



**Barcelona
Supercomputing
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Centro Nacional de Supercomputación

BSC Update

Oriol Jorba, Emanuele Emili, Jeronimo Escribano, Miriam Olid, Eleni Karnezi, Jayoung Yun, Guillaume Monteil, Andrea Piacentini, Ruben Sousse, Dene Bowdalo, Raphael Grodotzig, Hervé Petetin, Michael Orieux, James Petticrew, Carlos Pérez García-Pando

10-06-2026

ICAP 2026, Bonn, Germany

Outline

- MONARCH aerosol forecasts
 - ICAP global forecast update
 - MONARCH-dust SDS-WAS update
- JEDI DA activities
- Nitrate formation and the EMIT mineralogical dataset
- Surface observation representativeness for model evaluation
- Other highlights

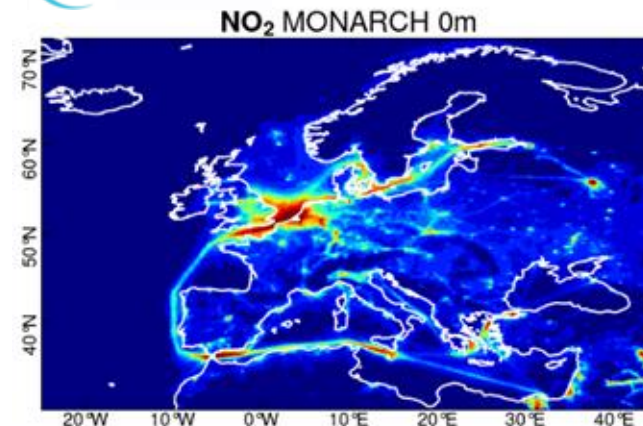
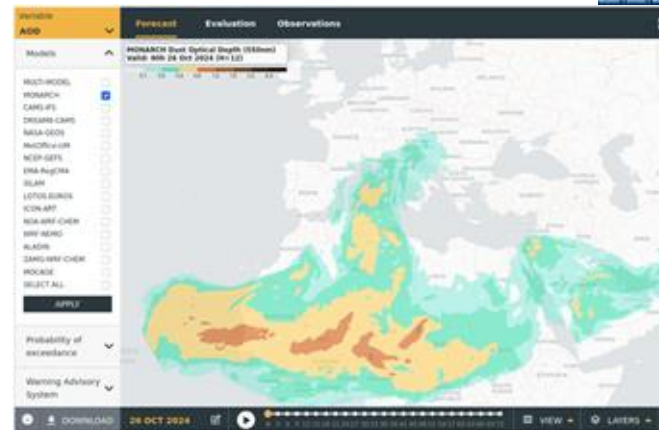
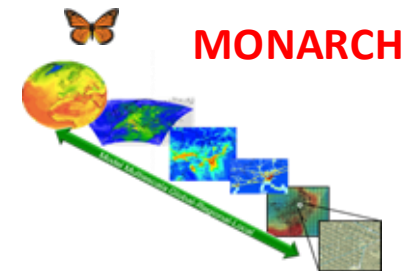
MONARCH aerosol forecasts



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Operational forecasts in 2026



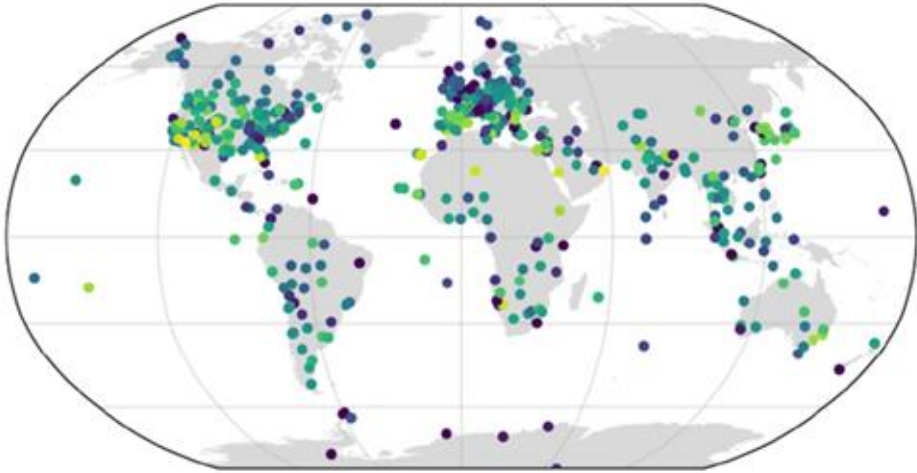
Global aerosols	Configuration
Meteorology	Inline NMMB
Initial condition	GFS 0.5x0.5 deg
Resolution	0.7x0.5 deg
Levels	48
Forecast range	5 days
Output frequency	6 hours
Species	Dust, Sea Salt BC, OC (POA,SOA) Sulfate
Size Bins	8 (dust, salt) bulk for others
Chemistry	Climatology
Antho. & Biogenic Emission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

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

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)

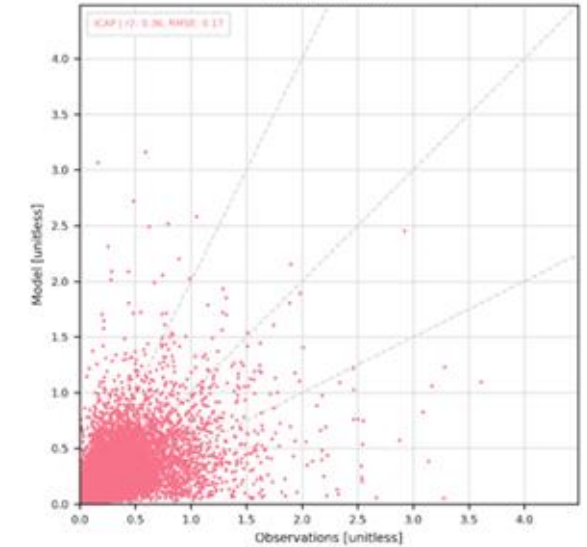
AERONET AOD evaluation of all ICAP upgrades-daily

All-All (604 stations)

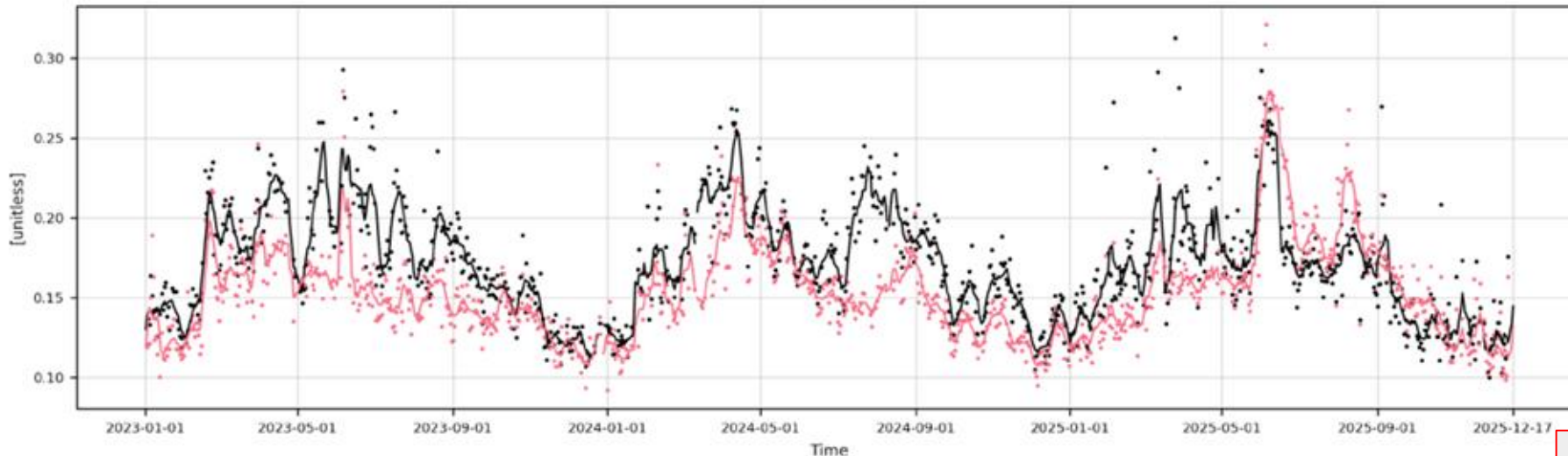


		Mean_bias	RMSE	r	MFB	MFE
All	ICAP	-0.02	0.17	0.60	-1.36	47.39
Europe	ICAP	-0.01	0.10	0.55	-3.56	44.01
Africa	ICAP	0.02	0.20	0.70	13.26	55.31
MiddleEast	ICAP	-0.06	0.23	0.55	-17.91	45.18
North America	ICAP	-0.00	0.14	0.48	2.29	42.61
South America	ICAP	-0.03	0.16	0.58	-20.60	55.99
North Asia	ICAP	-0.06	0.29	0.50	-5.64	52.73
South Asia	ICAP	-0.08	0.24	0.55	-17.54	49.83
Australia	ICAP	0.01	0.07	0.59	5.96	38.83

All-All (604 stations)



All-All (604 stations)



ICAP-old

ICAP-U1

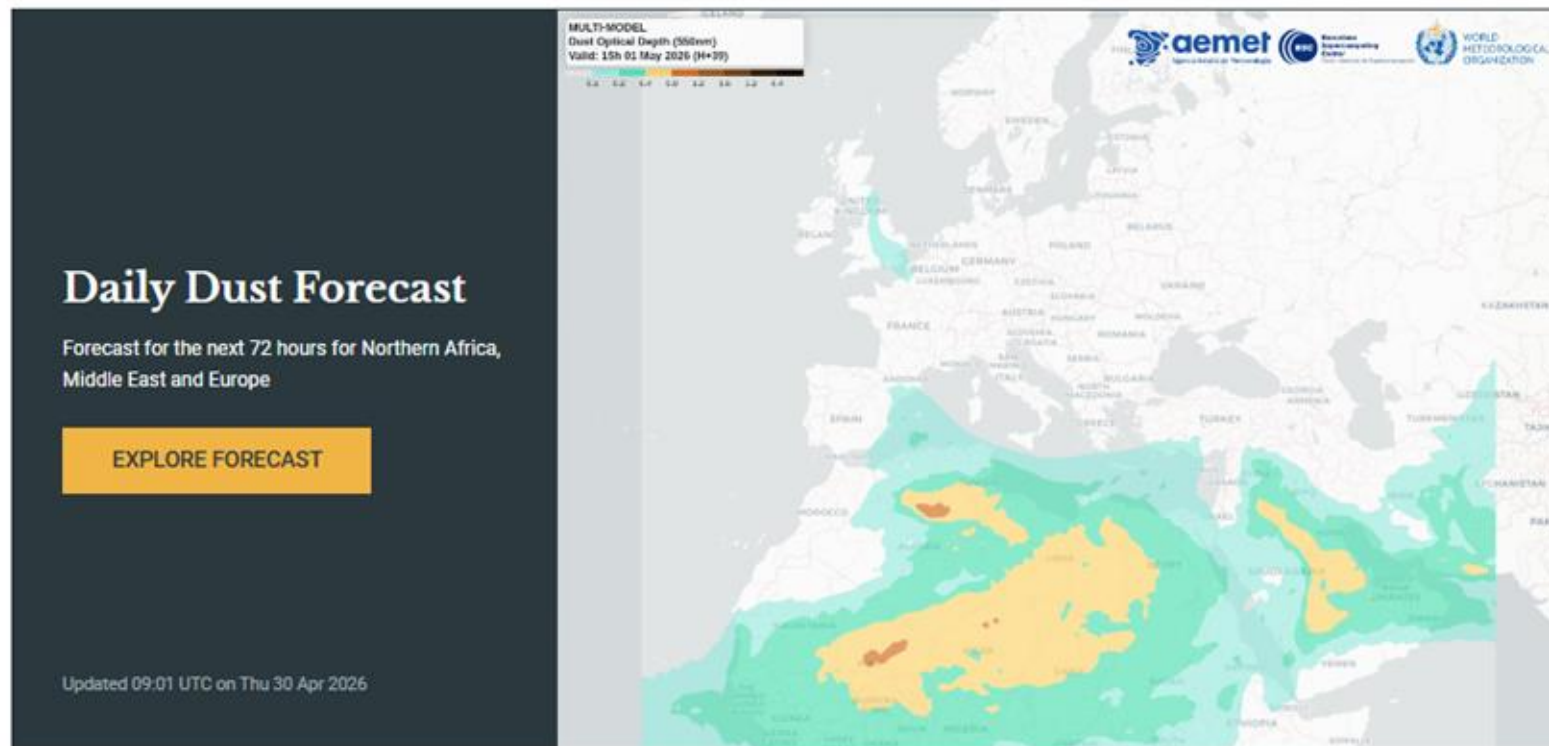
ICAP-U2

Production stopped to
be resumed in Summer
2026

Barcelona Dust Regional Center Update

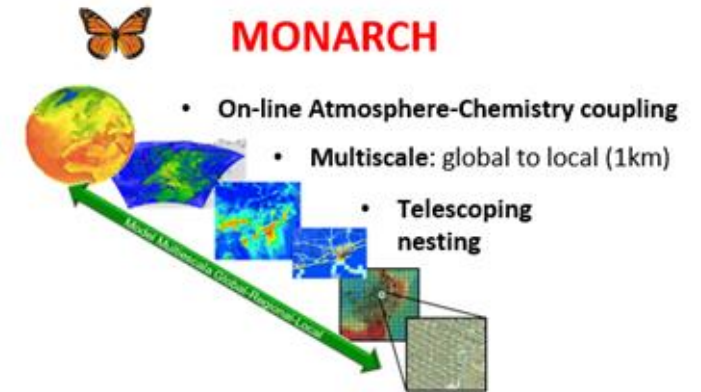


The screenshot shows the top navigation bar of the Barcelona Dust Regional Center website. On the left is the WMO logo and the text "Barcelona Dust Regional Center". On the right are links for "FAQ", "Contact Us", and "Log in", along with a search box. Below this is a dark navigation menu with "Products", "Research", "Resources", "News & Events", and "About Us". The main banner features a world map background and the text: "WMO SDS-WAS Regional Center for Northern Africa, Middle East and Europe, conducting research and providing operational products".

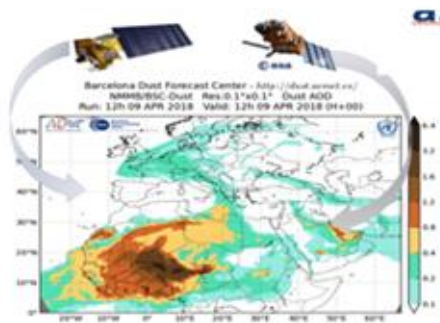


BDRC upgrades over the years

MONARCH Version	Date of deployment	Description of changes
v0.0.0	14th February 2012	<ul style="list-style-type: none"> • Pérez et al. (2011) version
v1.0.0	16th December 2020	<ul style="list-style-type: none"> • Introduction of different dust source functions • Introduction of different dust emission sources and emission schemes • Introduction of developments described in Perez et al. (2011), Spada (2015), Badia et al. (2017) and Di Tomaso (2017).
v2.1.0	15th June 2023	<ul style="list-style-type: none"> • Aerosol-radiation interaction allowed with dynamic coupling of dust-radiation • Introduction of spheroid particles • SNES postprocessor in the workflow



LETKF DA Ensemble based Data Assimilation system

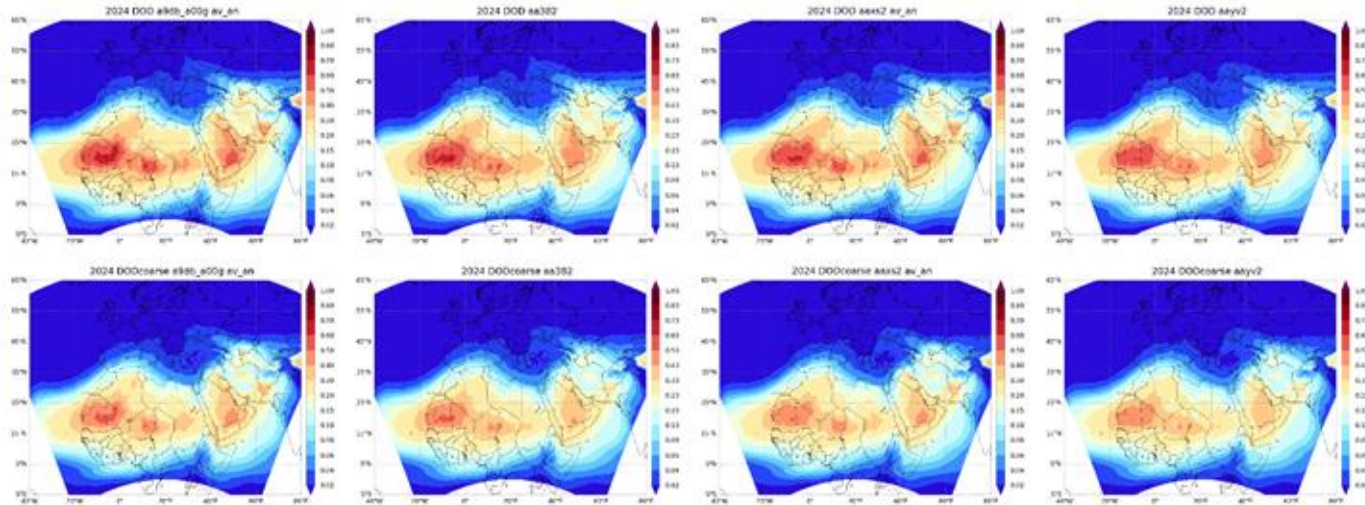


v2.7.2	25th July 2024	<ul style="list-style-type: none"> • Output of vertical layers of dust concentration • Correction in dry deposition • Change in threshold affecting wet scavenging below stratiform clouds
v2.11.0	22 nd July 2025	<ul style="list-style-type: none"> • Initialization with Data Assimilation of NOAA-20 VIIRS observations • Revision of dust emissions calibration factor • Bug-fix in the postprocessor for the expression of dust concentrations

BDRC next upgrade U4 Summer 2026

E. Emili,
E. Karnezi,
M. Olid

BDRC-U3-AN BDRC-U3-FC BDRC-U4-AN BDRC-U4-FC



AOD coarse (O'Neill) evaluation 2024

		Mean_bias	RMSE	r	MFB	MFE
Selected_BDRC_2021	BDRC_U3-AN	0.01	0.08	0.79	-58.87	99.53
	BDRC_U3-FC	0.00	0.08	0.77	-60.85	100.11
	BDRC_dcal-AN	5.91e-04	0.08	0.79	-62.71	100.02
	BDRC_dcal-FC	-0.00	0.08	0.77	-64.66	100.60
Mediterranean	BDRC_U3-AN	-0.02	0.06	0.77	-80.87	101.04
	BDRC_U3-FC	-0.02	0.06	0.74	-81.87	102.07
	BDRC_dcal-AN	-0.02	0.05	0.77	-84.79	102.63
	BDRC_dcal-FC	-0.02	0.06	0.74	-85.75	103.63
NorthAfrica	BDRC_U3-AN	0.05	0.14	0.75	12.48	82.58
	BDRC_U3-FC	0.05	0.14	0.72	11.84	83.26
	BDRC_dcal-AN	0.04	0.13	0.75	8.84	80.89
	BDRC_dcal-FC	0.04	0.13	0.72	8.07	81.58
Sub-SaharanAfrica	BDRC_U3-AN	0.03	0.10	0.85	-14.19	60.45
	BDRC_U3-FC	0.03	0.10	0.85	-14.36	60.48
	BDRC_dcal-AN	0.02	0.09	0.85	-18.01	59.60
	BDRC_dcal-FC	0.02	0.10	0.85	-18.48	59.74
MiddleEast	BDRC_U3-AN	0.04	0.10	0.76	1.83	68.95
	BDRC_U3-FC	0.02	0.10	0.75	-9.00	69.57
	BDRC_dcal-AN	0.03	0.10	0.76	-3.69	68.58
	BDRC_dcal-FC	0.02	0.09	0.75	-14.18	69.26
SouthernEurope	BDRC_U3-AN	-0.01	0.05	0.60	-114.61	134.23
	BDRC_U3-FC	-0.01	0.05	0.59	-114.00	133.96
	BDRC_dcal-AN	-0.02	0.04	0.60	-117.38	135.02
	BDRC_dcal-FC	-0.01	0.04	0.59	-116.78	134.73

Global calibration revised down

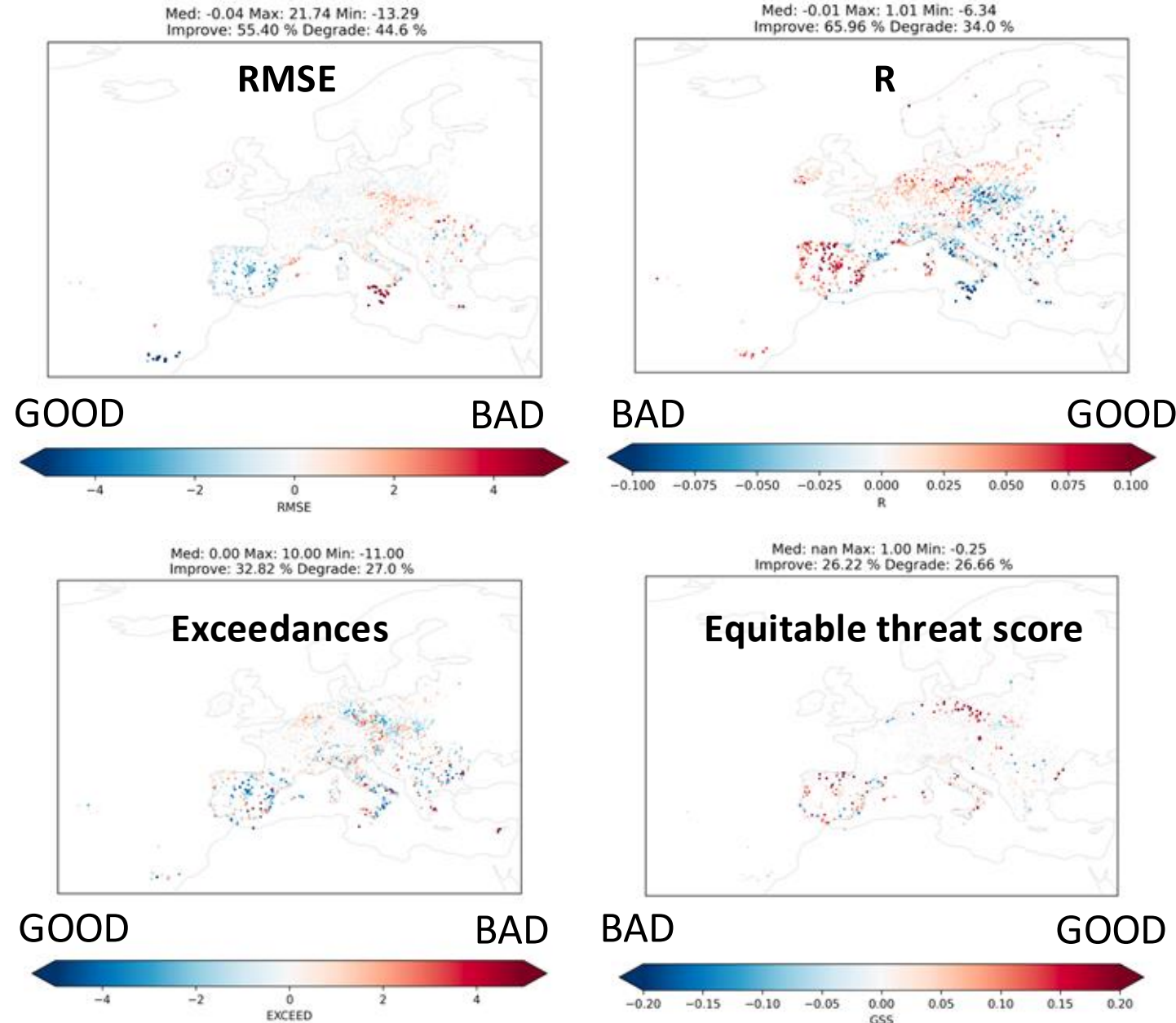
Workflow more robust to DA failures (use past days or propagate free ensemble)

Evaluating dust surface forecasts for EU AQ directive

- Contribution of natural aerosols (dust) to EU particulate pollution of growing concern
- Not yet proven impact of satellite data assimilation for Air Quality (AQ) applications
- Employed atmospheric composition models to account for **non-dust PM10** contribution
- Summed **dust-PM10** contribution from two MONARCH BDRC forecasts (**U2** no satellite assimilation, **U3** NOAA20-VIIRS assimilation)
- Computed usual skill scores (**RMSE**, **R**) against **EEA daily PM10 measurements** but also **50 mug/m3 exceedances** and corresponding scores (POD, FAR, GSS)

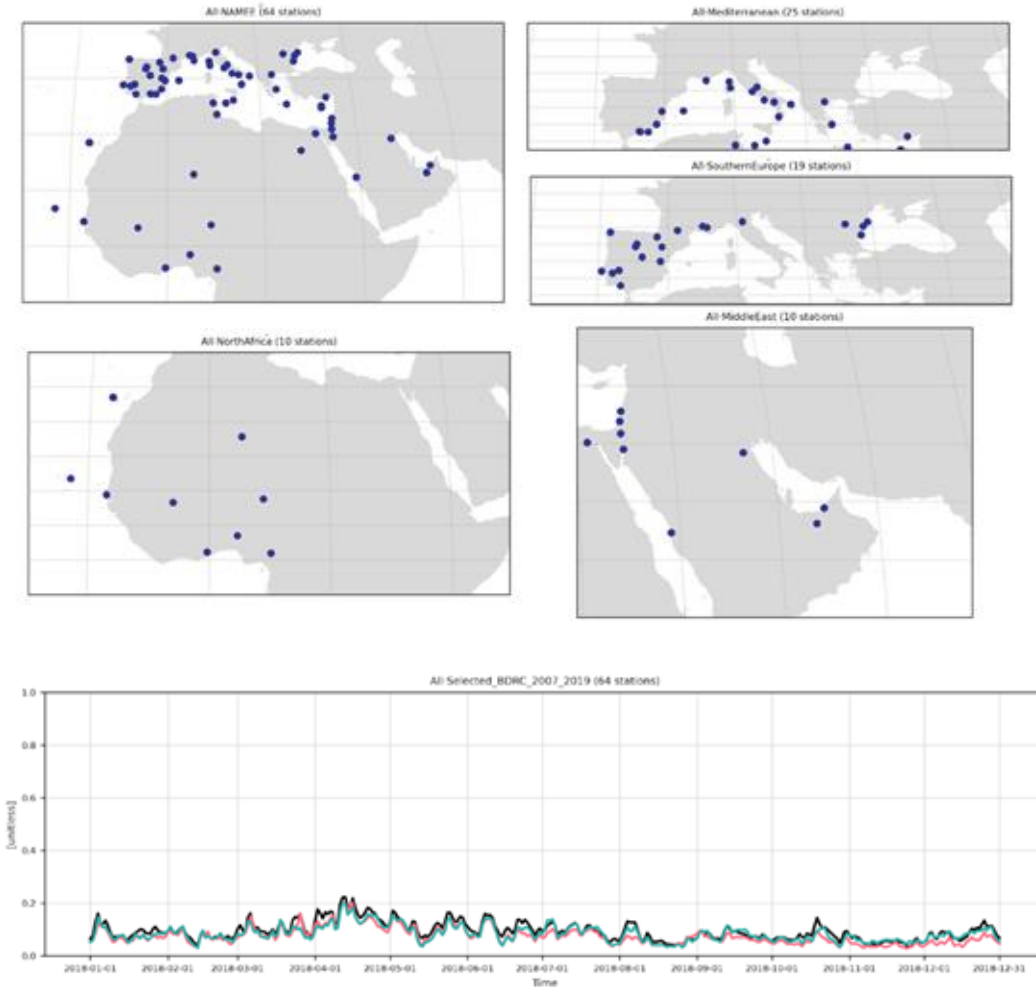
Result

- Impact of satellite dust assimilation on PM10 mostly positive in Western Europe and Canaries



- DustClim v1.0 2006 - 2018
- DustClim 2.0 2019
 - Aligned with BDRC U4
 - Dust emission scheme from Ginoux (2001) updated with friction velocity (Klose et al. 2020) ***instead of three different emission schemes in the original DustClim.***
 - OPAC tri-axial spheroids extinction coefficients ***instead of spherical particles in the original DustClim.***
 - The input meteorology (initial and boundary conditions) has been changed from ERA-Interim to ERA-5 (Hersbach et al. 2020).
 - NOAA-20 VIIRS NASA AOD for assimilation as last BDRC upgrade
 - Preparation production for the period 2020-2024

DustClim v2.0 vs v1.0 : AERONET evaluation (O'Neill product)



		NDAT A	r	RMSE	MB	MFB	MFE
NAMEE	DustClim	43628	0.79	0.10	-0.02	-82.4	107.5
	DustClim 2.0		0.83	0.08	-0.01	-72.2	101.9
Mediterranean	DustClim	15850	0.80	0.06	-0.02	-97.7	110.6
	DustClim 2.0		0.84	0.05	-0.01	-86.7	105.3
North Africa	DustClim	5358	0.83	0.16	-0.07	-58.3	73.8
	DustClim 2.0		0.84	0.15	-0.03	-30.2	64.8
Middle East	DustClim	7746	0.70	0.15	0.05	23.1	67.9
	DustClim 2.0		0.70	0.13	0.04	18.8	67.1
Southern Europe	DustClim	14674	0.69	0.05	-0.03	-130.4	137.3
	DustClim 2.0		0.83	0.04	-0.02	-120	130.1

JEDI DA activities

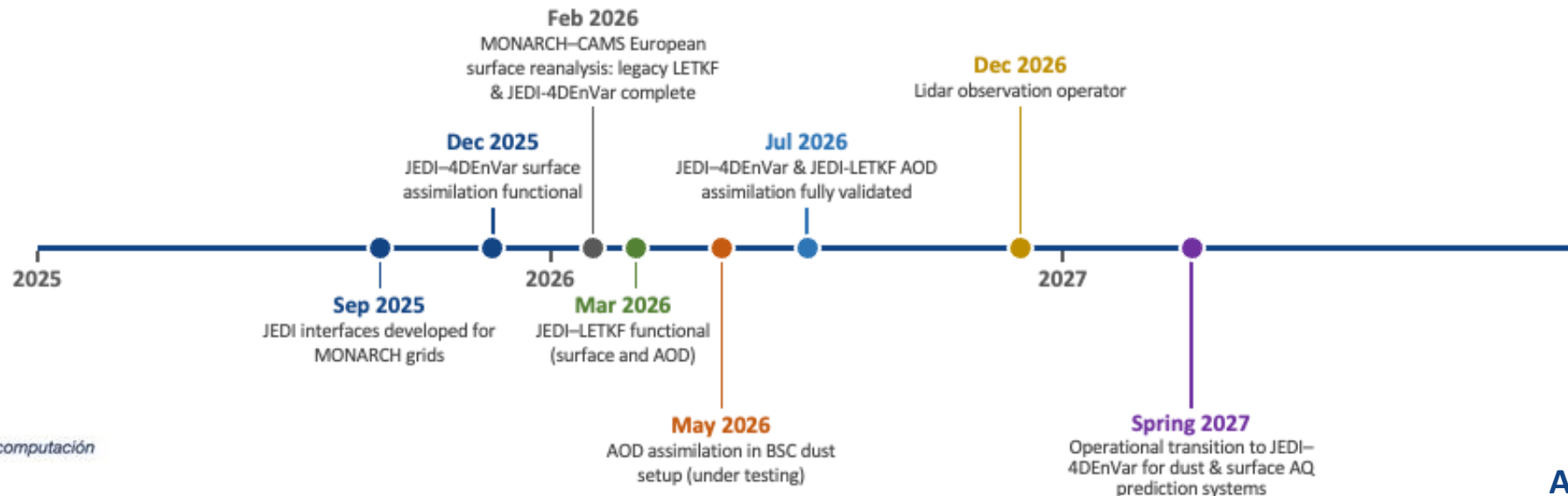


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Roadmap towards transitioning to JEDI at BSC

- The legacy LETKF code used at BSC was far from efficient and difficult to upgrade (e.g. new instruments, control variables, multi-compound assimilation)
- Aim to transition from LETKF to 4DEnVar:
 - Linearized observation operators should be more accurate than raw ensemble sensitivities (ensemble sizes smaller than 12 in our current operations)
 - Localization in model space (4DEnVar) instead of in observation space (LETKF) should help with non-local observations and multi-compounds assimilation
- Benefit from community developments on DA algorithm aspects that cannot be afforded in-house (covariance modeling, localization, minimizers, numerical optimizations ...)
- BSC aims to focus on aspects of JEDI-DA that relate to observation operators for atmospheric composition (UFO)



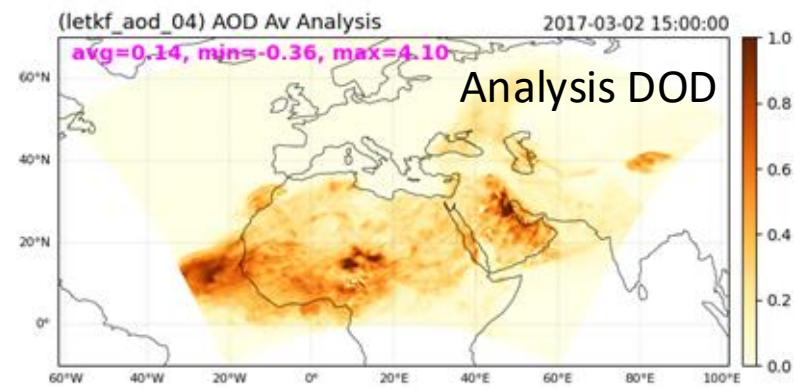
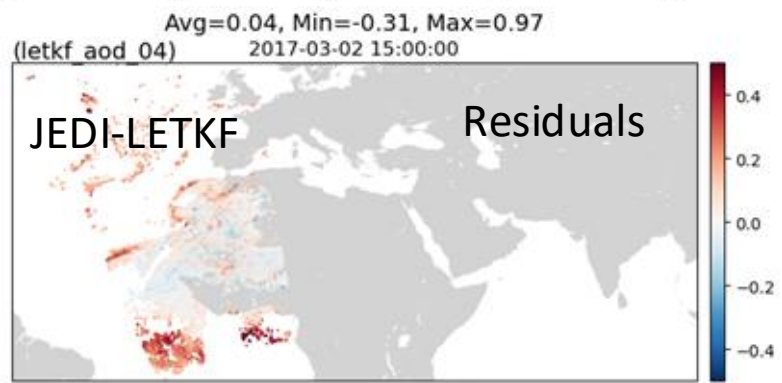
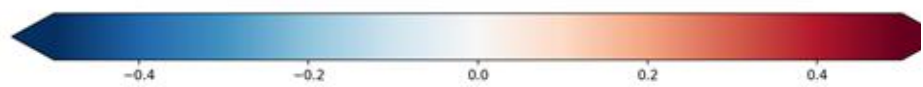
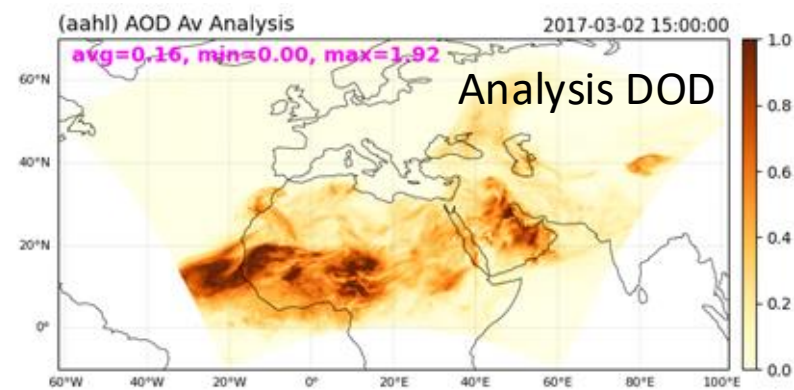
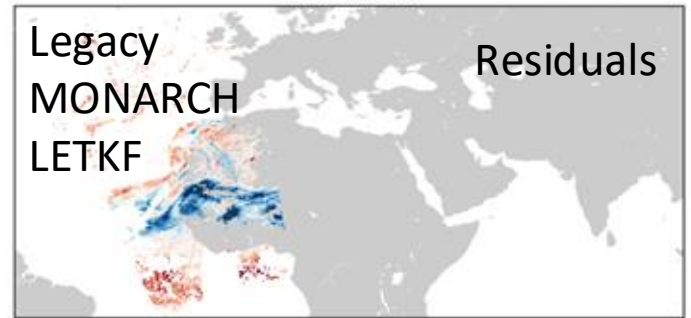
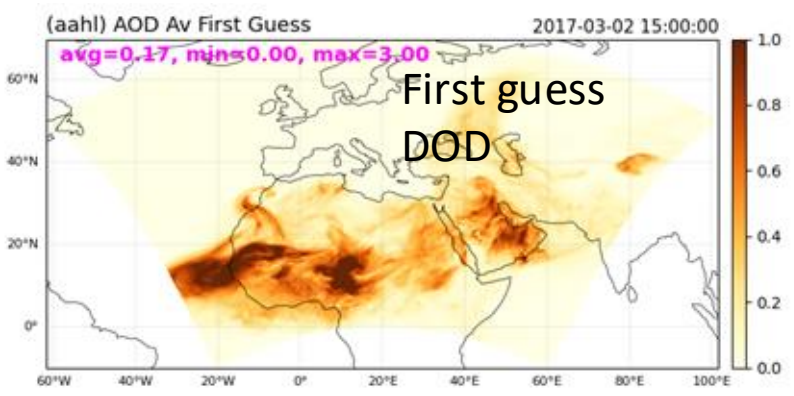
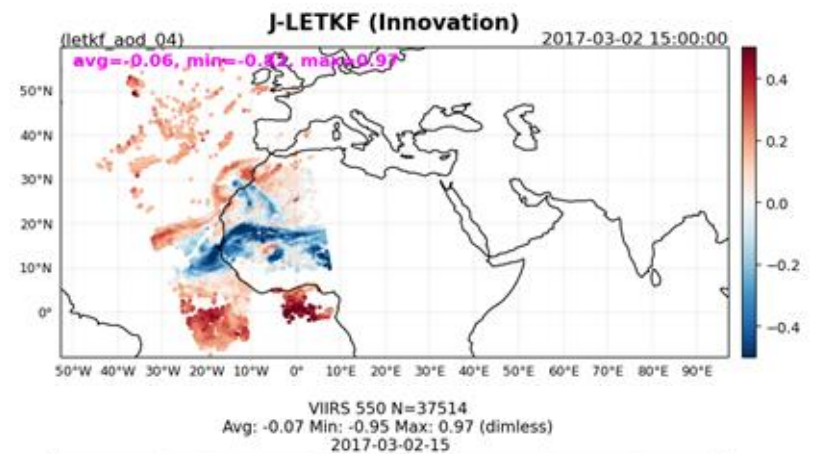
Jayoung Yun,
 E. Emili,
 G. Monteil,
 Andrea Piacentini

JEDI-LETKF vs Legacy MONARCH-LETKF

- NOAA-20 VIIRS AOD operational assimilation setup for the Barcelona Dust Regional Center (12 ensemble members)
- Identical setup experiments (legacy LETKF versus JEDI-LETKF)

Main algorithmic differences:

- Total dust mass (legacy-LETKF) versus resolved dust PSD (JEDI-LETKF) as control variable
- Miyoshi, T. and Y. Sato, 2007 vertical localization based on model extinction profile (legacy-LETKF) versus no vertical localization (JEDI-LETKF)



Nitrate formation and the EMIT dataset



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Nitrate heterogeneous formation

Ruben Sousse,
Oriol Jorba,
Carlos Pérez

- Incorporate a variety of mechanisms with different complexity in MONARCH
- Understand the role of dust heterogeneous chemistry processes
- Understand the role of mineralogical representation of dust
- Assess the impact on secondary inorganic aerosol formation and aerosol optical properties

Irreversible reactions		
Reaction	Process	
(R1) $DU_{(acr)} + H_2SO_{4(g)} \rightarrow SO_{4(aq)}^{2-}$	Condensation	
(R2) $SS_{(acr)} + H_2SO_{4(g)} \rightarrow SO_{4(aq)}^{2-}$	Condensation	
(R3) $DU_{(acr)} + SO_{2(g)} \rightarrow SO_{4(aq)}^{2-}$	UPTK (γ_1)	
(R4) $CaCO_{3(aer)} + 2HNO_{3(g)} \rightarrow Ca(NO_3)_{2(aer)} + H_2O + CO_2$	UPTK (γ_2)	
(R5) $SS_{(acr)} + HNO_{3(g)} \rightarrow NaNO_{3(aer)} + HCl_{(g)}$	UPTK (γ_3)	

Gas-particle equilibrium reactions		
Reaction	Process	
(R6) $HNO_{3(g)} + NH_{3(g)} \rightleftharpoons NH_4^+_{(aq)} + NO_3^-_{(aq)}$	TEQ	
(R7) $H_2SO_{4(g)} + NH_{3(g)} \rightleftharpoons NH_4^+_{(aq)} + SO_4^{2-}_{(aq)}$	TEQ	
(R8) $CaCO_{3(aq)} + 2HNO_{3(g)} \rightleftharpoons Ca^{2+}_{(aq)} + 2NO_3^-_{(aq)} + H_2O + CO_2$	TEQ	
(R9) $MgCO_{3(aq)} + 2HNO_{3(g)} \rightleftharpoons Mg^{2+}_{(aq)} + 2NO_3^-_{(aq)} + H_2O + CO_2$	TEQ	
(R10) $K_2CO_{3(aq)} + 2HNO_{3(g)} \rightleftharpoons 2K^+_{(aq)} + 2NO_3^-_{(aq)} + H_2O + CO_2$	TEQ	
(R11) $Na_2CO_{3(aq)} + 2HNO_{3(g)} \rightleftharpoons 2Na^+_{(aq)} + 2NO_3^-_{(aq)} + H_2O + CO_2$	TEQ	
(R12) $NaCl_{(aq)} + HNO_{3(g)} \rightleftharpoons Na^+_{(aq)} + NO_3^-_{(aq)} + HCl_{(g)}$	TEQ	

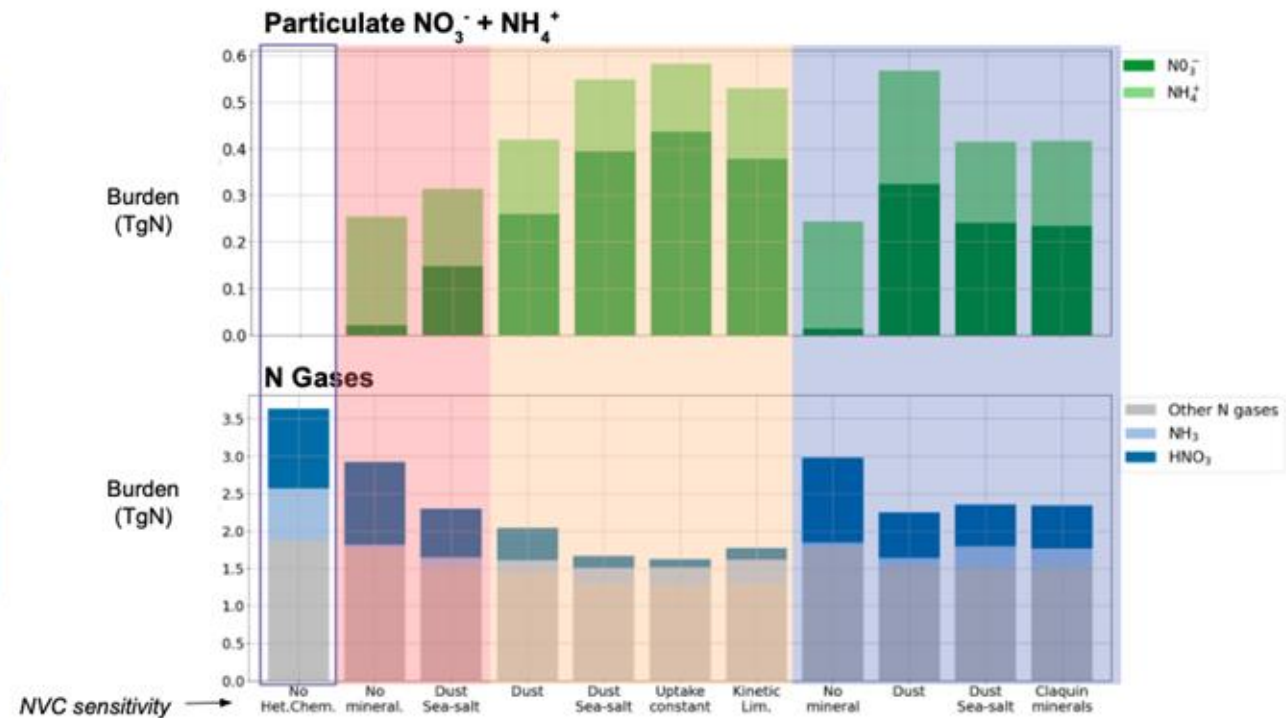
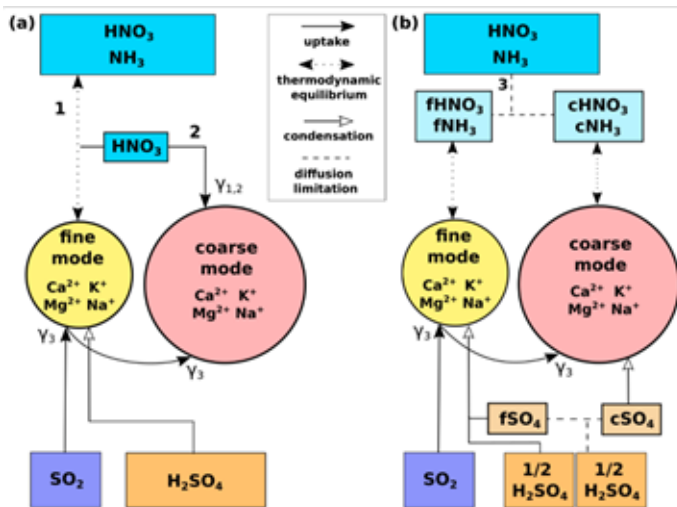
MECHANISMS

No Het. Chem.

Reversible fine SIA

Reversible fine SIA + Irreversible coarse SIA

Reversible fine & coarse SIA



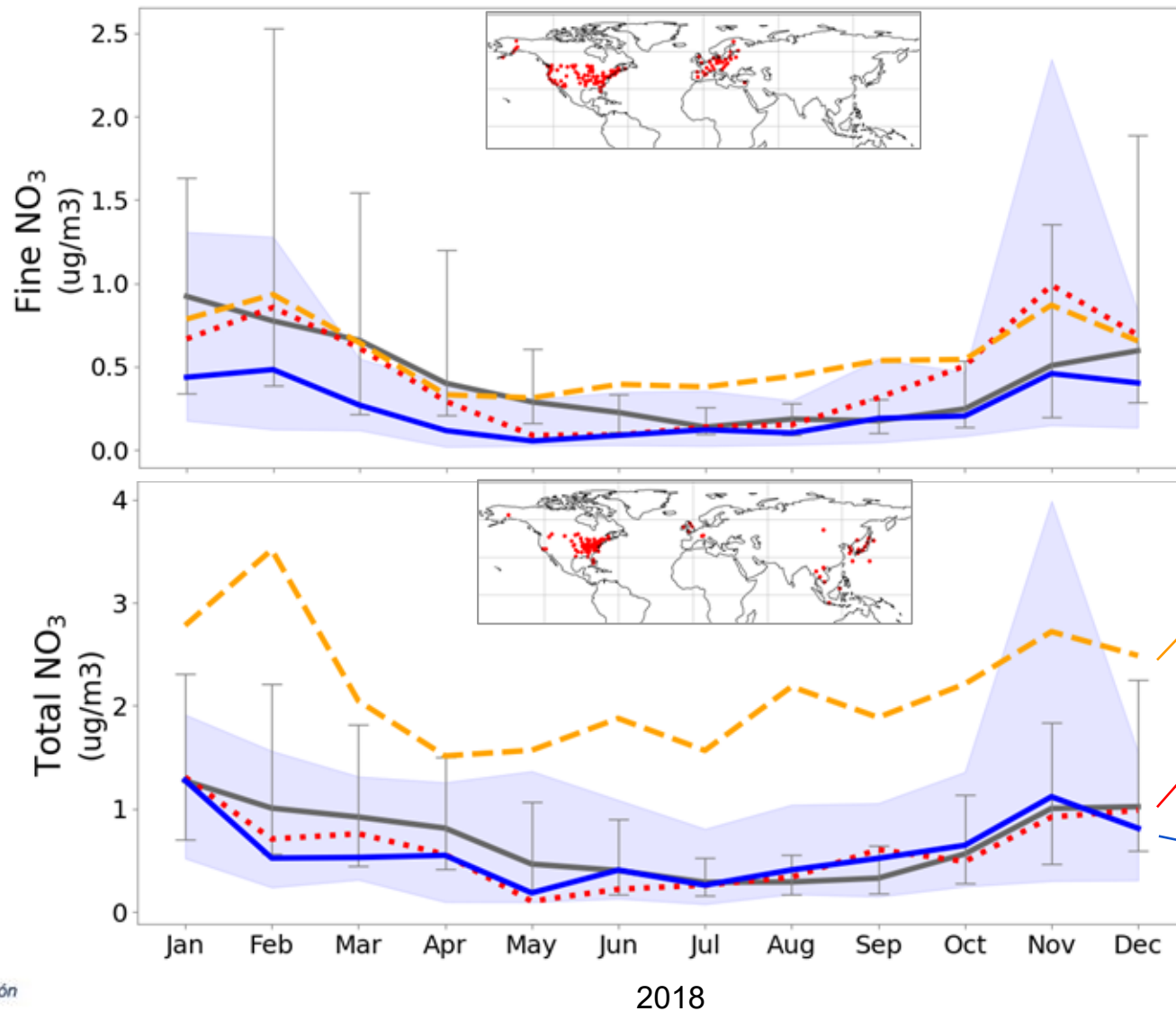
Evaluation of surface particulate nitrate

MECHANISMS

Reversible
fine SIA

Reversible
fine SIA
+
Irreversible
coarse SIA

Reversible
fine &
coarse SIA



Overestimates NO_3^-
Correlation ~ 0.6

Compensates for coarse NO_3^-
Correlation ~ 0.9

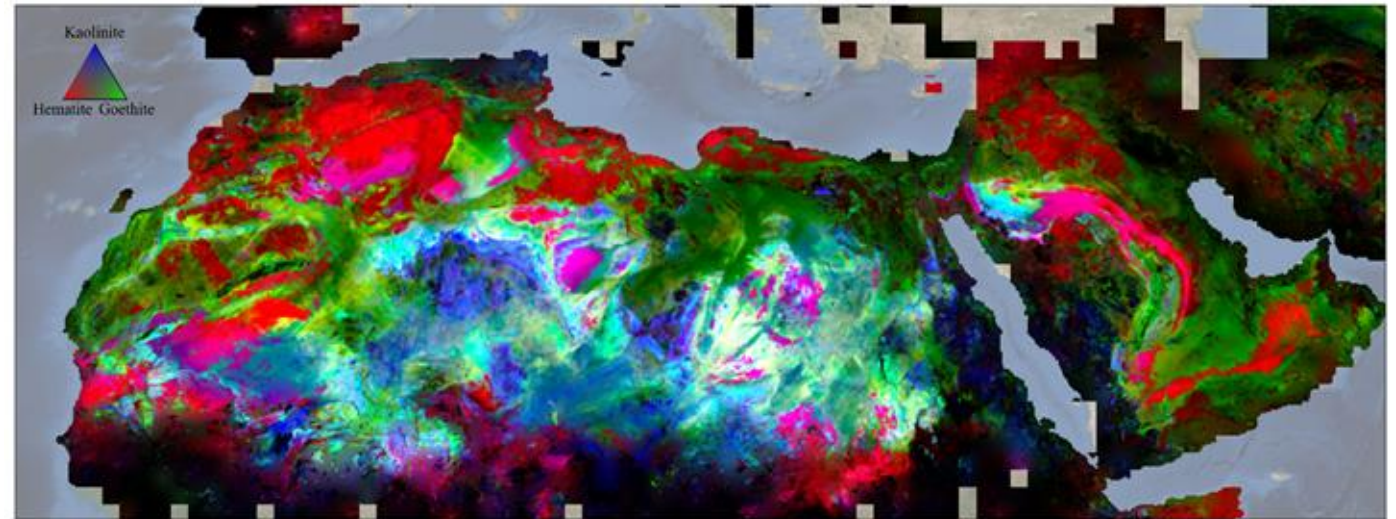
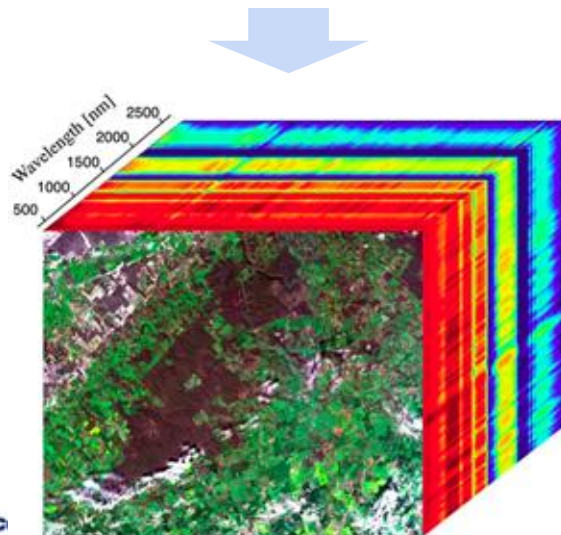
Balances accuracy and
size representation
Correlation ~ 0.8

The Earth Surface Mineral Dust Source Investigation (EMIT)

Green and Thompson 2020
Brodrick et al. 2025



- Imaging spectrometer
- Launched by NASA in 2022 onboard ISS
- Observationally constrained mineral soil-surface data
- High-resolution mineral characterization



Calcite representation using different datasets

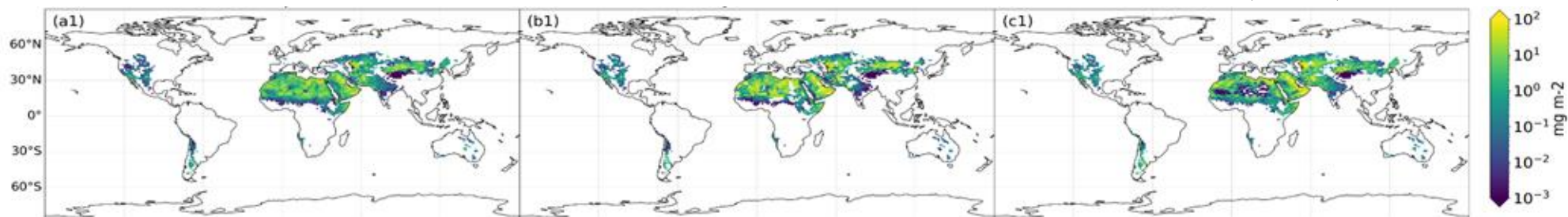
Comparison of mineral datasets

Claquin et al. 1999

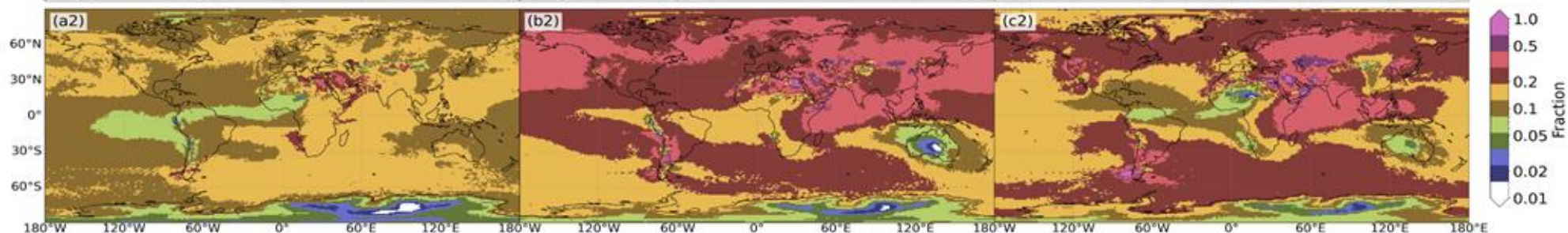
Journet et al. 2014

EMIT (2023)

Ca²⁺
emissions

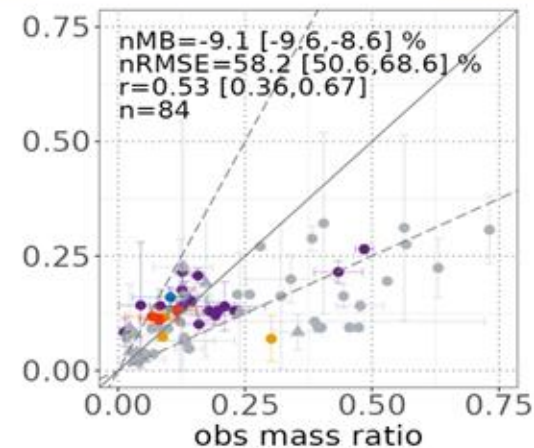
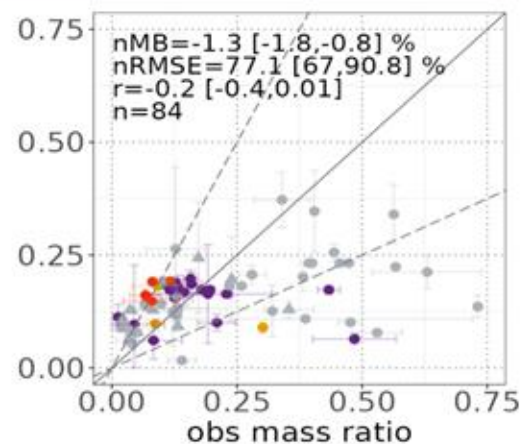
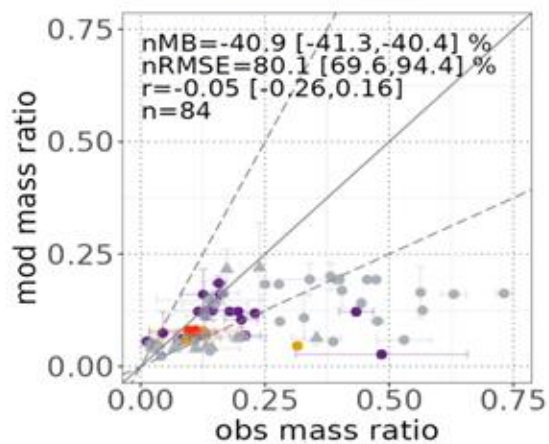


Ca²⁺ / dust
Surf. fraction



Evaluation
of CaCO₃

Perlwitz et al. 2015b
(1960s-present)

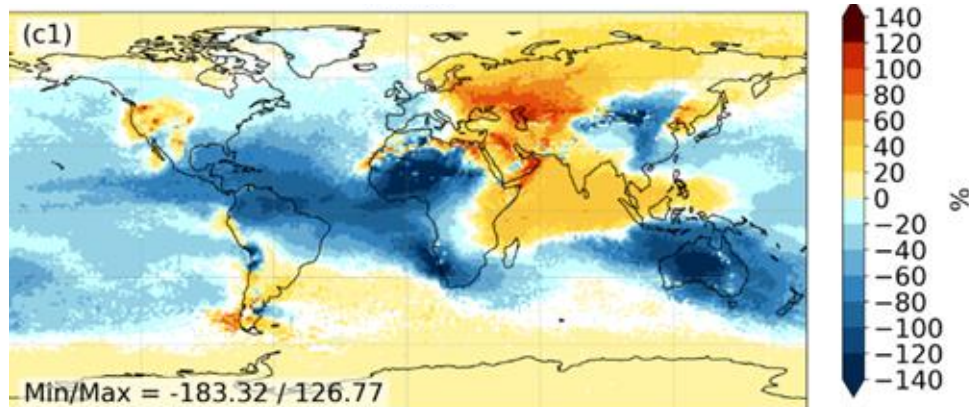


Size range
 • <2µm
 • <10µm
 • <20µm
 • bulk
 • 2-20µm

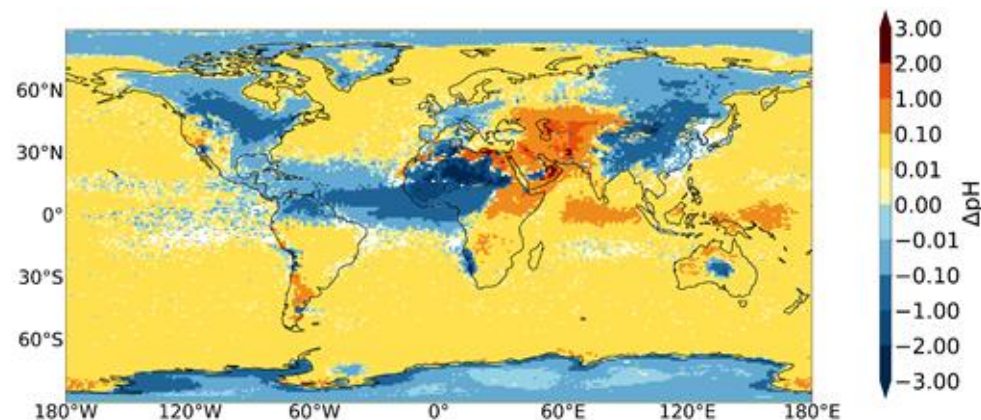
Impact on secondary inorganic aerosol and pH

Source-based CaCO_3 vs. Globally-averaged CaCO_3
 Ca^{2+} & SIA

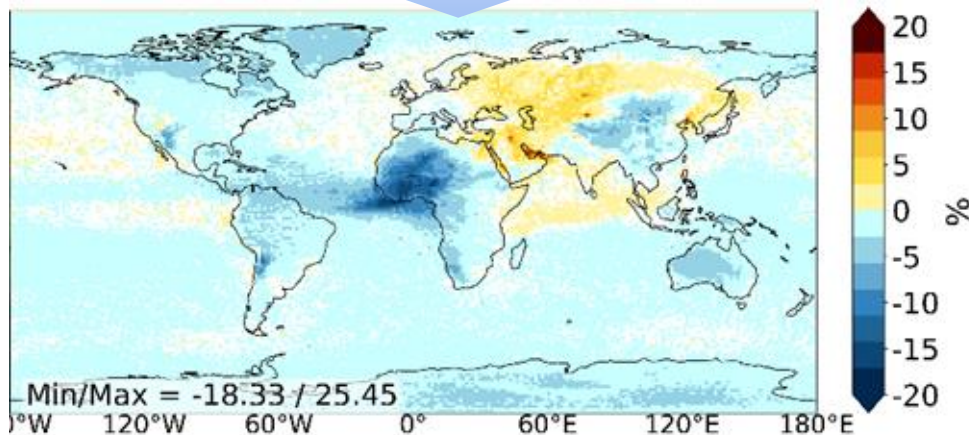
Differences % (PM20)
Source-based - Glob.Avg.



Surface total ΔpH
Source-based - Glob.Avg.



ΔSIA
Surf.Conc.



pH differences from **-4 to +3 units**

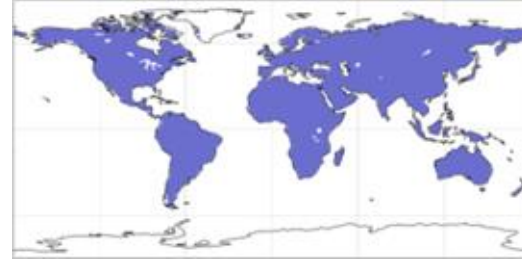
Impact on aerosol optical properties

- Implement EMIT mineralogy in MONARCH with two configurations:
 - **Globally-averaged** simplified mineralogy
 - **Source-based** “realistic” mineralogy
- Impacts on aerosol single-scattering albedo (SSA) due to:
 - Secondary inorganic aerosol (**SIA**) formation
 - Mineralogy (**Iron oxides**)

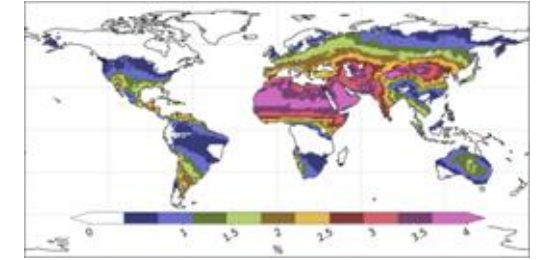
Result

- Secondary inorganic aerosols have a secondary effect on aerosol SSA.
- Iron oxides play a principal role in shaping aerosol SSA.

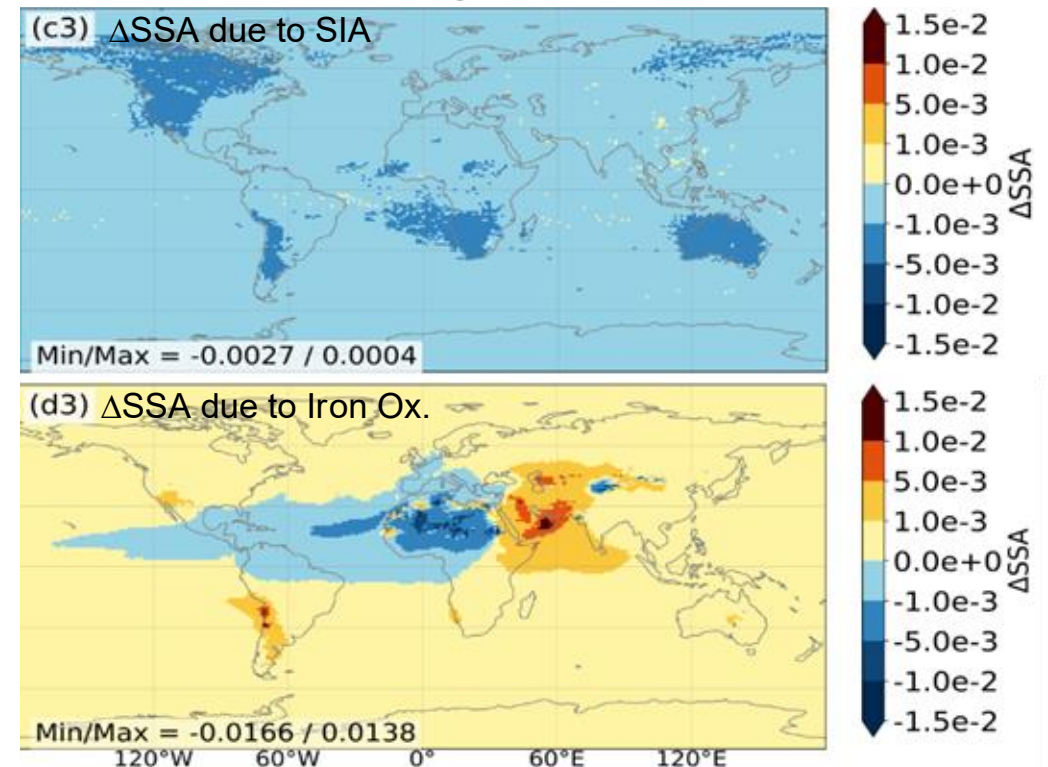
Globally-averaged mineralogy



Source-based mineralogy



vs.



Surface observation representativeness for model evaluation



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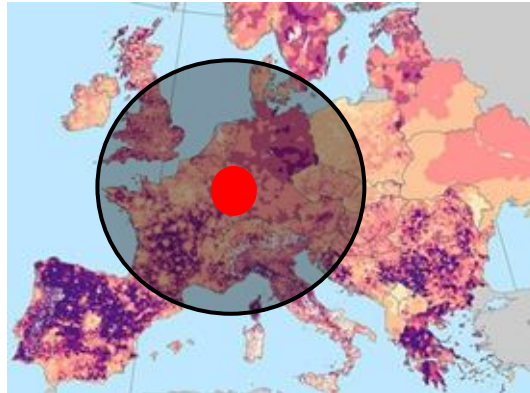
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In-situ observation representativeness for models

Spatial Representativity

Calculated using gridded proxies: *population density, nighttime lights, land cover, ruggedness etc.*

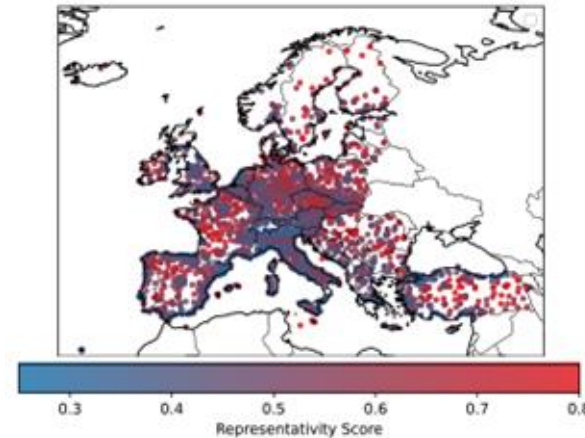
Calculate variance per station



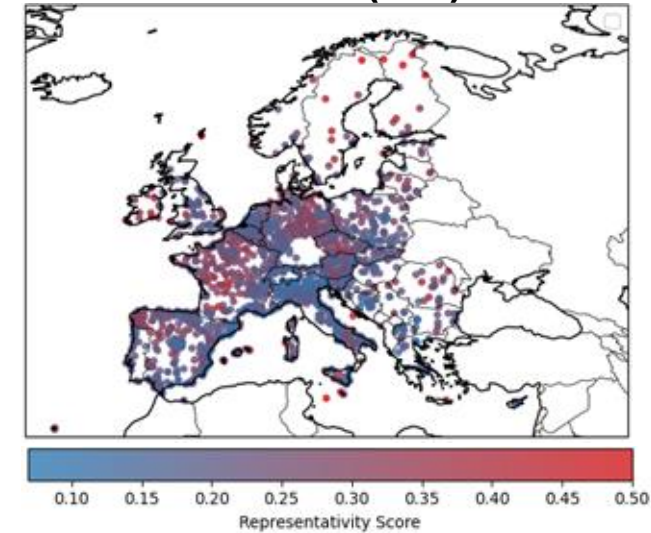
What is the spatial variability around each station at the model resolution?



Integrate variances in one score per station (0-1)

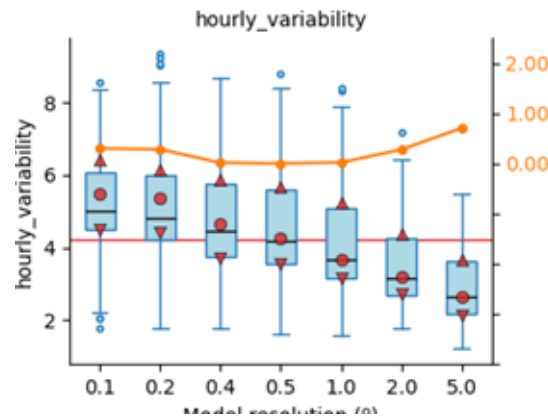


Total representativity per station (0-1)

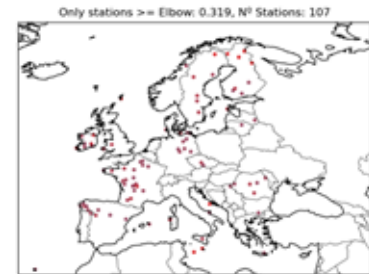
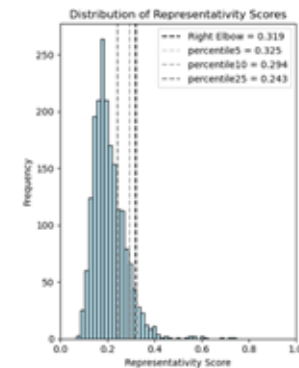
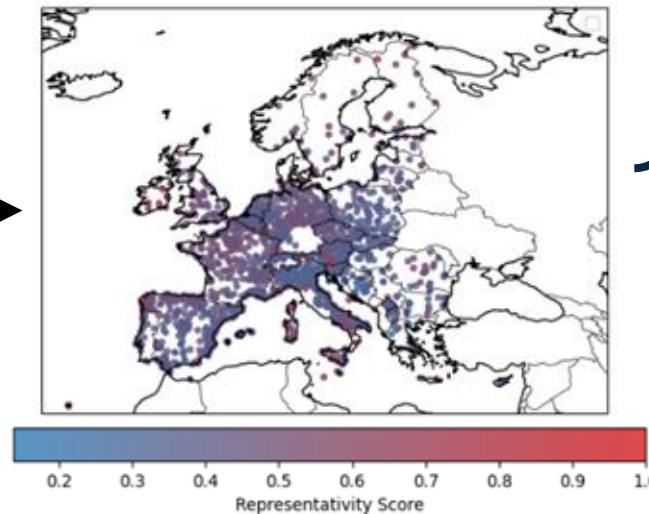


Temporal Representativity

Calculated using metrics: *hourly variability, daily variability, hourly spread etc.*



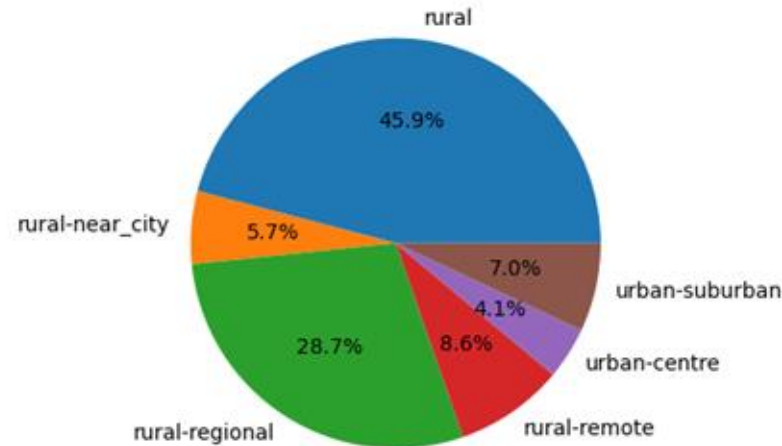
How similar is the temporal metric at each station with those surrounding it?



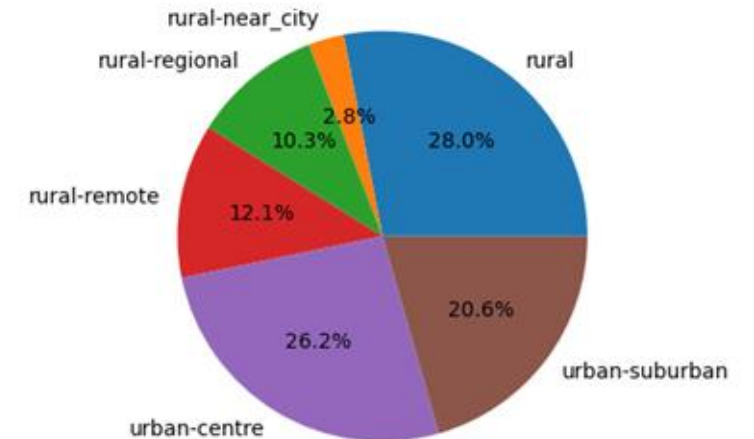
Selected station types for O₃

- Selected stations for model evaluation (with scores \geq elbow) are very different than those from Joly-Peuch (1-2).
- The Joly-Peuch method are 90% rural, whereas our method results in an almost 50/50% split between rural and urban stations.

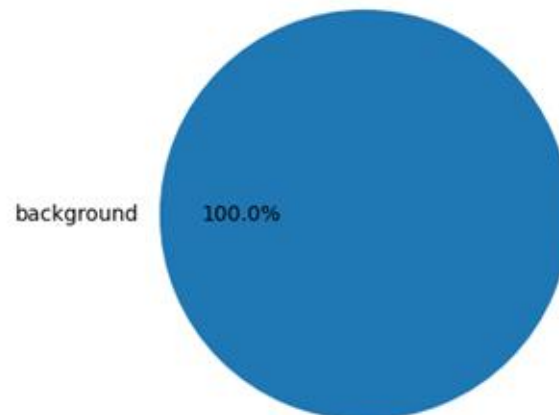
Area classification for JP_1-2 (total 244)



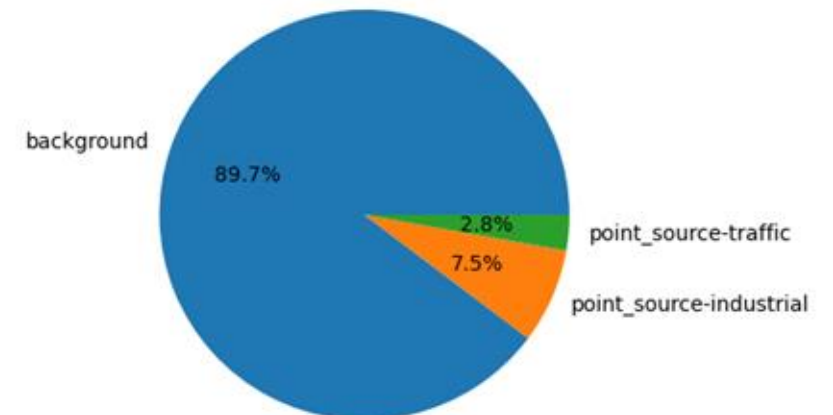
Area classification for Representativity \geq 0.319 (total 107)



Station classification for JP_1-2 (total 244)



Station classification for Representativity \geq 0.319 (total 107)



Global CAMS forecast evaluation – 24/25 DJF

O₃

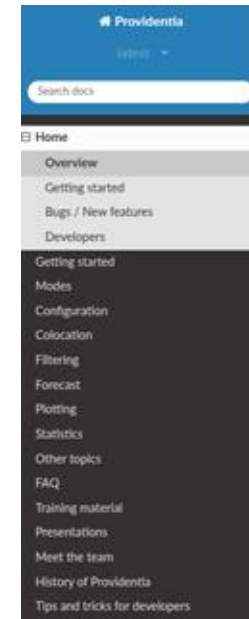
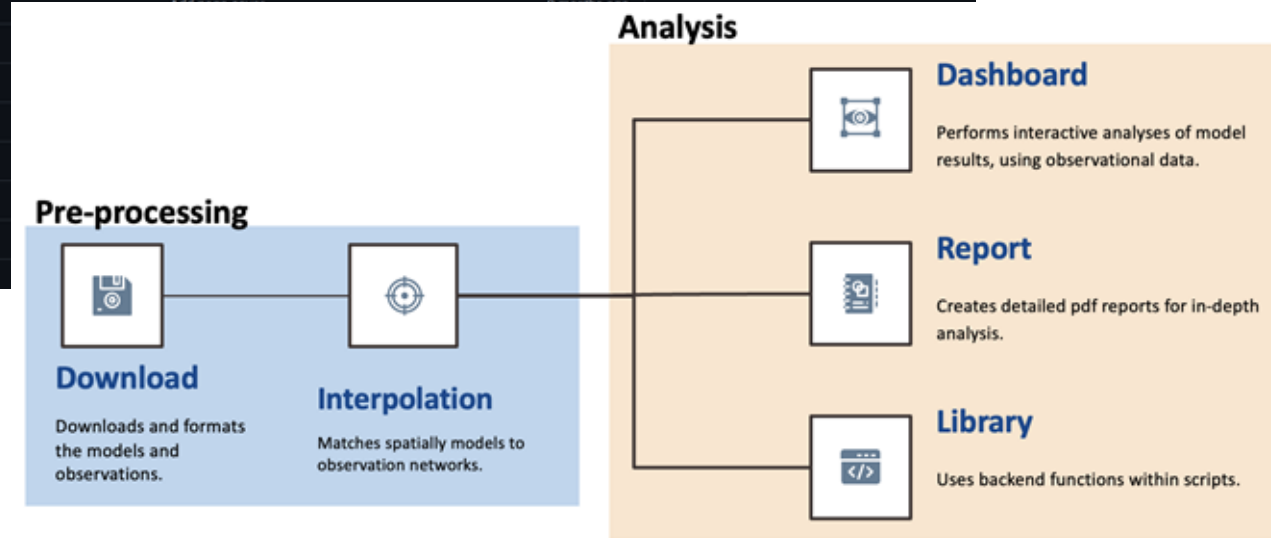
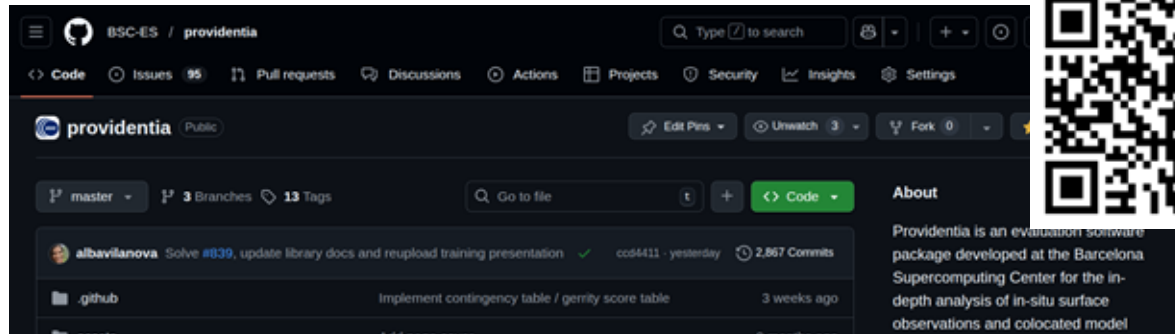
			Mean	StdDev	MFB	MFE	r	NStations
sconco3	all	camsf-day1	5.01	-1.63	29.38	39.75	0.68	1992.50
		camsf-day4	5.04	-1.49	29.48	41.80	0.62	1992.50
	JP_1-2-all	camsf-day1	-1.09	0.01	-3.54	22.77	0.64	237.00
		camsf-day4	-1.15	0.12	-3.62	24.46	0.58	237.00
	elbow	camsf-day1	2.56	-1.01	11.18	21.03	0.71	104.00
		camsf-day4	2.54	-0.92	9.92	22.99	0.65	104.00

- Method results in low model biases and high correlation scores.

NO₂

			Mean	StdDev	MFB	MFE	r	NStations
sconcno2	all	camsf-day1	-5.27	-2.78	-77.06	86.13	0.39	2743.00
		camsf-day4	-5.24	-2.75	-76.03	86.62	0.34	2743.00
	JP_1-2-all	camsf-day1	0.53	0.41	14.46	55.39	0.44	149.00
		camsf-day4	0.54	0.44	12.99	57.50	0.36	149.00
	elbow	camsf-day1	0.02	-0.08	1.02	54.33	0.46	111.00
		camsf-day4	-0.06	-0.06	0.20	57.20	0.40	111.00

Providentia: an evaluation package for atmospheric modeling



Repository: <https://github.com/bsc-es/providentia>

Documentation: <https://providentia.readthedocs.io/en/latest/>

OS: Linux and Mac. On Windows through WSL and virtual machines.

Other highlights

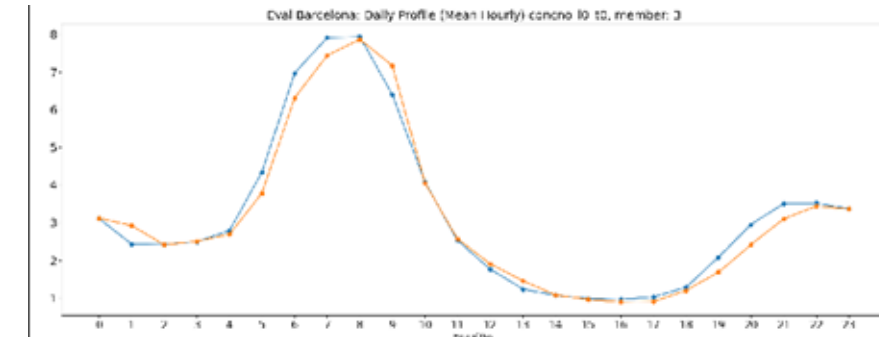
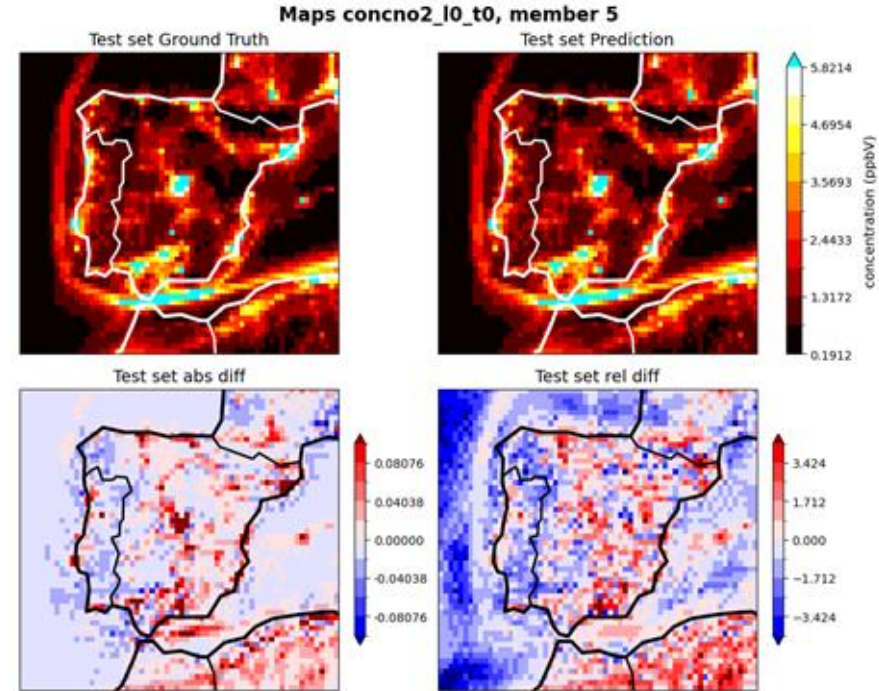
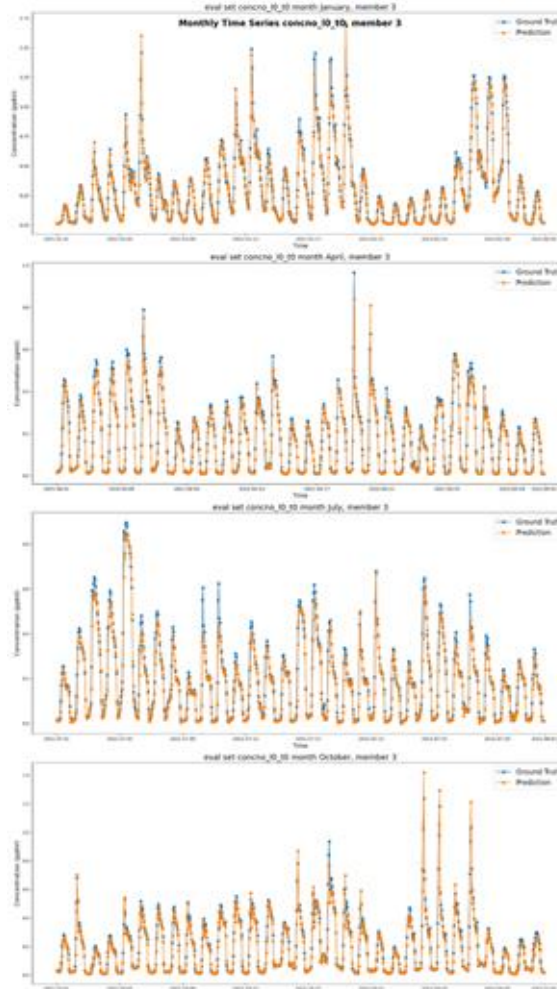
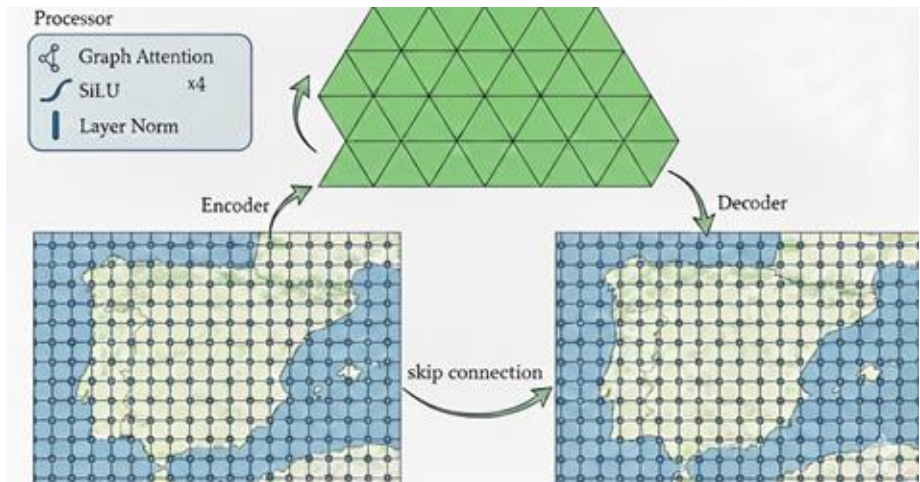


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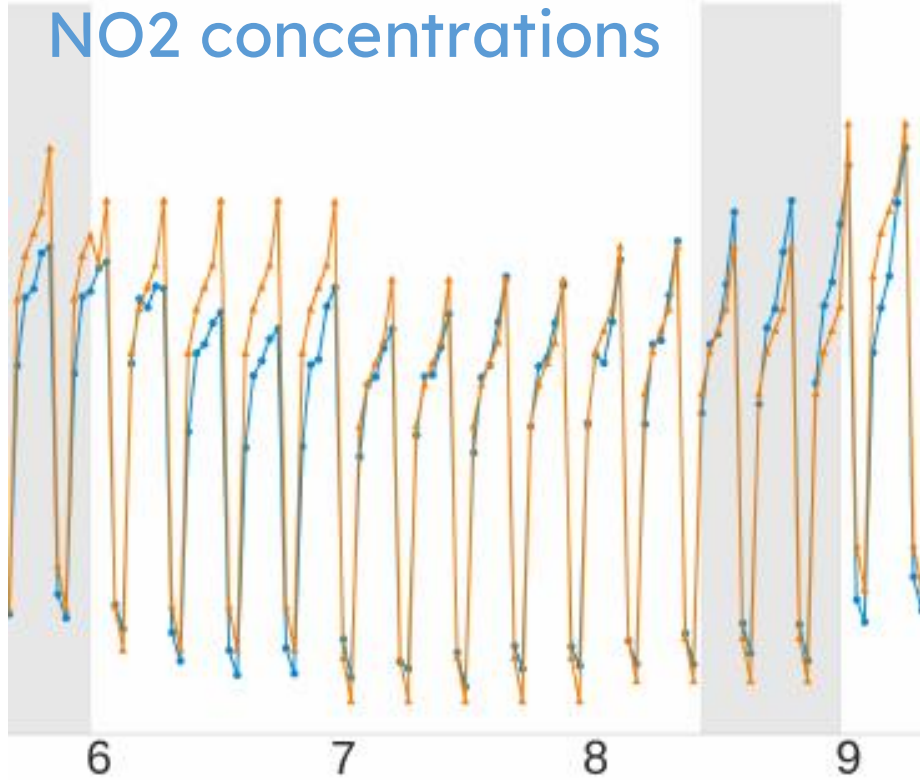
Result from eMONARCH with Graph Neural Networks (GNN)

GNN: Deep learning architecture relying on Graphs and message passing



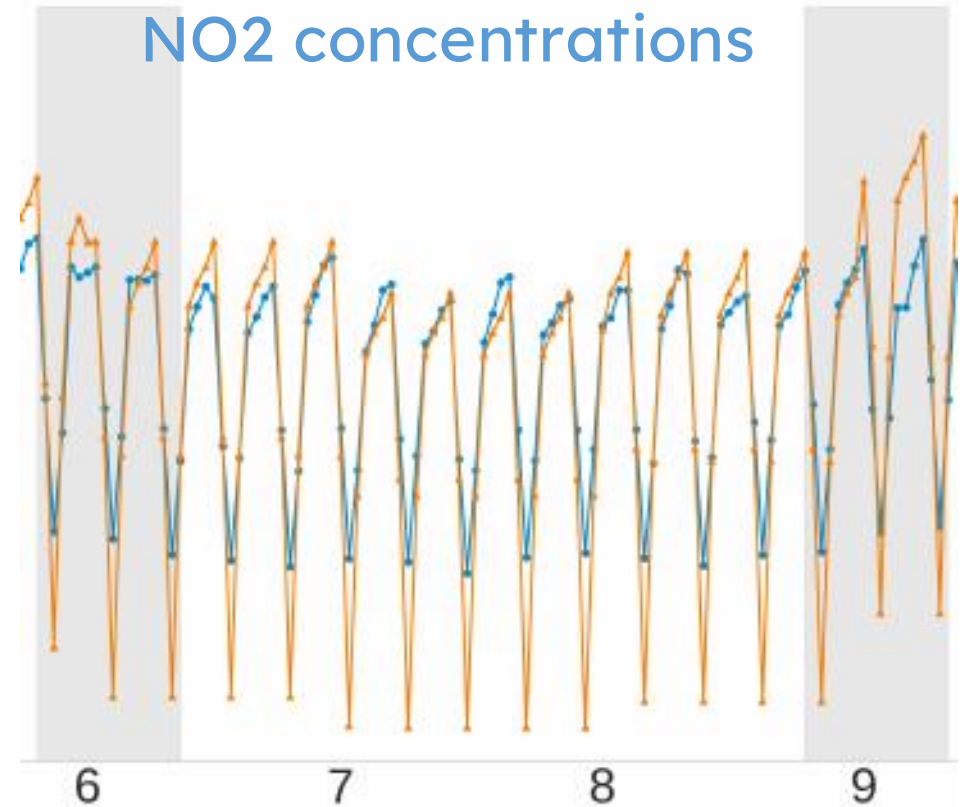
Moving from predicting emissions with daily-averaged NO2 concentrations to predicting with instantaneous 1330 concentrations

Using daily-averaged NO2 concentrations



NOx emissions flux

Using instantaneous 1330 NO2 concentrations



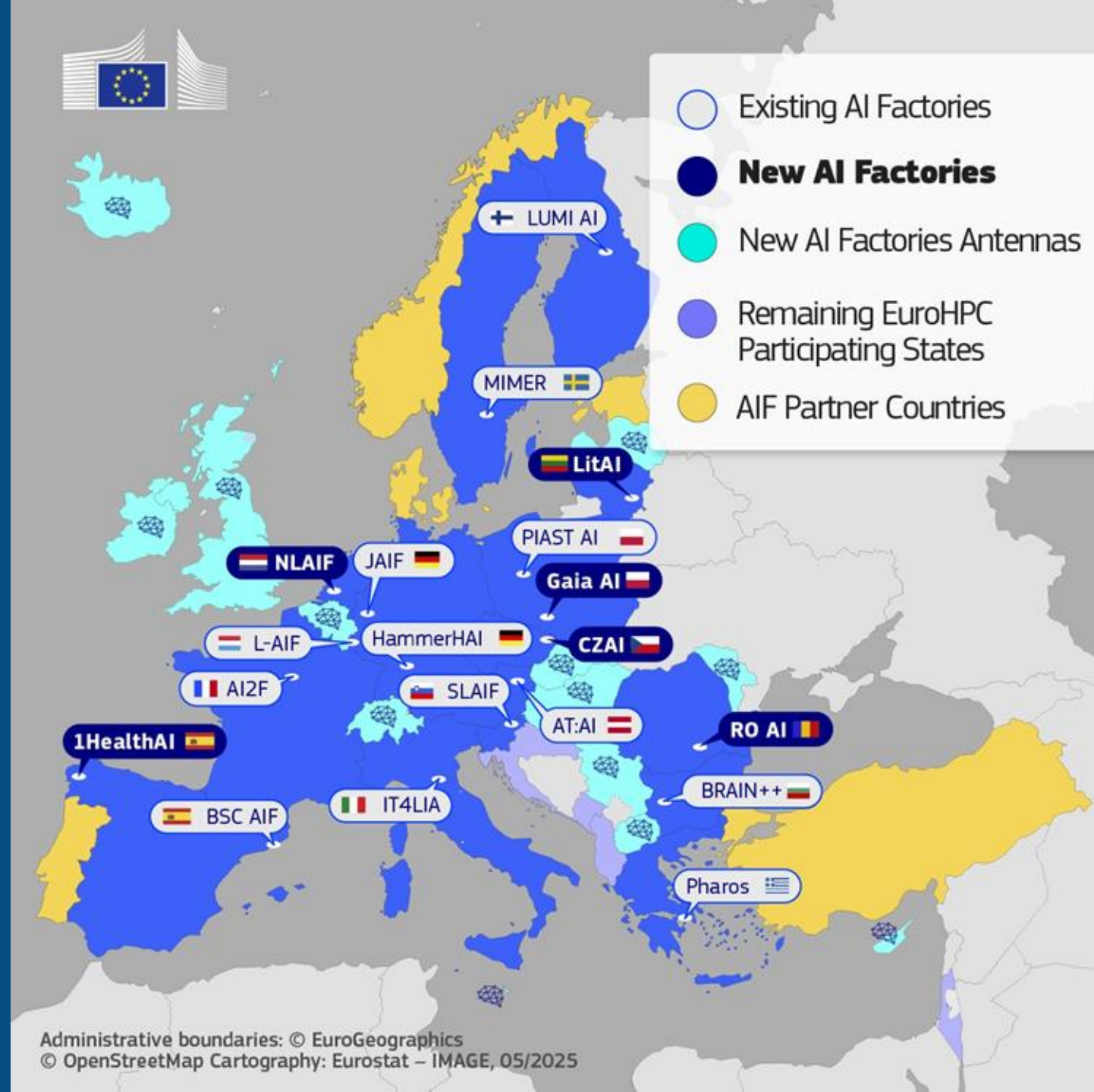
Space-averaged NOx emission predictions over Spain from June-September 2017

- Change in median-scaled RMSE from 5.7% to 11.3%
- Change in median scaled bias from -0.9% to -0.6%

AI FACTORY



- Dynamic ecosystems built around AI-optimised supercomputers
- Provide computing power and expert support to:
 - European industry
 - European scientific users
- Enable the development of large AI models that leverage Europe's AI capabilities
- Foster skills, knowledge, and innovation in the AI domain across the EU



Thank you!

We acknowledge support from the European Research Council (FRAGMENT, grant no. 773051), the AXA Research Fund through the AXA Chair on Sand and Dust Storms at the Barcelona Supercomputing Center (BSC), the World Meteorological Organization through the Barcelona Dust Regional Center managed by BSC and AEMET, the Copernicus Programme through different CAMS services, the ACTRIS project, as well as 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 their 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. R.S. was supported by the predoctoral programme AGAUR-FI Joan Oró (2025 FI-3 01106), funded by the Secretariat of Universities and Research of the Department of Research and Universities of the Generalitat of Catalonia and the European Social Plus Fund.

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