BSC Update

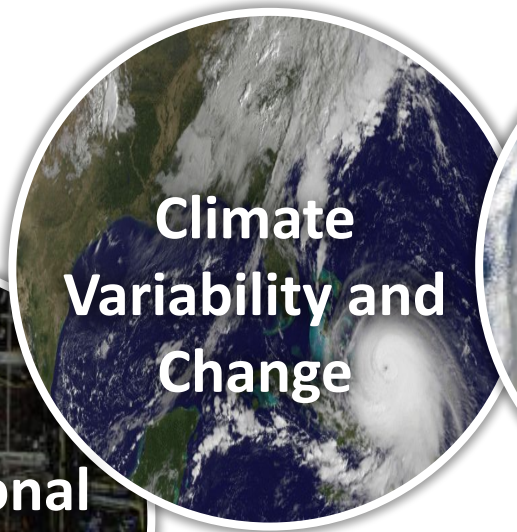
J. Escribano, E. Emili, and the
Atmospheric Composition Group

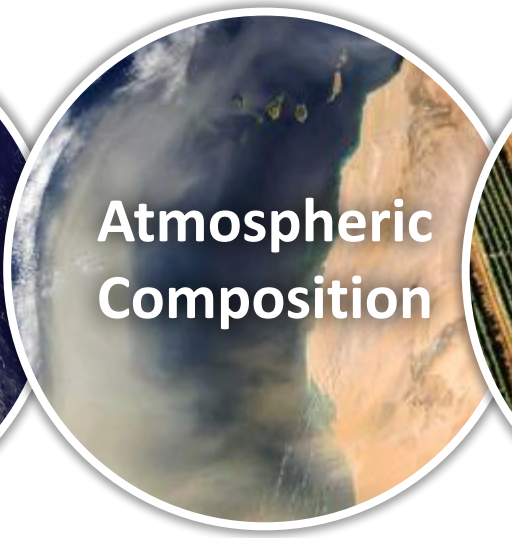
8 November 2023

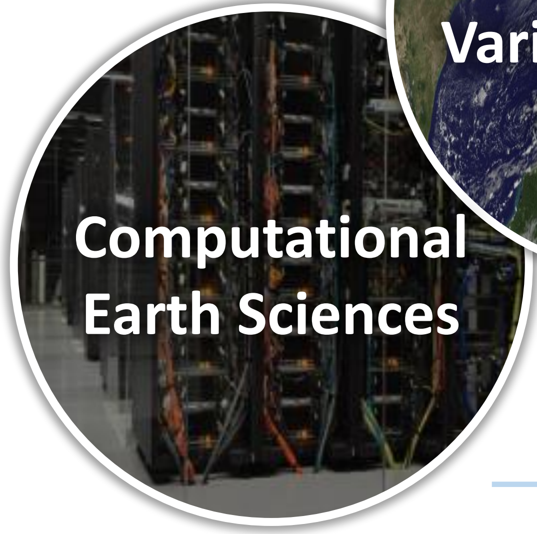
ICAP Darmstadt 2023

Earth Sciences Department

Environmental modelling and forecasting using process-based and artificial intelligence models, with a particular focus on weather, climate and air quality. This includes transferring solutions to support the main societal environmental challenges through data applications







- ~160 people
- Funding from EC, Copernicus, private sector, ESA, Spanish and regional governments
- Four ICREA, closer link to local universities

The BSC Atmospheric Composition group (Nov. 2023)

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

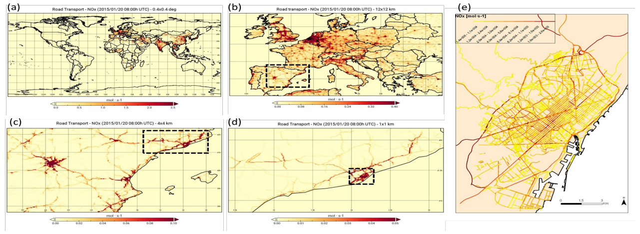
Understand, constrain and predict the spatiotemporal variations of atmospheric pollutants across scales along with their effects upon air quality, health, weather and climate

- About **30** people working on air quality, emissions, atmospheric chemistry and aerosols.

Model and Tool developments

HERMESv3

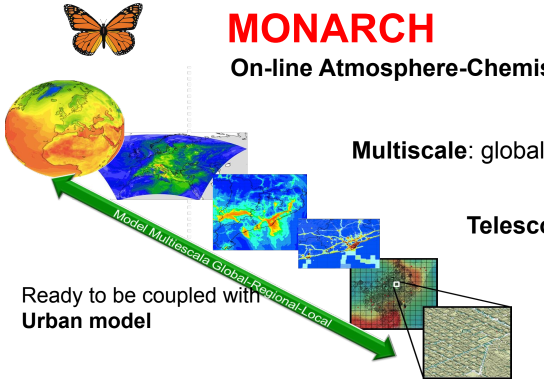
A **python-based, open source, parallel and multiscale** emission model



Guevara et al. (2019, GMD)
Guevara et al. (2020, GMD)
Guevara et al. (2021, ESSD)

MONARCH

On-line Atmosphere-Chemistry coupling



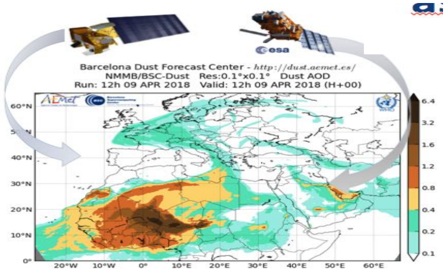
Multiscale: global to local (1km)

Telescoping nesting

Badia et al. (2017, GMD)
Peng et al. (2019, QJMRS)
Klose et al. (2021, GMD)

LETKF DA

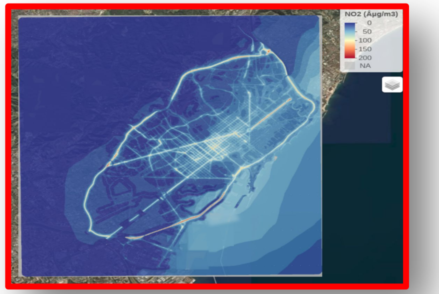
Ensemble based Data Assimilation system



Di Tomaso et al. (2017, GMD)
Escribano et al. (2022, ACP)
Di Tomaso et al. (2022, ESSD)

CALIOPE-Urban

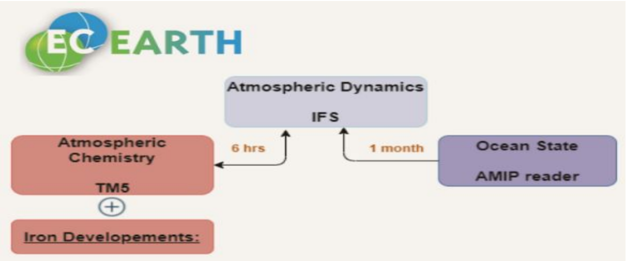
Street-scale dispersion model



Benavides et al. (2019, GMD)
Benavides et al. (2021, ERL)
Rodriguez-Rey et al. (2021, TR-RES)
Rodriguez-Rey et al. (2021, STOTEN)

EC-Earth3-Iron

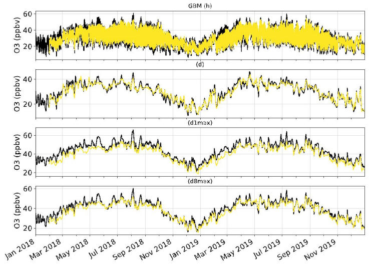
Atmospheric iron cycle in EC-Earth



Myriokefalitakis et al. (2021, GMD)
Bergas-Masso et al. (2023, Earth's Future)

Model Output Statistics

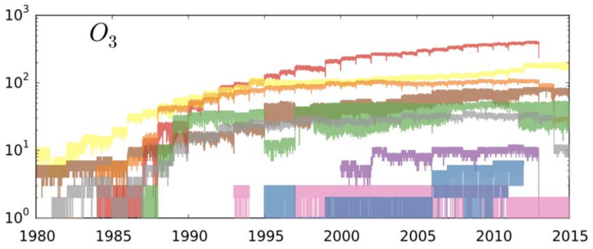
Including machine learning



Petetin et al. (2020, ACP)
Petetin et al. (2022, ACP)

GHOST

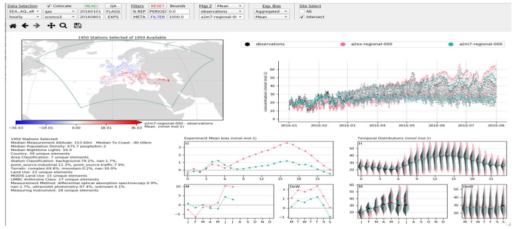
Harmonised treatment of observations



Bowdalo et al. (2023, subm. ESSD)
Bowdalo et al. (2021, ERL)

Providentia

Dynamic/flexible evaluation system



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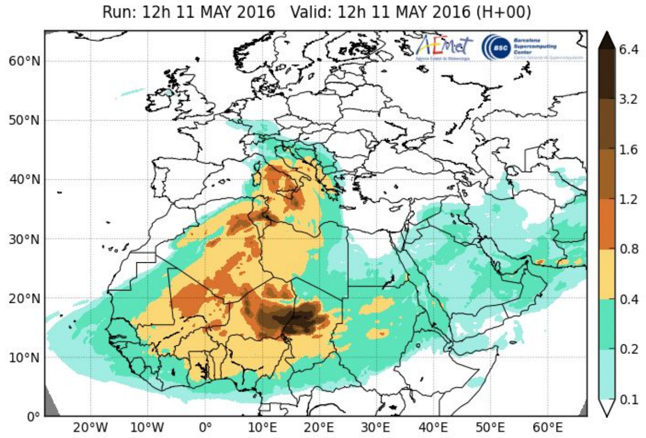
Centro Nacional de Supercomputación

In collaboration with CES, ESS and CVC

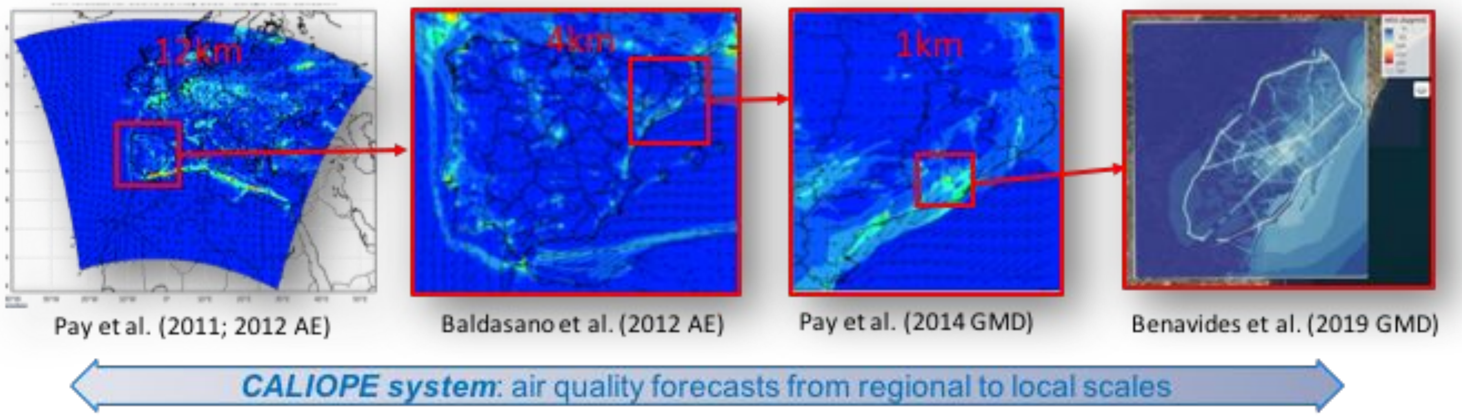
Forecasts, reanalysis and impact assessment

WMO Dust Regional Centers

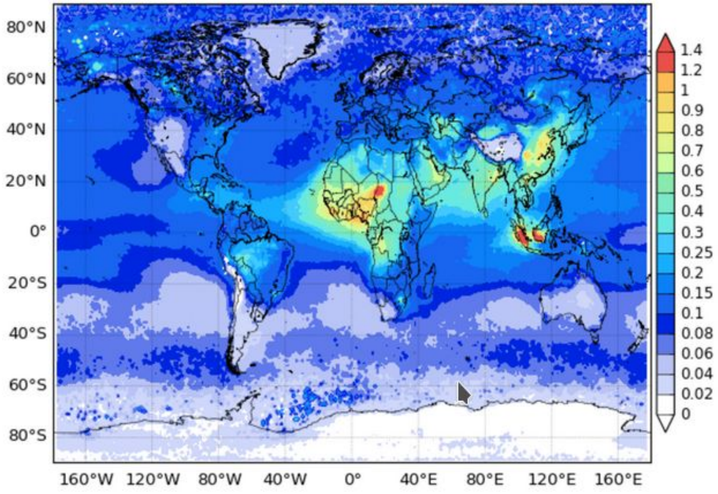
Dust forecasts and and renalysis



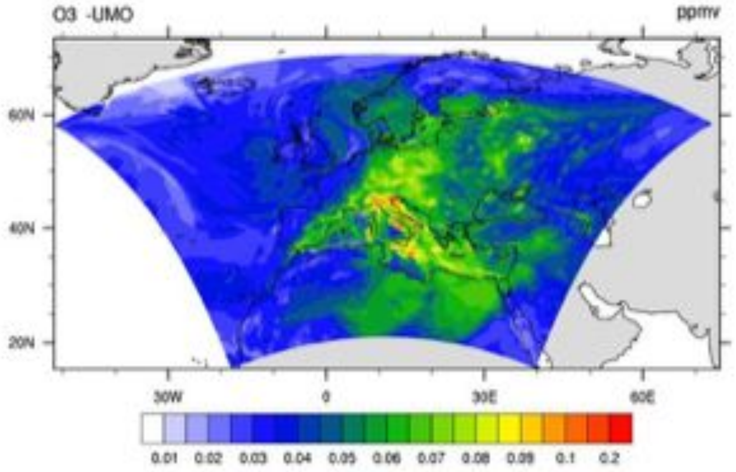
CALIOPE Forecast system



ICAP global aerosol ensemble



Copernicus CAMS Europe air quality



In collaboration with CES and ESS

Barcelona Dust Regional Center
MONARCH operational dust forecasts

V1.0.0 (June 2020-2023):

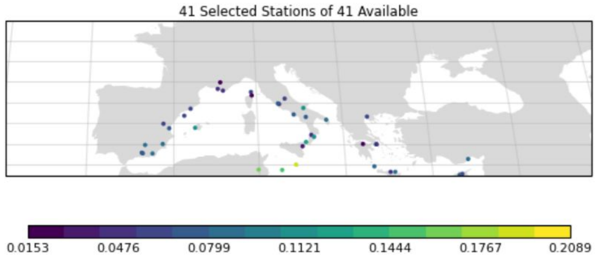
- Introduced MODIS DB dust preferential sources atlas (Ginoux et al. 2012)
- Switched dust emission scheme to Ginoux et al. 2001 [G01]

V2.1.0 (since June 2023):

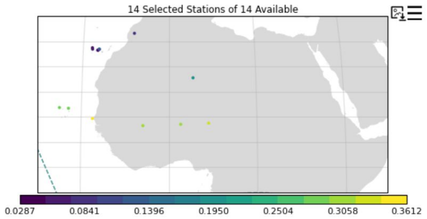
- Introduced spheroid particles to compute optical properties (and PMs)
- Activated online coupling of dust radiation with meteorology

https://dust.aemet.es/

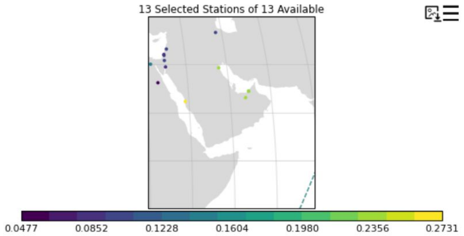
Evaluation against AERONET coarse AOD (O’Neill) in 2021



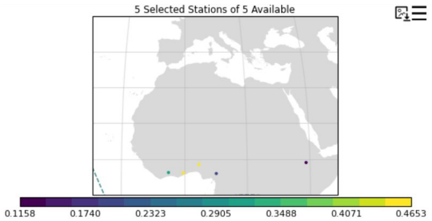
	Bias	RMSE	MNMB	FGE	r
V1.0.0	-0.01	0.09	-101.2	119.9	0.79
V2.1.0	-0.01	0.08	-97.7	118.1	0.80



	Bias	RMSE	MNMB	FGE	r
V1.0.0	0.09	0.22	-5.2	95.9	0.68
V2.1.0	0.09	0.21	-1.4	96.3	0.68



	Bias	RMSE	MNMB	FGE	r
V1.0.0	0.02	0.13	-17.4	61.4	0.70
V2.1.0	0.01	0.12	-16.1	59.3	0.71



	Bias	RMSE	MNMB	FGE	r
V1.0.0	-0.10	0.23	-53.9	69.8	0.77
V2.1.0	-0.12	0.25	-60.2	73.9	0.76

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E. Emili, E. Karnezi

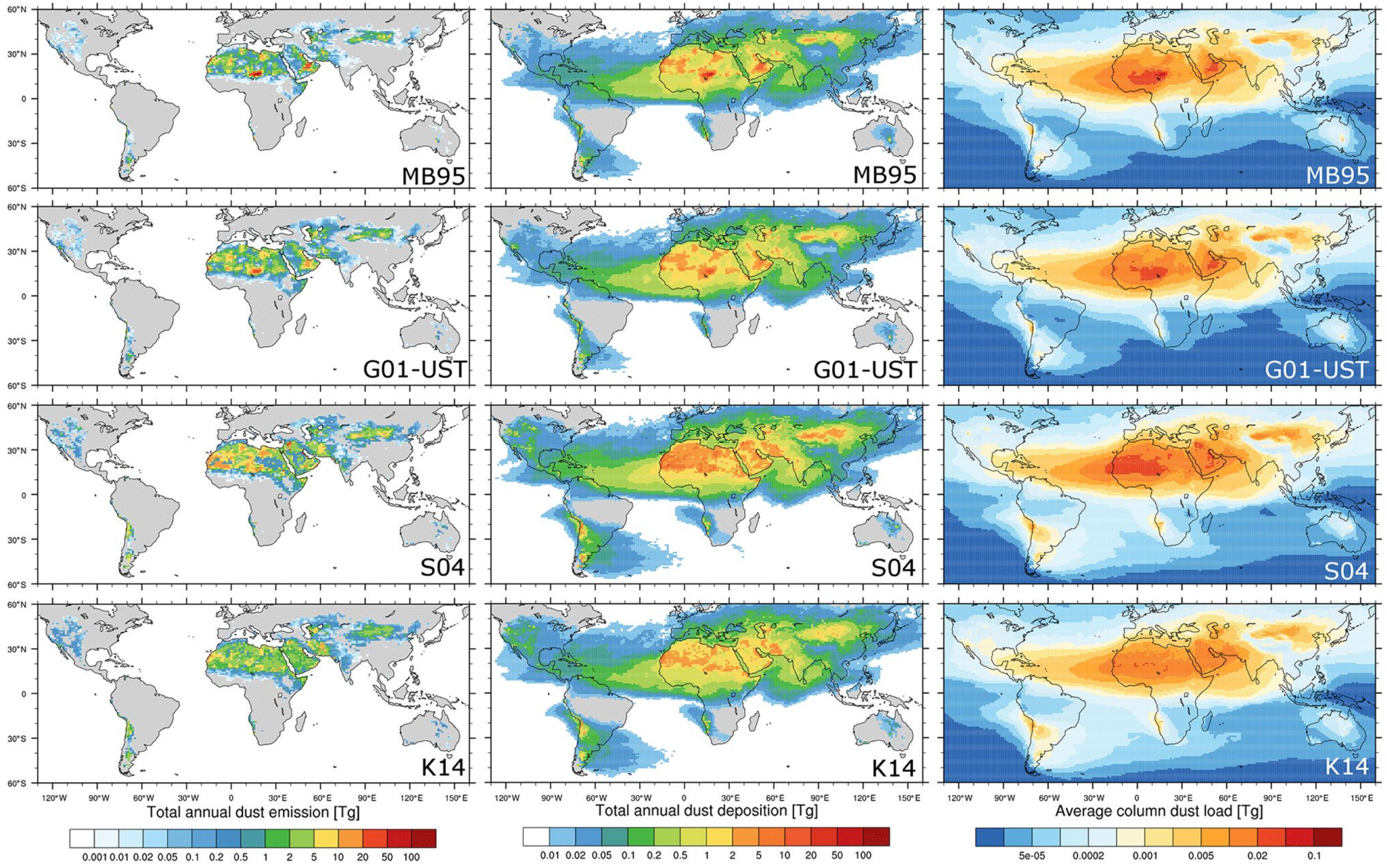
MONARCH ICAP upgrades for early 2024

Marenostrum4 to Marenostrum5 --> upgrade of the MONARCH - ICAP forecast system

- Climatological gaseous precursors –> full online CB05 Chemistry
- SOA (antro, fires), Nitrates
- Emissions (coupled with HERMESv3) : HTAPv2 –> CAMS_GLOBv4.2
- TBD: horizontal resolution / computing resources (preparation for AOD Ens DA)

Dust emission upgrades [Klose et al., 2021 GMD]:

- 4 dust schemes available: from strongly simplified to physics-based parameterizations
- Static and dynamic roughness length dependencies upon emission
- Size-dependent index of refraction based on mineralogy
- Ellipsoidal particle shape in optical properties



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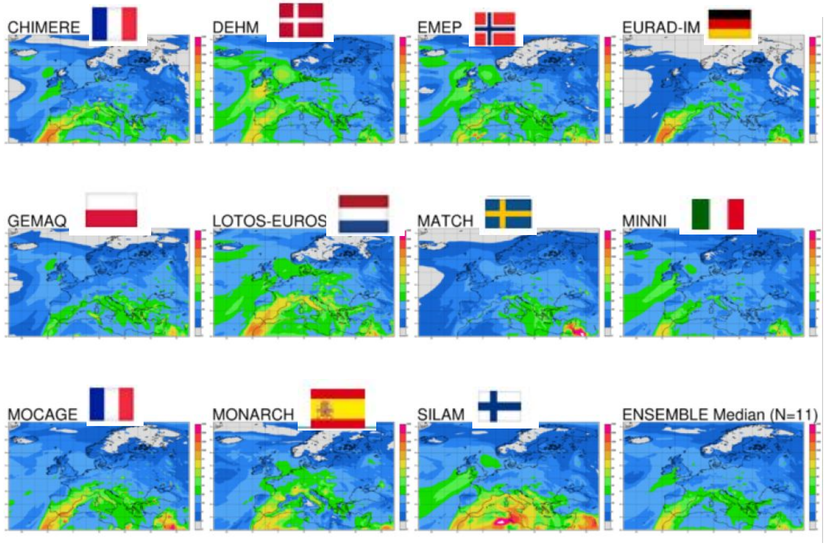
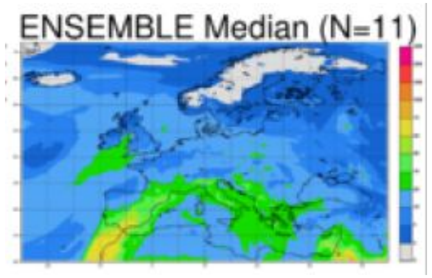
Copernicus Programme: Regional Air Quality Products

Operational Europe-wide Air Quality Service based on:

11 operational AQ models



1 ENSEMBLE model



How? Median of the individual results for each grid-cell
Why? Reliable, robust, performing

New operational models June 2022

MINNI (ENEA)
MONARCH (BSC)

Users

NRT Forecasts and Analyses Daily	Interim & Validated Reanalyses Annually
METEO FRANCE	INERIS

Barcelona Supercomputing Center
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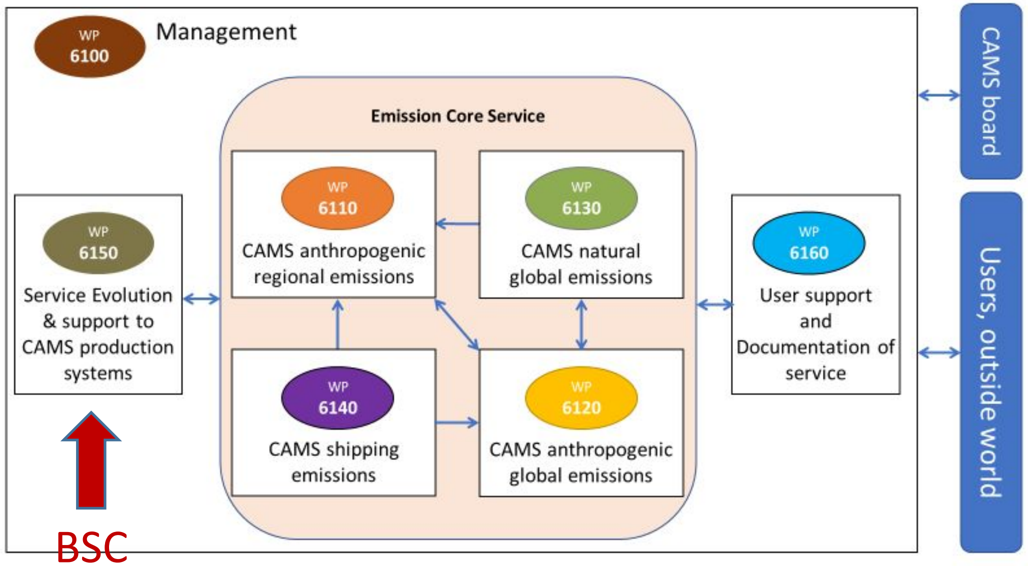
https://atmosphere.copernicus.eu

opernicus Europe's eyes on Earth
European Commission

Global and European emission inventories: CAMS2_61

- To provide gridded distributions of anthropogenic (global and Europe) and natural emissions (global only) for reactive gases, aerosols and greenhouse gases.
- **Monthly, weekly and diurnal temporal profiles will have to be delivered, so that variations can be accounted for in the CAMS systems.**
- **Provide support and guidance to the CAMS global and regional production chains in the implementation and evaluation of the new emission products developed.**



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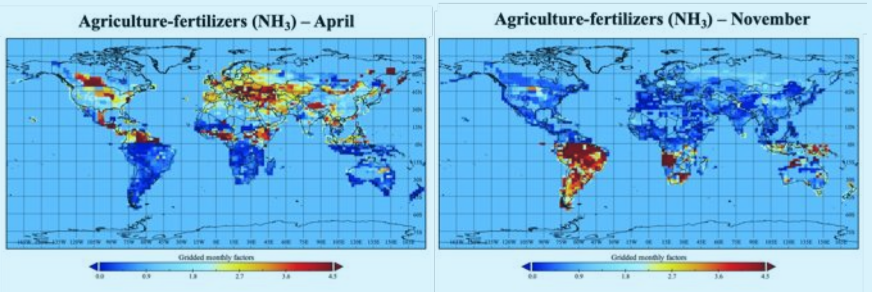
Copernicus Europe's eyes on Earth — European Commission

New CAMS-TEMPO profiles

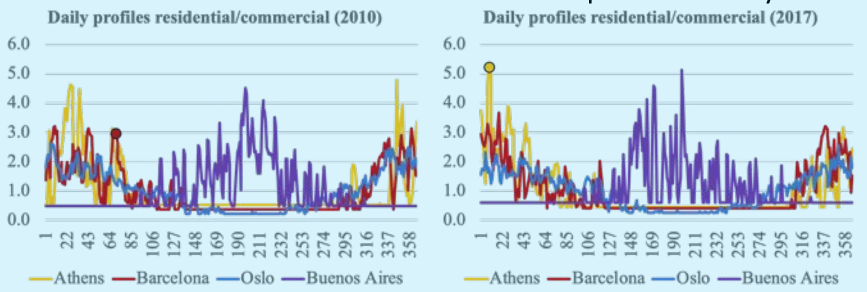
New Features:

- Use of global/national/local up-to-date datasets
- Reported as spatial variant profiles (gridded data)
- Use of meteorological parametrizations
- Consideration of cultural aspects & pollutant dependencies

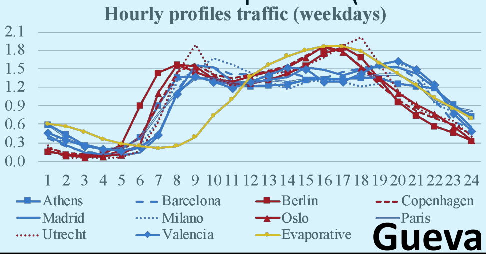
Fertilizers: Influence of national crop calendars



Residential combustion: Influence of temperature and year



Traffic: Influence of behaviour & process (exhaust vs. evaporative)



Guevara et al. (2021 ESSD)

GHOST: Globally Harmonised Observations in Space & Time

N° Processed Measurements: **~7 billion**

N° Components: **227**

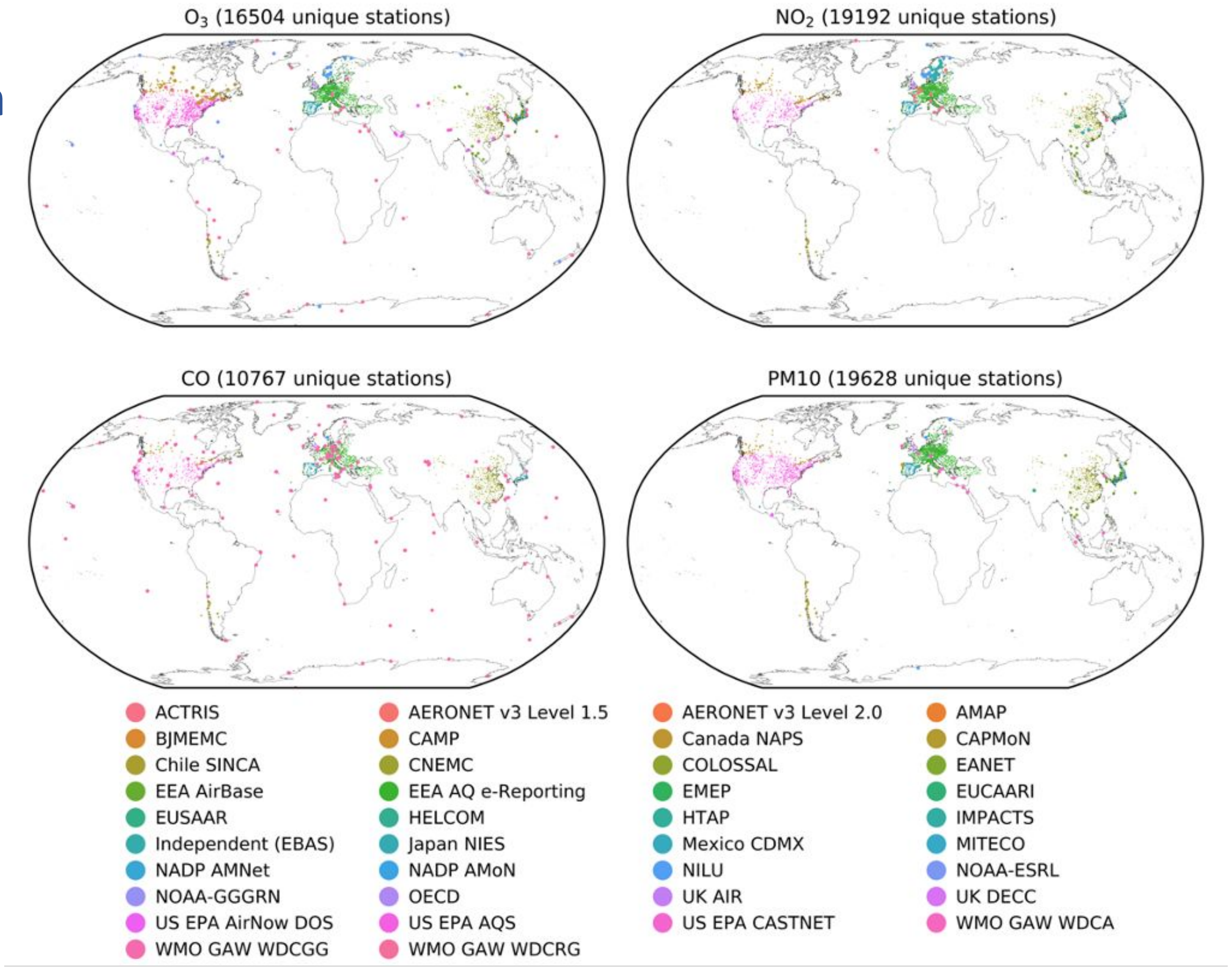
N° Networks: **38**

Temporal range: **1970-2023**

Paper submitted:

Bowdalo et al., 2023, ESSD

Publicly available data as netCDFs



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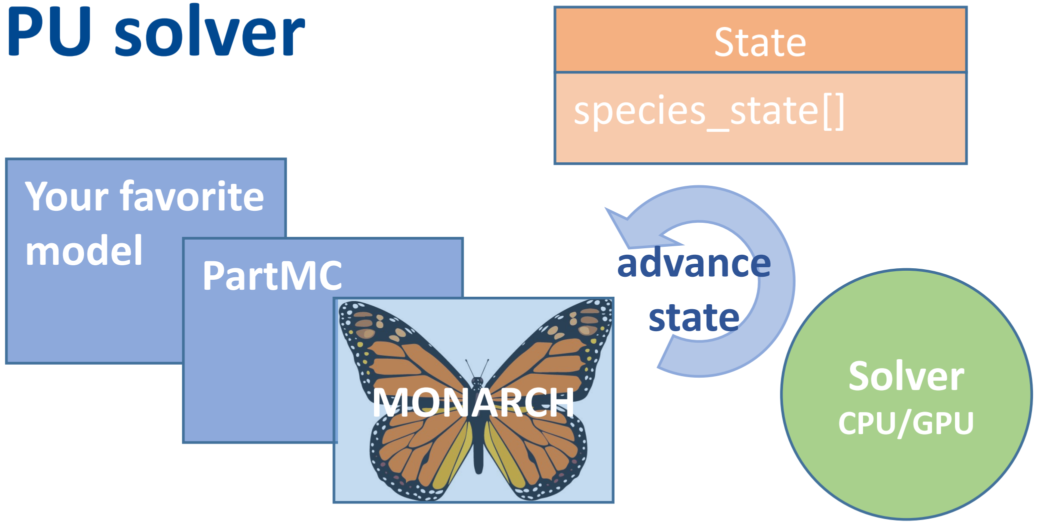
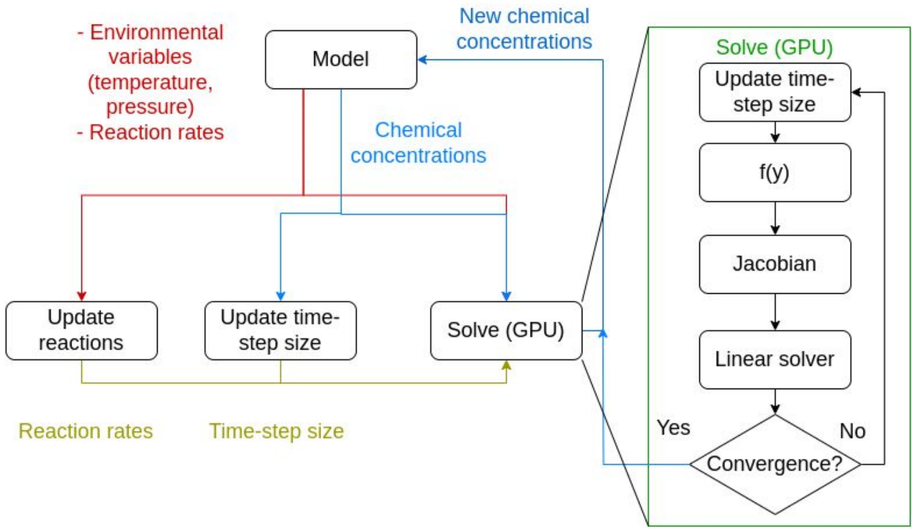
CAMP: Chemistry Across Multiple Phases - GPU solver



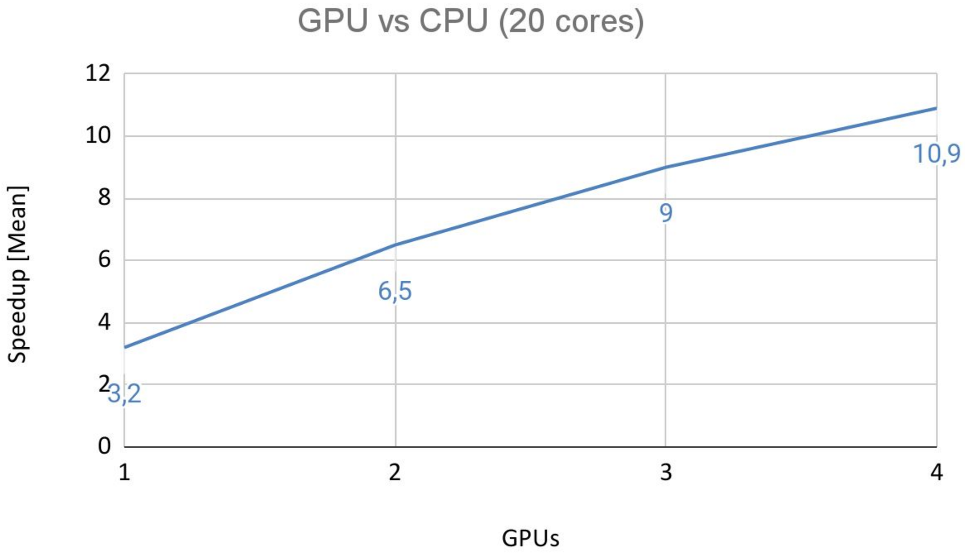
- Scalable kinetics treatment for chemistry in multi-phase models
- Change the chemical mechanism ***without recompiling***
- Run with ***multiple GPUs*** per CPU. The speedup close to linear with the number of GPUs.

Dawson et al. (2021 GMD)



Guzman et al. (2023 ICICT)

CB05 chemical mechanism
test with 100.000 cells



The CAMP library is available at: https://github.com/open-atmos/camp

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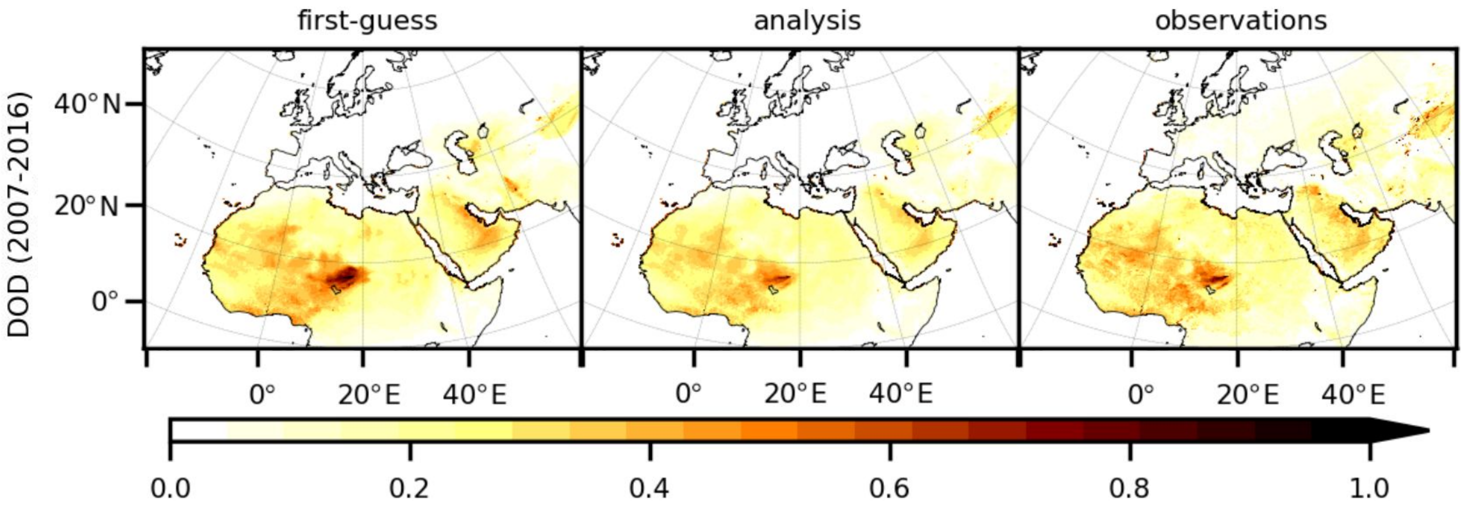
The MONARCH high-resolution reanalysis of desert dust aerosol over Northern Africa, the Middle East and Europe

A complete and consistent, four dimensional, regional reconstruction of desert dust in a recent decade (2007-2016) [in process: 2017, 2018]

- ➔ Unprecedented **high resolution**: 0.1º x 0.1º
- ➔ Specific **dust observational constraint**
- ➔ **Uncertainty estimates** in the reanalysis output
- ➔ Link to specific **air quality** and **climate services**
- ➔ **FAIR** data guidelines



Open access. To request access to the repository, please contact reanalysis.access@bsc.es

Dataset PID: http://hdl.handle.net/21.12146/c6d4a608-5de3-47f6-a004-67cb1d498d98

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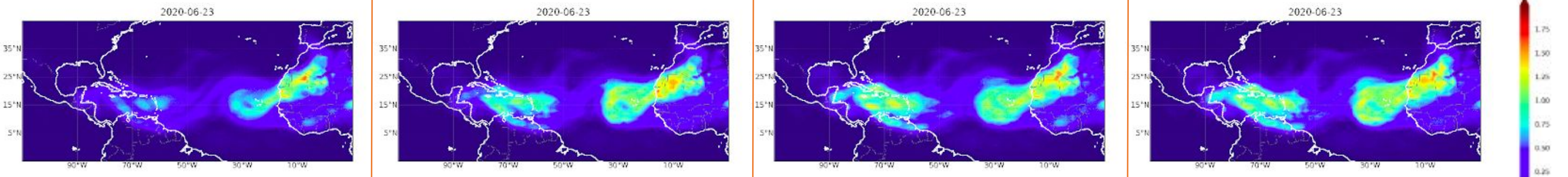
DustClim
ERA4CS European Research Area for Climate Services

Di Tomaso et al., 2022, ESSD,
doi:10.5194/essd-14-2785-2022

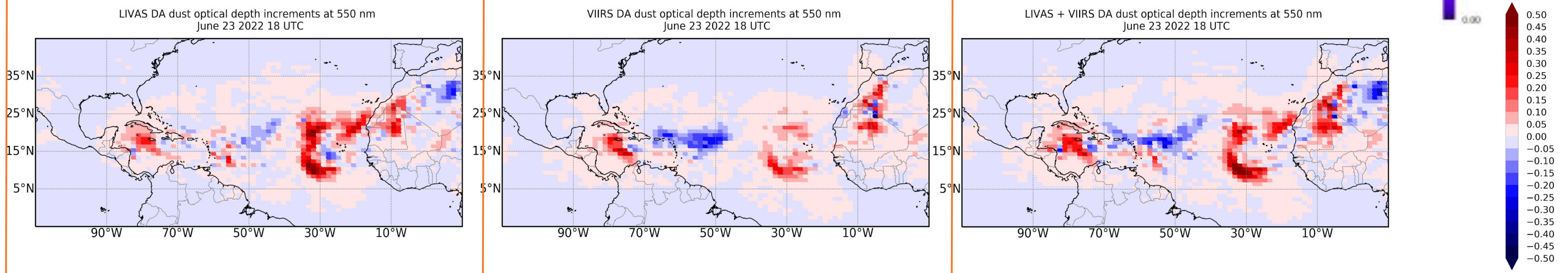
Assimilation Dust AOD + lidar : “Godzilla” June 2020 case

	free run	LIVAS dust ext. coef. DA	VIIRS DOD DA	LIVAS + VIIRS DA

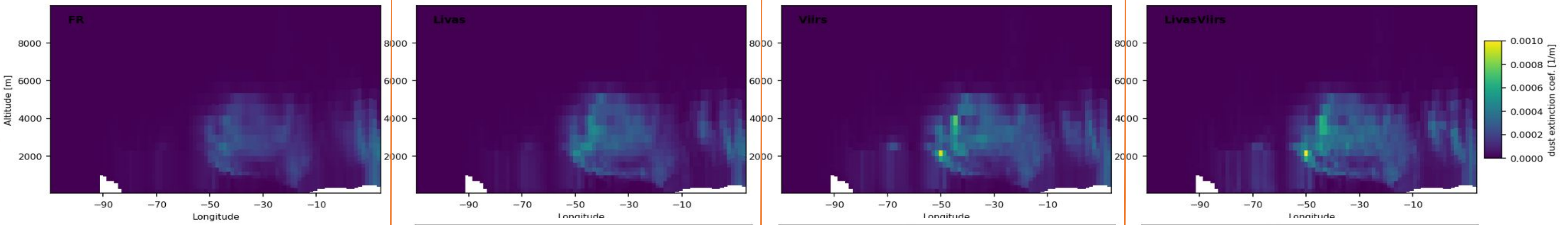
DOD



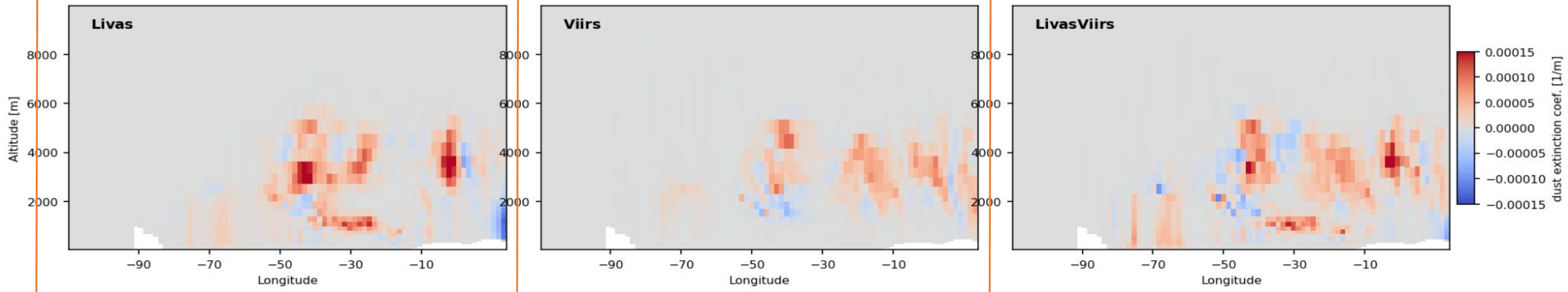
DOD increments



Dust extinction coef. (15 N)



Dust extinction coef. increments



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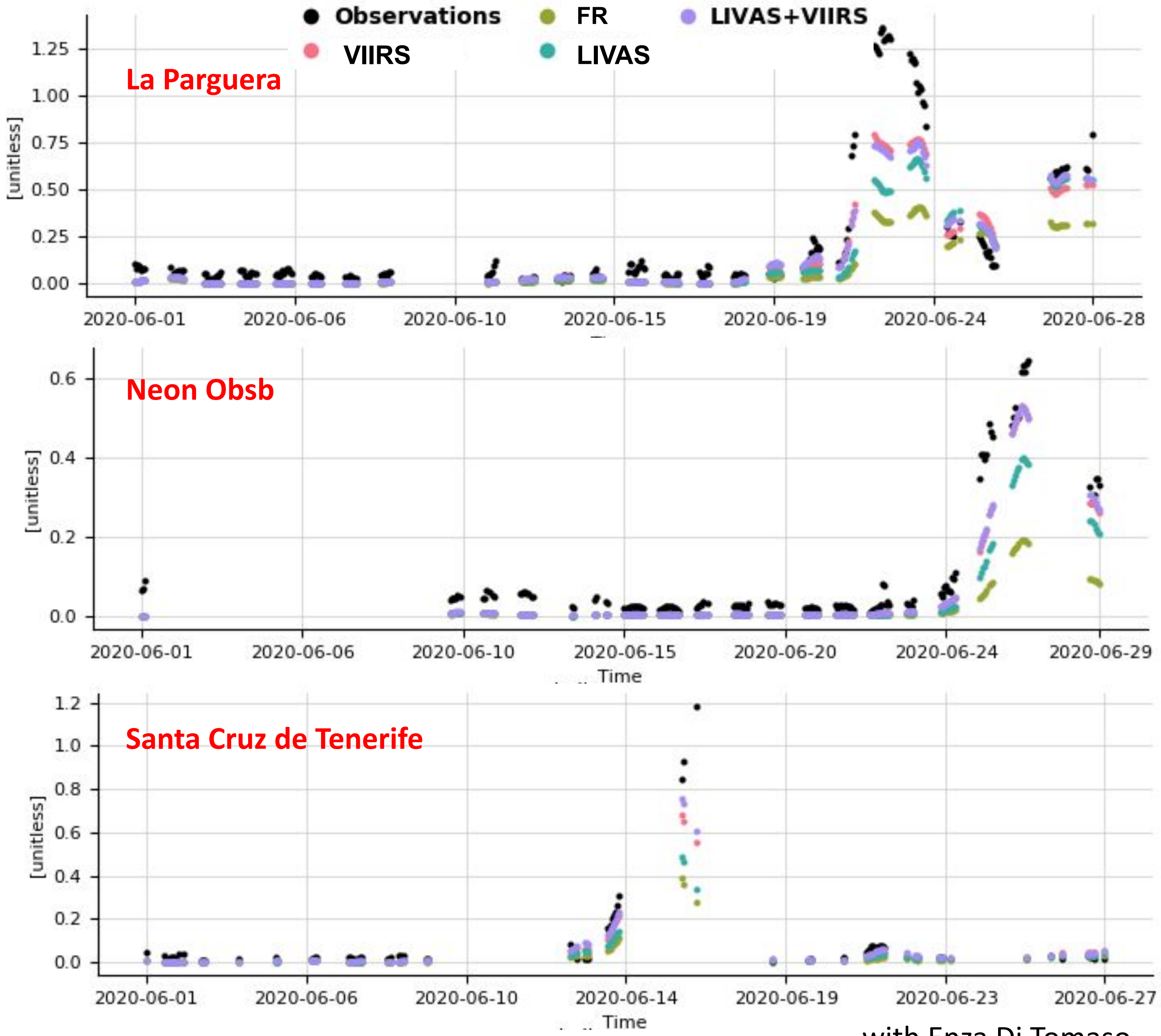
with Enza Di Tomaso

Simulated coarse DOD at 550 nm and AERONET SDA coarse AOD at 500 nm

The information provided by the different retrievals is not redundant

The two sensors CALIOP and VIIRS work synergistically when assimilated together

The assimilation in all the experiments brings the model simulations closer to AERONET retrievals



with Enza Di Tomaso

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DOMOS

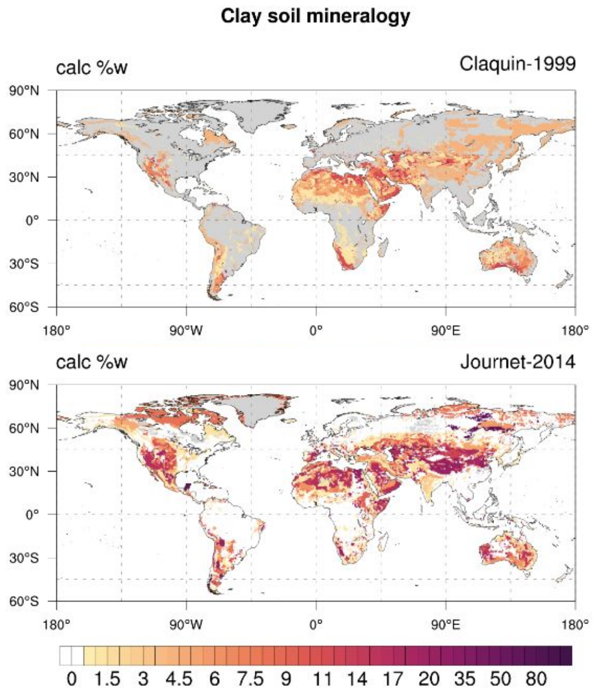
Research on dust mineralogy and its impacts on the Earth System

MONARCH has been developed to explicitly represent dust mineralogy, with the aim of improving our knowledge on its impacts in the Earth System (e.g. interaction with radiation, atmospheric chemistry).

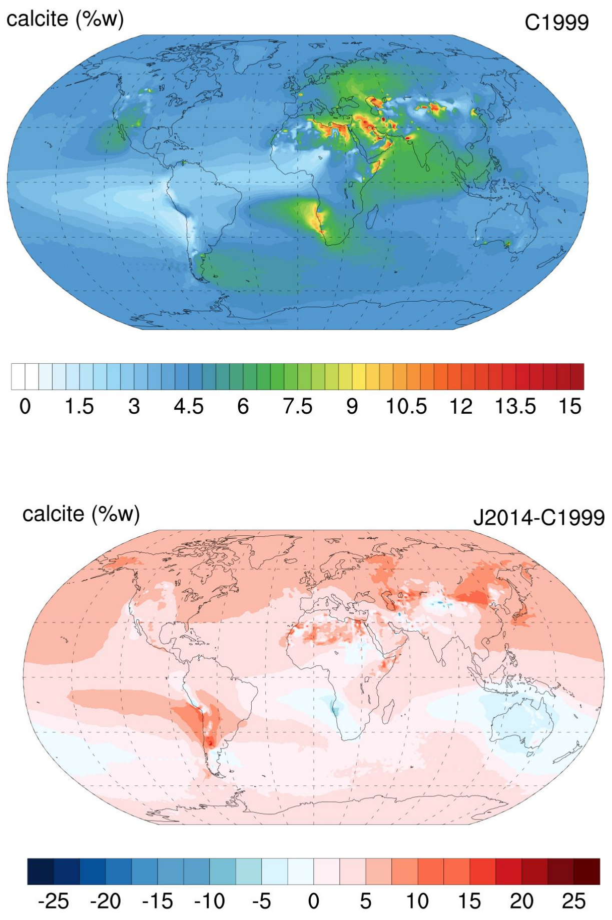
2 state of the art Mineralogy Atlases:

Claquin et al. (1999), Nickovic et al. (2012)
8 minerals:
Illite, smectite, kaolinite, quartz, feldspars, calcite, gypsum and hematite (iron oxides).

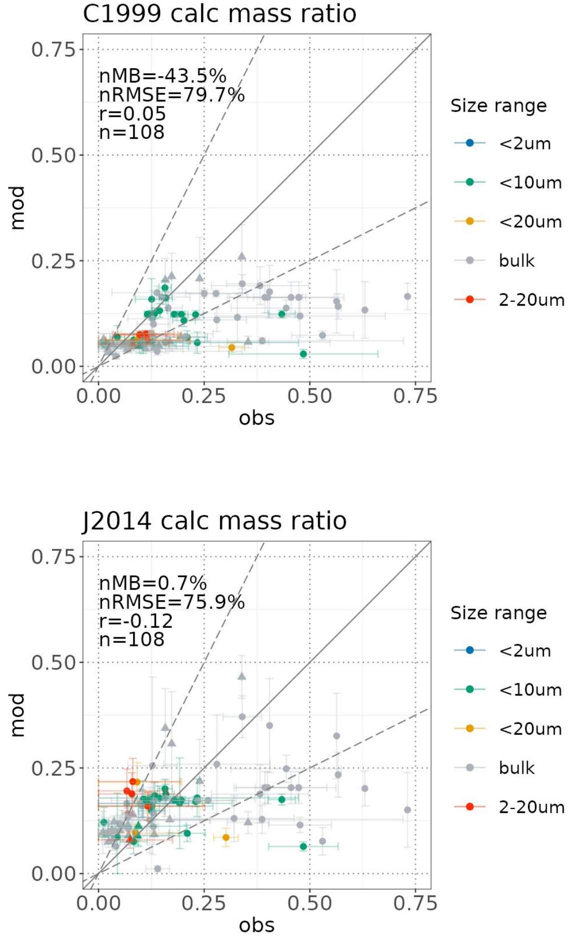
Journet et al. (2014)
12 minerals:
Illite, smectite, kaolinite, vermiculite, chlorite, mica, quartz, feldspars, calcite, gypsum, hematite and goethite.



Mineral fraction at surface conc.
(MONARCH 2006-2010, %w)



Evaluation against observations
(following Perlwitz et al. 2015)



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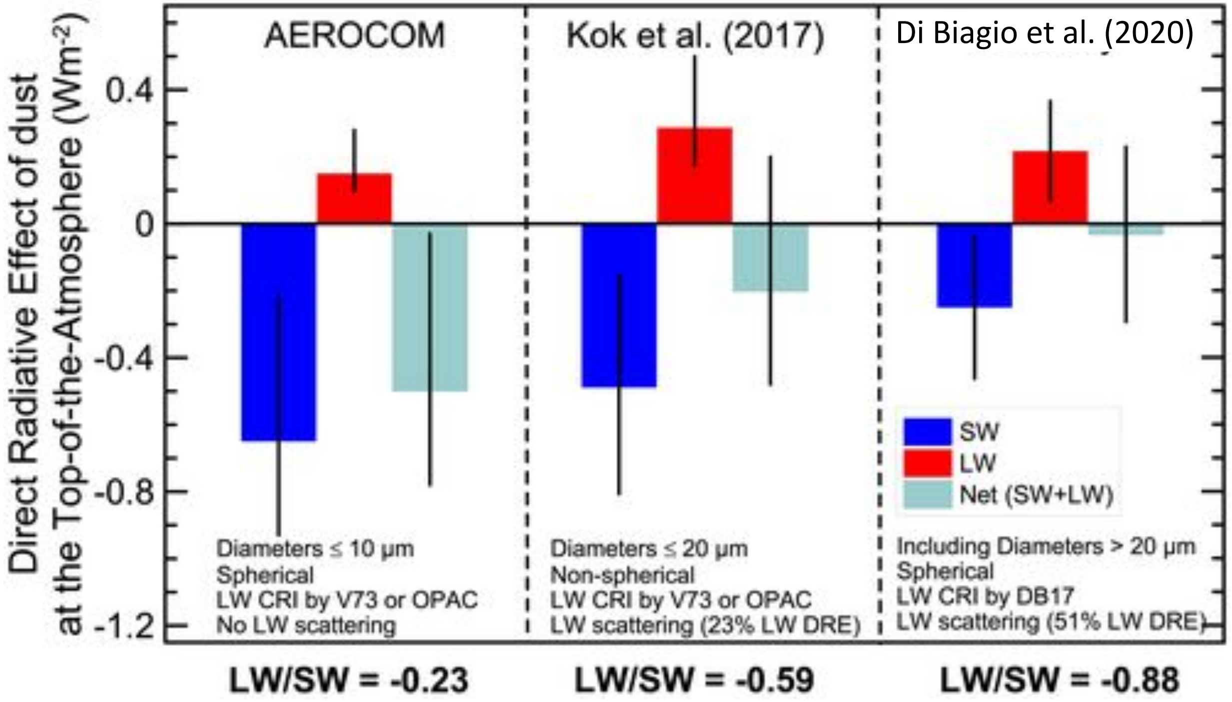
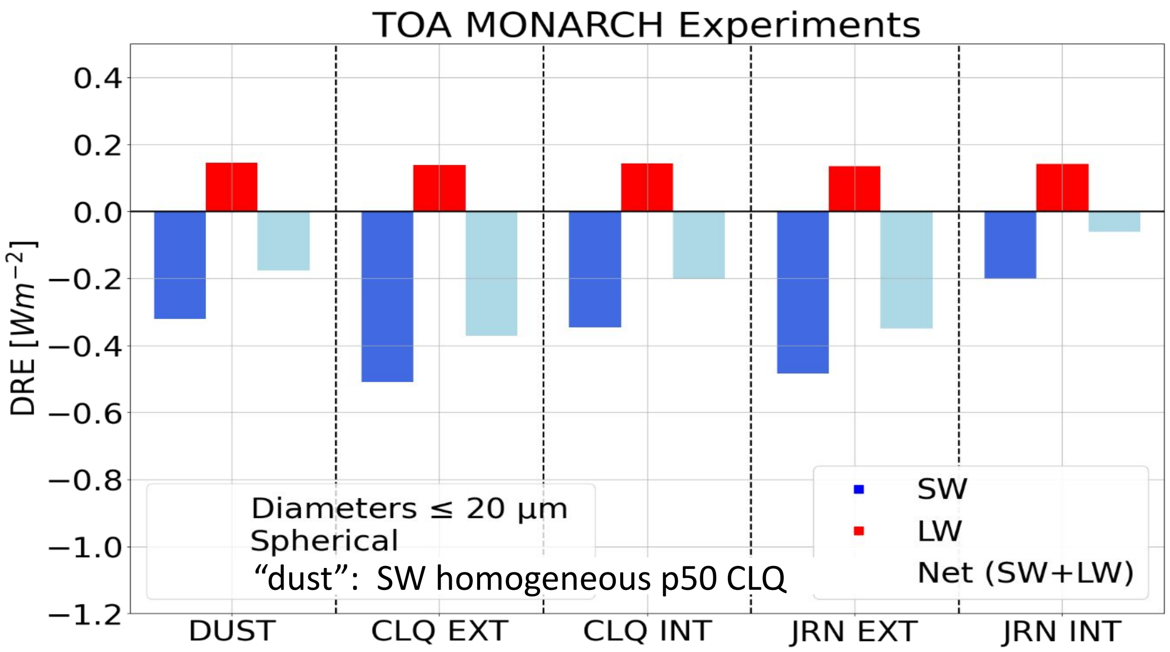
M. Gonçalves Ageitos, et al., 2023 ACP

Dust direct radiative effect: mineralogy



Di Biagio et al. (2020)



- Di Biagio:
  - Reduced DRE in SW with inclusion of large particles
- MONARCH:
  - Similar DRE reduction with JRE INT
  - Reduced DRE in DUST run compared to CLQ INT

- Additional Experiments to test:
  - Internal mixing with goethite 50% imaginary RI
  - Runs with partly external/partly internal mixing

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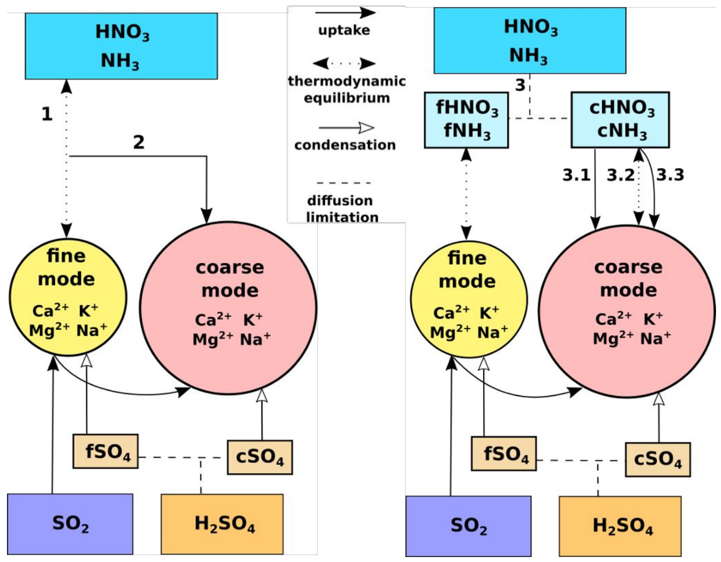
Luka Ilić

Nitrate formation on coarse particles

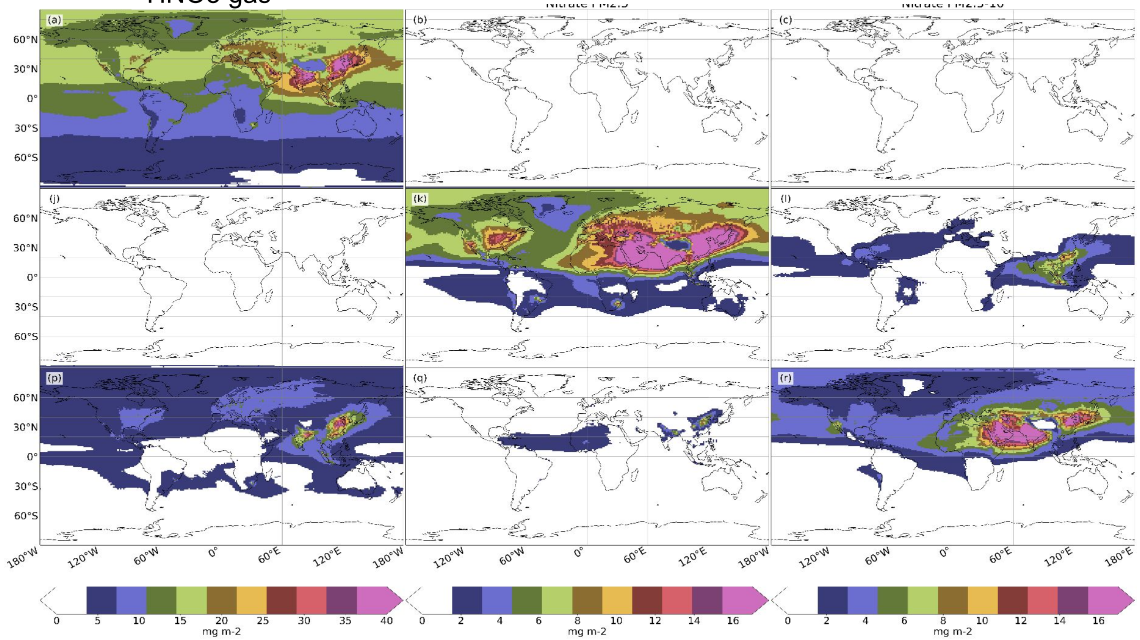
- **Implementation of nitrate heterogeneous chemistry mechanisms in the MONARCH model**
- **Sensitivity to dust and sea salt alkalinity and reversible uptake of nitrate**



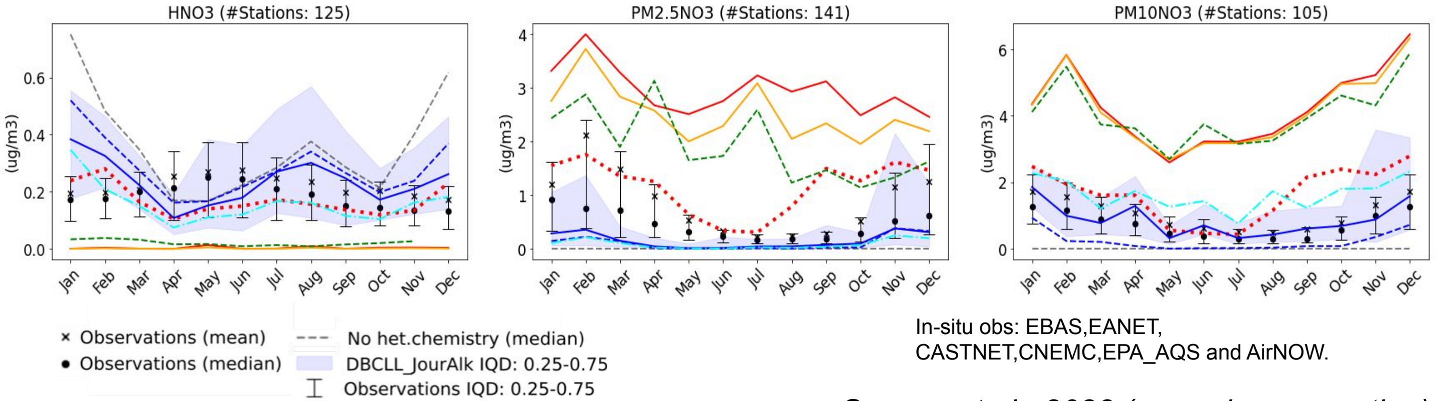
1	fTEQ_noAlk fTEQ_Alk	**Thermodynamic equilibrium (ISORROPIA)** only on fine mode of dust and sea salt, with/without alkalinity (Alk & noAlk).
2	HYB	**Hybrid**: fTEQ + uptake reaction of HNO_3 on coarse mode.
3.1	HYB_DL	Like HYB using diffusion kinetic limitation (Pringle et al., 2010).
3.2	DBCLL_noAlk DBCLL_JourAlk	**Double Call:** TEQ on fine and coarse with diffusion kinetic limitation w/o alkalinity (noAlk & JourAlk).
3.3	DBCLL+UPTK	Like DBCLL (case 3.2) with uptake of the leftover HNO_3 gas on coarse mode of dust.

Global runs 1º
Year 2018

Column average concentration (mg m-2) for 2018



Global average surf. concentrations (ug m-3) for 2018



In-situ obs: EBAS,EANET, CASTNET,CNEMC,EPA_AQS and AirNOW.

Sousse et al., 2023 (paper in preparation)

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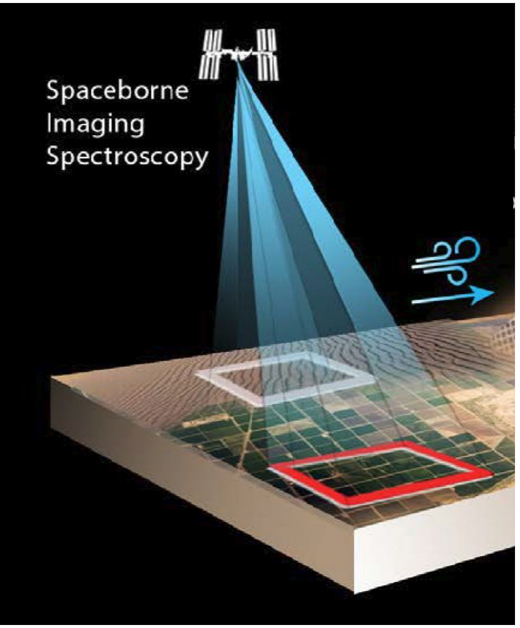
Sousse et al, in prep

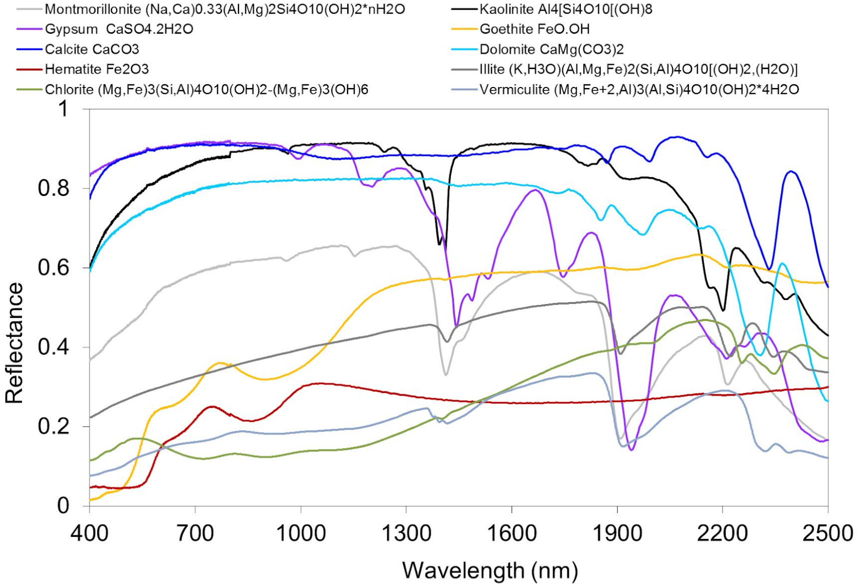
New mineralogy maps from NASA EMIT

(Green et al. 2020)

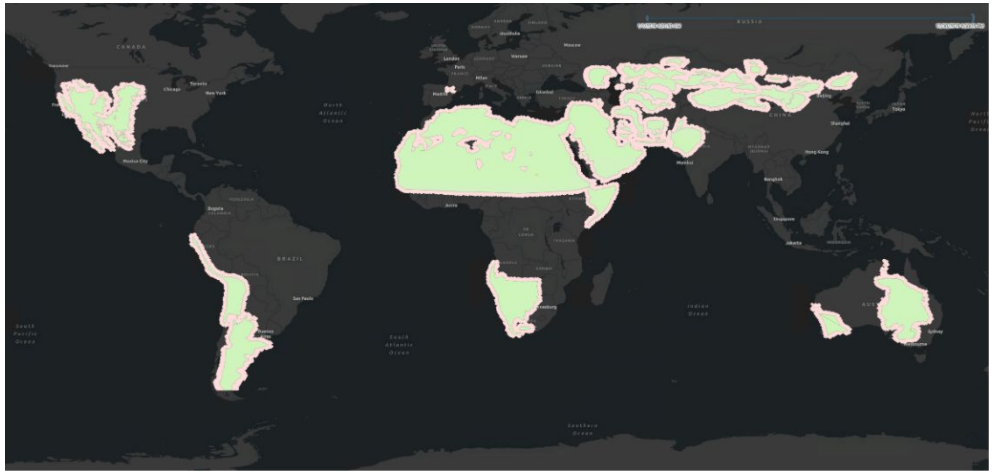


The EMIT instrument is measuring from the ISS since July 14, 2022.

VSWIR Spectra of Dust Source Minerals



Dust Minerals have distinct spectral signatures



Target mask for EMIT retrievals covering arid land regions

Level 3 products – map of 10 (+2) minerals to be used within ESMs

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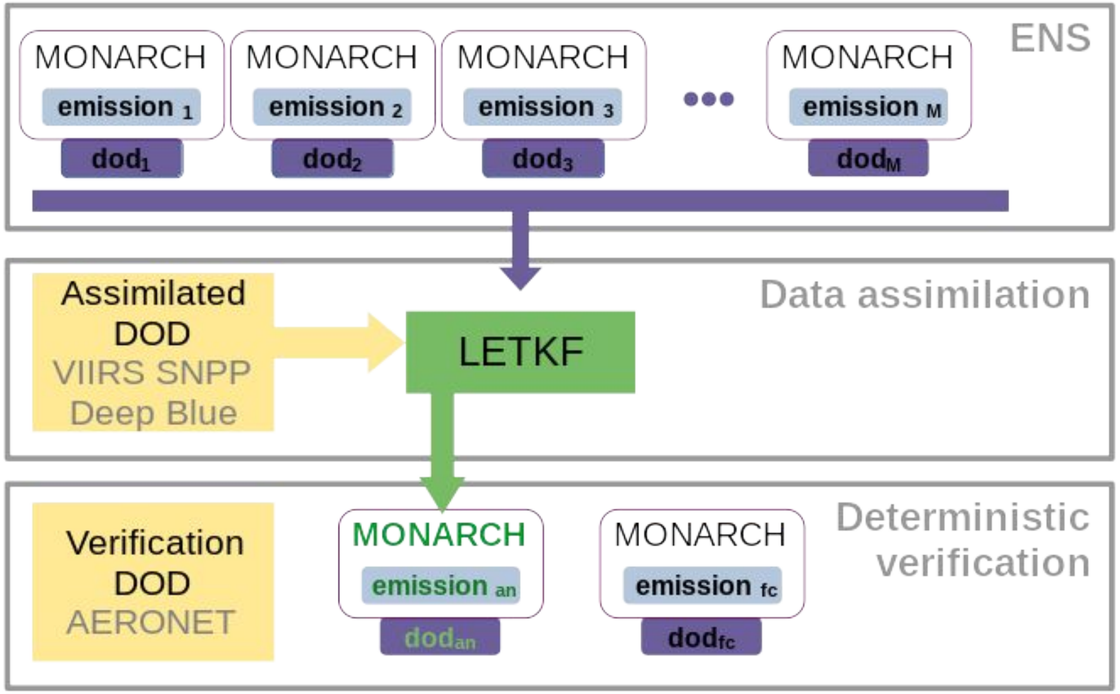
California Institute of Technology

Constraining spatio-temporal variations in dust emission at global scale with ensemble data assimilation of satellite optical depth retrievals



3 dust schemes

5 years: 2017-2021

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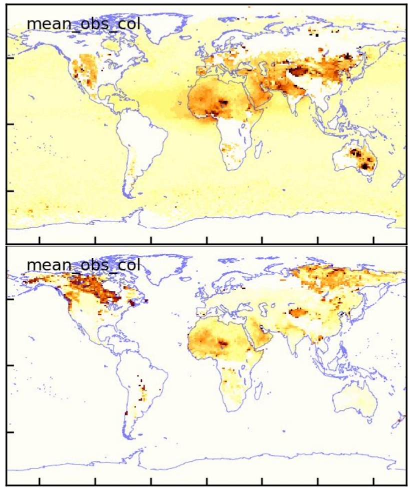
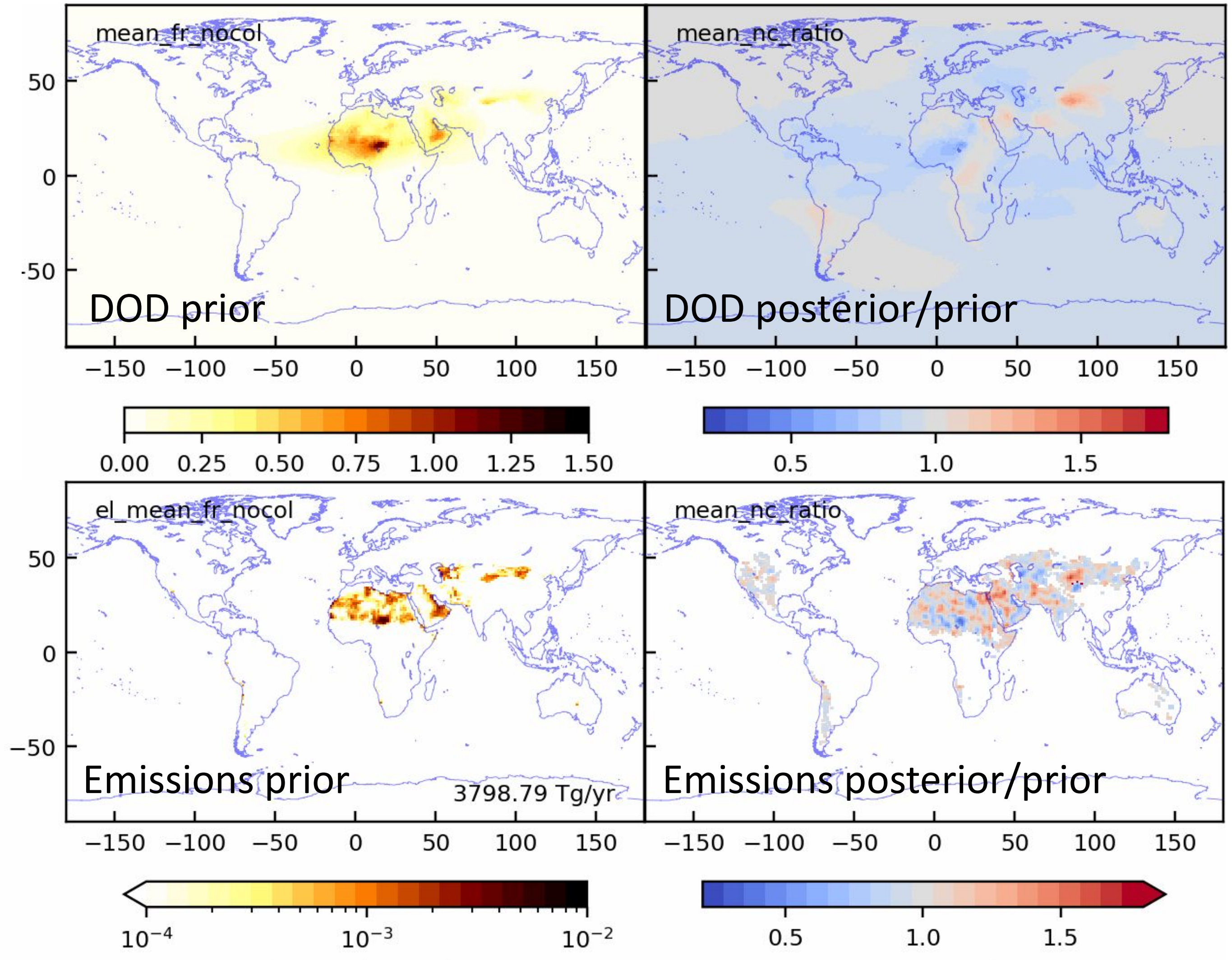
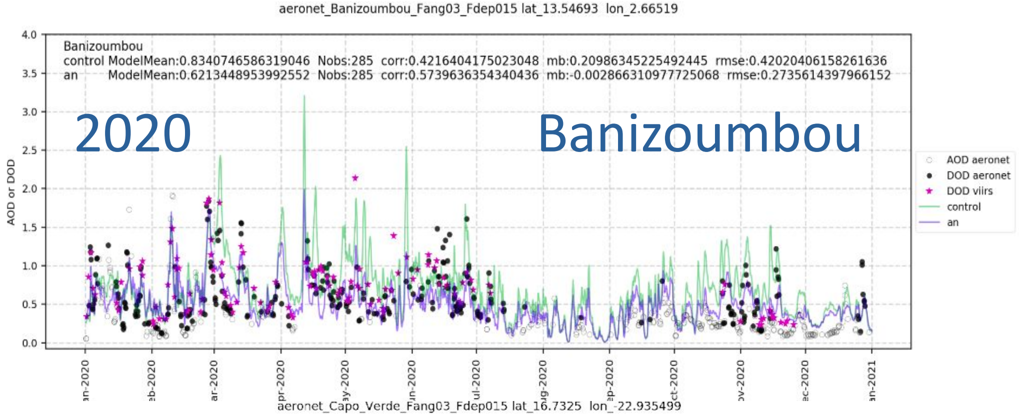


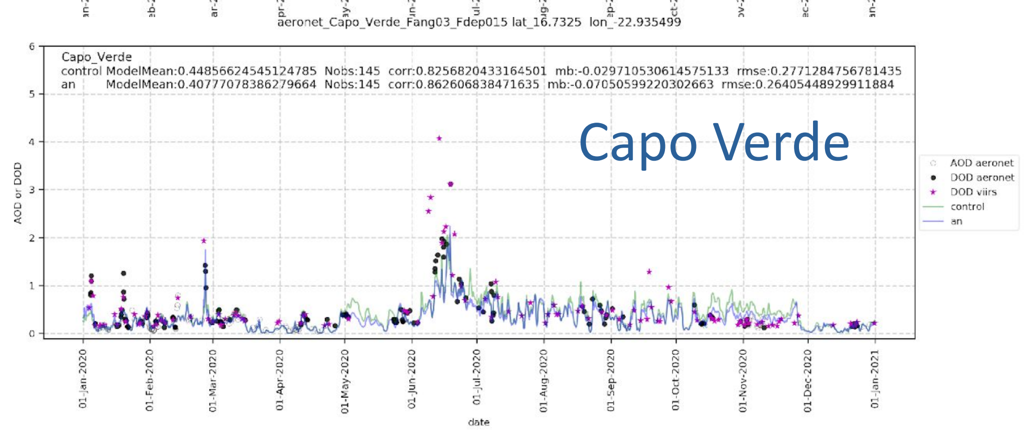
VIIRS DB total and coarse DOD

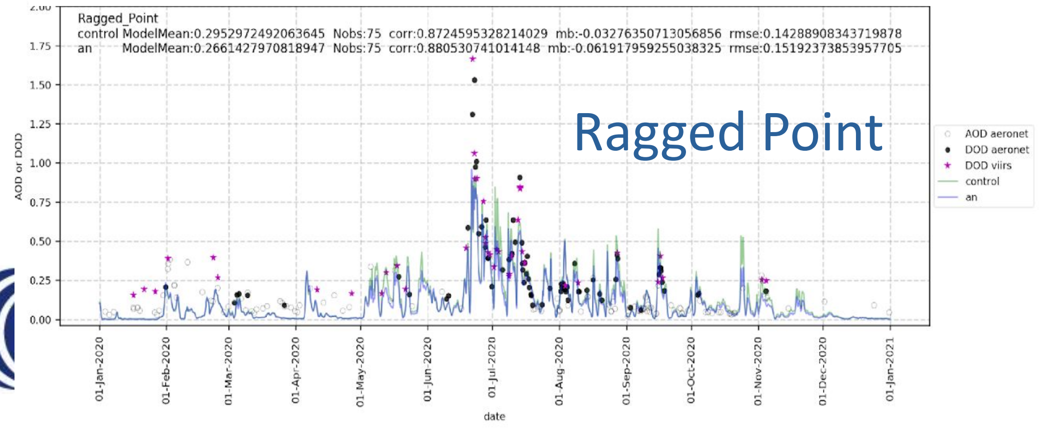


with M. Klose, S. Basart, E. Di Tomaso

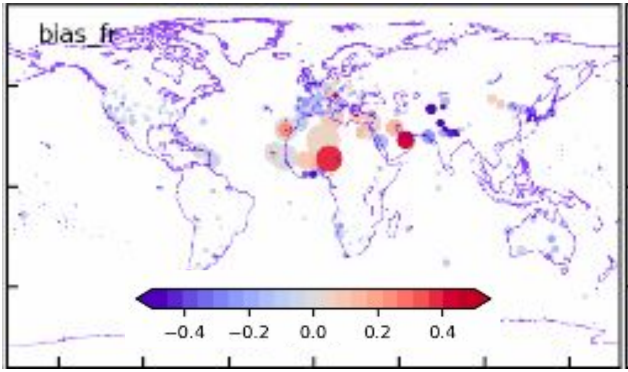
Verification with filtered AOD from AERONET ($\text{ång}<0.3$, $d_{1020}>0.15$) : G2001, Total DOD DA

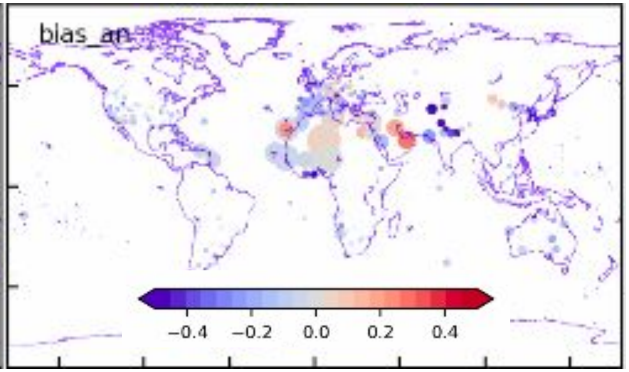




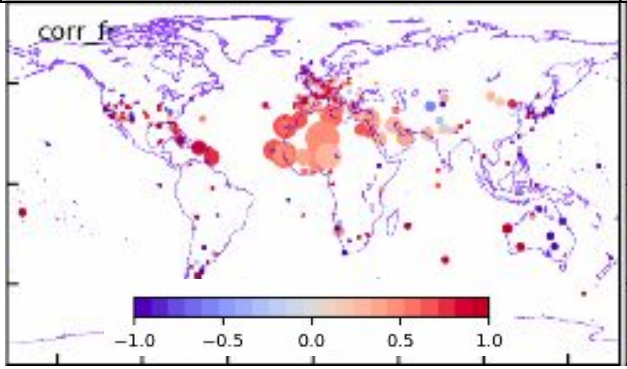


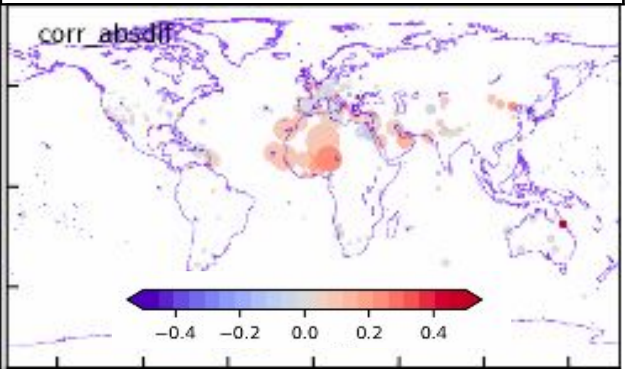
Bias control	Bias analysis



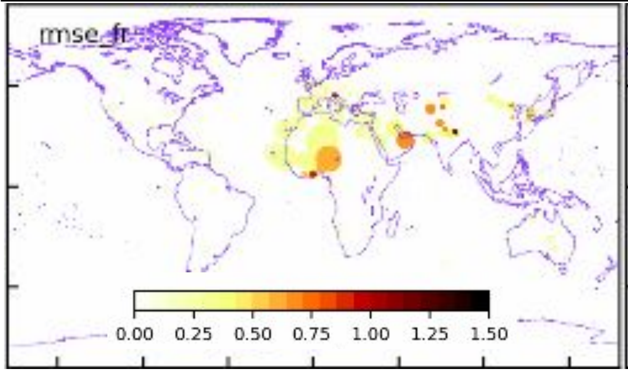


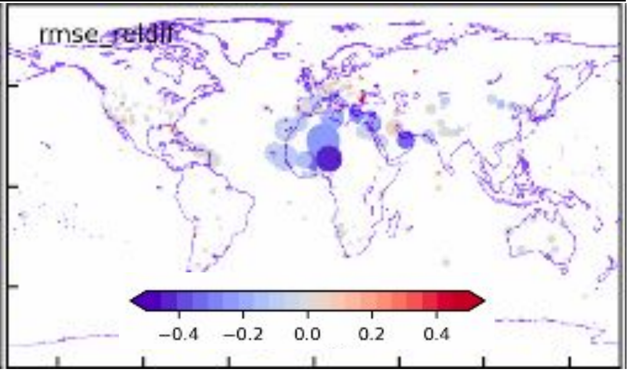
Correlation control	Corr. analysis - corr. control





RMSE control	(RMSE_a - RMSE_c)/RMSE_c

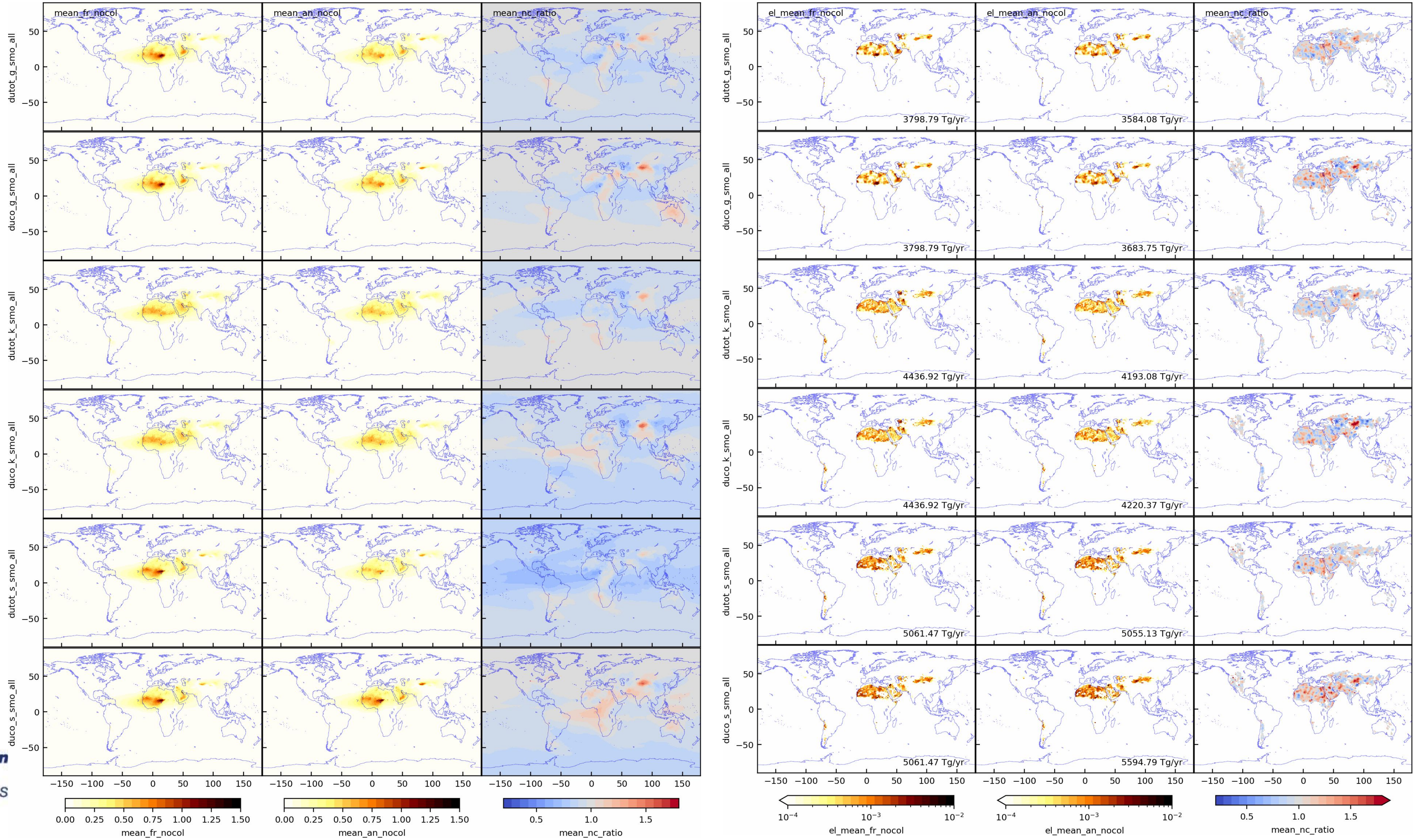




Results: Time averaged dust optical depth and dust emissions

Dust emission	Assim. DOD
Ginoux 2001	Total
	Coarse
Kok 2014	Total
	Coarse
Shao 2004	Total
	Coarse

Control DOD	Analysis DOD	Analysis/Control	Control emissions (kg/m2/day)	Analysis emissions	Analysis/Control



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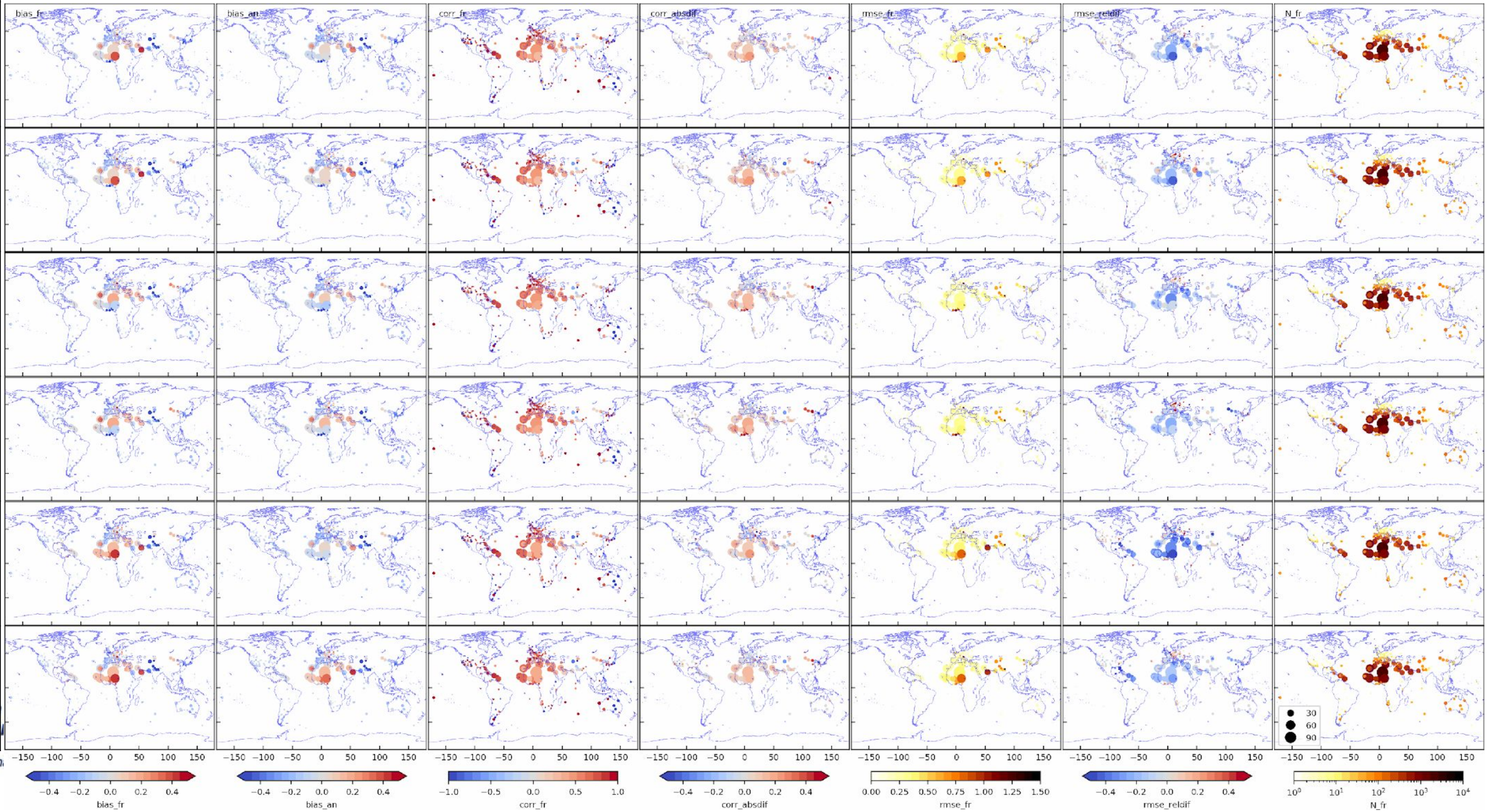
Verification with filtered AOD from AERONET (ång<0.3, d_{1020}>0.15)

Dust emission	Assim. DOD	Bias control	Bias analysis	Correlation control	Corr. analysis –Corr. control	RMSE control	(RMSE_analysis - RMSE control)/RMSE control	Number obs
Ginoux 2001	Total							
	Coarse							
Kok 2014	Total							
	Coarse							
Shao 2004	Total							
	Coarse							



constraining dust emissions

- ➔ Better agreement of analysis AOD with dust filtered ground-based AOD from AERONET with respect to their controls.
- ➔ It is able to constrain emissions in scale of hundreds of km
- ➔ Dust AOD and emission changes depend on the emission scheme <u>and</u> on the assimilated observation: Need better constrain and QA on assimilated observation
- ➔ Unresolved tasks: LETKF ensemble perturbation length scale determines the correction length scales-> Multi-scale constraints, etc

Why to continue ?

- Emission estimates for better constraint total dust optical depth
- Regional emission constraints to better estimate airborne mineral dust mineralogy
  - New data from EMIT
  - Meaningful sensitivity of DRE to dust mineralogy, total dust load and size distribution.
  - Impact of mineralogy on Dust-cloud interactions (e.g. INP)
  - Nitrate formation sensitivity to dust mineralogy
- Assimilation with variables related to emissions in the control vector to improve the accuracy of the forecasts
- Can detect systematic errors in emission schemes or input data

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Questions?

and thank you!

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