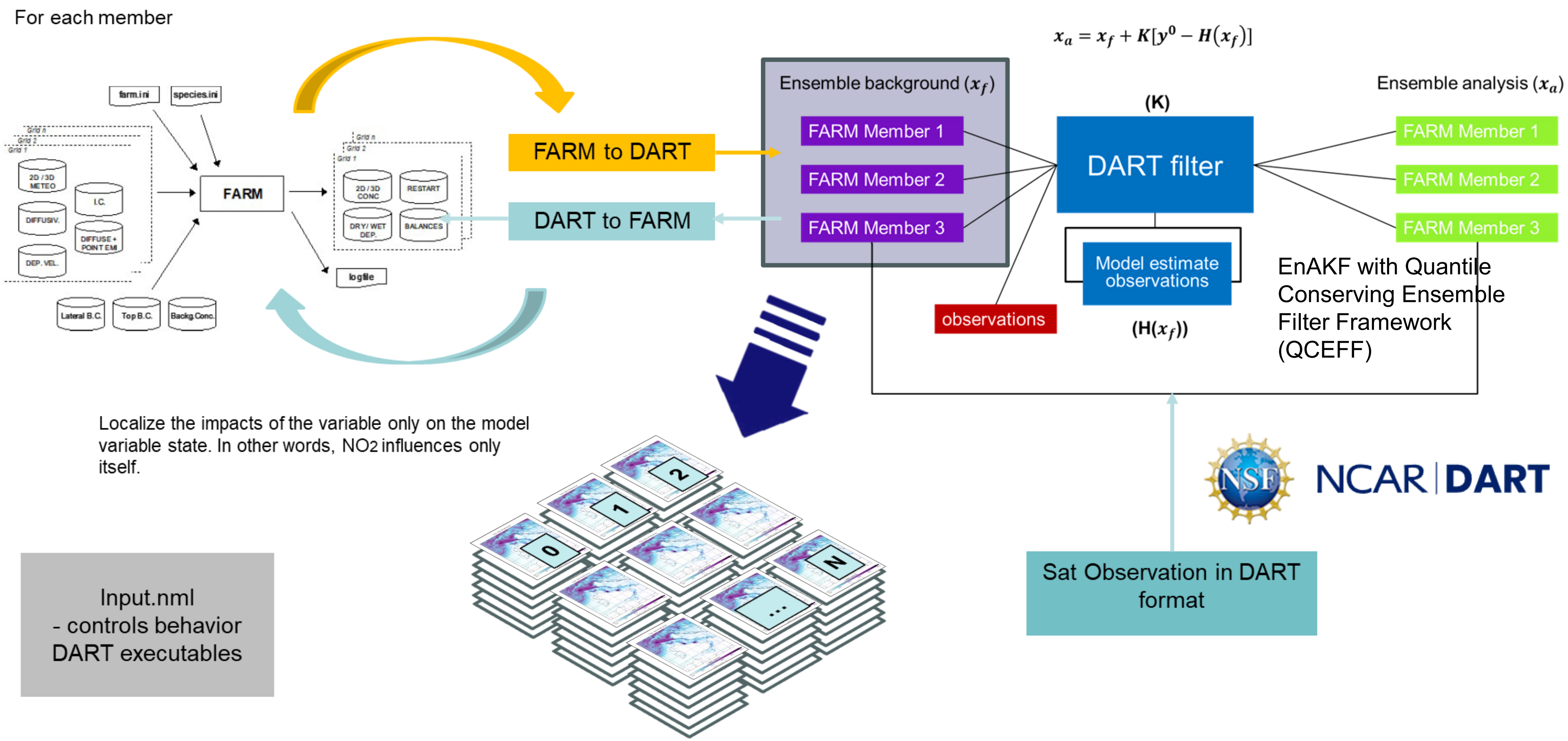
POLITECNICO MILANO 1863

Machine Learning methodology for generating ensemble members in Data Assimilation of Earth Observations

Alessandro D'Ausilio (ARIANET-SUEZ), **Giorgia De Moliner** (PhD Candidate, Politecnico di Milano), **Camillo Silibello** (ARIANET-SUEZ), **Giovanni Lonati** (Professor, Politecnico di Milano)

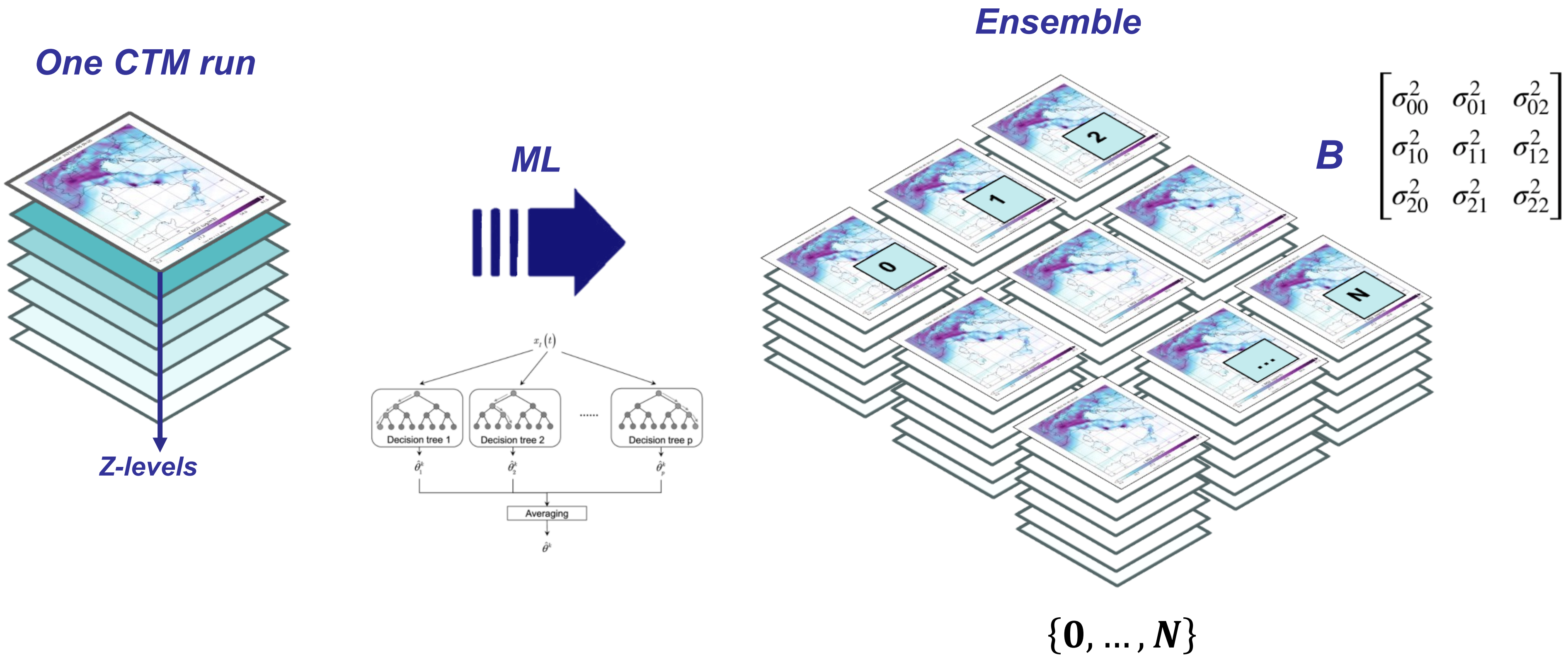
iride
GOVERNO ITALIANO | ASI | ESA

MEEO
Meteorological Environmental Earth Observation


For each member
farm.ini
species.ini
FARM
logfile
FARM to DART
DART to FARM
$x_a = x_f + K[y^0 - H(x_f)]$
Ensemble background (x_f)
FARM Member 1
FARM Member 2
FARM Member 3
(K)
DART filter
Model estimate observations
observations
($H(x_f)$)
Ensemble analysis (x_a)
FARM Member 1
FARM Member 2
FARM Member 3
EnAKF with Quantile Conserving Ensemble Filter Framework (QCEFF)
Localize the impacts of the variable only on the model variable state. In other words, NO2 influences only itself.
Input.nml
- controls behavior
DART executables
0
1
2
...
N
Sat Observation in DART format
NCAR | DART

Scope of the work

I. To generate a stationary ensemble of perturbated, realistic 3D concentration fields that provide a realistic estimate of the model uncertainties, without the need to run the model multiple times
II. To enable computationally-feasible, operational Data Assimilation (EnOI) of satellite data



IRIDE project

ARIANET
A SUEZ company

- A constellation of **Low Earth Orbit** (LEO) **satellites** to advance **environmental monitoring** and management from space

- Equipped with **optical**, **multispectral**, and **radar** technologies

- **High spatio-temporal resolution**, focused on the Mediterranean region

Funded by the European Union
NextGenerationEU

MEEO
Meteorological Environmental Earth Observation

ASI
Agenzia Spaziale Italiana

esa

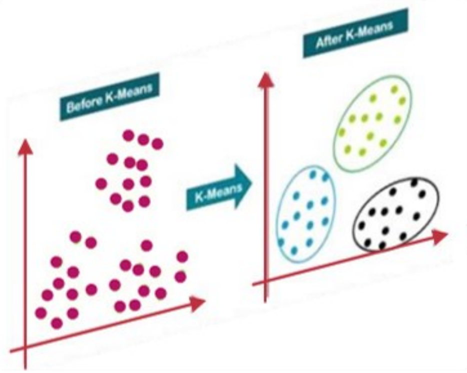
iride
GOVERNO ITALIANO | ASI | ESA

Methodology

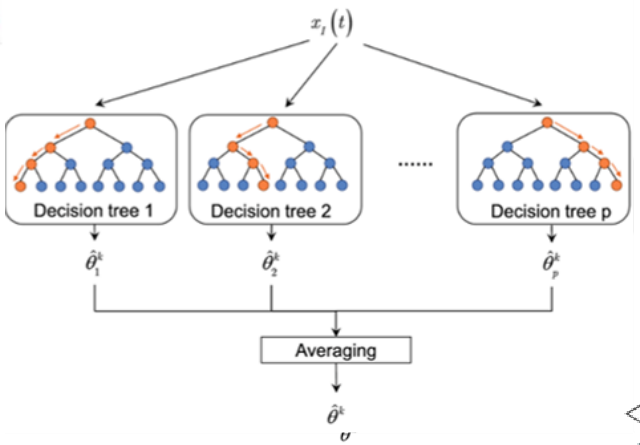
t_0	$C_{NO2,(t_0)}$	$C_{i,(t_0)}$	$P_{(t_0)}$	REL	$T_{(t_0)}$	$Sp_{(t_0)}$	$C_{NO2,(t_0-1)}$	$C_{NO2,(t_0-2)}$	…	$C_{NO2,(t_0-N)}$	…	$T_{(t_0-N)}$
2021-01-01 00:00:00												
2021-01-01 01:00:00												
…												
202x-xx-xx xx:xx:xx												

1. Inference Datasets Generation

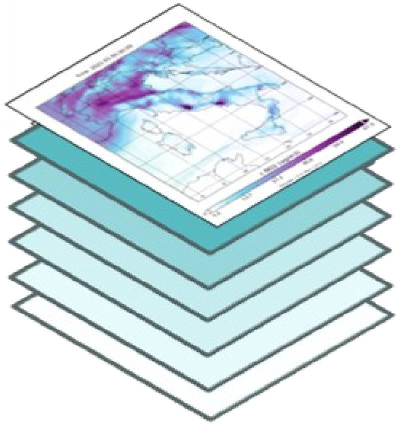
2. Dimensionality reduction



3. Models Training



4. Prediction and 3D field assembly



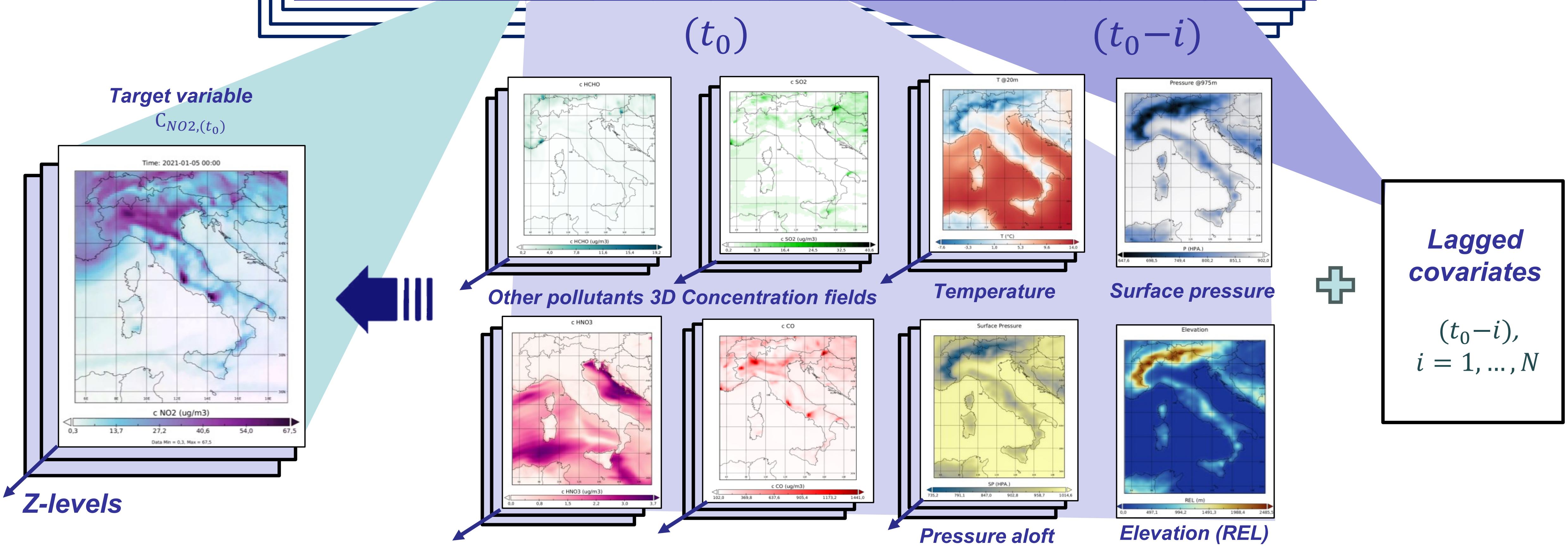
Step 1 : Inference Dataset Generation

ARIANET
A SUEZ company

Target variable | *Predictors*

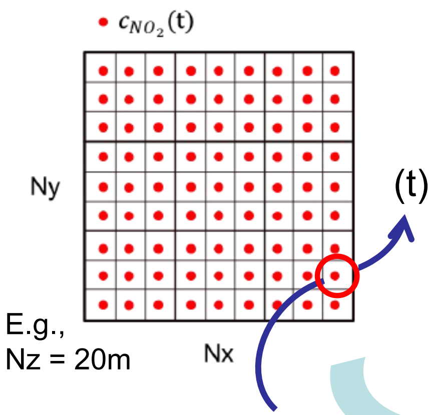
t_0	$C_{NO2,(t_0)}$	$C_{i,(t_0)}$	$P_{(t_0)}$	REL	$Sp_{(t_0)}$	$T_{(t_0)}$	$C_{NO2,(t_0-1)}$	$C_{NO2,(t_0-2)}$	…	$C_{NO2,(t_0-N)}$	…	$T_{(t_0-N)}$
2021-01-01 00:00:00												
2021-01-01 01:00:00												
…												
202x-xx-xx xx:xx:xx												

Z-levels



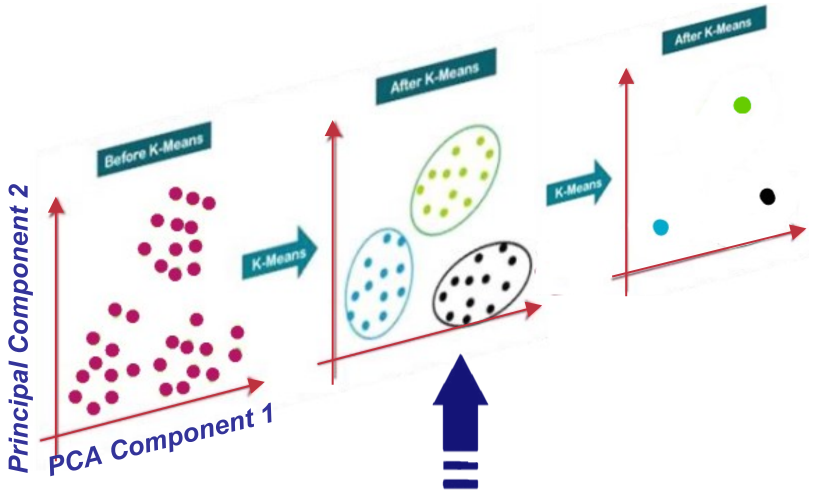
Step 2: PCA/K-Means Clustering

→ Training features reduced from O(10^7) to O(10^5)



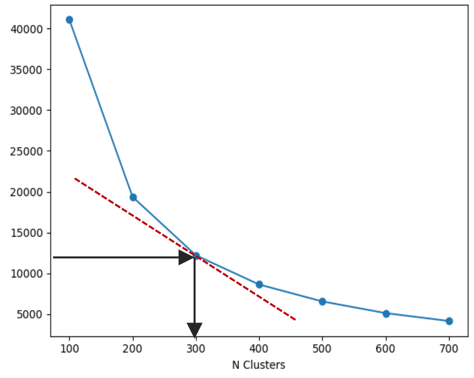
PCA

Time series with similar characteristics are grouped together



Mean cluster values are extracted as representatives of the entire cluster

Elbow method to define optimal number of clusters



Step 3: Models Training

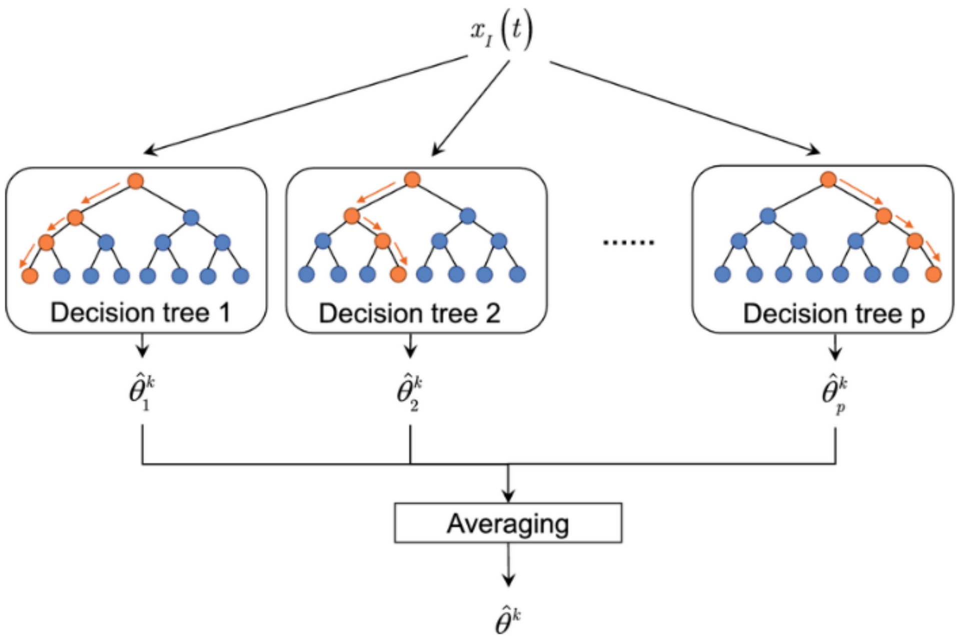
Target variable — *Predictors*

t_0	$\bar{C}_{NO2,(t_0)}$	$\bar{C}_{i,(t_0)}$	$\bar{P}_{(t_0)}$	$\bar{T}_{(t_0)}$	$\overline{S_P}_{(t_0)}$	$\bar{C}_{NO2,(t_0-1)}$	$\bar{C}_{NO2,(t_0-2)}$	…	$\bar{C}_{NO2,(t_0-N)}$	…	$\bar{T}_{(t_0-N)}$
2021-01-01 00:00:00											
2021-01-01 01:00:00											
…											
202x-xx-xx xx:xx:xx											

→ Reduced subset of features:
Instances of each cluster-representative timeseries

Z-levels

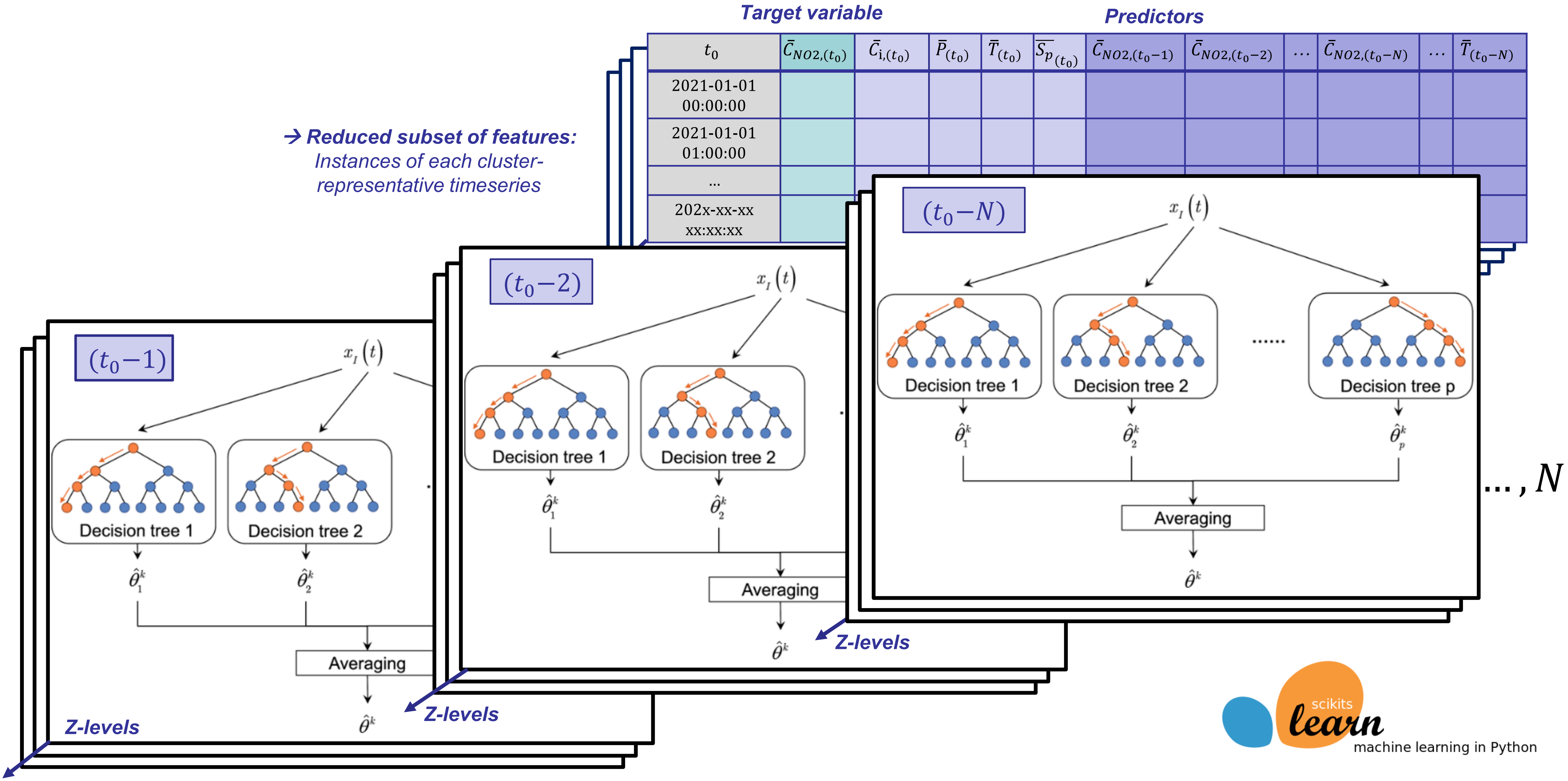
$$C_{NO2,(t_0)} \sim RF\left(predictors_{(t_0-k)}\right), \quad k = 0,1,\dots,N$$



scikits learn
machine learning in Python

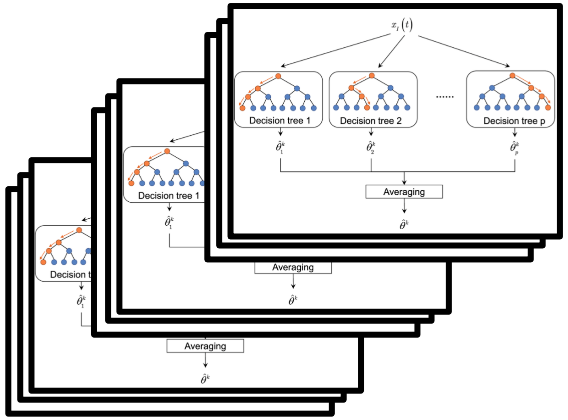
Step 3: Models Training

→ Reduced subset of features:
Instances of each cluster-representative timeseries

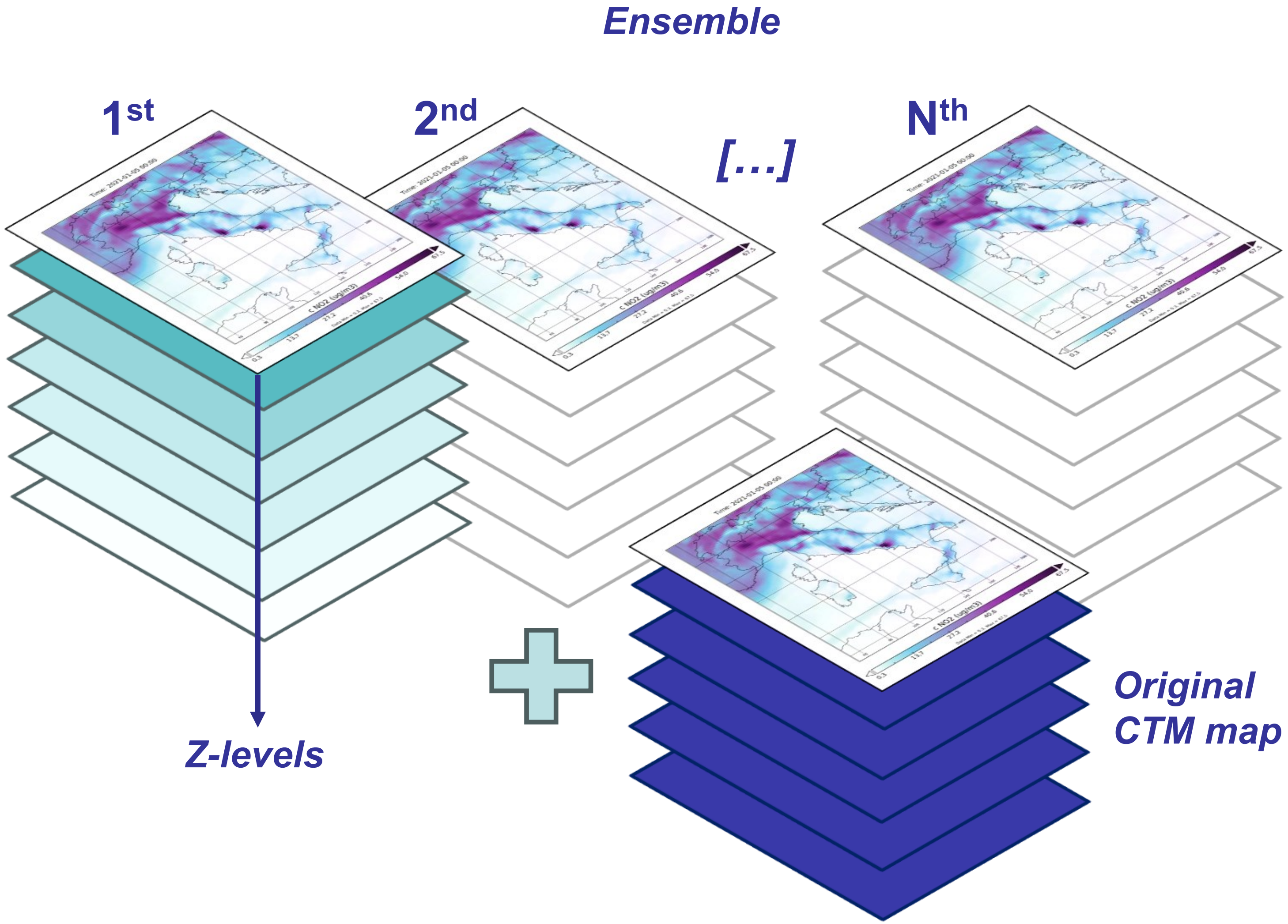


Step 4: Prediction and 3D field assembly

$$C_{NO2,(t_0)} \sim RF$$



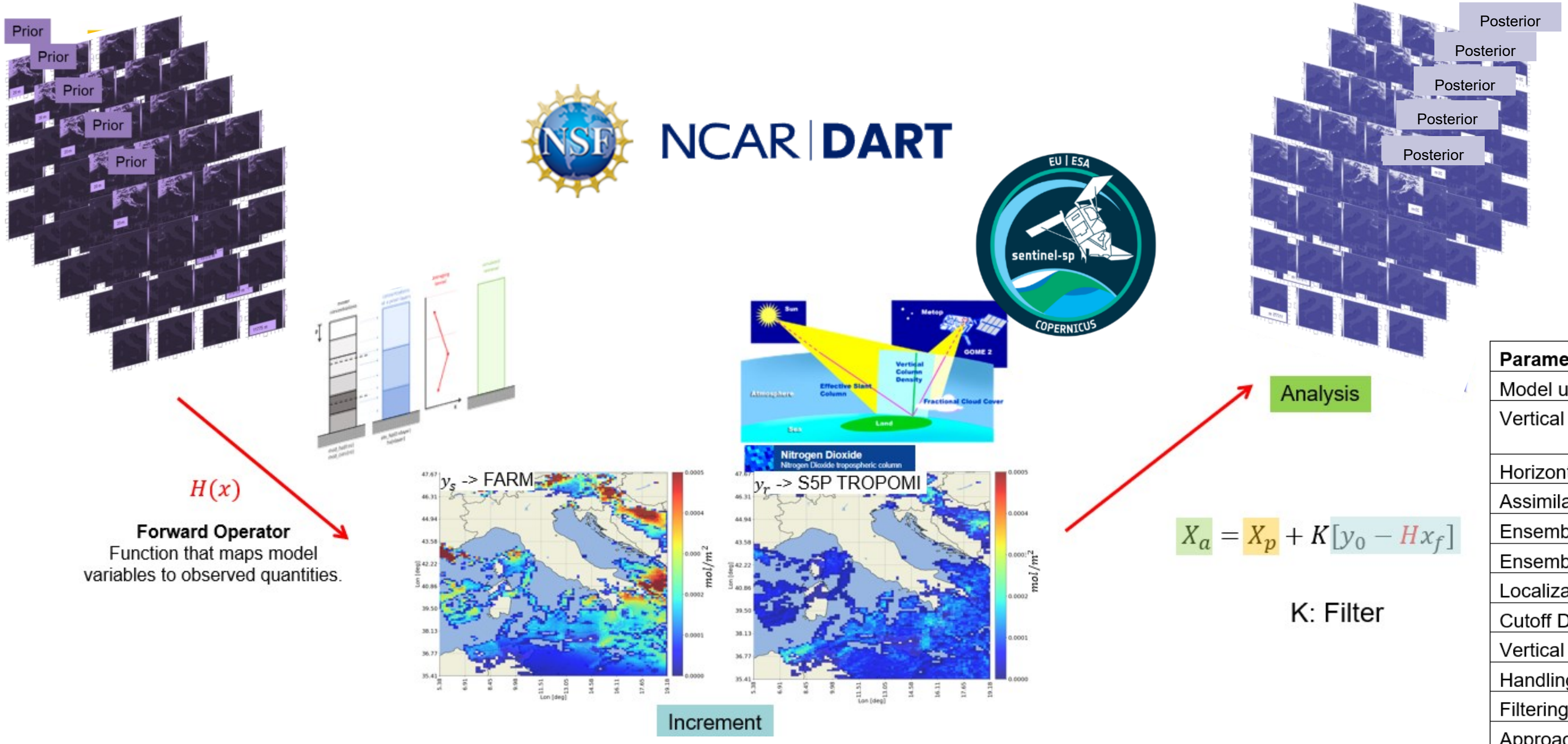
$$\{0, \ldots, N\} \; x \; \{0, \ldots, Z\}$$



Data Fusion experiment

→ The ML-generated ensemble was tested in an offline Data Assimilation of S5p **tropospheric NO_2 total columns** observations in a FARM model simulations over the Italian domain during a **two-month winter period**.

→ **Data Fusion/OI** as the analysis isn't used to update initial conditions for subsequent runs, viable under the hypothesis that **model uncertainties grow quickly → Stationary B**

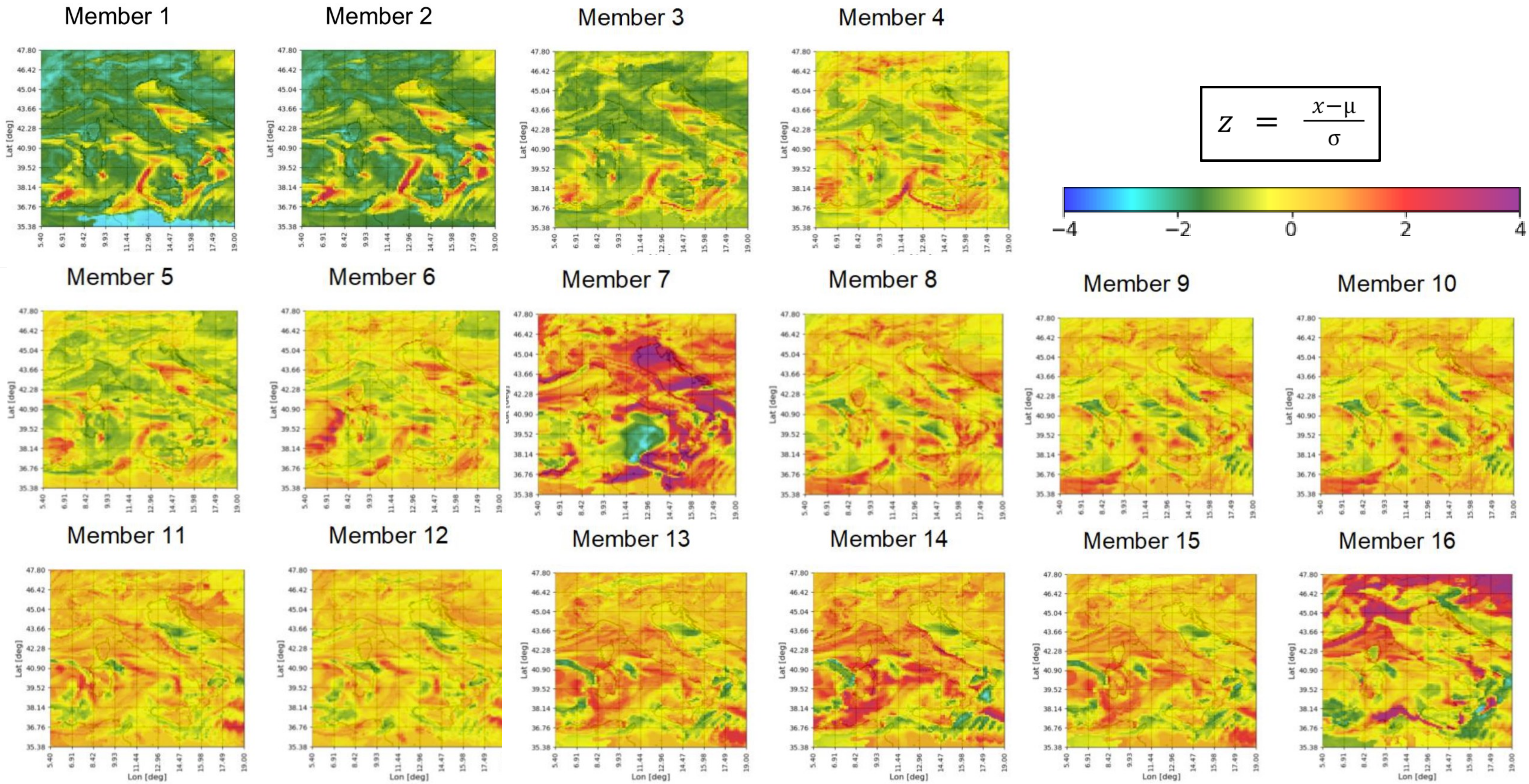


FARM-DART

Parameter	Description
Model used	FARM
Vertical Levels	16 levels rangin from 20m near the surface to 9290 m at the top level
Horizontal Resolution	0.104° x 0.15°
Assimilation Tool	DART
Ensemble	17 members provided as netCDF files
Ensemble Spread Management	Not applied
Localization Function	Gaspari-Cohn
Cutoff Distance / Horizontal Influence	0.0025 (~30km / 0.25°)
Vertical Influence	3.6 km
Handling Negative Concentrations	Quantile-Conserving Ensemble Filter (QCEFF)
Filtering Method	Ensemble Adjustment Kalman Filter (EAKF)
Approach	Data Fusion: The analysis does not influence the next timesteps. Background Covariance Matrix considered as static: EnOI

Figure 19. Summary Data Fusion experiment.

Ensemble insight – z-scores



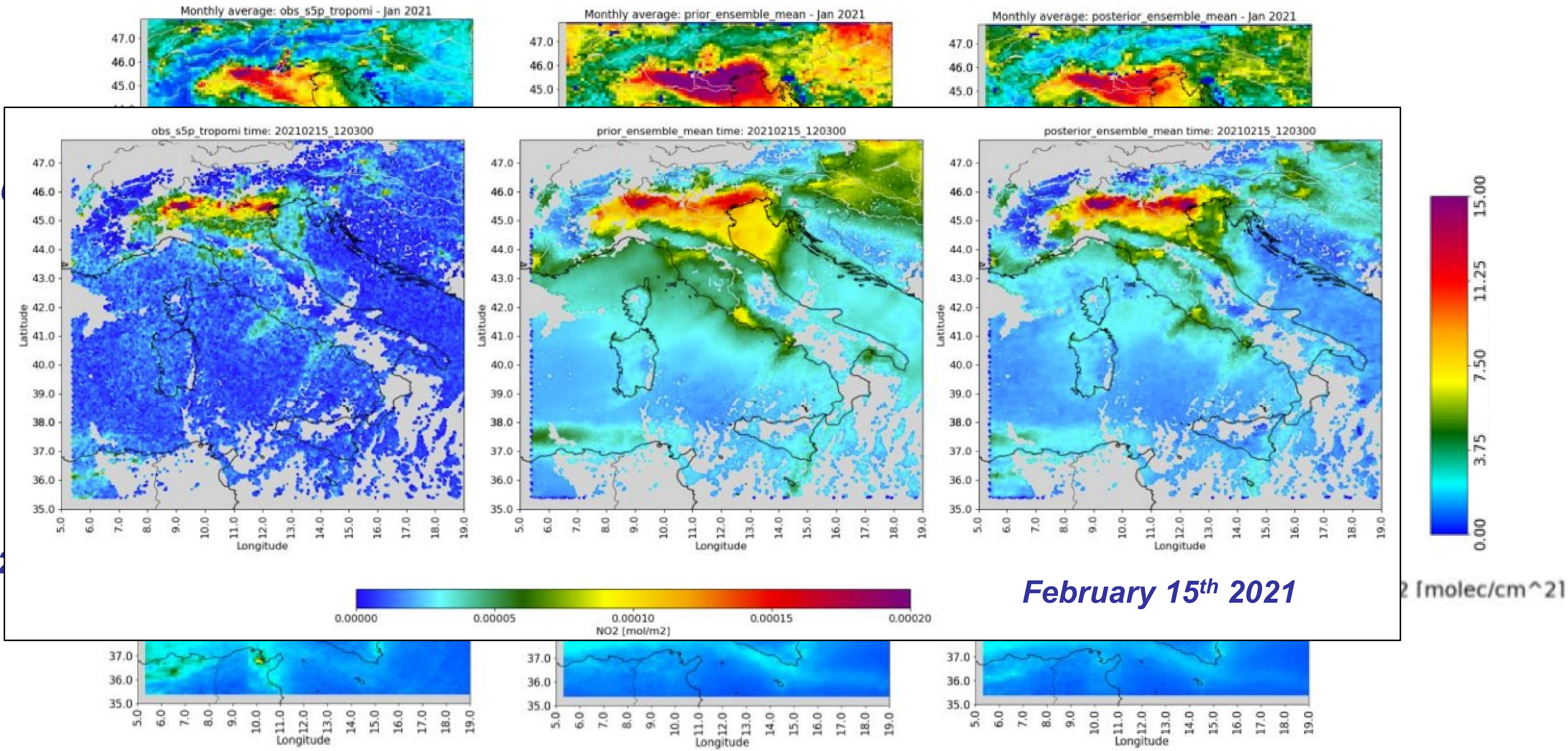
$$z = \frac{x - \mu}{\sigma}$$

Data Fusion Results – 1

S5p NO2 vcd observations | **Prior NO2 vcd ensemble mean** | **Posterior NO2 vcd ensemble mean**

January 2

February 2

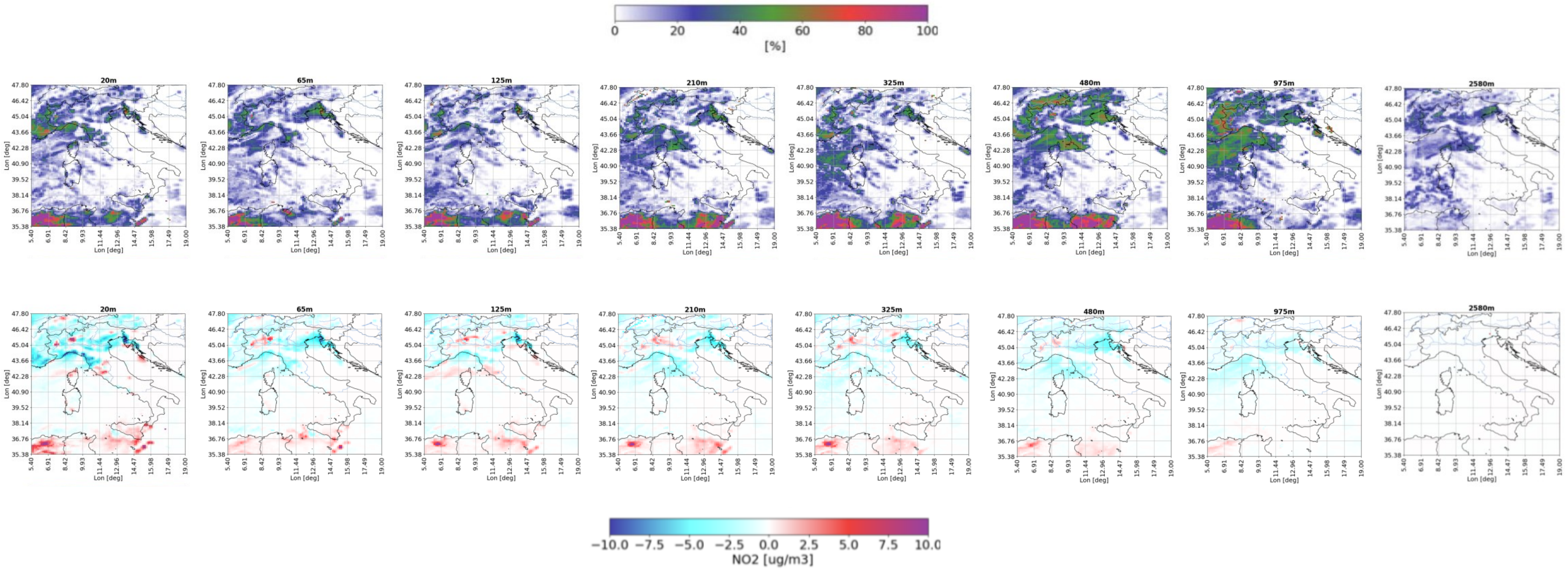


February 15th 2021

Monthly means

Data Fusion Results – 2

(prior-posterior)/prior



prior-posterior

Conclusions

- A **computationally efficient** alternative to conventional **ensemble generation** methods has been presented
- Leveraging on **multiple RF regressors**, an ensemble of CTM runs was synthetized; a statistical representation of the **uncertainties in the model's forecast** can be drawn
- Preliminary results show the presented methodology can capture **both diagonal and off-diagonal covariance matrix terms**
- By avoiding the computational burden of starting N perturbated runs, **operational DA** of satellite data for air quality applications can be feasible for national level's PAs→ *towards geostationary Sentinel-4*
- Further work will focus on enabling **online DA**, as well as on anchoring the ensemble mean to the original CTM run

ARIANET

A SUEZ company

10th International Symposium on Data Assimilation
Kobe, Japan
October 21-25, 2024

POLITECNICO MILANO 1863

Machine Learning methodology for generating ensemble members in Data Assimilation of Earth Observations

Alessandro D'Ausilio (ARIANET-SUEZ), **Giorgia De Moliner** (PhD Candidate, Politecnico di Milano), **Camillo Silibello** (ARIANET-SUEZ), **Giovanni Lonati** (Professor, Politecnico di Milano)

iride

GOVERNO ITALIANO | ASI | ESA

MEEO
Meteorological Environmental Earth Observation