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Supercomputing
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Centro Nacional de Supercomputación



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The Atmospheric Composition Group in a nutshell

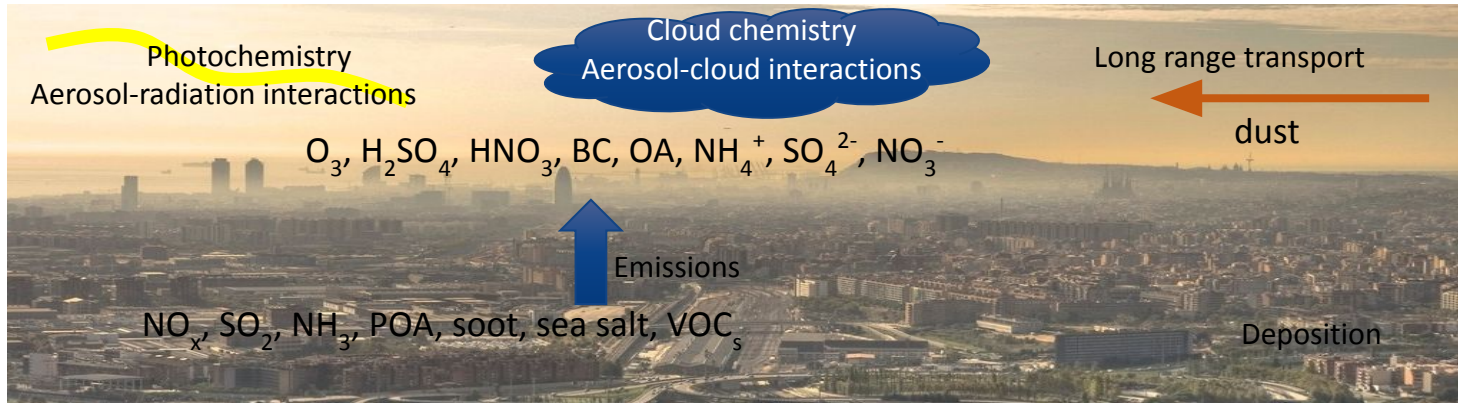


Department Day meeting

27/05/2021

Main goal

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



Keywords

Emission inventories, natural emissions, source apportionment

Ozone, mineral dust, secondary organic aerosols, iron cycle

Variability and trends, aerosol chemistry, aerosol-radiation-cloud, climate

Model development, global, mesoscale, urban

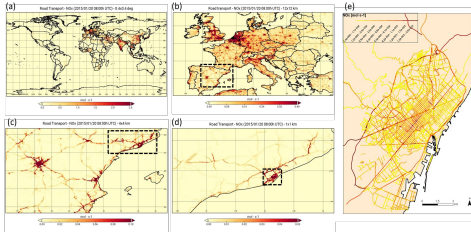
Forecasting, reanalysis, data assimilation, machine learning, observations

Field campaigns, health effects

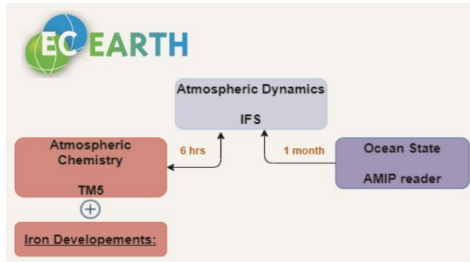
Model and tool developments

HERMESv3

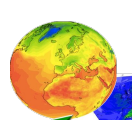
A python-based, open source, parallel and multiscale emission model



EC-Earth3-Iron

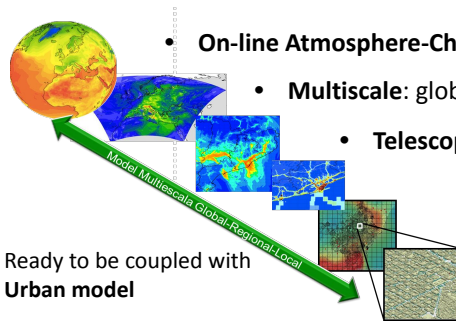


MONARCH



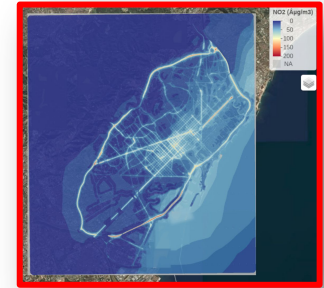
- On-line Atmosphere-Chemistry coupling
- Multiscale: global to local (1km)
- Telescoping nesting

Ready to be coupled with Urban model



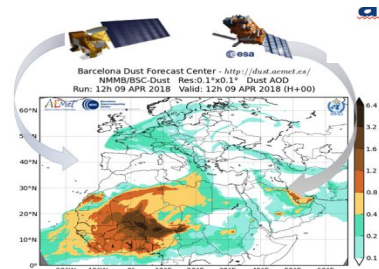
CALIOPE-Urban

Street-scale dispersion model



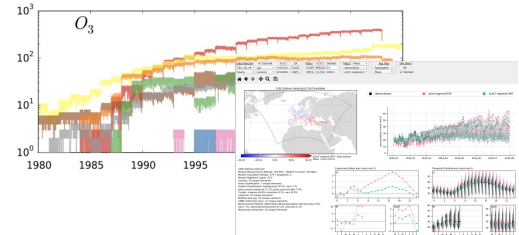
LETKF DA

Ensemble based Data Assimilation system



GHOST/Providentia

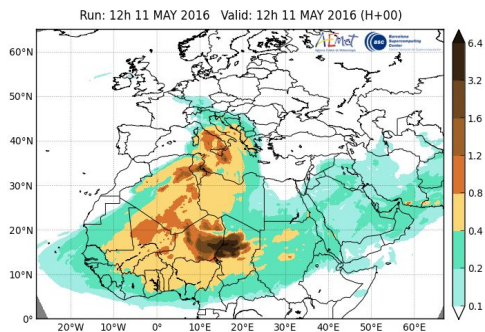
Harmonised treatment of observations and dynamic/flexible evaluation system



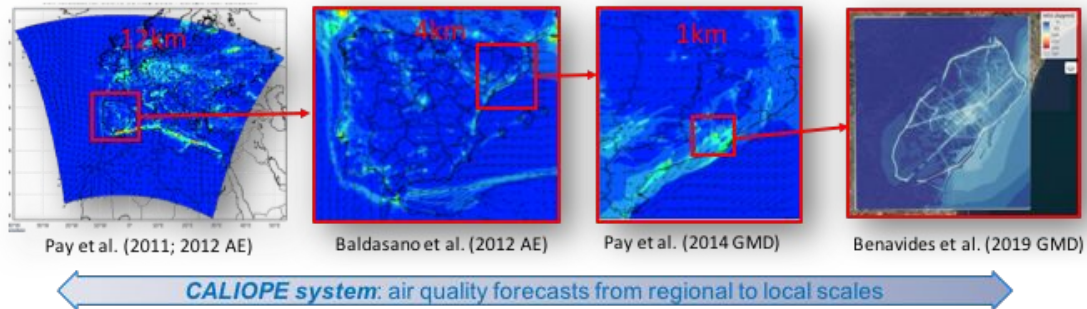
Forecasts, reanalysis, services

WMO Dust Regional Centers

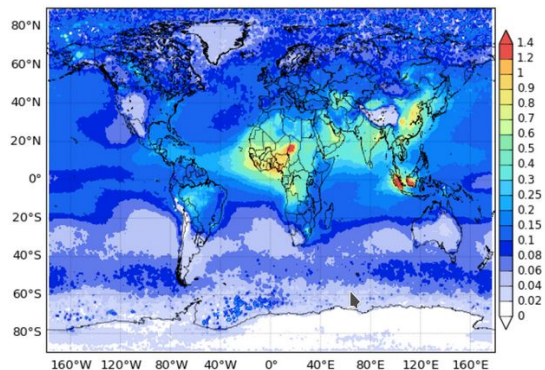
Dust forecasts and reanalysis



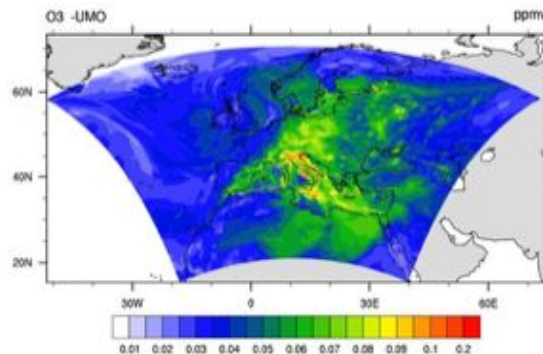
CALIOPE Forecast system



ICAP global aerosol ensemble



Soon joining the CAMS air quality regional ensemble



In collaboration with CES and ESS

Ongoing and near-future projects

AXA Research Fund	AXA Chair on Sand and Dust Storms
ERC Consolidator	FRAGMENT
NASA	EMIT
H2020	SOLWARIS, FORCES, AQ-Watch, CoCO2
CAMS	43, 50, 61, 81, 84, COP_66, COP_79, 2_35, 2_40
ERA4CS	DustClim
ESA	CCI, DOMOS
National Retos	NUTRIENT, BROWNING, VITALIZE
Cost Action	InDust
Contracts and other	Encomienda Dust, Service agreement, Sedema, Generalitat

COVID-19

Health effects

THE LANCET
Planetary Health

CORRESPONDENCE | VOLUME 4, ISSUE 7, E268, JULY 01, 2020

Reduction in air pollution and attributable mortality due to COVID-19 lockdown

Hicham Achekab · Hervé Petetin · Marcos Quijal-Zamorano · Dene Bowdalo · Carlos Pérez García-Pando ·

Joan Ballester

Open Access · Published: July, 2020 · DOI: [https://doi.org/10.1016/S2542-5196\(20\)30148-0](https://doi.org/10.1016/S2542-5196(20)30148-0)

NO₂ reductions, in situ, Spain

Atmos. Chem. Phys., 20, 11119–11141, 2020
<https://doi.org/10.5194/acp-20-11119-2020>
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Atmospheric
Chemistry
and Physics



Meteorology-normalized impact of the COVID-19 lockdown upon NO₂ pollution in Spain

Hervé Petetin¹, Dene Bowdalo¹, Albert Soret¹, Marc Guevara¹, Oriol Jorba¹, Kim Serradell¹, and Carlos Pérez García-Pando^{1,2}

NO₂ reductions, satellite, models, Europe

Atmos. Chem. Phys., 21, 7373–7394, 2021
<https://doi.org/10.5194/acp-21-7373-2021>
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Atmospheric
Chemistry
and Physics



Estimating lockdown-induced European NO₂ changes using satellite and surface observations and air quality models

Jérôme Barré¹, Hervé Petetin¹, Augustin Colette¹, Marc Guevara², Vincent-Henri Peuch¹, Laurence Rouil³, Richard Engelen⁴, Antje Inness⁵, Johannes Flemming¹, Carlos Pérez García-Pando^{1,2}, Dene Bowdalo², Frederik Meulen⁶, Camilla Geels⁷, Jesper H. Christensen⁸, Michael Gauss⁹, Anna Benedictow¹⁰, Svetlana Tsyro⁶, Elmar Friese¹¹, Joanna Struzewska¹², Jacek W. Kaminski¹³, John Douras¹⁴, Renske Timmermans¹⁵, Lennart Robertson¹², Mario Adani¹³, Oriol Jorba², Mathieu Joly¹⁴, and Rostislav Kouznetsov¹⁵

Emission reductions

Atmos. Chem. Phys., 21, 773–797, 2021
<https://doi.org/10.5194/acp-21-773-2021>
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Atmospheric
Chemistry
and Physics



PM, O₃ changes and implications



Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv



Contents lists available at ScienceDirect

Environmental Pollution

journal homepage: www.elsevier.com/locate/envpol

Time-resolved emission reductions for atmospheric chemistry modelling in Europe during the COVID-19 lockdowns

Marc Guevara¹, Oriol Jorba¹, Albert Soret¹, Hervé Petetin¹, Dene Bowdalo¹, Kim Serradell¹, Carles Tena¹, Hugo Denier van der Gon², Jeroen Kuenen², Vincent-Henri Peuch³, and Carlos Pérez García-Pando^{1,4}

Lessons from the COVID-19 air pollution decrease in Spain: Now what?

Xavier Querol^{a,*}, Jordi Massagué^{a,b}, Andrés Alastuey^a, Teresa Moreno^a, Gotzon Gangoiti^c, Enrique Mantilla^d, José Jaime Duéñez^d, Miguel Escudero^e, Eliseo Monfort^f, Carlos Pérez García-Pando^{g,h}, Hervé Petetin^g, Oriol Jorba^g, Víctor Vázquez^h, Jesús de la Rosa^k, Alberto Campos^l, Marta Muñoz^l, Silvia Monge^l, María Hervás^l, Rebeca Javato^l, María J. Cornide^l



Trade-offs between short-term mortality attributable to NO₂ and O₃ changes during the COVID-19 lockdown across major Spanish cities*

Hicham Achekab^{a,b,*}, Hervé Petetin^c, Marcos Quijal-Zamorano^a, Dene Bowdalo^c, Carlos Pérez García-Pando^{c,d}, Joan Ballester^a

Who are we?



Carlos P.



Oriol J.



María G.



Enza Di T.



Marc G.



Sara B.



Jerónimo E.



Dene B.



Montse C.



Arnau B.



Santiago E.



Roger G.



Franco L.



Hector N.



Ruben S.



Elisa B.



Adolfo G.



Cristina G.



Visitors ex-BSC and collaborators

+ *long list of close collaborators from CES, ESS and CP*
Thanks!

+ ***4 Open positions***

Today

**Aerosol modeling
MONARCH**



Hector N.

**Iron modeling
EC-Earth**



Ruben S.



Elisa B.

**Dust field campaigns
FRAGMENT**



Adolfo G.



Cristina G.



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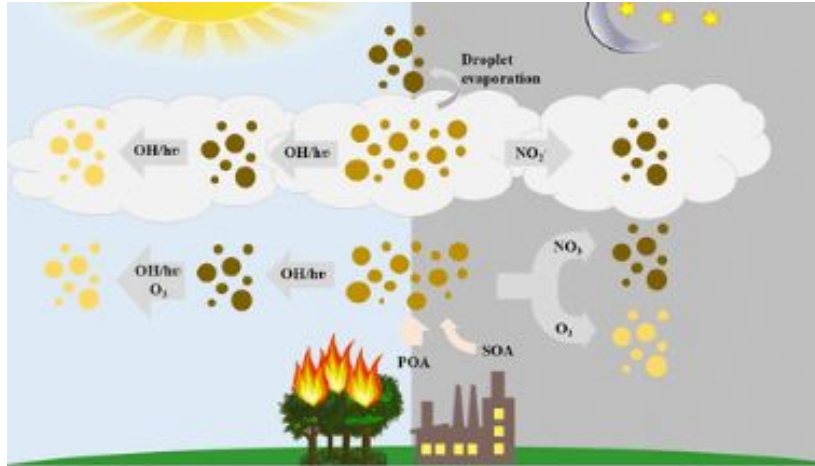
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MONARCH: organic aerosol and dust heterogeneous chemistry

Hector Navarro - PhD Student

Ruben Sousse - PhD Student

Why studying Organic aerosol (OA) ?



Sources and chemistry of OA (Hems et al., 2021)

- OA represents in some places more than 50% of total aerosols mass.
- Chemistry of OA is currently not well understood.
- Certain primary and secondary OA have a strong influence on radiative effect absorbing solar radiation. This type of OA is known as **Brown Carbon (BrC)**.

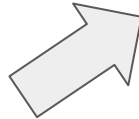
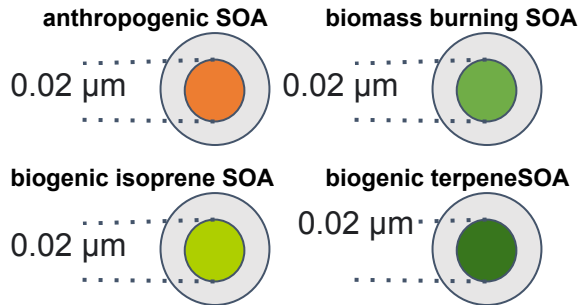
OA and BrC representation in MONARCH

OA scheme based on [Pai et al. \(2020\)](#):

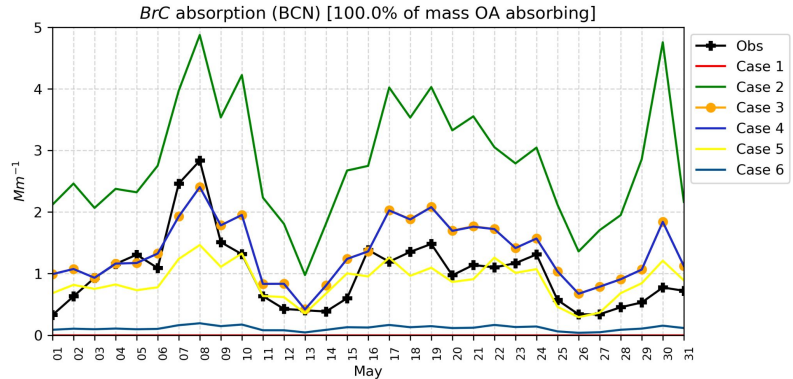
1) Primary Organic Aerosols (POA)



2) Secondary Organic Aerosols (SOA)



We have performed sensitivity tests with different BrC fractions of OA to reproduce observations over Barcelona, Montseny, and Montsec EGAR stations:



In collaboration with:

Dust heterogeneous chemistry

Assessing role of dust mineralogy in atmospheric chemistry
(as part of the **FRAGMENT (ERC) project**)

1 Different sources →
different dust mineralogies

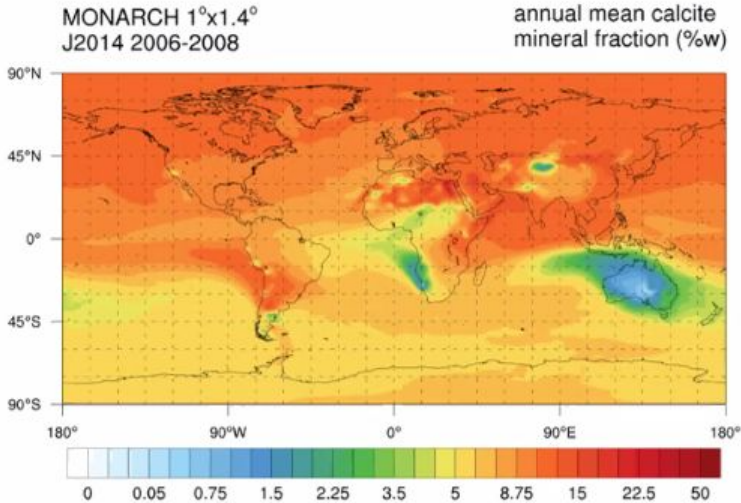
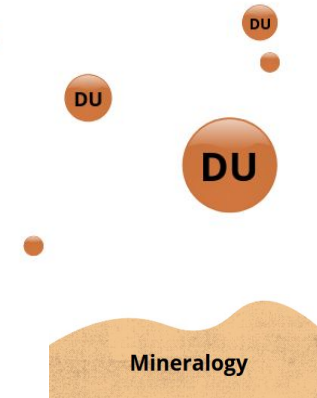
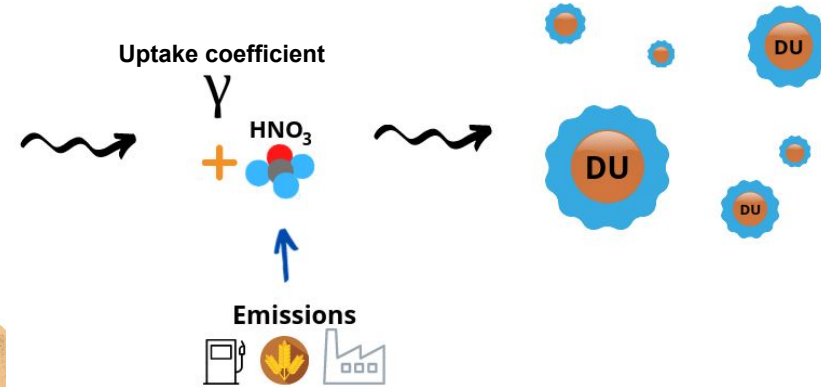


Image credit: Maria Gonçalves

2 Dust is emitted and
transported into the atmosphere

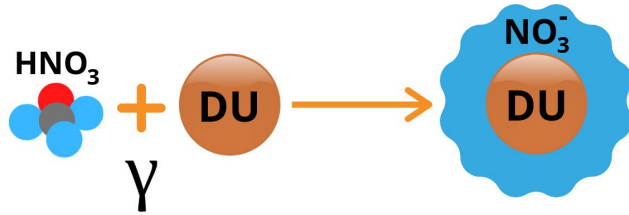


3 Heterogeneous chemical reactions
forming liquid coatings



MONARCH implementation

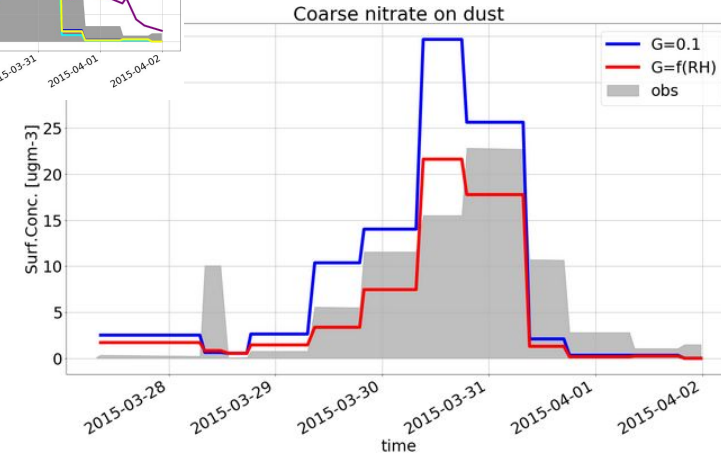
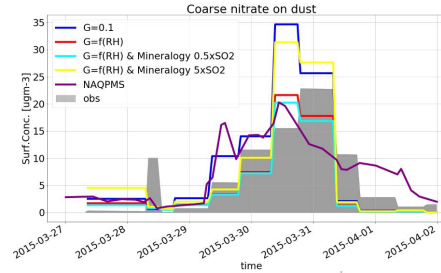
4 In MONARCH we implemented the HNO_3 heterogeneous reaction on dust surface:



Uptake coefficient (γ) depends on:

- Dust mineralogy (source)
- Ambient humidity
- etc.

5 Sensitivity studies are performed and evaluated with observations



6 Implementations are used in other FRAGMENT working groups (i.e. **aerosol radiation, aerosol cloud interaction**)



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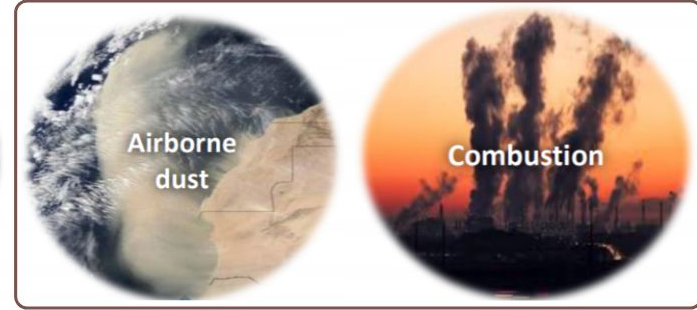
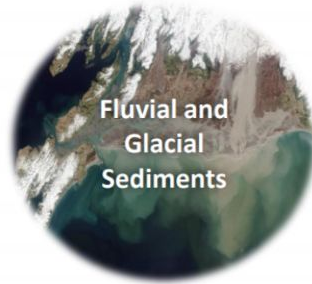
Iron Modeling - EC-Earth

Elisa Bergas-Massó - PhD Student

The Atmospheric Iron Cycle

Ocean productivity (specially in ocean remote regions) **relies upon bioavailable Fe** for photosynthesis, respiration, and nitrogen fixation, which makes the **Fe biogeochemical cycle a key modulator of the ocean's ability to uptake atmospheric CO₂**.

1 Emissions

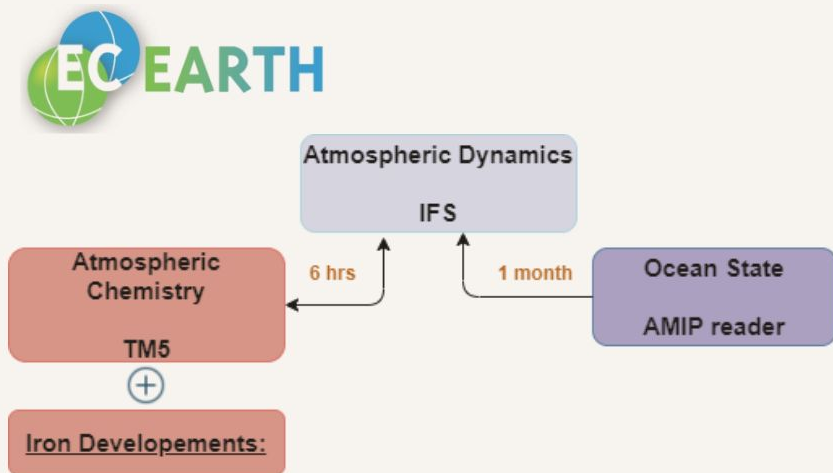


2 Atmospheric Processing



3 Wet & Dry Deposition

Iron CMIP6 Scenarios



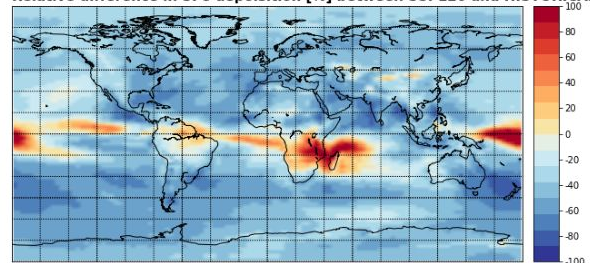
- Anthropogenic Emissions
- Atmospheric Acidity
- Soluble-Fe Deposition



SSP126

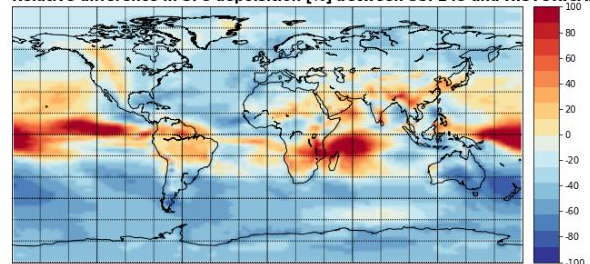
Relative differences with PD

Relative difference in SFe deposition [%] between SSP126 and HISTORICAL



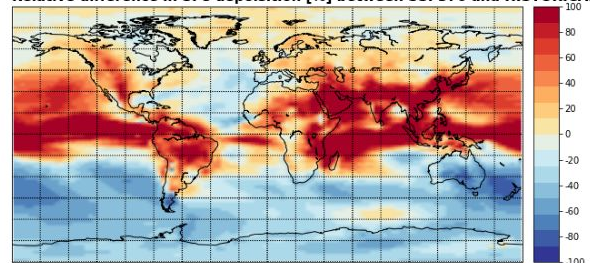
SSP245

Relative difference in SFe deposition [%] between SSP245 and HISTORICAL



SSP370

Relative difference in SFe deposition [%] between SSP370 and HISTORICAL





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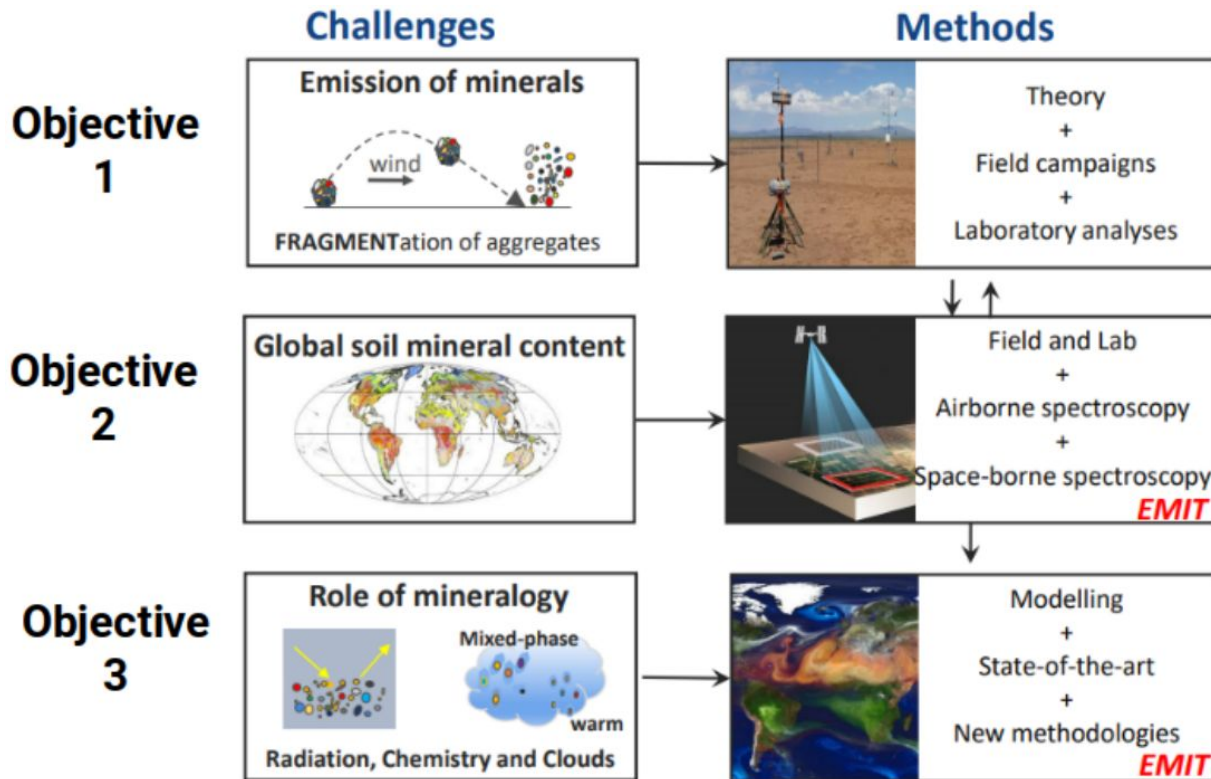
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Field campaigns in FRAGMENT

Cristina González Flórez - PhD Student

Adolfo González Romero - PhD Student

Frontiers in dust mineralogical composition and its Effects upon climate (FRAGMENT)



Host institution:



Partner institutions:



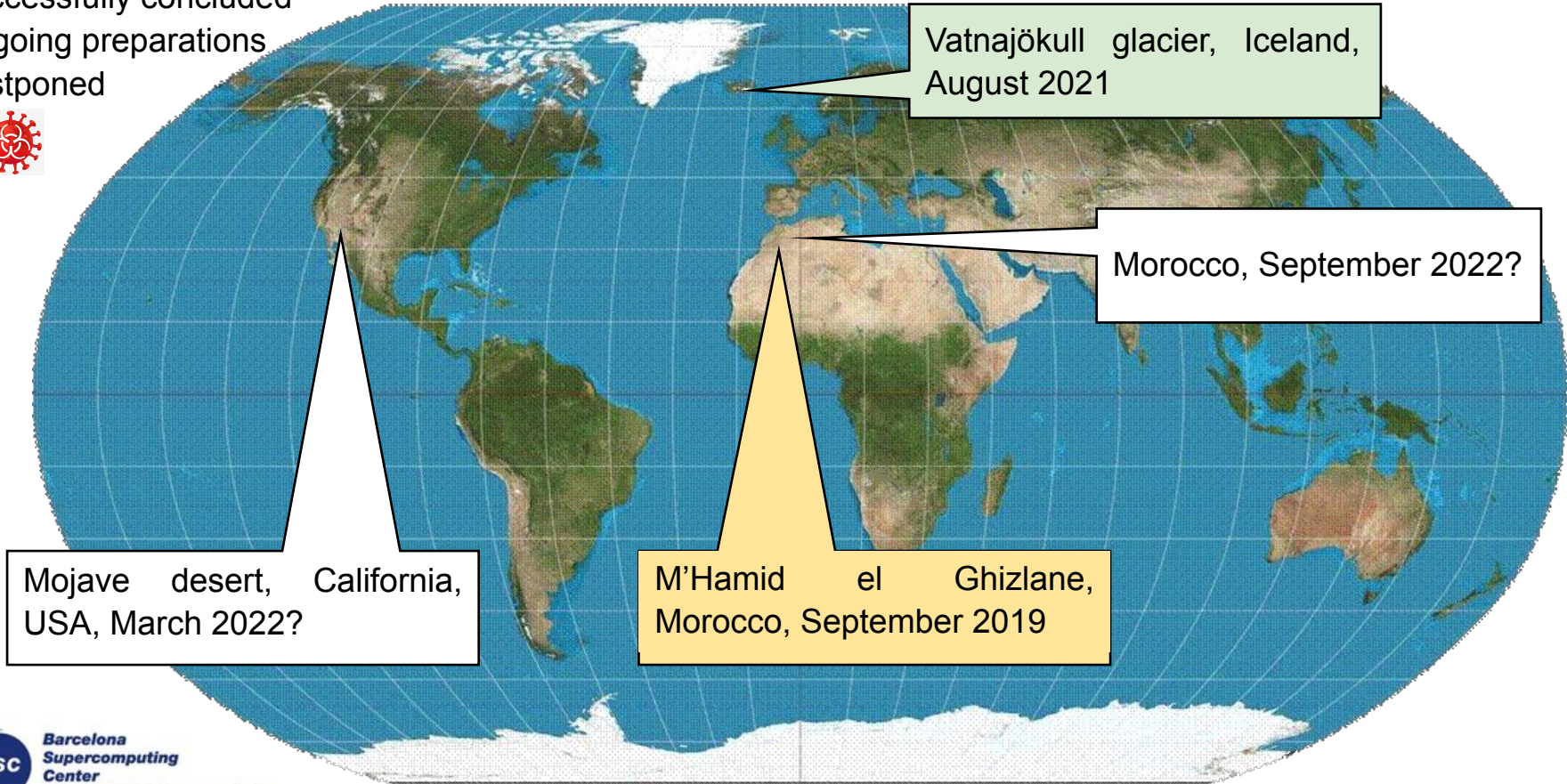
Other collaborators:



Image credit: C. Pérez García-Pando (PI of FRAGMENT)

Field campaigns in FRAGMENT

- Successfully concluded
- Ongoing preparations
- Postponed



Experimental setup

AUGUST 2019						
SUN	MON	TUE	WED	THU	FRI	SAT
				1	2	3
4	5	6	7	8	9	10
11	12	13	14	15	16	17
18	19	20	21	22	23	24
25	26	27	28	29	30	31

Arrival

Regional exploration

SEPTEMBER 2019						
SUN	MON	TUE	WED	THU	FRI	SAT
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30					

Setup

Measures

OCTOBER 2019						
SUN	MON	TUE	WED	THU	FRI	SAT
		1	2	3	4	5
6	7	8	9	10	11	12

Take-down

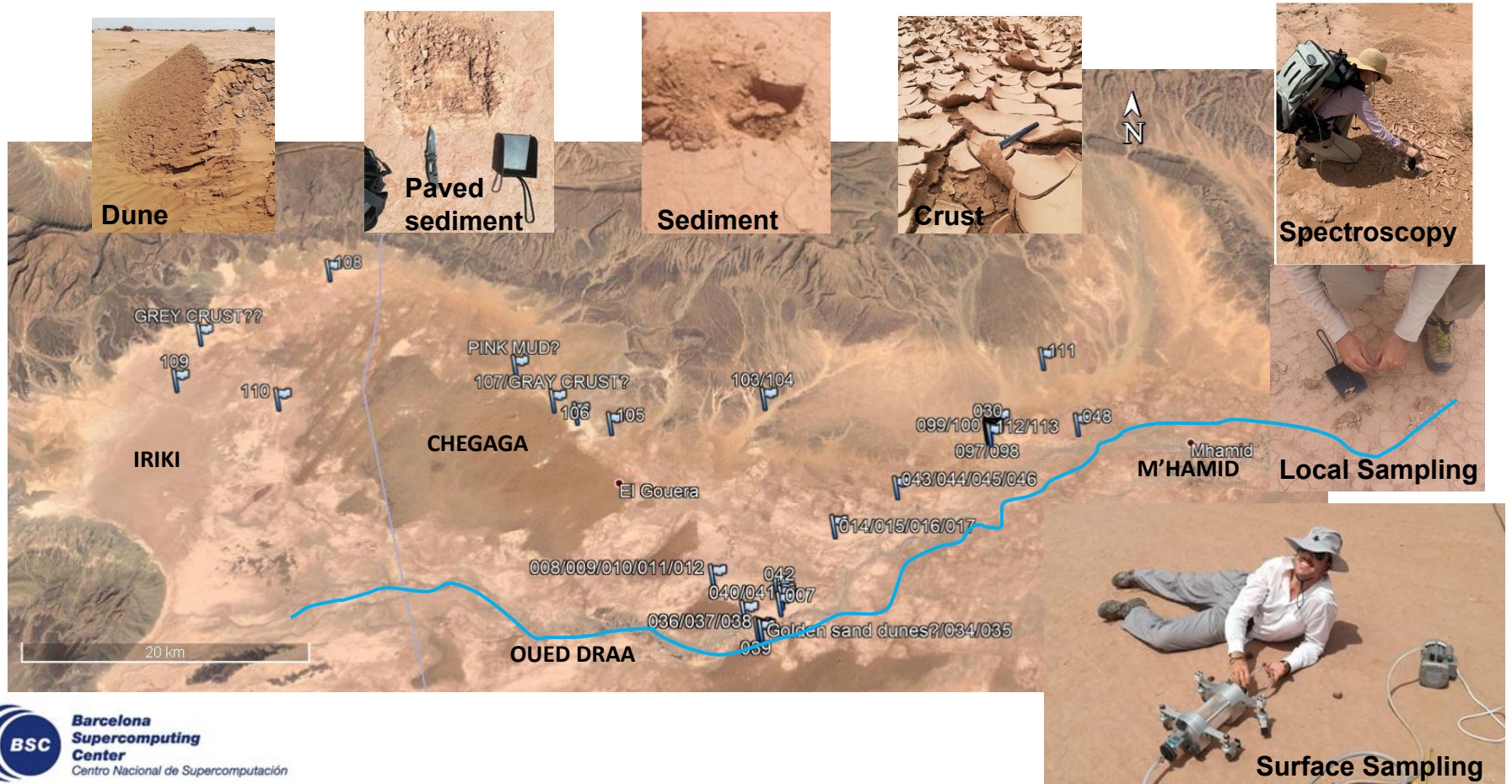
Return



Meteorological & airborne measurements



Local & regional soil sampling



AUGUST 2019						
SUN	MON	TUE	WED	THU	FRI	SAT
				1	2	3
4	5	6	7	8	9	10
11	12	13	14	15	16	17
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Arrival

Regional exploration

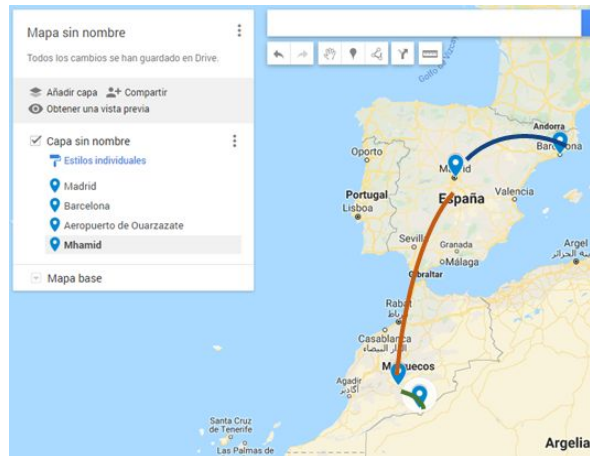
SEPTEMBER 2019						
SUN	MON	TUE	WED	THU	FRI	SAT
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Setup

Measures

OCTOBER 2019						
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Return



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Arrival

Regional exploration

SEPTEMBER 2019						
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22	23	24	25	26	27	28
29	30					

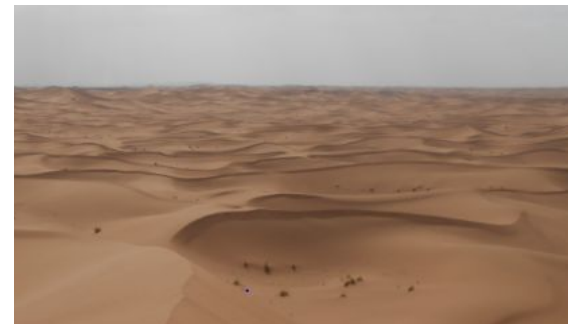
Setup

Measures

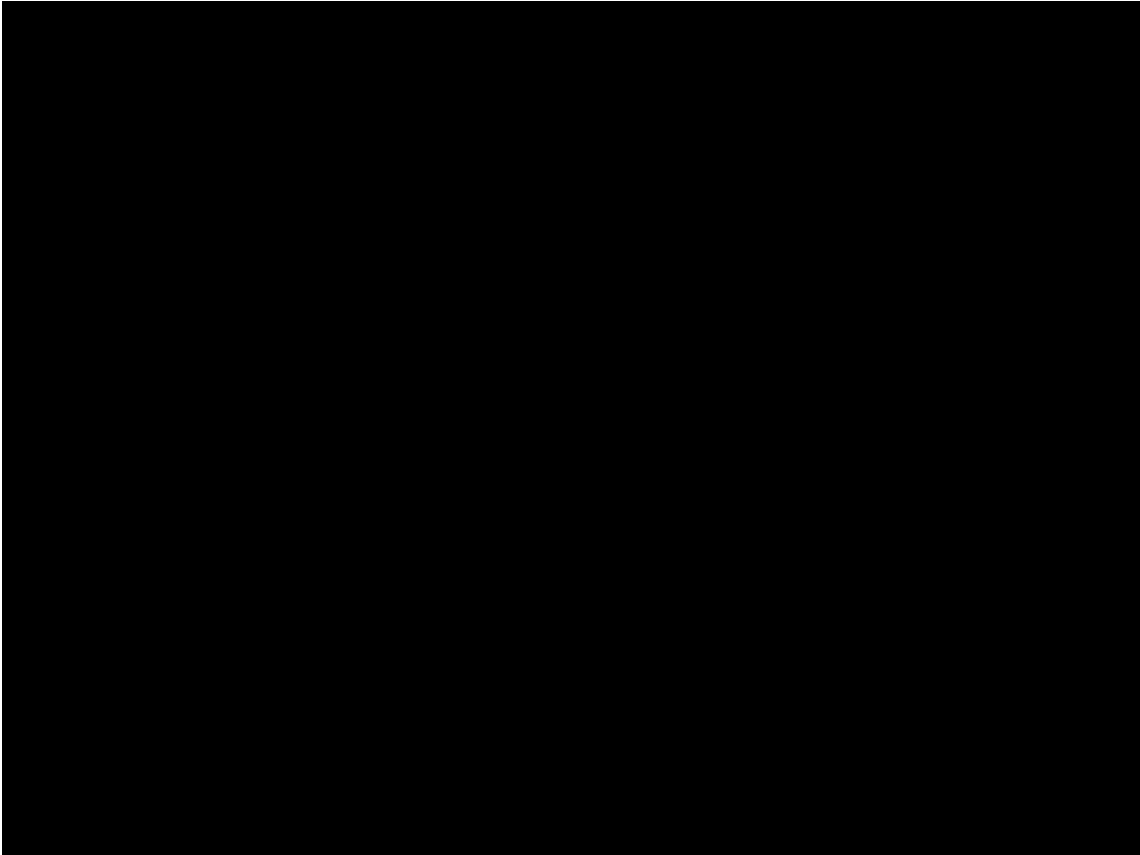
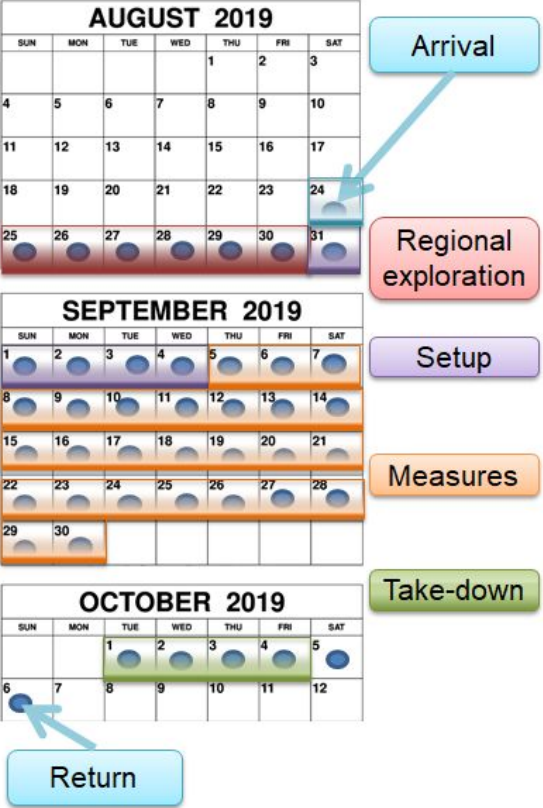
OCTOBER 2019						
SUN	MON	TUE	WED	THU	FRI	SAT
		1	2	3	4	5
6	7	8	9	10	11	12

Take-down

Return



Dust event



The main goal of these campaigns is to evaluate, monitor and sample dust events on the source area

Next challenge....

Iceland





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Thank you!!