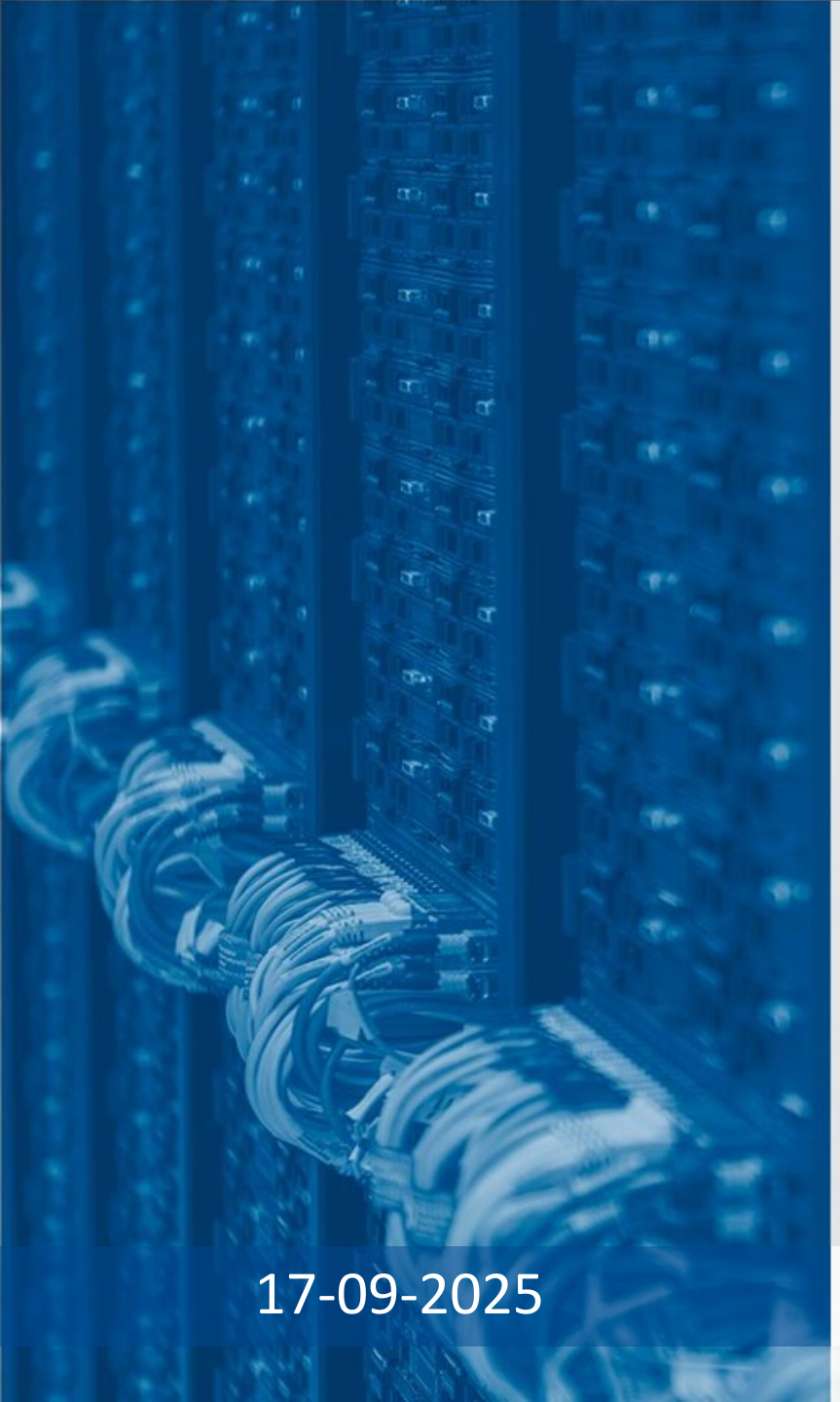


Barcelona Supercomputing Center
Centro Nacional de Supercomputación

BSC Update

Jeronimo Escribano, Emanuele Emili, Oriol Jorba, Miriam Olid, Eleni Karnezi, Rafaela Cruz Alves, Carlotta Gilè, Guillaume Monteil, Jayoung Yun, Andrea Piacentini, Miguel Hortelano, Carlos Pérez García-Pando

17-09-2025

ICAP 2025, Fukuoka, Japan

Outline

- Atmospheric composition group at BSC

- MONARCH aerosol forecasts
  - ICAP global forecast updates
  - MONARCH-dust SDS-WAS contribution: Update on DA and new products

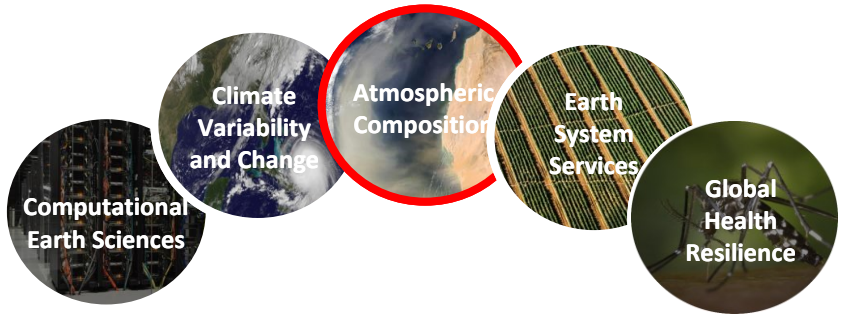
- Other highlights
  - Joint Surface PM and AOD assimilation
  - JEDI (AQ) 4DEnVar implementation for assimilation of surface
  - Forecasts of AOD from observations

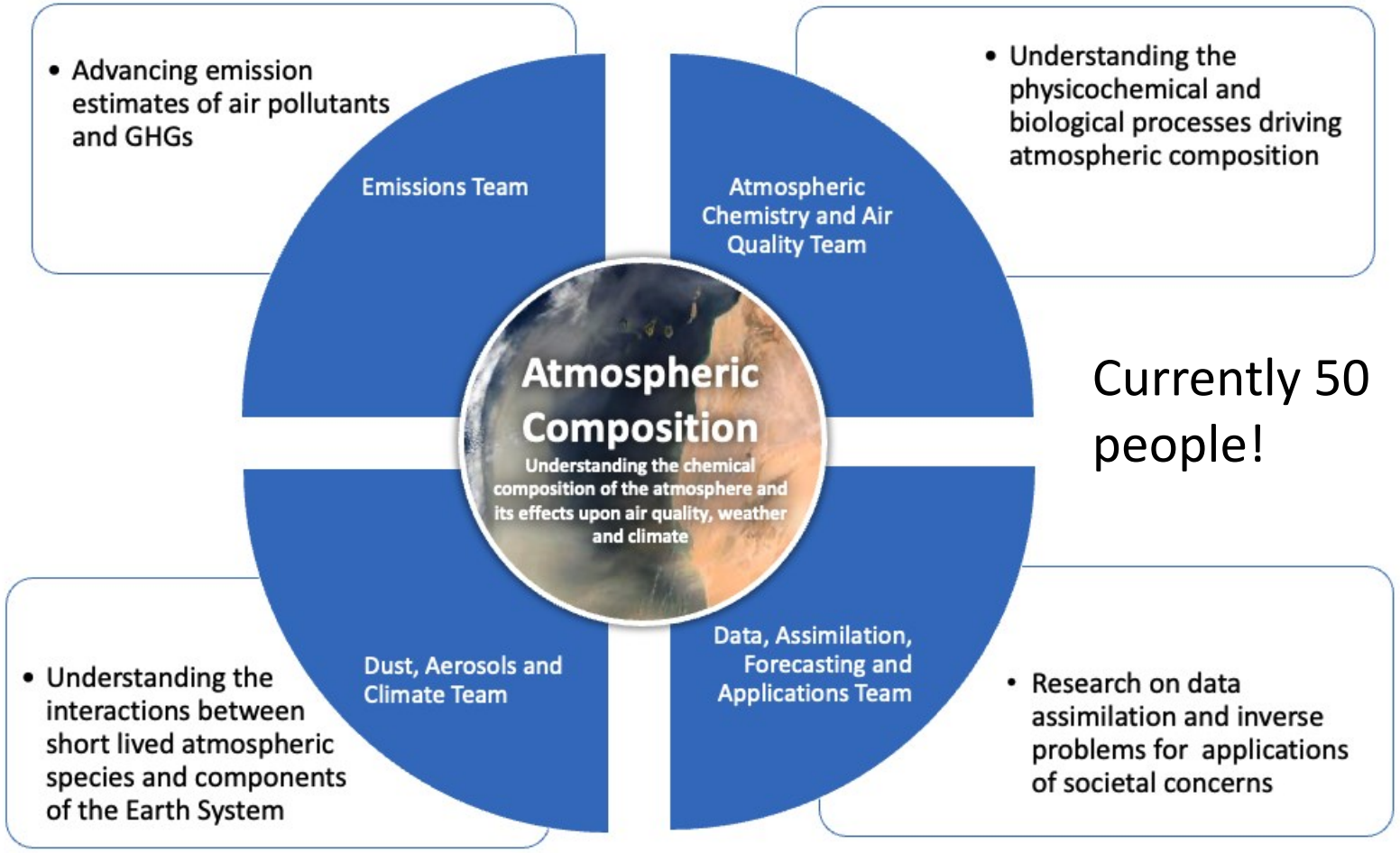
The Atmospheric Composition group at BSC

Understand, constrain and predict the spatiotemporal variations of atmospheric pollutants across scales along with their effects upon air quality, health, weather and climate.

BSC Earth Science department:

- ~250 people
- Rely on competitive funding from EC, Copernicus, private sector, ESA, Spanish and regional governments





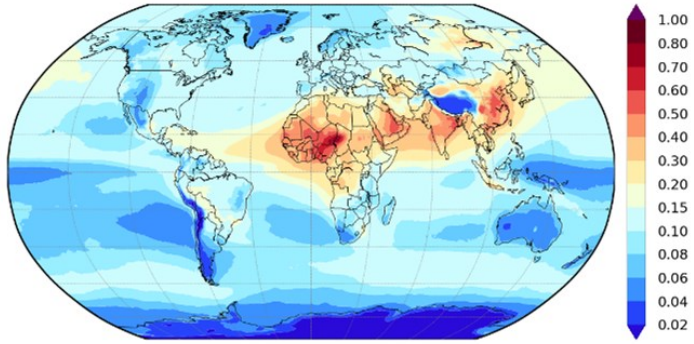
Currently 50 people!

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

MONARCH aerosol forecasts

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Operational forecasts in 2025

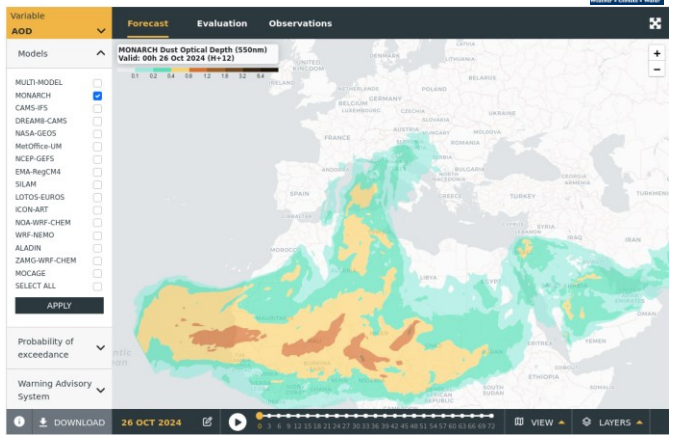


Global aerosols	Configuration
Meteorology	Inline NMMB
Initial condition	GFS 0.5x0.5 deg
Resolution	0.7x0.5 deg
Levels	48
Forecast range	5 days
Output frequency	6 hours
Species	Dust, Sea Salt BC, OC (POA,SOA) Sulfate
Size Bins	8 (dust, salt) bulk for others
Chemistry	Climatology
Antho. & Biogenic Emission	CAMS-GLOB-ANTv4.2 (anthro) HTAPv2 (aviation), MEGANv2.04 (biogenic)
Bio. Burn. Emissions	GFAS (daily)

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

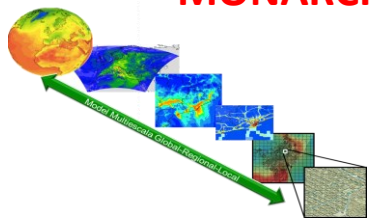
aemet Agencia Estatal de Meteorología

World Meteorological Organization

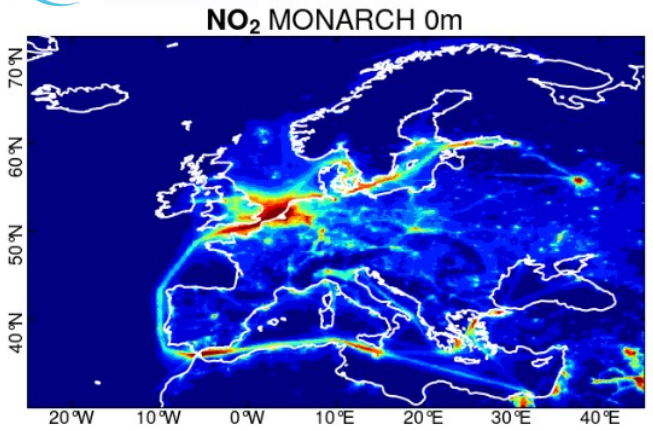


SDS-WAS	Configuration
Meteorology	Inline NMMB
Initial and boundary conditions	GFS 0.5x0.5 deg
Resolution	0.1x0.1 deg
Levels	40
Forecast range	3 days
Output frequency	3 hours
Species	Dust
Size Bins	8
Antho. & Biogenic Emission	NA
Bio. Burn. Emissions	NA

MONARCH



Atmosphere Monitoring Service



CAMS regional	Configuration
Meteorology	Inline NMMB
Initial and boundary conditions	IFS and CAMS GLOB
Resolution	0.15x0.15 deg
Levels	24
Forecast range	4 days
Output frequency	hourly
Species	Dust, Sea Salt BC, OC (POA,SOA) Sulfate, Ammonium, Nitrate
Size Bins	8 (dust, salt), 3 nitrate, bulk BC, OA, ammonium, sulfate
Chemistry	CB05 plus chlorine chemistry, Fast-J photolysis
Antho. & Biogenic Emission	CAMS-REGv6.1 (anthro), MEGANv2.04 (biogenic)
Bio. Burn. Emissions	GFAS (hourly)

ICAP MONARCH model upgrades

Emanuele Emili, Miriam Olid, Oriol Jorba

U1 (April 2024)

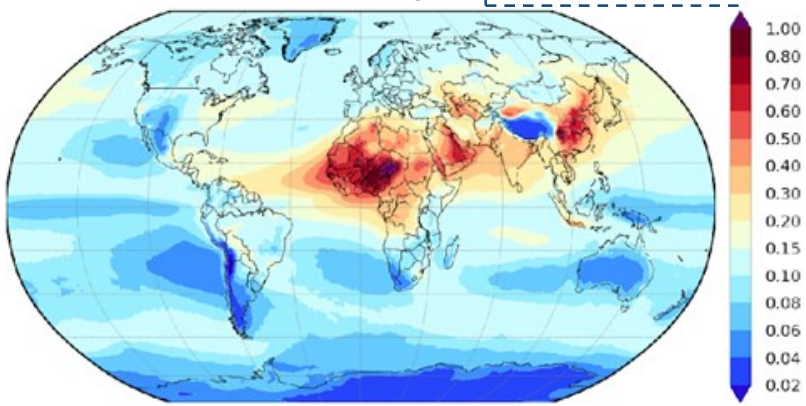
- Climatological gases -> Full online chemistry (CB05 mechanism)
- 72 gases and 34 aerosols tracers
- Inclusion of ammonium and nitrate aerosols
- Heterogeneous chemistry on coarse particles (dust and sea salt, EQSAM + irreversible uptake on coarse)
- Updated anthropogenic emissions (CAMS-GLOB v4.2)
- Updated SOA formation, desert dust (emission scheme, spheres -> spheroids), sea salt (emissions)
- Increased outputs (gases, speciated PMs) and frequency (6h -> 3h)
- *Same aerosols-chemistry scheme as in the MONARCH Copernicus air-quality regional forecasts*

U2 (Dec 2024)

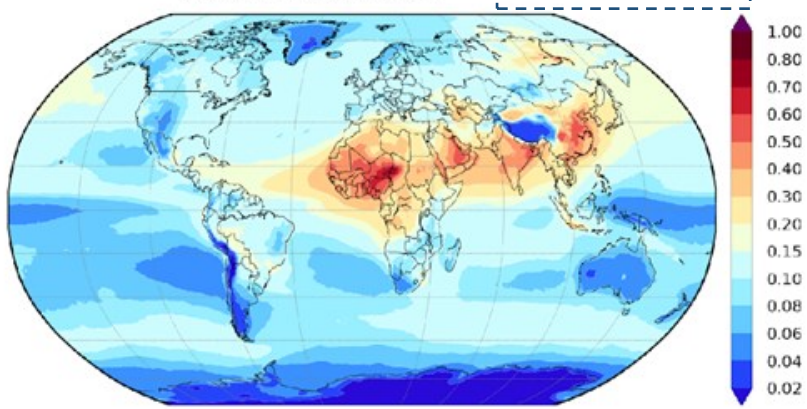
- Minor bug fixes
- PM10 and PM2.5 outputs
- Fix on BB emission factors
- Same dust scheme as in the MONARCH SDS-WAS regional forecasts

2021

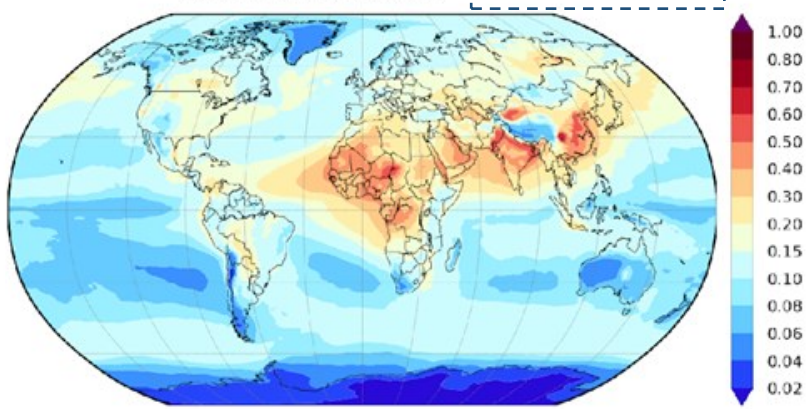
Previous



U1



MERRA-2

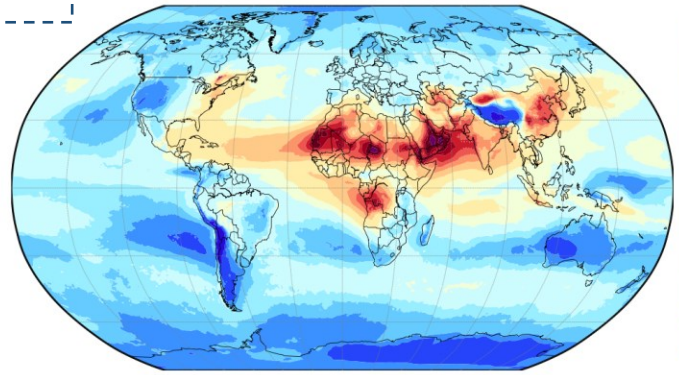


E. Emili, E. Karnezi

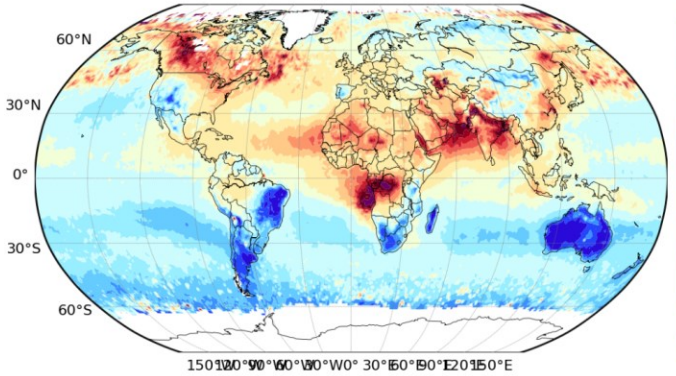
Previous

(2023)

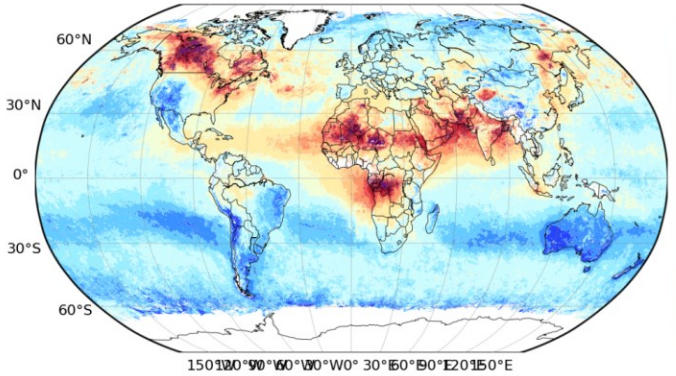
JJA_2023 aod_total a0yha



2023 JJA MODIS AOD



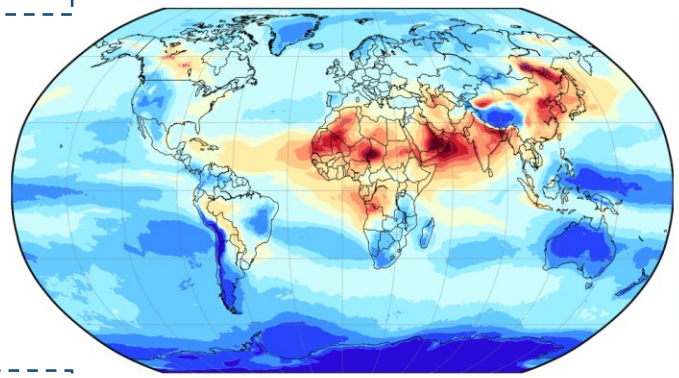
2023 JJA VIIRS AOD



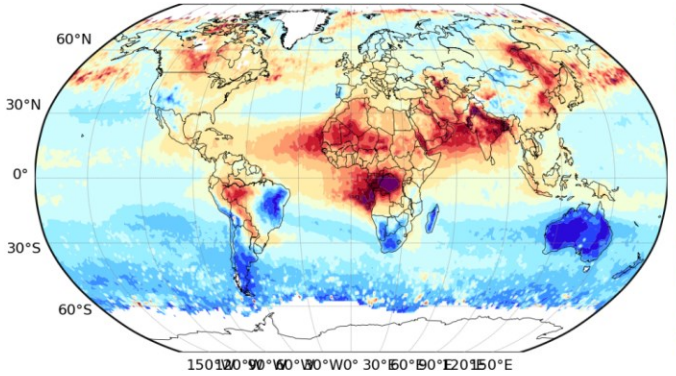
U1

(2024)

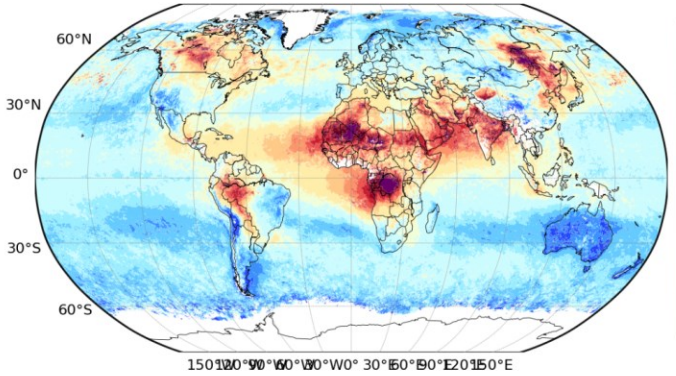
JJA_2024 aod_total a7eja



2024 JJA MODIS AOD



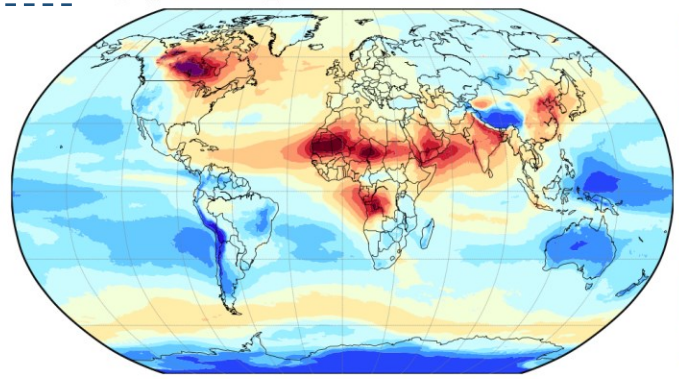
2024 JJA VIIRS AOD



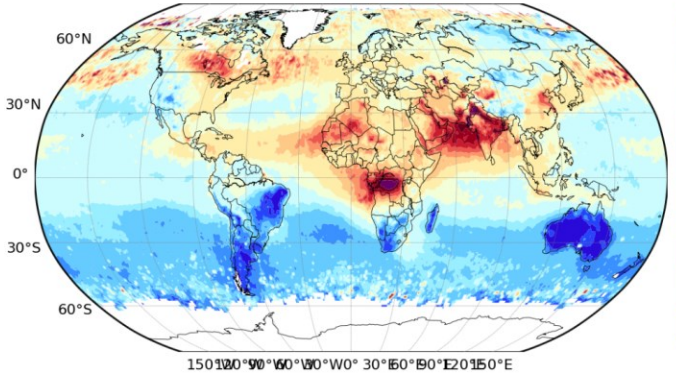
U2

(2025)

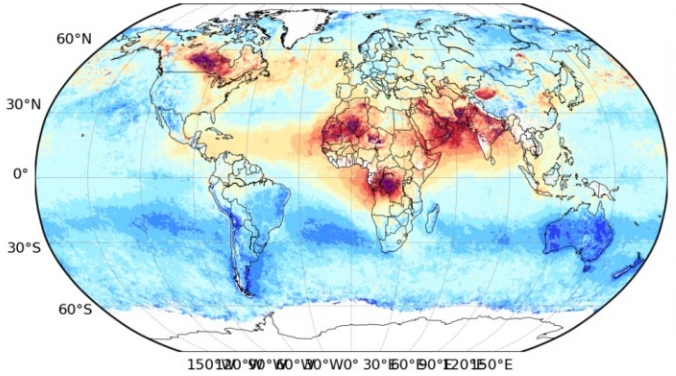
JJA_2025 aod_total a8mwa



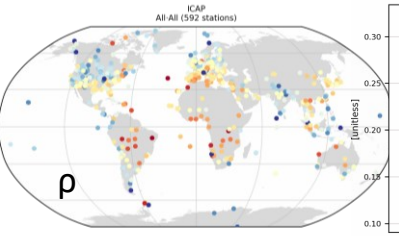
2025 JJA MODIS AOD

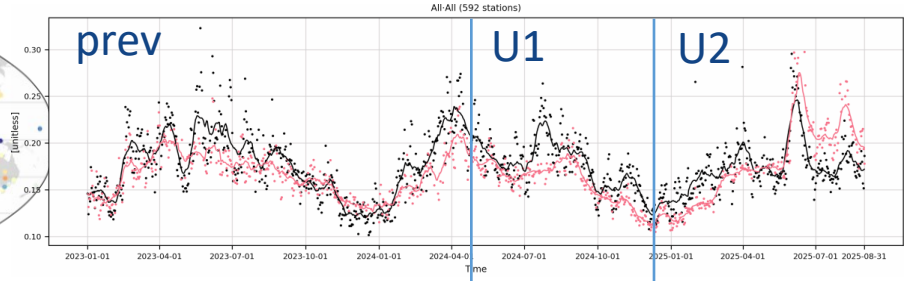


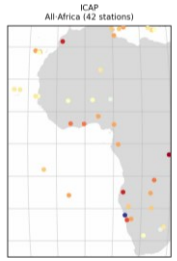
2025 JJA VIIRS AOD

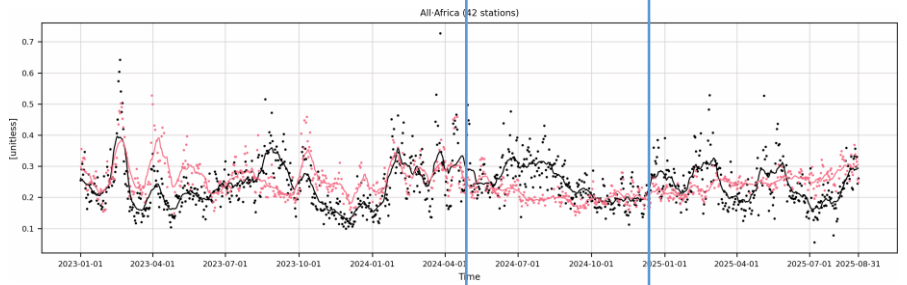


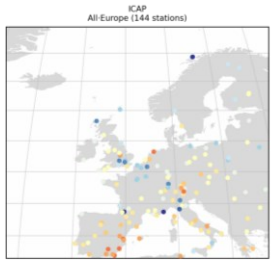
AOD (AERONET)

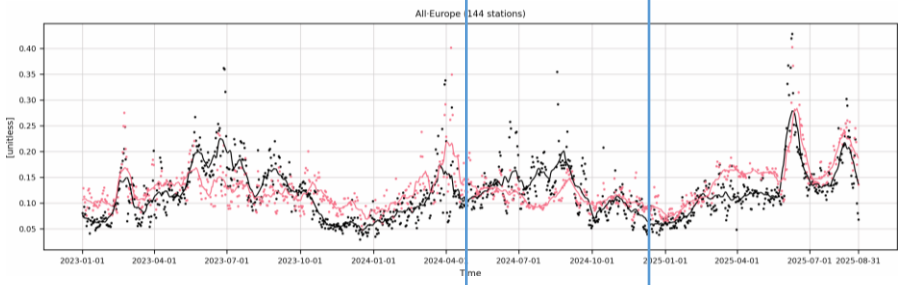


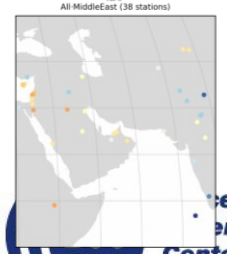


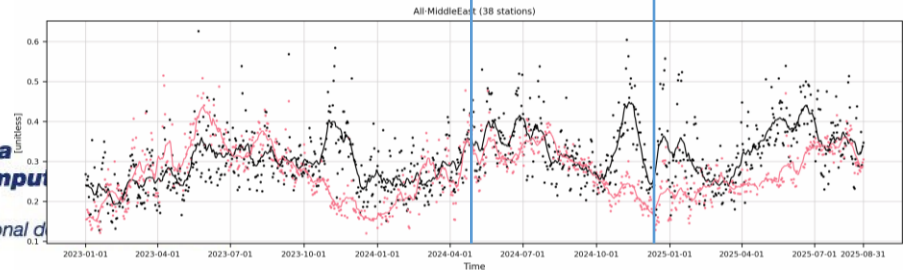


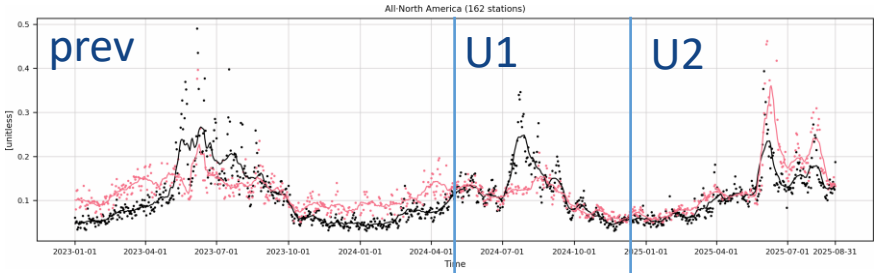


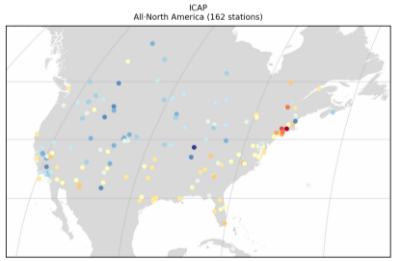


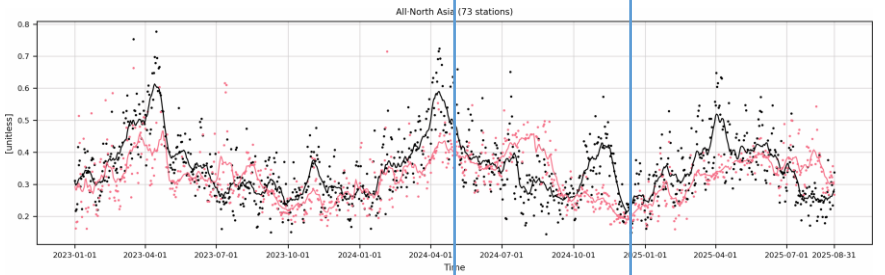


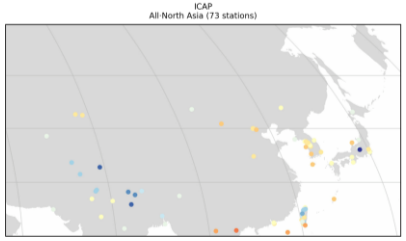


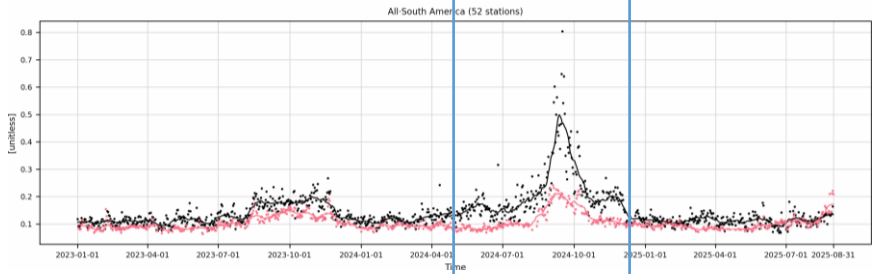


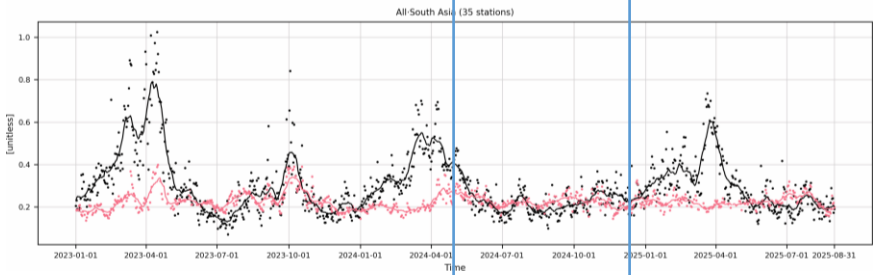


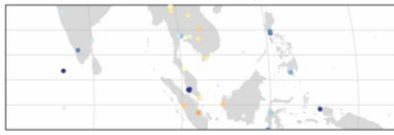


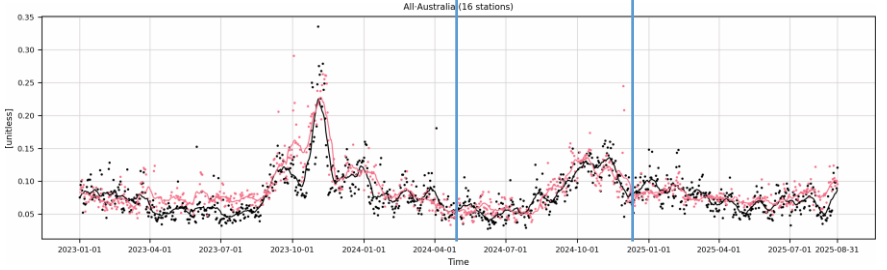


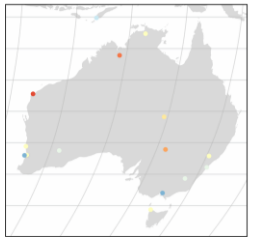










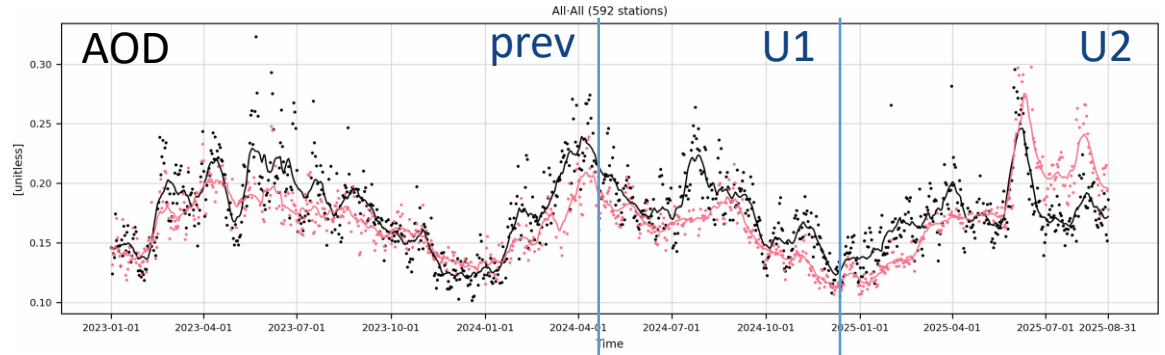


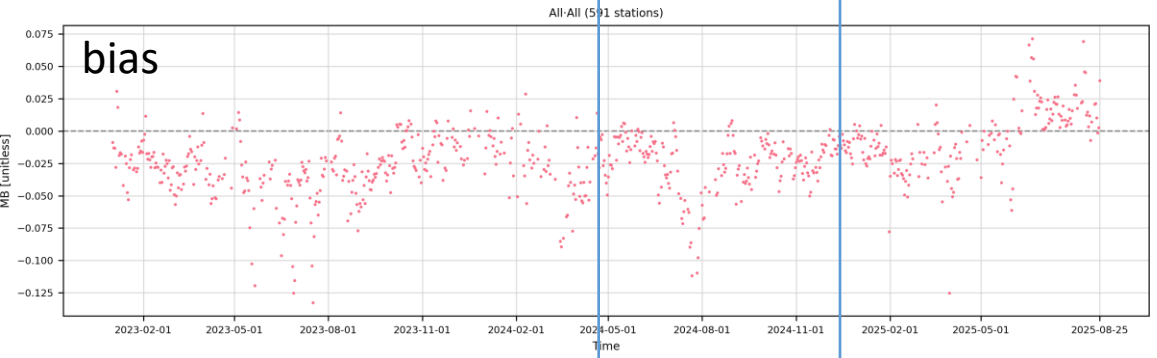
Barcelona Supercomputing Center
Centro Nacional de

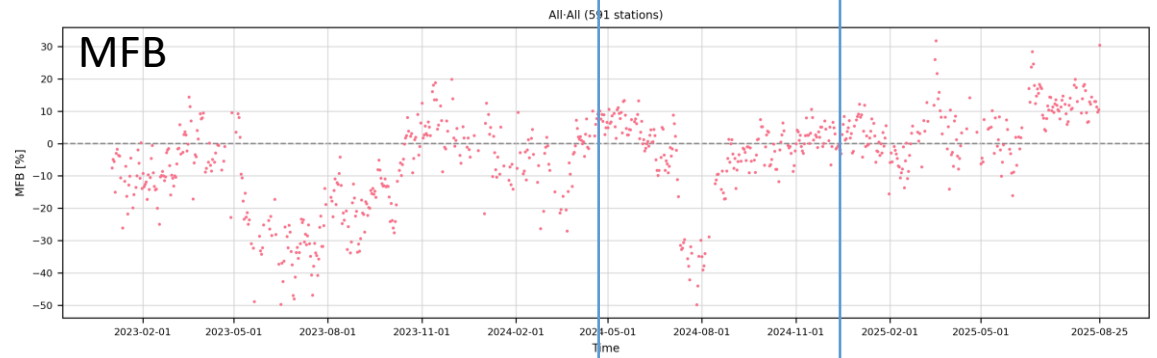
E. Emili, E. Karnezi

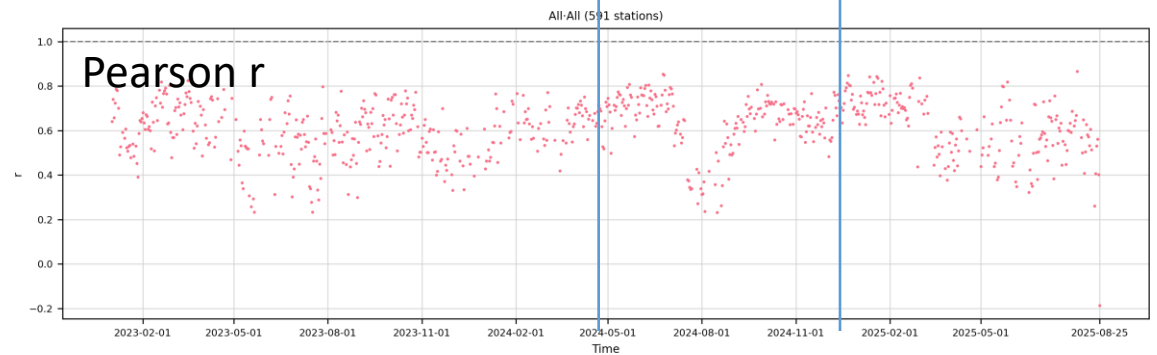
AOD - scores

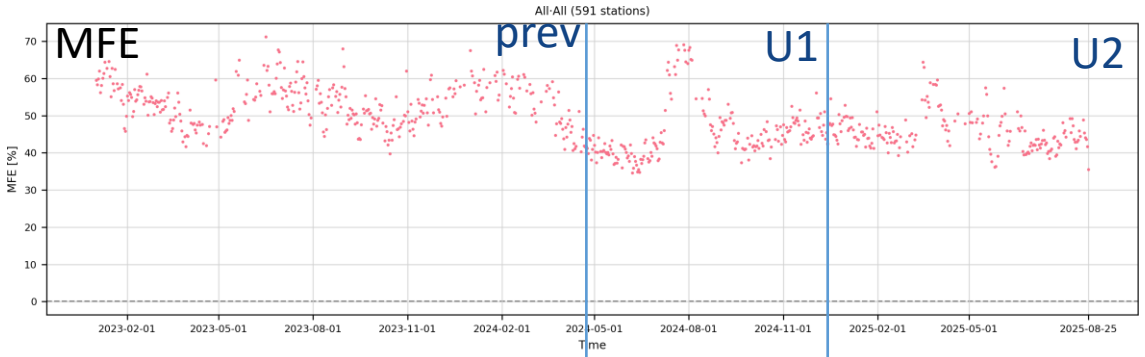
		bias	RMSE	r	MFB(%)	MFE(%)
old	(2023/01/01) - 2024/04/20	-0.03	0.20	0.59	-12.91	53.01
U1	2024/04/21 - 2024/12/12	-0.03	0.17	0.61	-4.08	45.66
U2	2024/12/12 – 2025/09/01	0.00	0.18	0.55	6.16	45.66

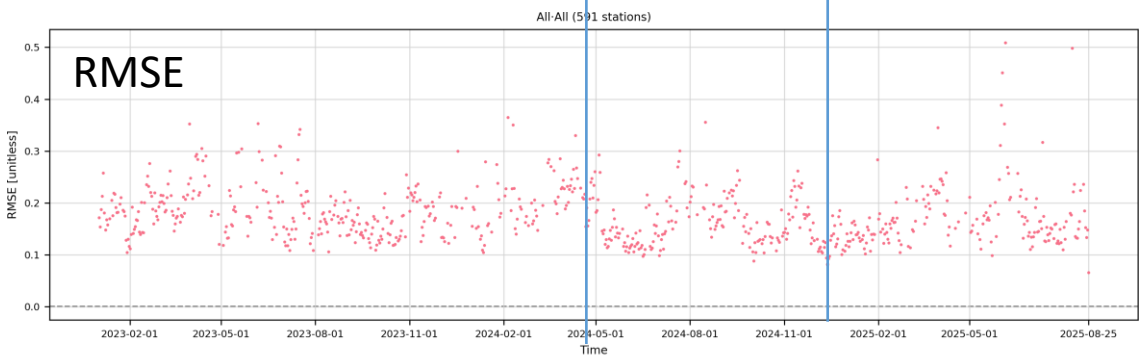












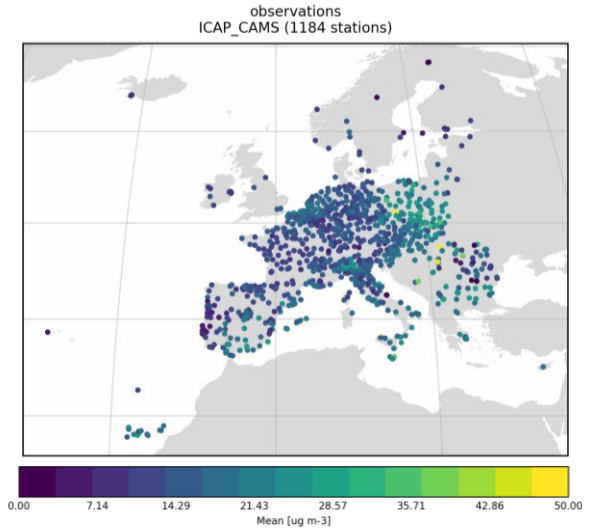
E. Emili, Rafaela Cruz

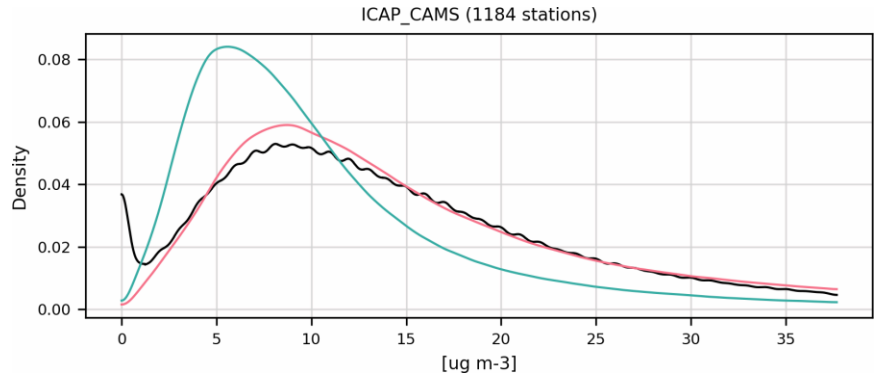
Surface PM10 over Europe

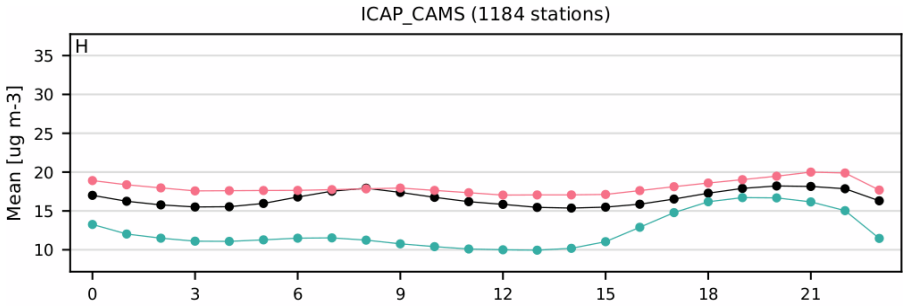
PM10 over Europe
(2024/07 – 2025/08)

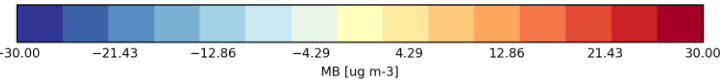
MONARCH CAMS
Regional ensemble
(0.15x0.15 deg)

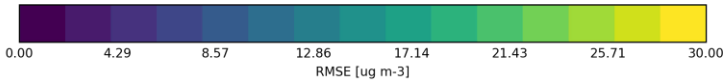
MONARCH ICAP global
(0.7x0.5 deg)

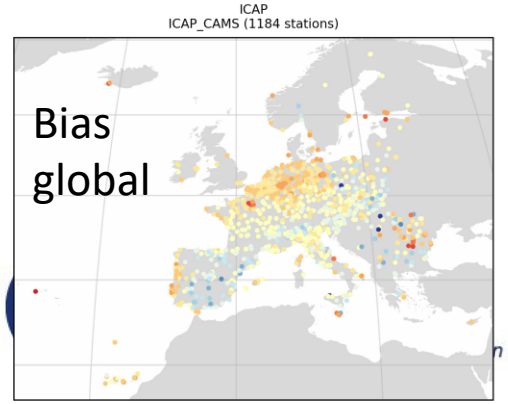


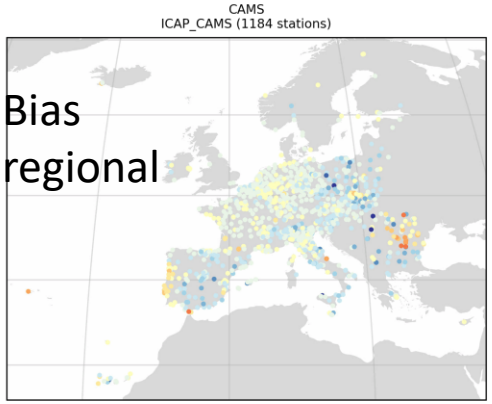


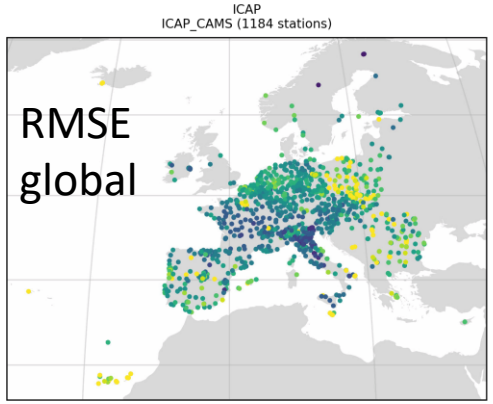


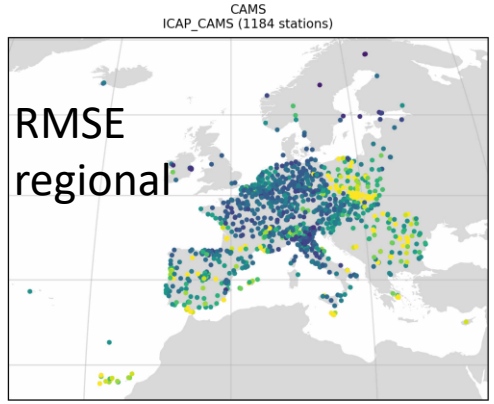












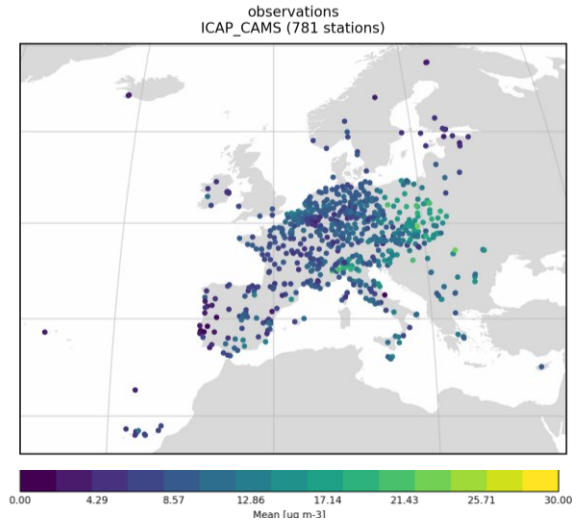
E. Emili, Rafaela Cruz

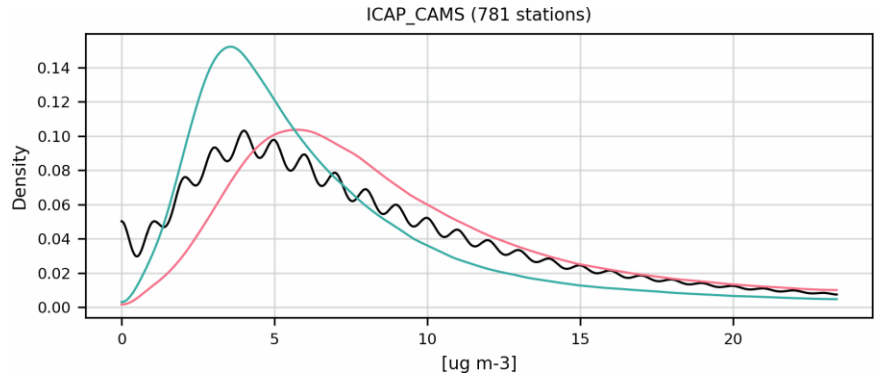
Surface PM2.5 over Europe

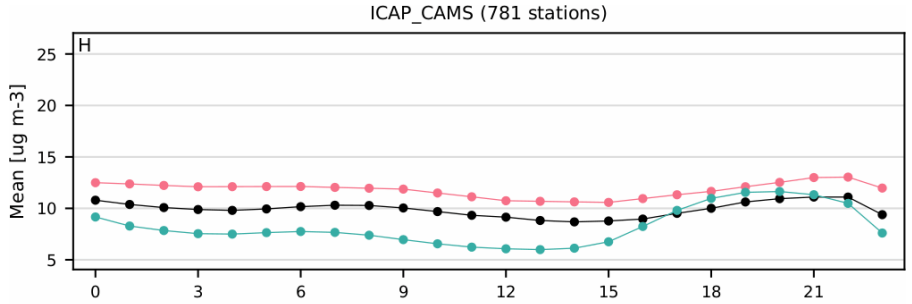
PM2.5 over Europe
(2024/07 – 2025/08)

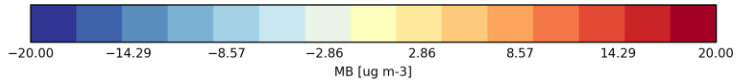
MONARCH CAMS
Regional ensemble
(0.15x0.15 deg)

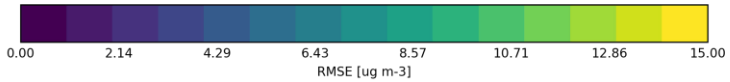
MONARCH ICAP global
(0.7x0.5 deg)

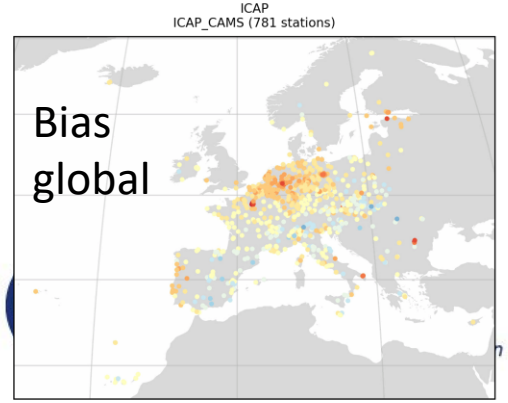


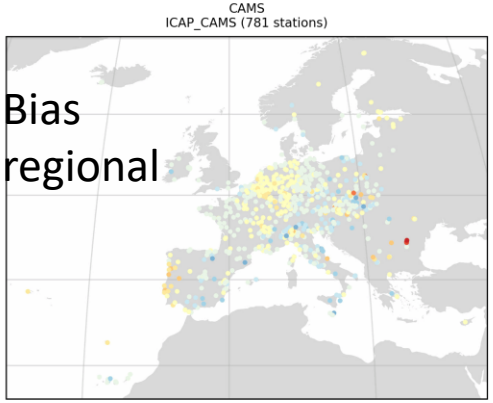


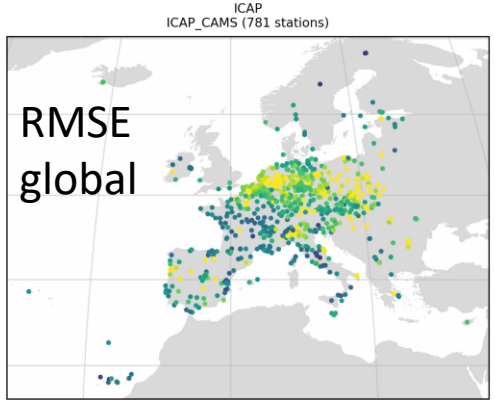


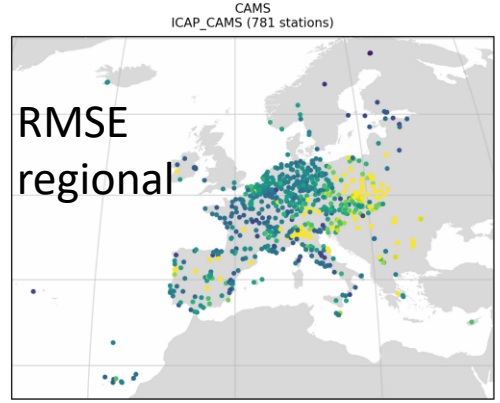








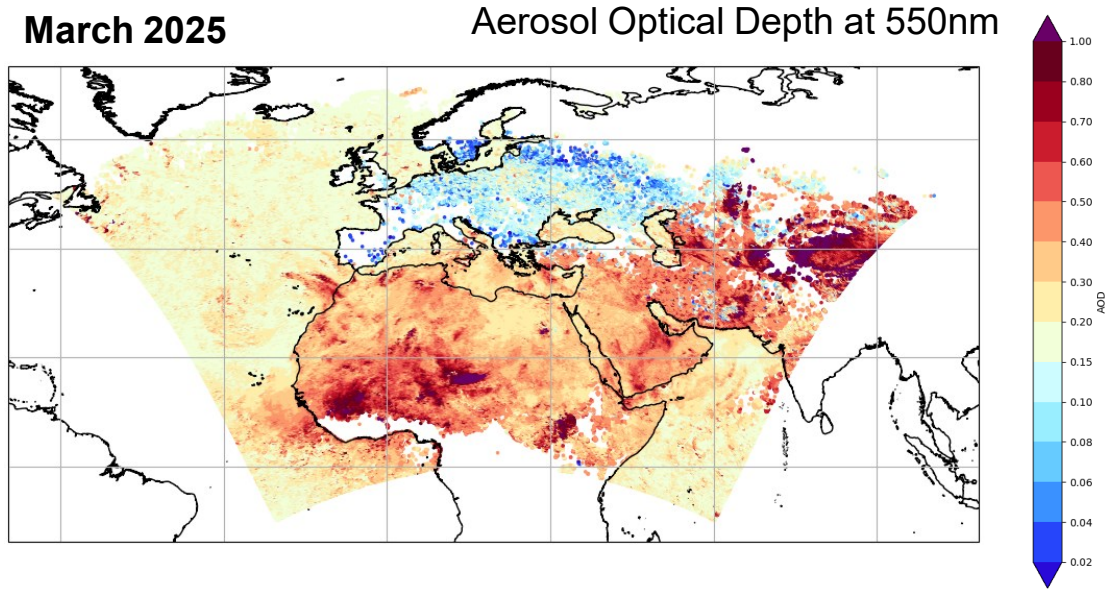


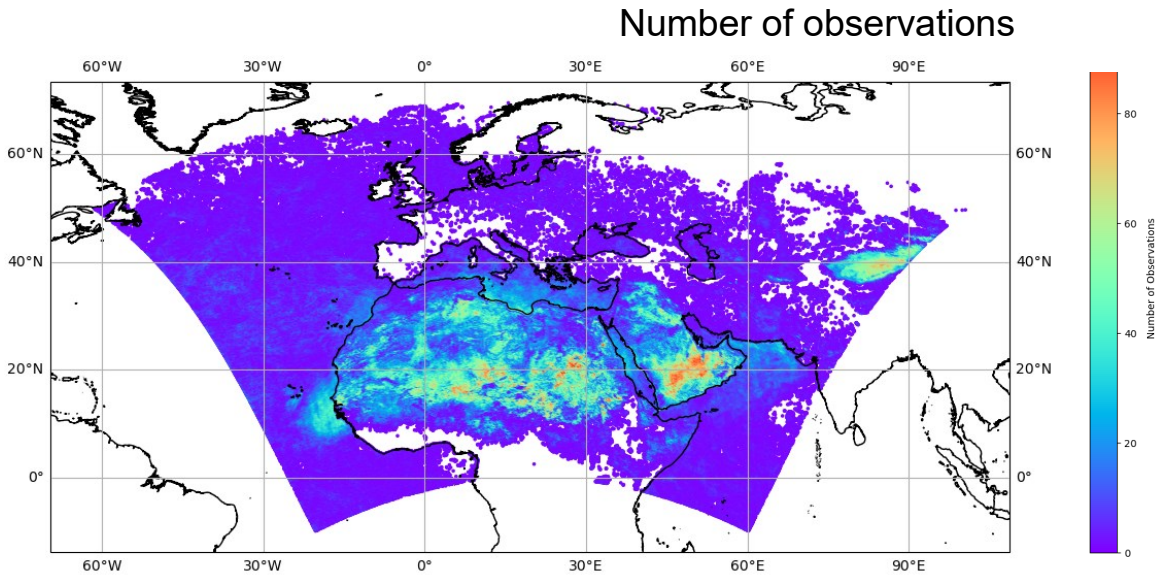


Emanuele Emili

Dust AOD assimilation in SDS-WAS NAMEE domain

- The **SDS-WAS** (Sand and Dust Storm Warning Advisory and Assessment System) aims to establish a coordinated global network of SDS research and forecasting centers to enhance operational SDS forecasts through technology transfer from research (**WMO**)
- **MONARCH** is the reference forecast model of the **Barcelona Dust Regional Center node**
- Satellite data assimilation shown to improve dust optical depth forecasts [Di Tomaso et al, 2017] but only used in research projects since then
- A **new** operational MONARCH e-suite assimilates NOAA-20 VIIRS AOD **since October 2024**
- **o-suite since July 2025**





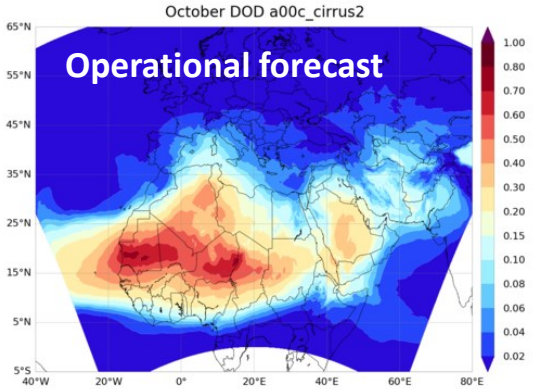
- NMMB-MONARCH + LETKF
  - 0.1 deg resolution, NAMEE domain
  - Only dust aerosols
- Ensemble: 12 members with dust emission perturbations
- Observations: VIIRS Deep Blue v2 550nm AOD from NOAA-20, dust-flagged, QA.

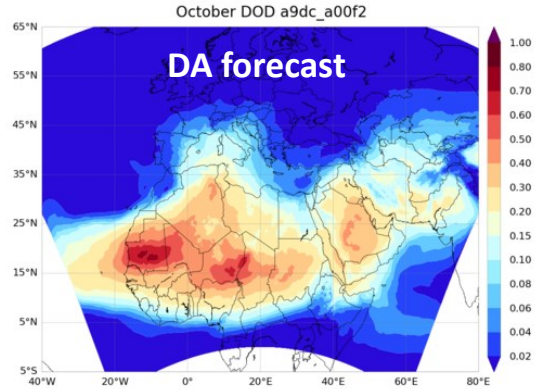
Barcelona Supercomputing Center
Centro Nacional de Supercomputación

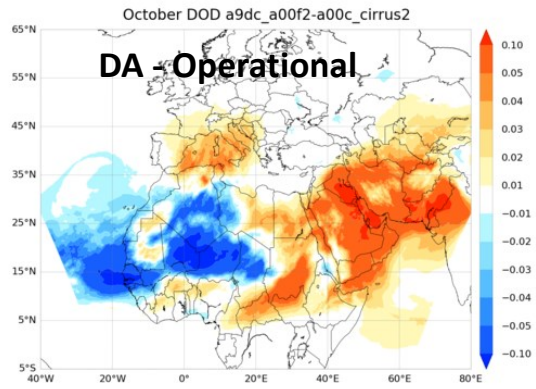
Emanuele Emili

Dust AOD assimilation in SDS-WAS NAMEE domain

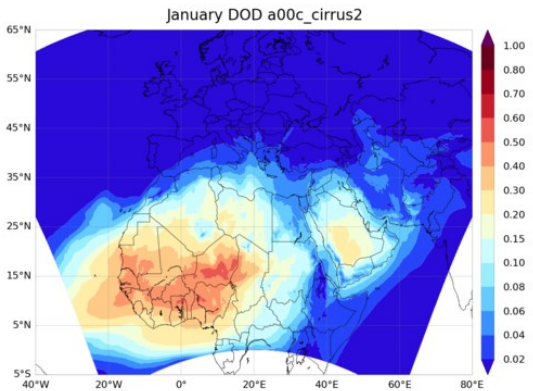
October 2024

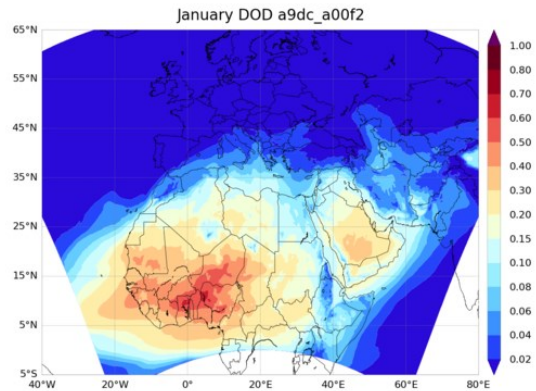


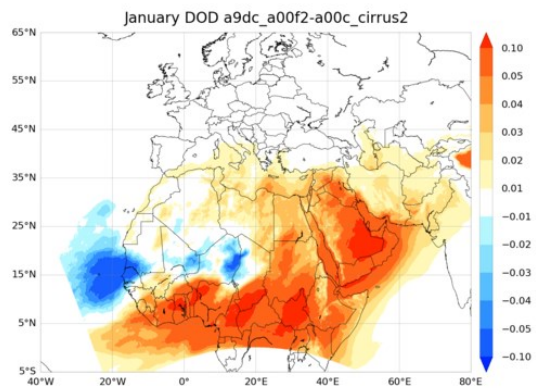




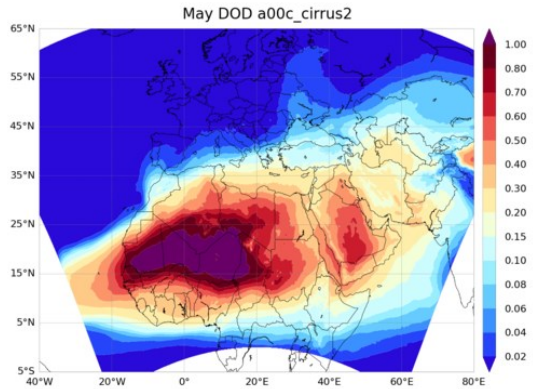
January 2025

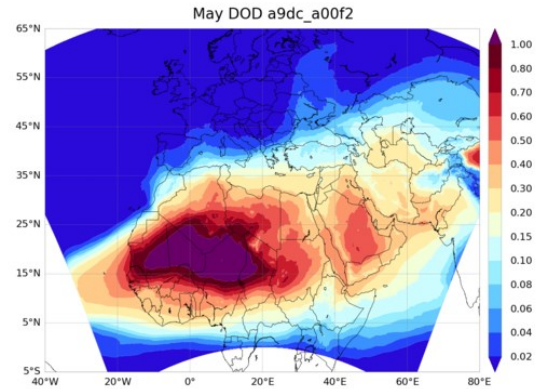


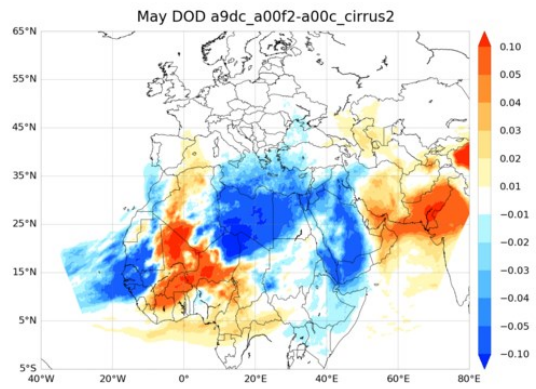




May 2025





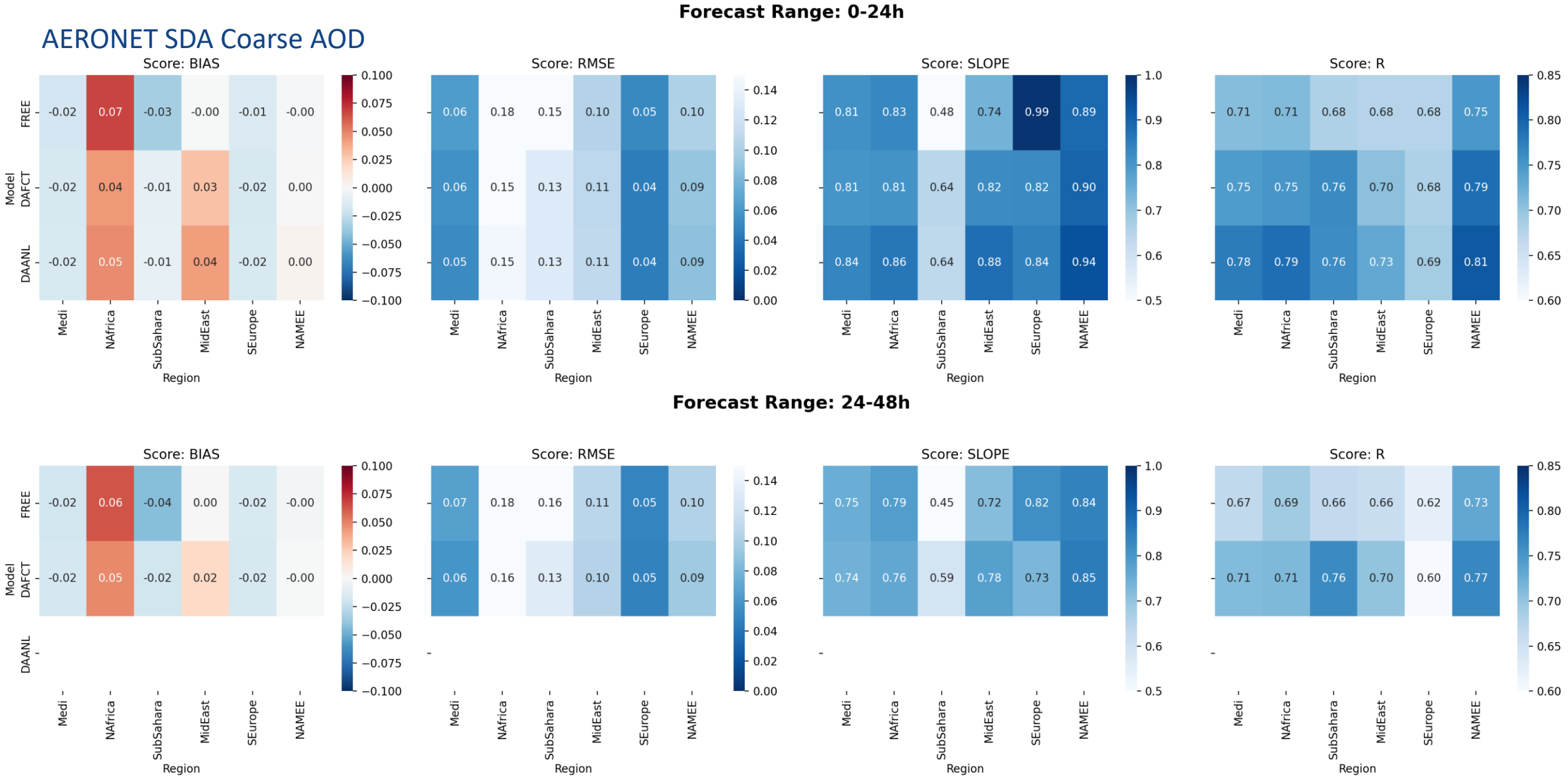


Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Emanuele Emili

Dust AOD assimilation in SDS-WAS NAMEE domain

AERONET SDA Coarse AOD

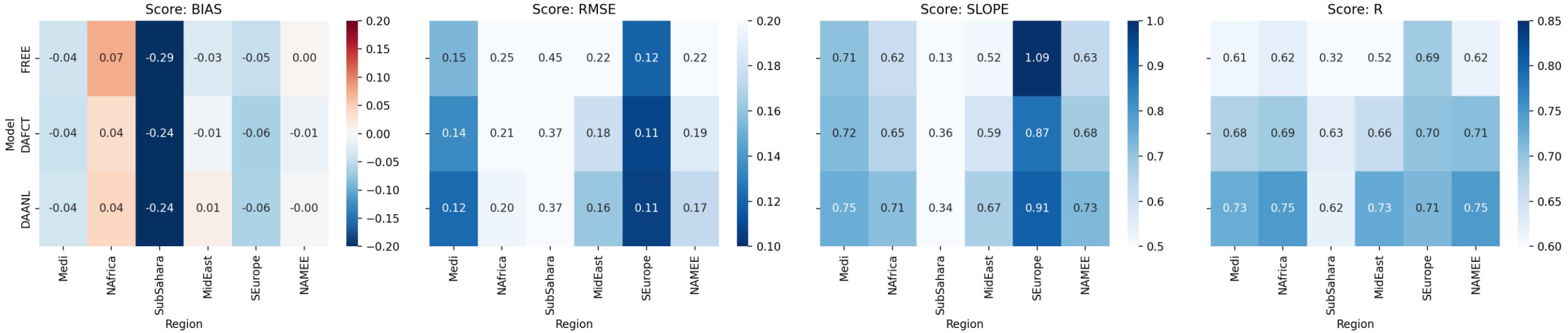


Emanuele Emili

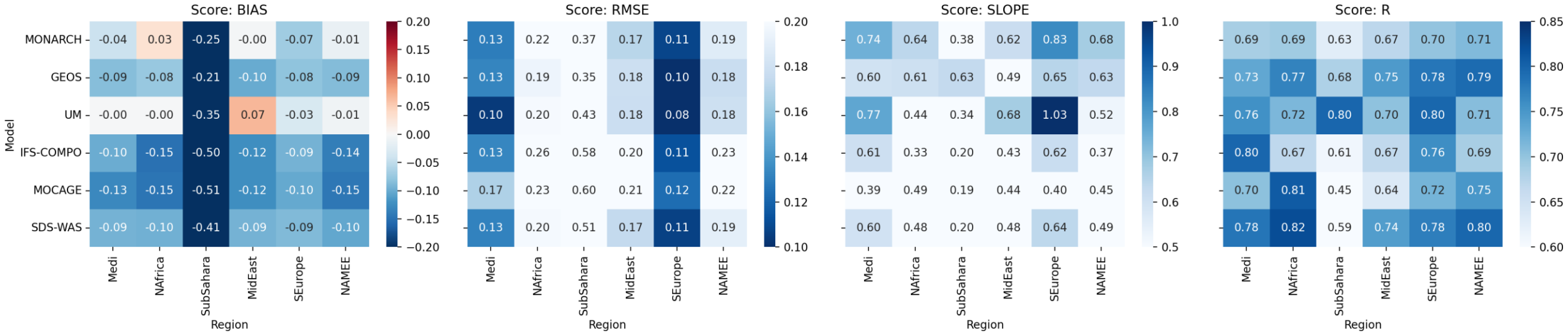
Dust AOD assimilation in SDS-WAS NAMEE domain

AERONET AOD, Ångström < 0.6

Forecast Range: 0-24h



Forecast Range: 0-24h

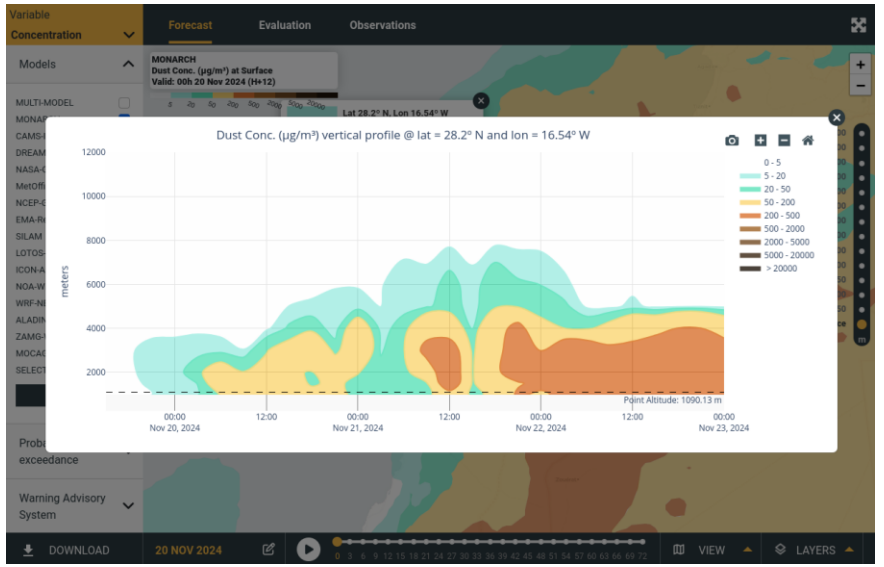


Carlotta Gilè

MONARCH dust SDS-WAS NAMEE: vertical profiles

Since July 2024, MONARCH provides mass mixing ratio of dust in the NAMEE node of the WMO SDS-WAS

- Data is sampled every 3 hours
- 13 altitude levels: 250, 500, 750, 1000, 1500, 2000, 3000, 4000, 5000, 6000, 8000, 10000, 12000 m.



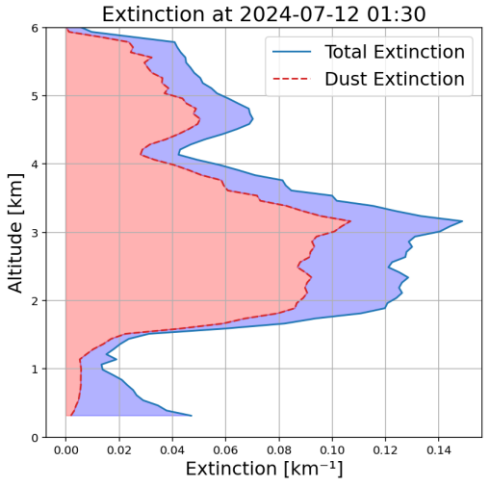
We use NASA **MPLNET** data and the POLYPHON (Tesche 2009, JGR) algorithm to estimate dust extinction coefficient at 3 sites

$$\alpha_{\lambda,d}(z) = S_{\lambda,d} \cdot \beta_{\lambda,d}(z) \quad \left[\frac{1}{km}\right]$$

$$\beta_{\lambda,d}(z) = \beta_{\lambda,p}(z) \frac{(\delta_{\lambda,p}(z) - \delta_{\lambda,nd})(1 + \delta_{\lambda,nd})}{(\delta_{\lambda,d} - \delta_{\lambda,nd})(1 + \delta_{\lambda,p}(z))} \quad \left[\frac{1}{km}\right]$$

$$\delta_{\lambda,d} = 0.31$$
$$\delta_{\lambda,nd} = 0.05$$
$$S_{\lambda,d} = 56\,\mathrm{sr}$$

"nd" and "d" stands for non-dust and dust respectively, "S" represents the lidar ratio

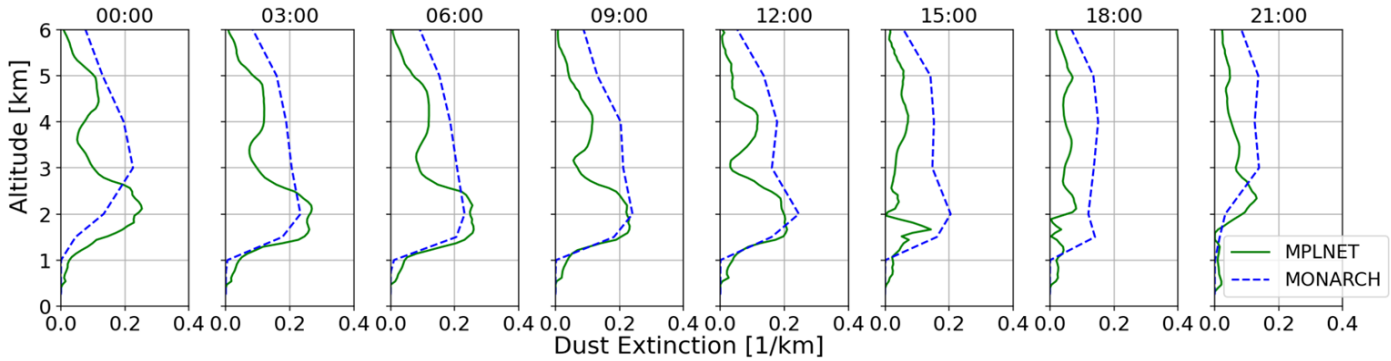


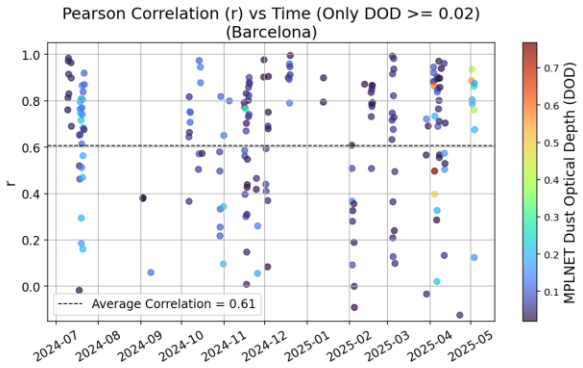
Barcelona Supercomputing Center
Centro Nacional de Supercomputación

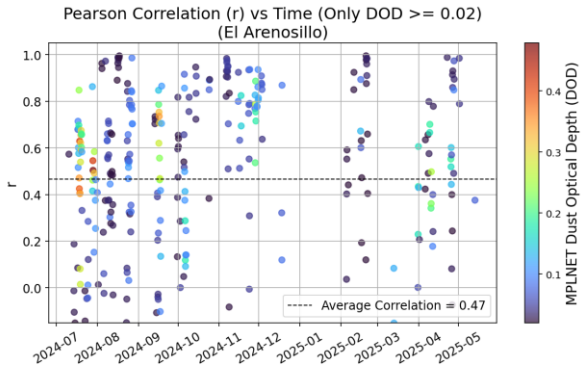
Carlotta Gilè

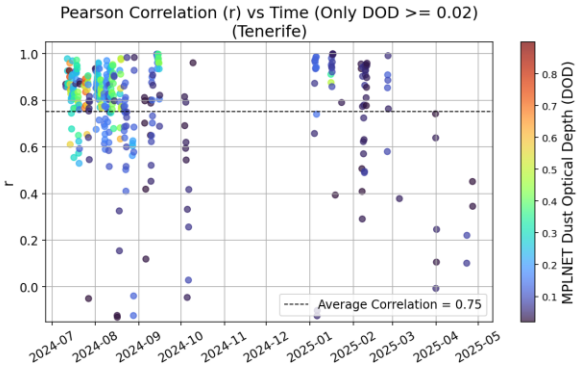
MONARCH dust SDS-WAS NAMEE: vertical profiles

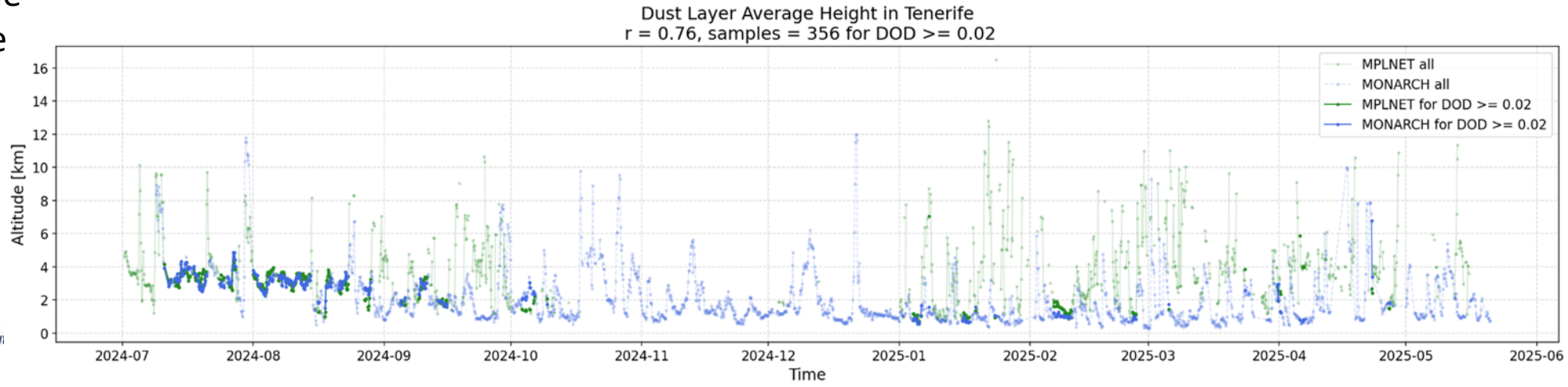
- Fair agreement of profile shapes (as seen by ρ)
- Overestimation of MONARCH DOD
- Fair agreement in the mean altitude of the dust mass for dust events











Barcelona Supercomputing Center
Centro Nacional de Supercomput

Other highlights

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Guillaume Monteil

Joint assimilation of VIIRS total AOD and surface data in MONARCH-DA

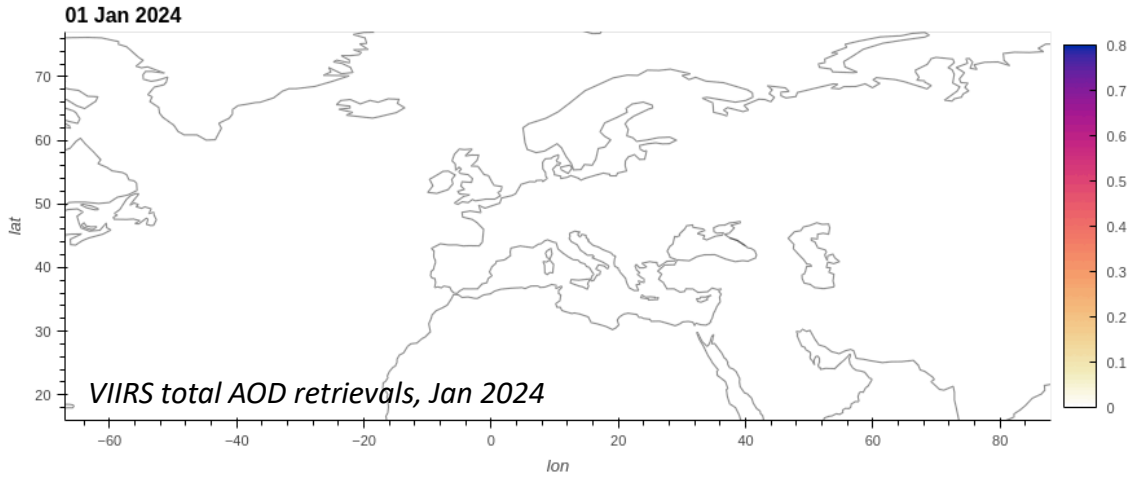
Do satellite AOD retrieval help modelling (and forecasting) surface air quality?

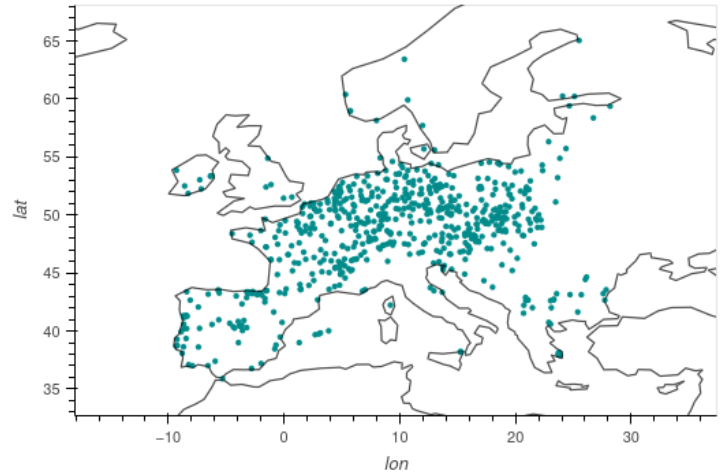
The MONARCH-DA system:

- NMMB-MONARCH model: **7 aerosol species, with 1-7 bin/species**
- LETKF data assimilation algorithm
- Joint assimilation of **surface PM10** observations and **VIIRS 550 nm total AOD retrievals**

Experimental setup:

- One month assimilation, in January 2024
- 6-member ensemble (i.e. operational CAMS setup)
- “offline” assimilation (no propagation of the analysis)





Surface observation sites (validation sites in red)

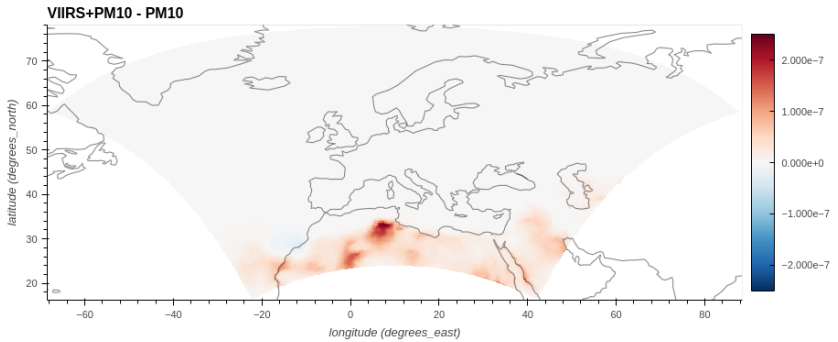
Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Guillaume Monteil

Joint assimilation of VIIRS total AOD and surface data in MONARCH-DA

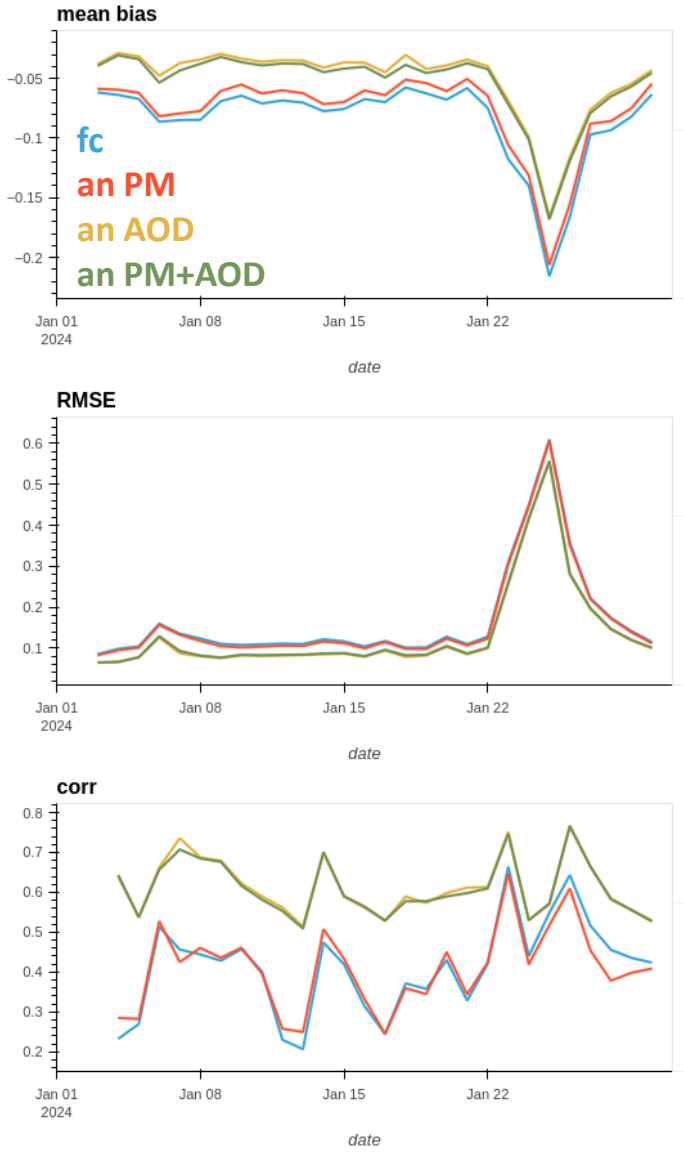
- MONARCH-DA is capable of jointly assimilating surface and satellite observations of aerosols
  - Fit to both obs datasets is improved
  - The DA is capable of accomodating both constraints by small adjustments in the vertical profiles, when needed.

- So far, this doesn't translate into measurable improvements in surface air quality estimates

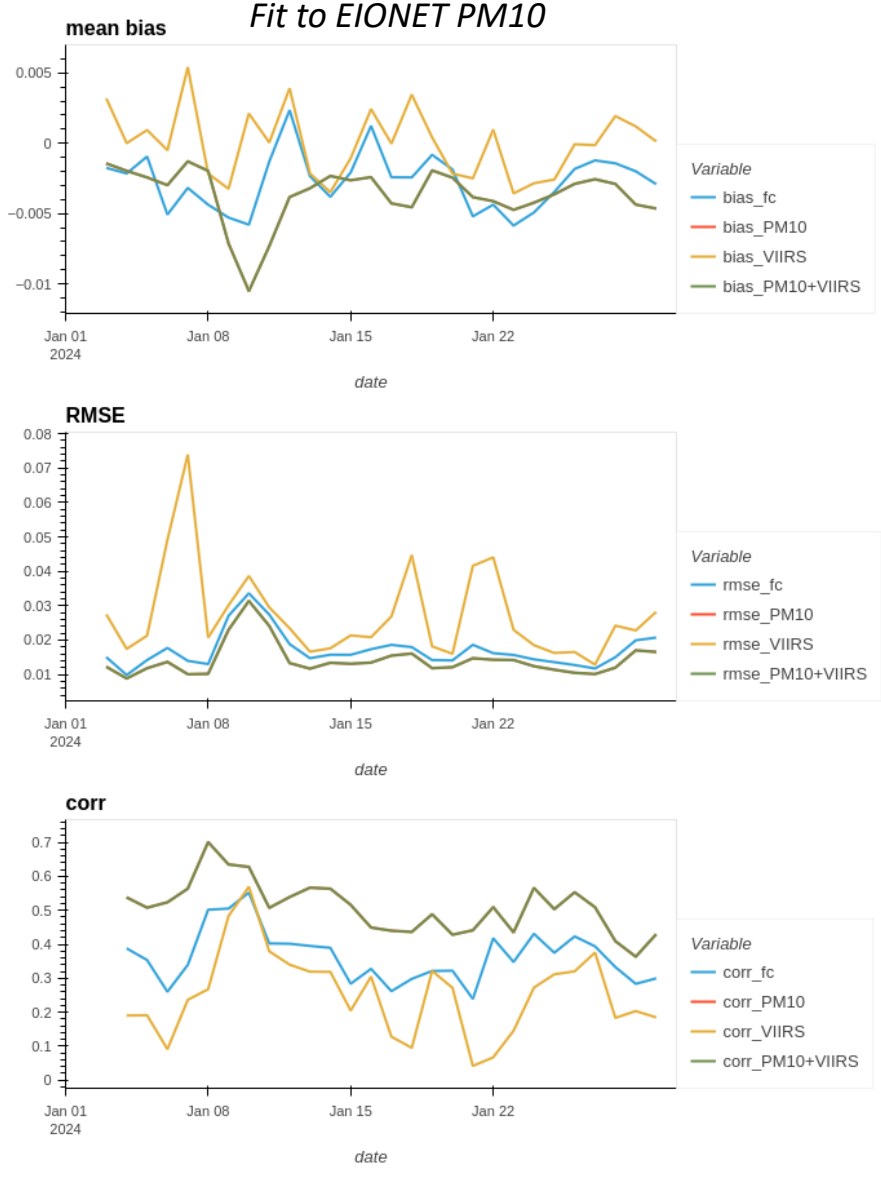


Difference between DA of VIIRS+PM10 and DA of PM10 on surface PM10 levels (jan 2024 average)

Fit to VIIRS AOD



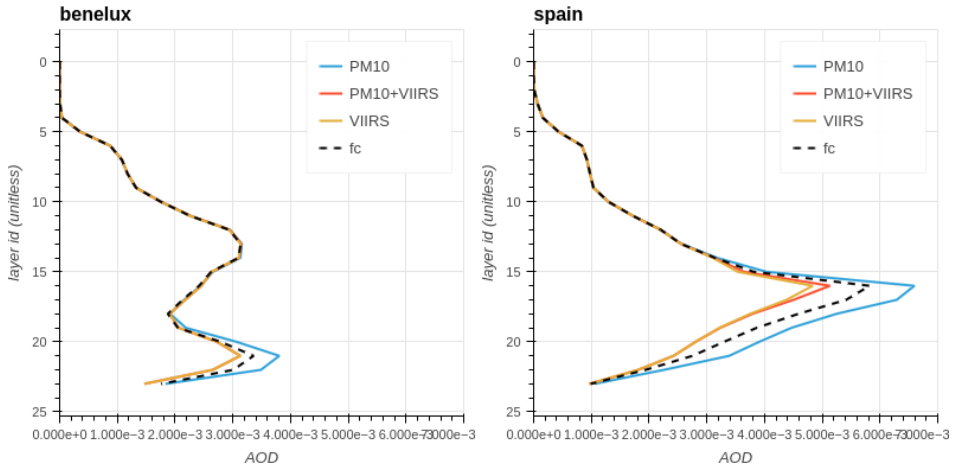
Fit to EIONET PM10



Guillaume Monteil

Joint assimilation of VIIRS total AOD and surface data in MONARCH-DA

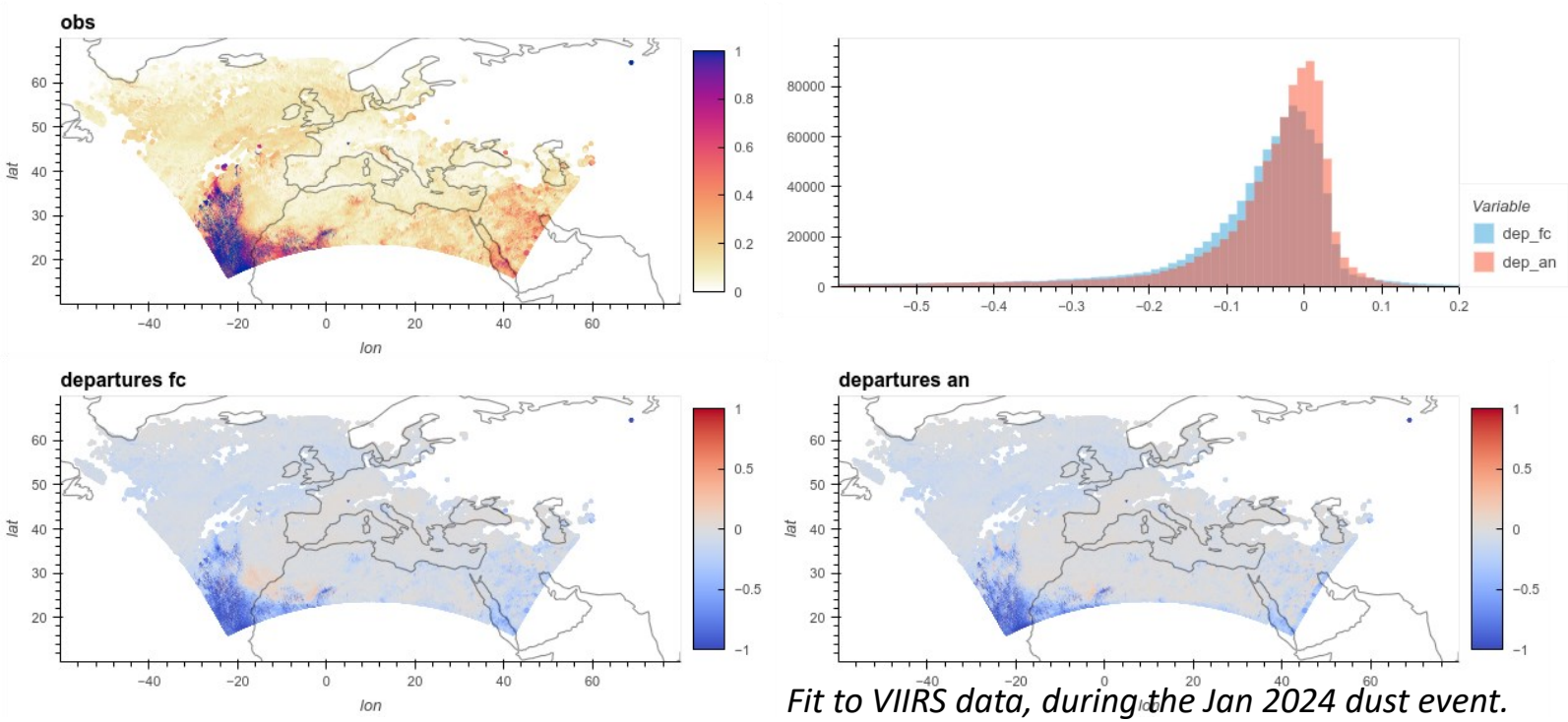
- MONARCH-DA is capable of jointly assimilating surface and satellite observations of aerosols
  - Fit to both obs datasets is improved
  - The DA is capable of accomodating both constraints by small adjustments in the vertical profiles, when needed.



AOD profiles 10-20 jan 2024

an PM
an PM+AOD
an AOD
fc

- So far, this doesn't translate into measurable improvements in surface air quality estimates
  - Large contribution of the mid to upper troposphere in the AOD corrections?
  - Ensemble lacks size and variability?
  - January 2024 may not be the best month (few VIIRS observations over Europe), few surface observations to evaluate the DA over North Africa, where it has an impact



Fit to VIIRS data, during the Jan 2024 dust event.
Not enough ensemble variability to match the obs over the ocean

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Implementation of JEDI (AQ) 4DEnVar

Jayoung Yun, E. Emili, Andrea Piacentini

Implementation of “AQ” version of JEDI in MONARCH model

Regional grid, 6 ens. member (CAMS-regional configuration)

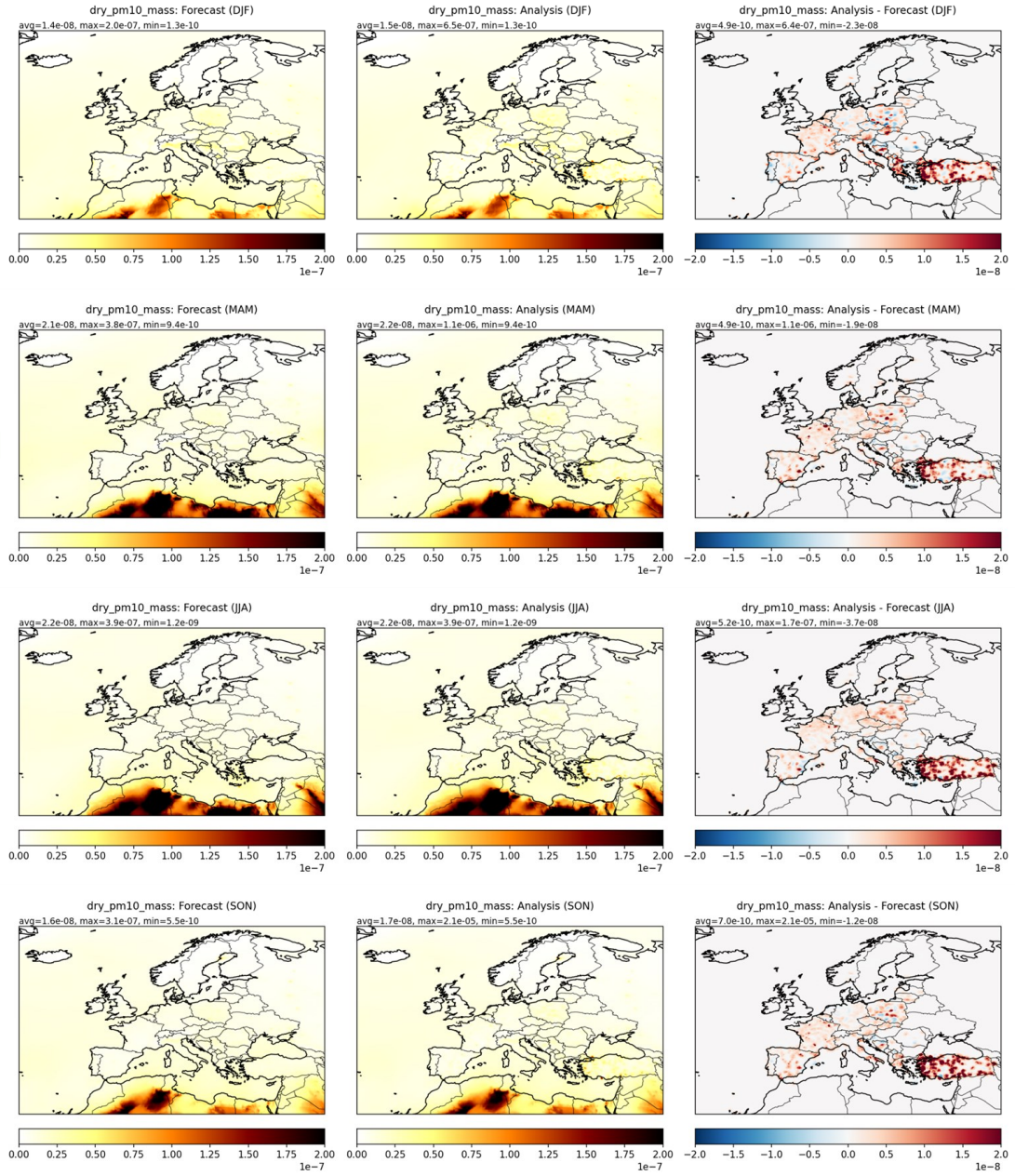
Assimilation of surface stations (as provided in CAMS2_40) : PM2.5, PM10, NO2, O3, CO, SO2

Aiming to move to operations in 2026/2027

Working on implementing the official JEDI release

Extending to AOD and others OO

PM10

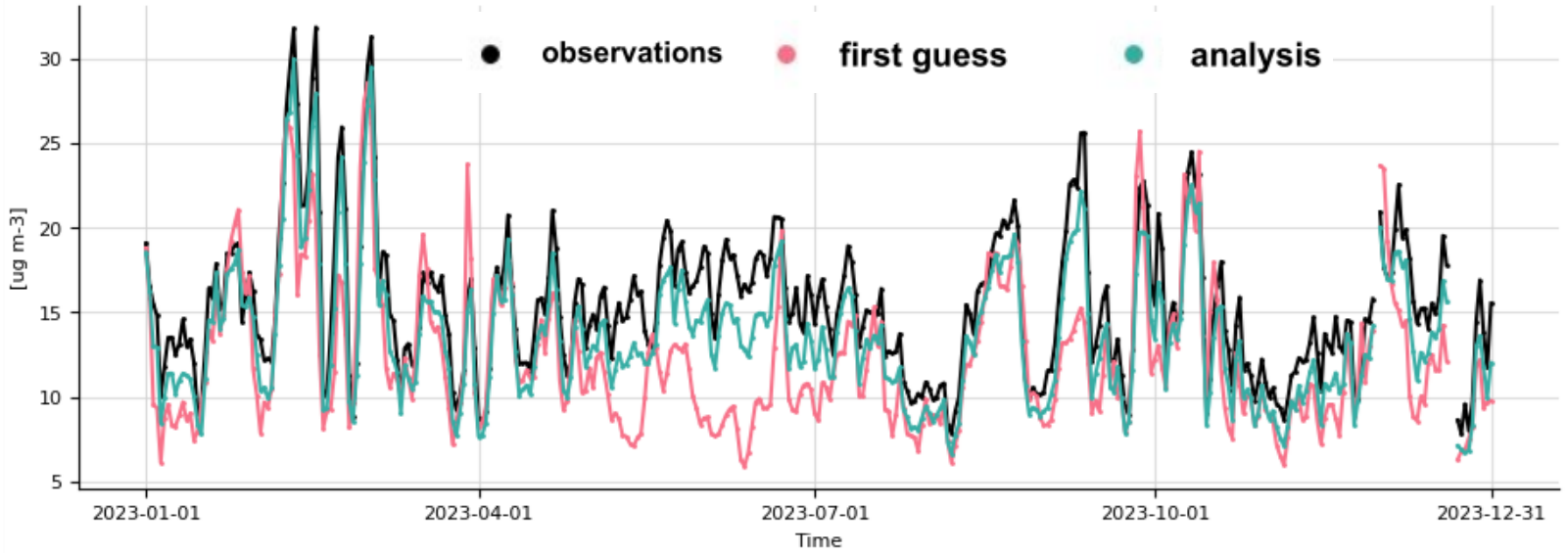


Barcelona Supercomputing Center
Centro Nacional de Supercomputación

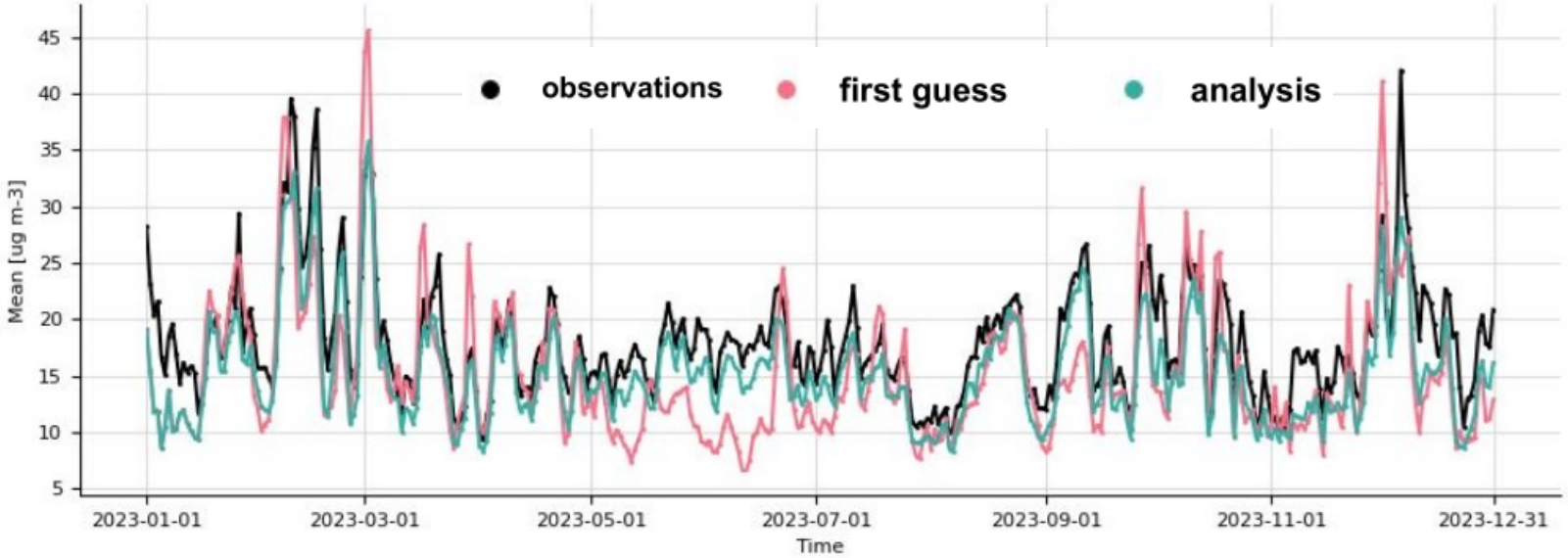
Implementation of JEDI (AQ) 4DEnVar

Jayoung Yun, E. Emili,
Andrea Piacentini

JEDI-4DEnVar



MONARCH-LETKF



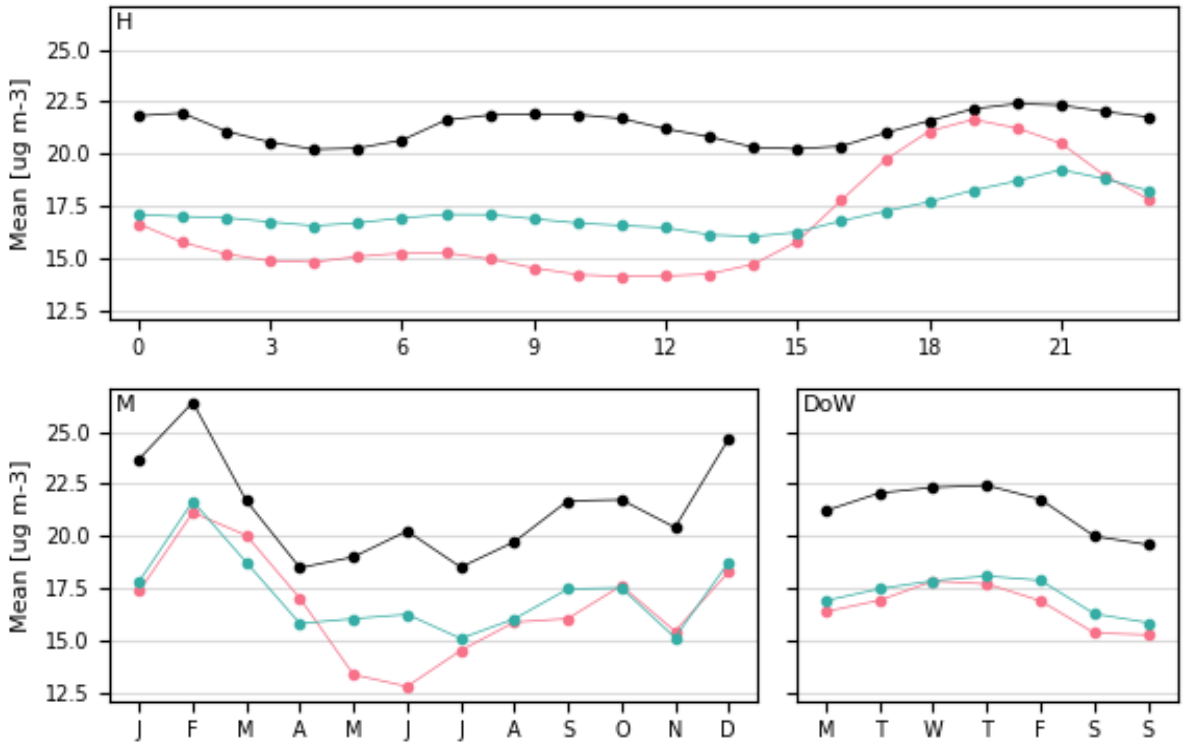
LETKF *excluded observations from some countries (e.g., Romania, Türkiye), while* ***JEDI-4DEnVar*** *used all observations from the* ***Ineris*** *network.*

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Implementation of JEDI (AQ) 4DEnVar

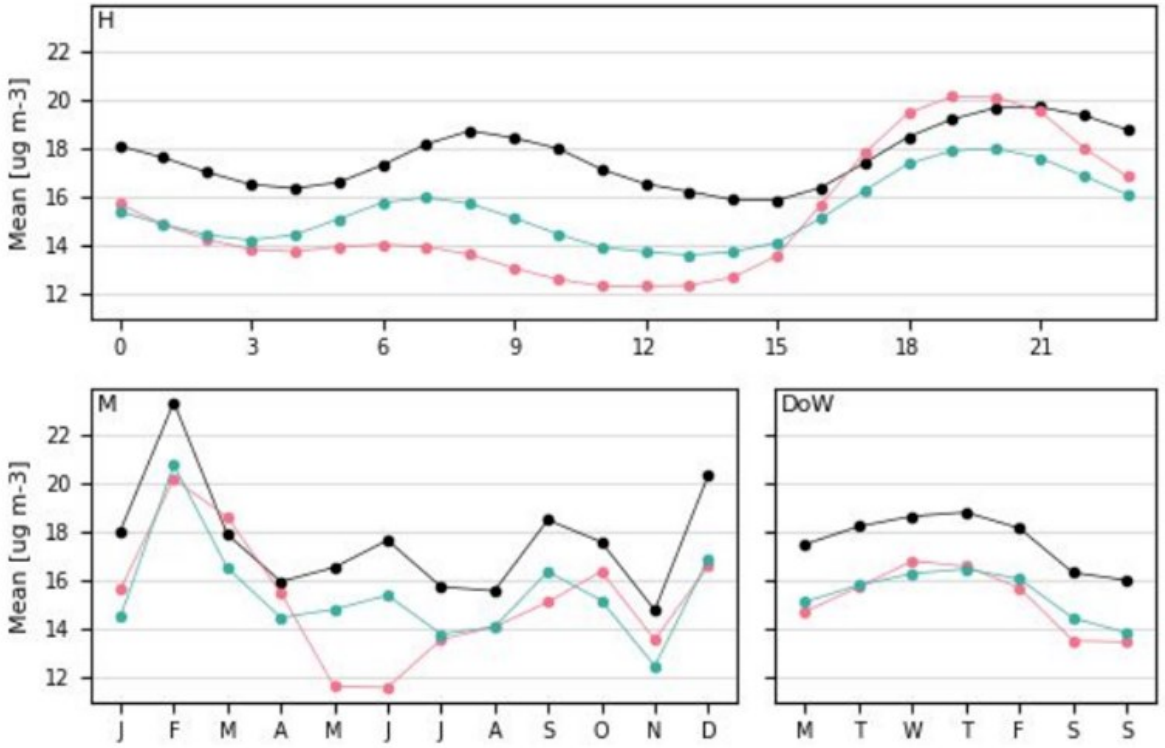
Jayoung Yun, E. Emili, Andrea Piacentini

JEDI-4DEnVar



	Mean	StdDev	NMB	NME	RMSE	r
a9j4-regional-av	-4.13	-13.01	-20.17	53.06	30.75	0.23
jedi_a2023-regional-000	-3.82	-14.20	-18.65	36.61	29.33	0.30

MONARCH-LETKF



	Mean	StdDev	NMB	NME	RMSE	r
a9j4-regional-av	-2.47	-9.28	-13.97	60.42	31.65	0.20
a9j4-regional-av_an	-2.25	-14.86	-12.73	40.20	28.39	0.29

observations first guess analysis

Supercomputing Center
Centro Nacional de Supercomputación

statistics mode: flattened, temporal collocation with daily resampling for JEDI-4DEnVar

ML Dust AOD forecasts

Miguel Hortelano

Data used

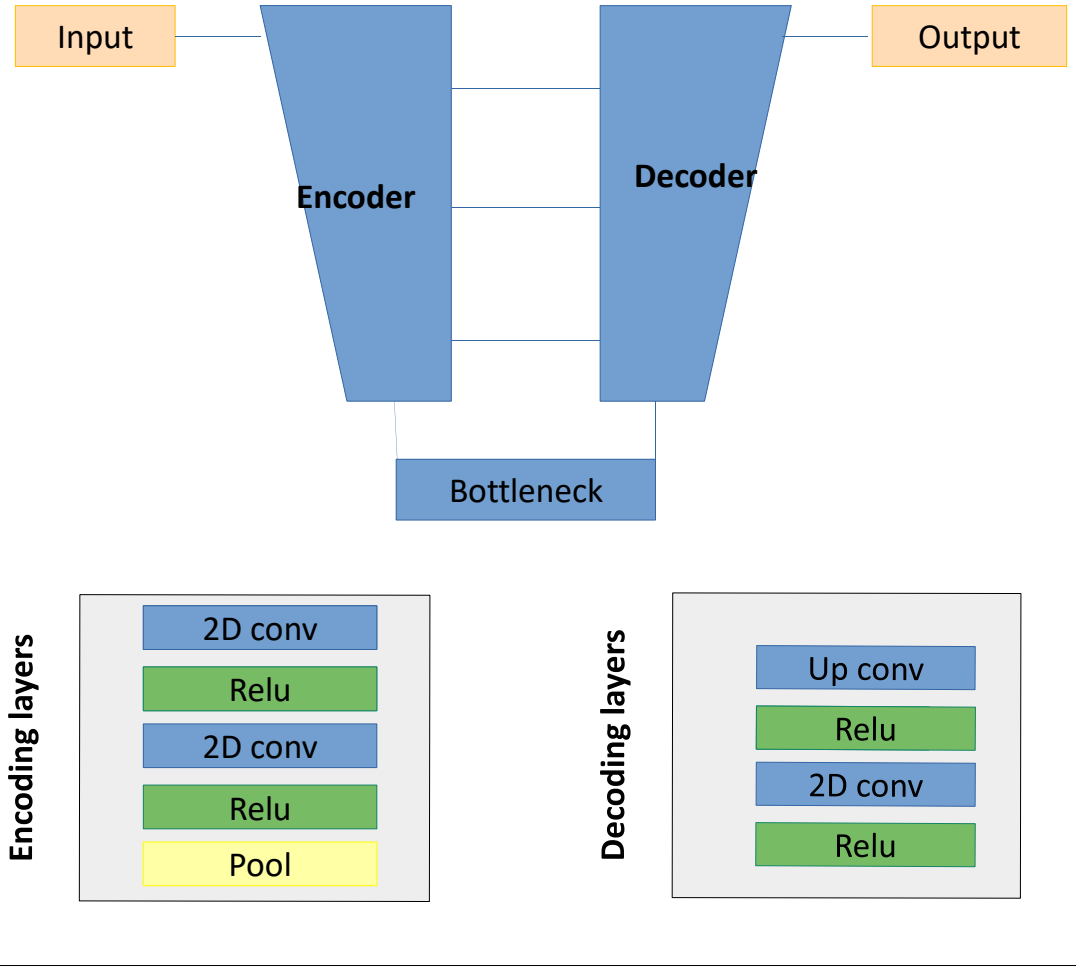
- VIIRS NOAA20 DBv2 550nm AOD L2
- GFS weather forecasts
  - 3 levels (500, 850 & 1000 hPa)
  - Dimensions (UGRD, VGRD, VVEL, T & RH)
- Terrain elevation
- Time encoding

Data split

Total instances 4281

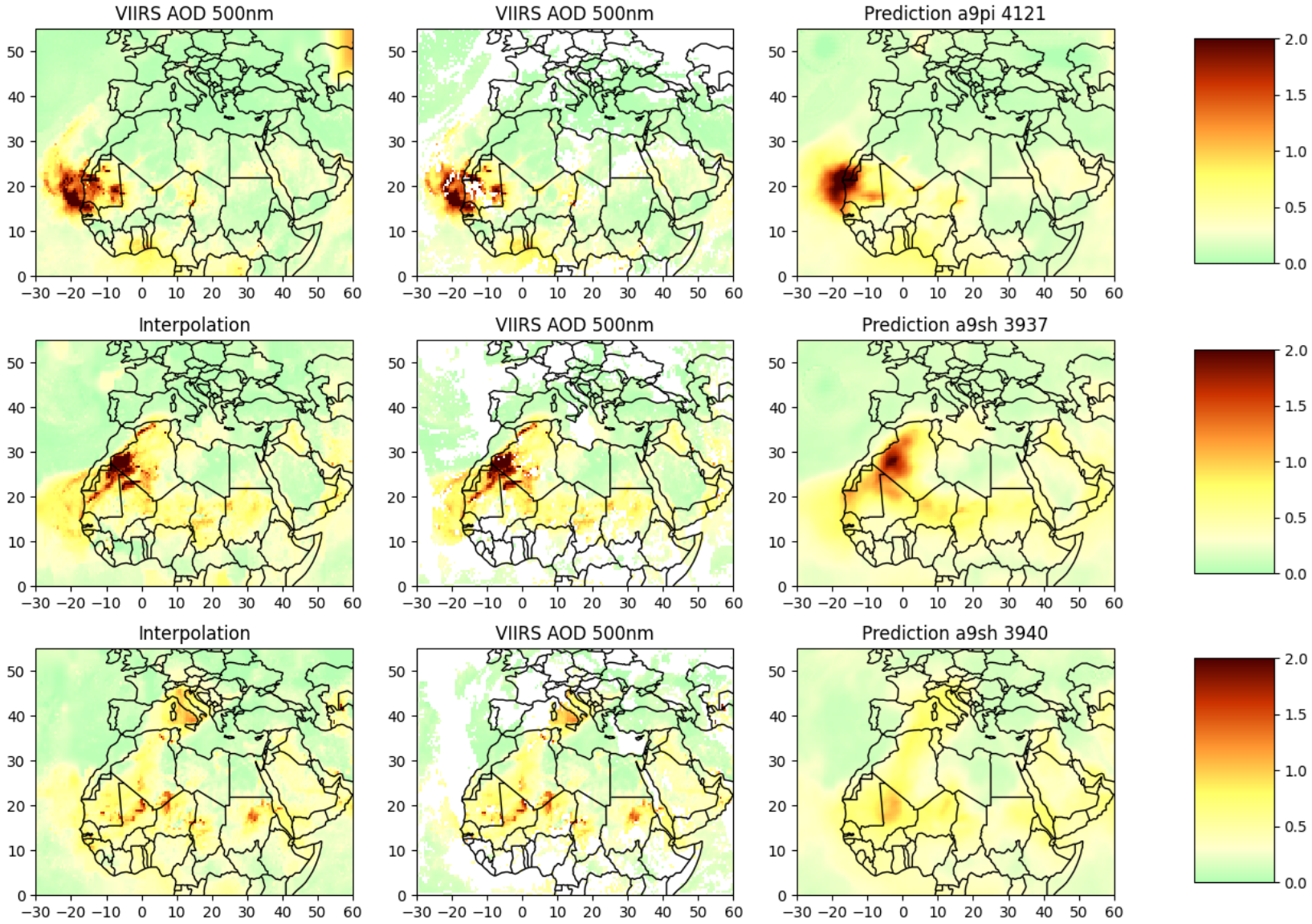
- Training set 70% (2996)
- Validation 20% (848)
- Test set 10% (437)

Network architechture



ML Dust AOD forecasts

Miguel Hortelano

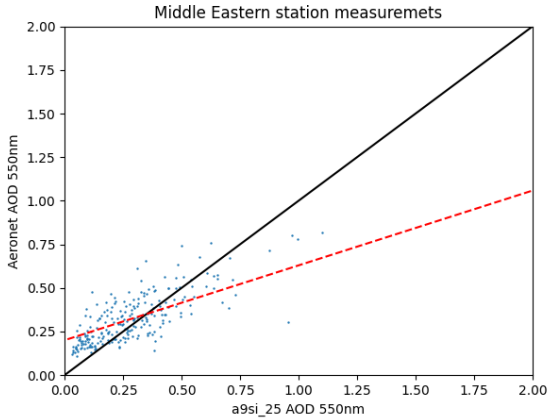


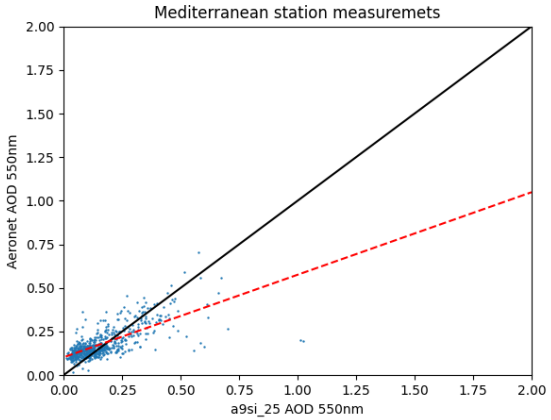
Barcelona Supercomputing Center
Centro Nacional de Supercomputación

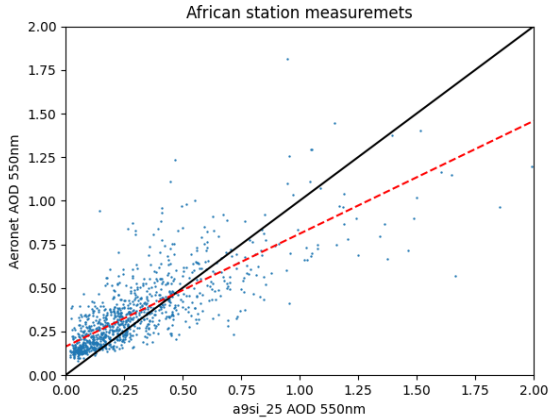
ML Dust AOD forecasts

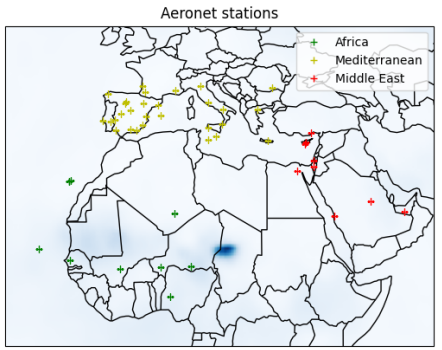
Miguel Hortelano

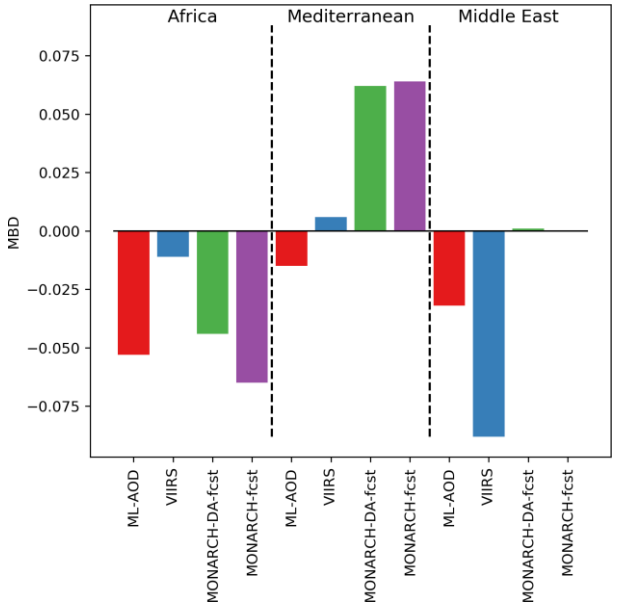
Model comparison

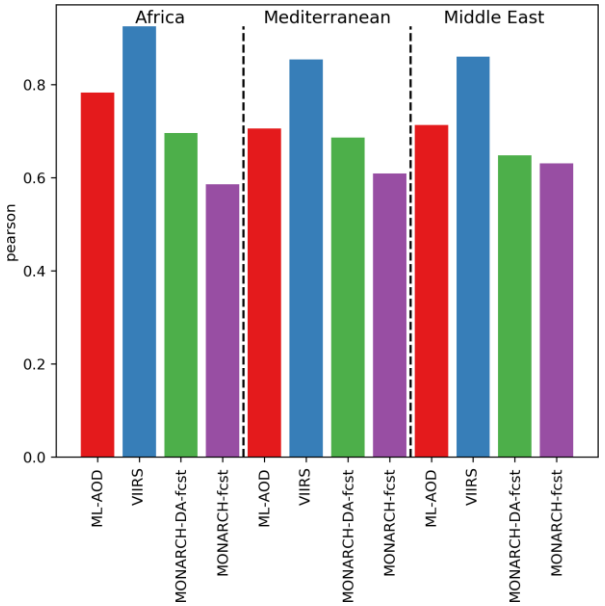


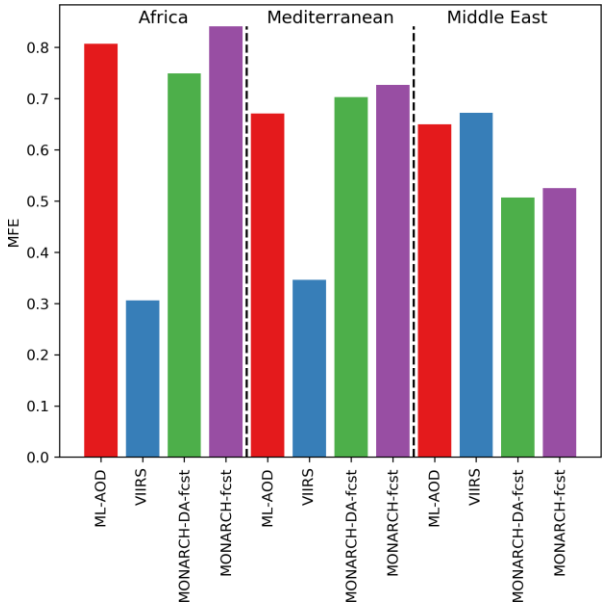


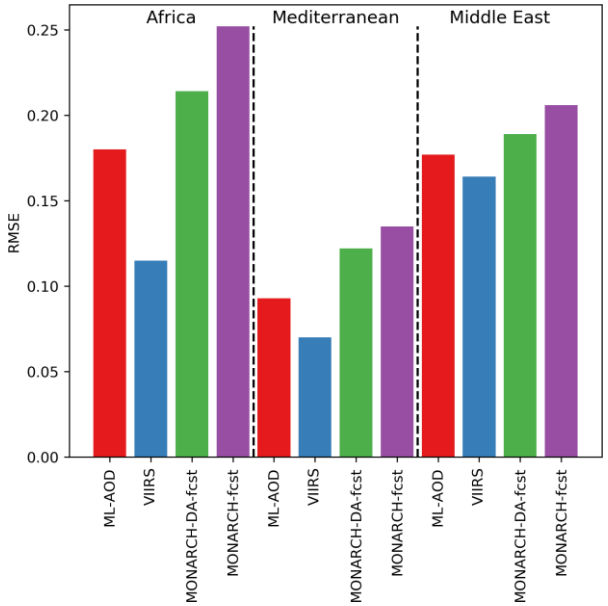












Other AI research in the BSC's Atmospheric Composition group

- Emulation of the atmospheric chemistry numerical solver
- Inversion of NOx emissions from satellite observations
- Emulation of MONARCH chemistry-transport model
- Observation-model data fusion
- Downscaling of atmospheric composition

- Porting our in-house CAMP multiphase chemistry library to GPUs to accelerate simulations

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Thank you!

We acknowledge the RESPIRE project, which is part of the Recovery, Transformation and Resilience Plan (Plan de Recuperación, Transformación y Resiliencia, PRTyR) funded by the European Union – NextGenerationEU. JE and EE acknowledge his AI4S fellowship within the “Generación D” initiative by Red.es, Ministerio para la Transformación Digital y de la Función Pública, for talent attraction (C005/24-ED CV1), funded by NextGenerationEU through PRTR. We also acknowledge support from the AXA Research Fund through the AXA Chair on Sand and Dust Storms at the Barcelona Supercomputing Center (BSC).

jeronimo.escribano@bsc.es