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EMS2023-261

An air quality multi-model prediction system for the Basque Country

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1. Introduction

Context:

- ✓ The problem of air pollution in the Autonomous Community of the Basque Country (BAC) has been very important throughout past century, with Bilbao area being one of the most affected zones.
- ✓ Air quality has improved substantially during this century, due to different factors (environmental policies applied, general socio-economic context, …) although the evolution has been different for different types of pollutants* and punctual poor quality episodes are still produced.
- ✓ An air quality control network and hourly pollutants concentration data are available in the Territory.
- ✓ Air quality community models are available and mature.
- ✓ Numerical weather modeling expertise and computing infrastructure are present in Tecnalia and Euskalmet.
- ✓ Increasing focus on operational impact weather and health effects.

This context (and other factors) arises to the need and opportunity to implement a system that extend operational Euskalmet forecast capabilities (weather, oceno-meteorology, …) to air quality.

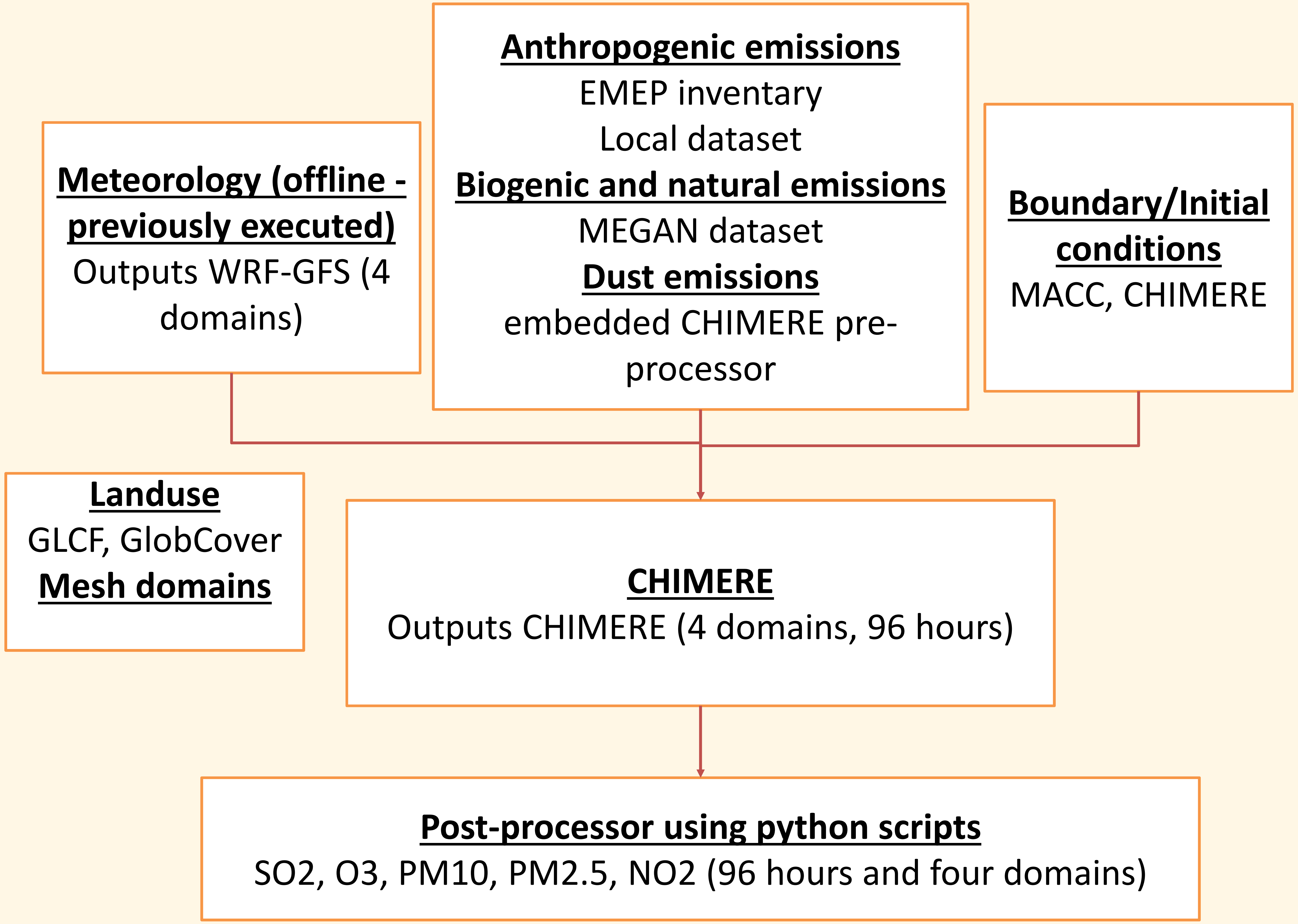
* In general, during the 21st century the air quality in BC has been improving over the years, due to the environmental policies applied and the general socio-economic context. Episodes of moderate or poor air quality due to the impact of SO2 (industrial, diesel, power generation) have been reduced and have almost disappeared; those related to CO (traffic) are nearly nonexistent; NO2 episodes (traffic, energy, heating) , which mainly affect urban areas, have been reducing for years; moderate or poor quality events with high PM10 and PM2.5 (antrophogenic and natural, direct and indirect), shows a systematic decrease; in the case of O3 (photochemical secondary pollutant) an increase in episodes in recent years with a growing trend is observed.

1. Introduction

- Here we introduce an **air quality multi-model prediction system that we have implemented in the Basque Country** for air quality forecast at local level, based on **CHIMERE and WRF-CHEM**.
- The final objective is the **hourly prediction** of air quality in the domain of the Basque Country based on forecasted values of main pollutants concentrations (**CO, NO_2, O_3, PM_{10}, $PM_{2.5}$ and SO_2**).
- We present some aspects of the implementation, post-processing, validation and some conclusions from pre-operational and operational experiences.

2. Implementation - CHIMERE (1/3)

- The CHIMERE multi-scale model is primarily designed to produce daily forecasts of ozone, aerosols and other pollutants and make long-term simulations for emission control scenarios.
- CHIMERE runs over a range of spatial scales from the regional scale to the urban scale. It can run with several vertical resolutions, and with a wide range of complexity. It can run with several chemical mechanisms, simplified or more complete, with or without aerosols.
- The chimere2014b was implemented over Linux OS. The following libraries were required, Fortran 95 compiler, GNU bash Bourne shell, awk and make, Unidata NetCDF library, Open MPI and the NCO libraries
- Forecast are available for 96 hours.

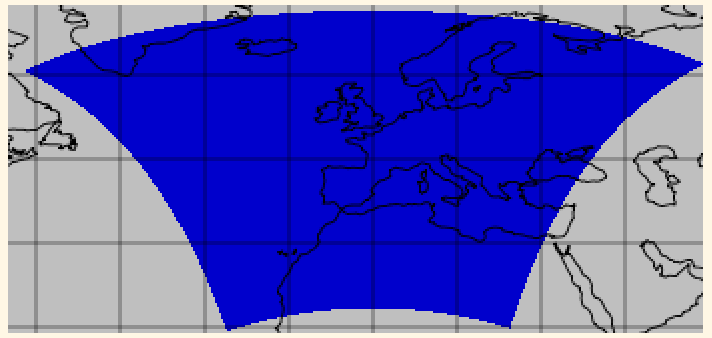


2. Implementation - CHIMERE (2/3)

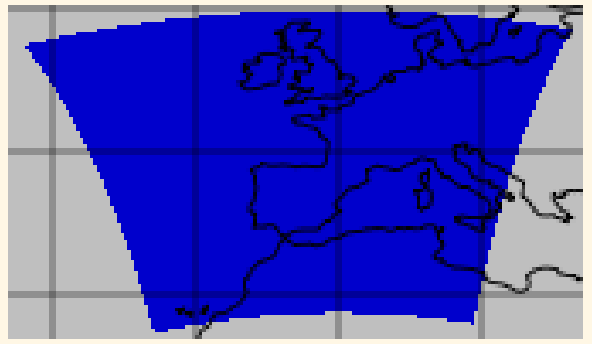
CHIMERE meteorology

Four WRF nested domains are executed daily (GFS 1º 00h)

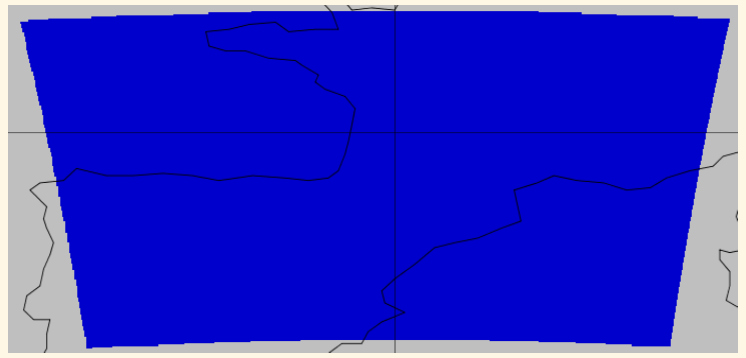
D1 -81x81km



D2 – 27x27 km



D3 – 9x9 km

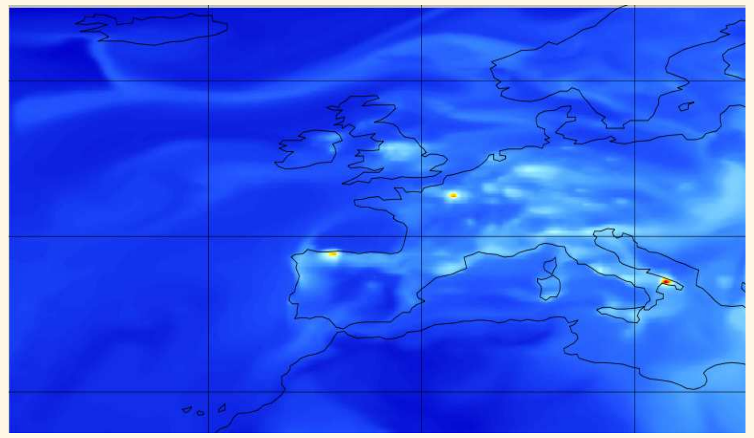


D4 -3x3 km

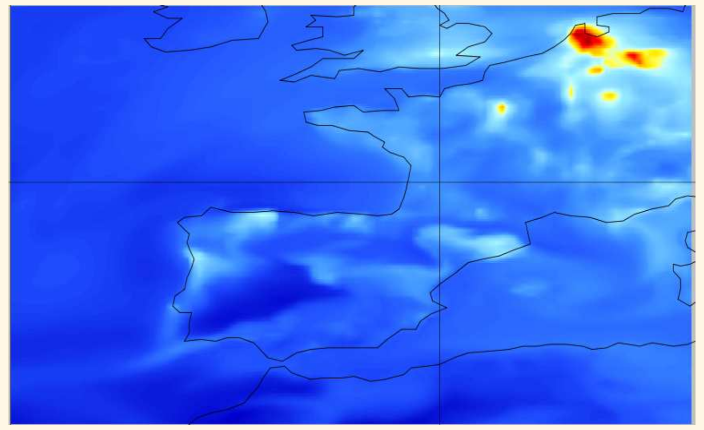
CHIMERE domains

Domain	NX	NY	DX	DY	XMIN	YMIN
DCH.1	193	153	0.27	0.27	-29	26
DCH.2	120	105	0.2	0.2	-15	33
DCH.3	100	60	0.1	0.1	-7	40
DCH.4	140	91	0.014	0.014	-3.5	42.35

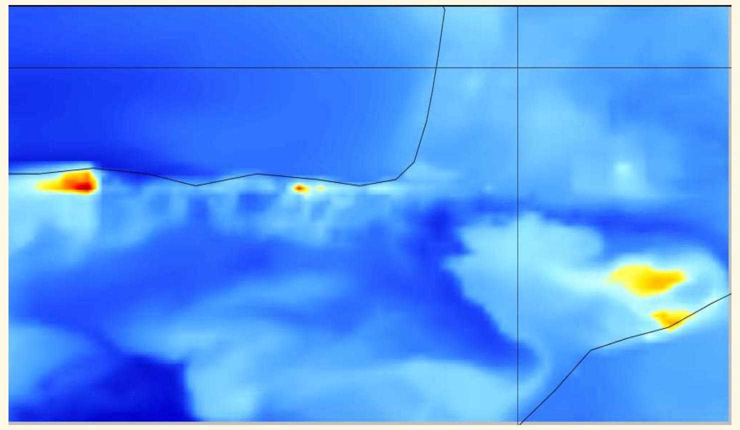
D1 ~0.27ºx0.27º (20 km aprox)



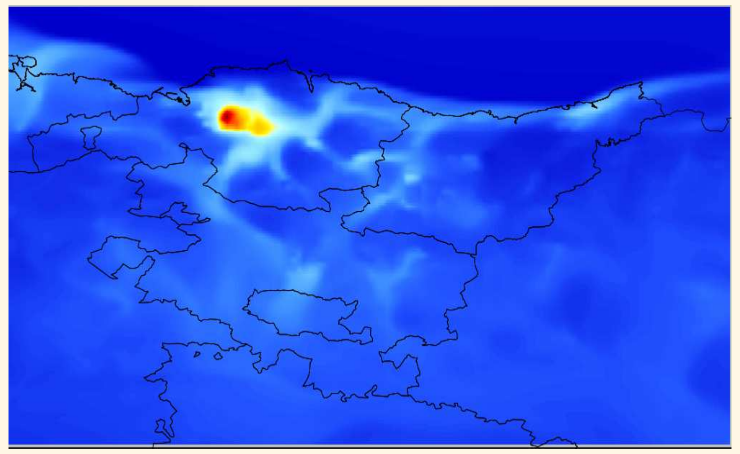
D2 ~ 0.2x0.2º (15 km aprox)



D3 ~ 0.1x0.1º (7km aprox)



D4 ~0.014ºx0.014º (1km aprox) km



2. Implementation - CHIMERE (3/3)

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CHIMERE emissions

EMEP datasets is processed with emi-surf.sh)

```
# WebDab output on Wed Jun  8 09:16:29 2016
# Format: ISO2;YEAR;SECTOR;POLLUTANT;LONGITUDE;LATITUDE;UNIT;NUMBER/FLAG
PL;2014;S1;CO;13.5;53;Mg;1.5561
PL;2014;S2;CO;13.5;53;Mg;73.06
PL;2014;S3;CO;13.5;53;Mg;3.2838
PL;2014;S4;CO;13.5;53;Mg;0
PL;2014;S5;CO;13.5;53;Mg;0
PL;2014;S6;CO;13.5;53;Mg;0
PL;2014;S7;CO;13.5;53;Mg;23.9837
PL;2014;S8;CO;13.5;53;Mg;2.6325
PL;2014;S9;CO;13.5;53;Mg;0.832
```

EMIS.DCH.4.01.APINEN.s.nc
EMIS.DCH.4.01.BaP_fin.s.nc
EMIS.DCH.4.01.BbF_fin.s.nc
EMIS.DCH.4.01.BCAR_coa.s.nc
EMIS.DCH.4.01.BCAR_fin.s.nc
EMIS.DCH.4.01.BkF_fin.s.nc
EMIS.DCH.4.01.C2H4.s.nc
EMIS.DCH.4.01.C2H5OH.s.nc
EMIS.DCH.4.01.C2H6.s.nc
EMIS.DCH.4.01.C3H6.s.nc
EMIS.DCH.4.01.C5H8.s.nc
EMIS.DCH.4.01.CH3CHO.s.nc
EMIS.DCH.4.01.CH3COE.s.nc
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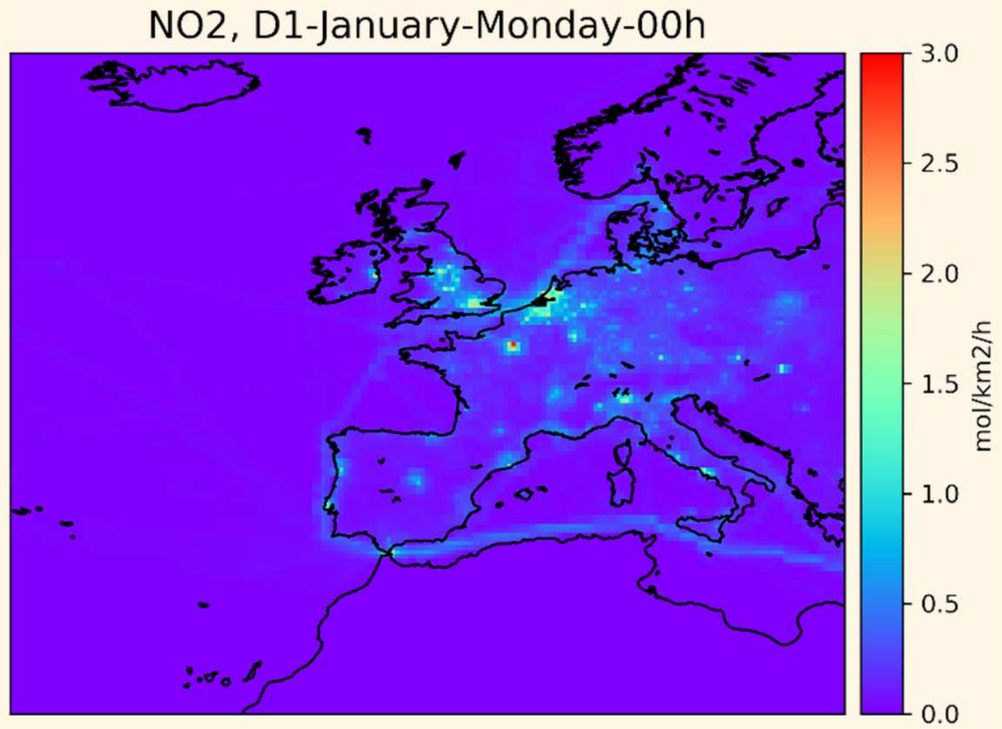
EMIS.DCH.4.01.CH4.s.nc
EMIS.DCH.4.01.CO.s.nc



Local datasets are included in netcdfs generated by emis-surf.sh

UTM

```
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1,1000001,502741.6249165630,4790590.5170839900,,,,,7644,10.2000000000,A-8,55.36,45.56,3.68
2,1000002,502747.3326734160,4790582.3071819000,,,,,7644,10.2000000000,A-8,55.36,45.56,3.68
3,1000003,502753.4000560090,4790574.3600116800,,,,,7644,10.2000000000,A-8,55.36,45.56,3.68
4,1000004,502759.9019258730,4790566.7648612800,,,,,7644,10.2000000000,A-8,55.36,45.56,3.68
5,1000005,502766.8830690290,4790559.6083801400,,,,,7644,10.2000000000,A-8,55.36,45.56,3.68
```
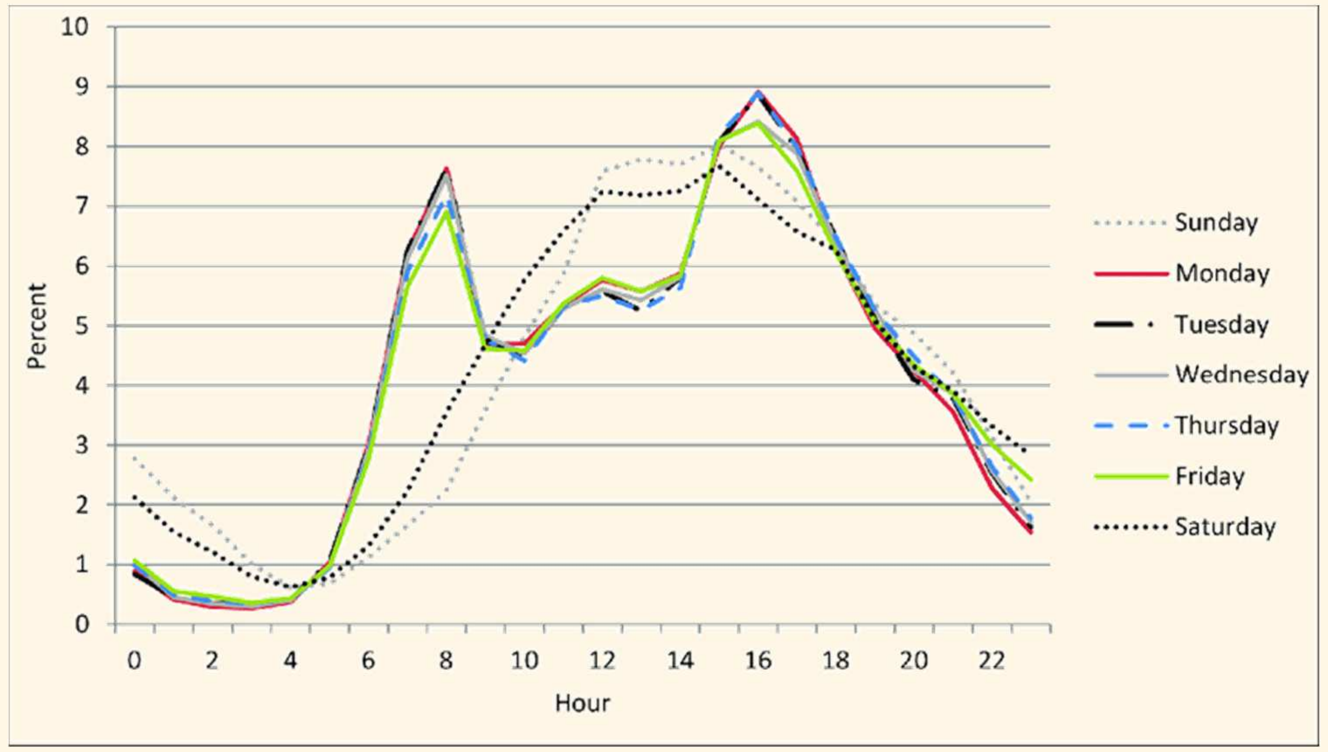
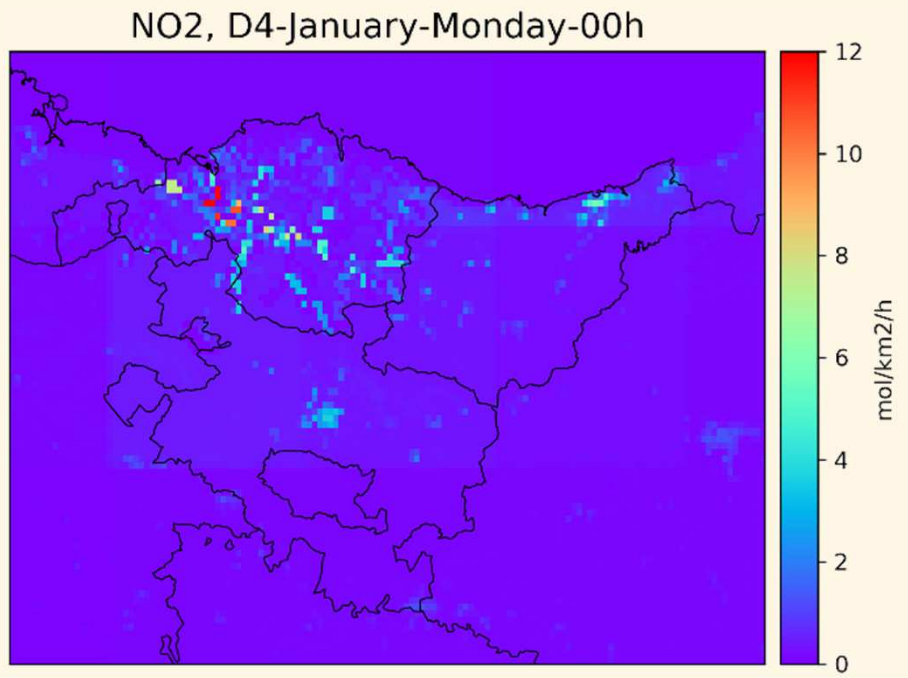
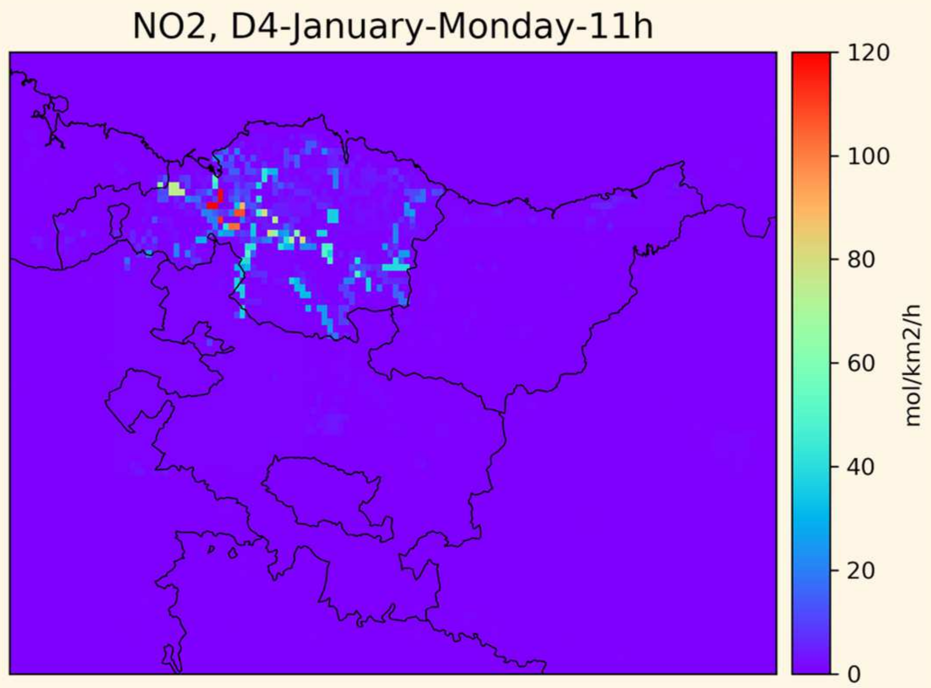

PM_{10}, g/day

CO, g/day

NOx, g/day

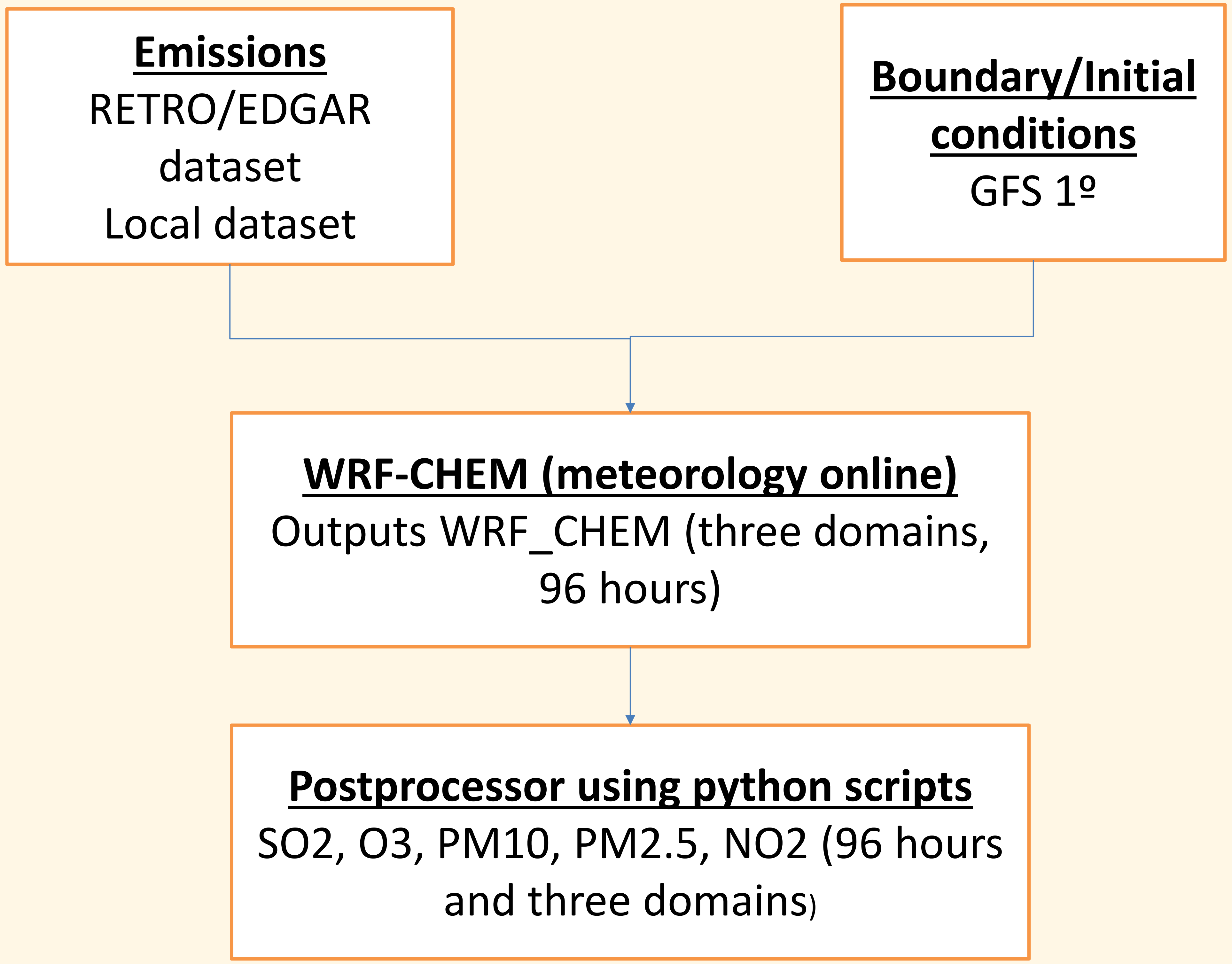






2. Implementation – WRF-CHEM (1/3)

- The WRF-Chem model is a multi-scale model, fully integrated on WRF, that produces forecasts of different pollutants (ozone, aerosols, ...)
- Chemistry part of the model needs to be provided by additional gridded input data related to emissions.
- This additional input data is provided either by the WPS (dust emission fields), or read in during the real.exe initialization (e.g., biomass burning, biogenic emissions, GOCART background fields, etc.), or read in during the execution of the WRF solver (e.g., anthropogenic emissions, boundary conditions, etc.).

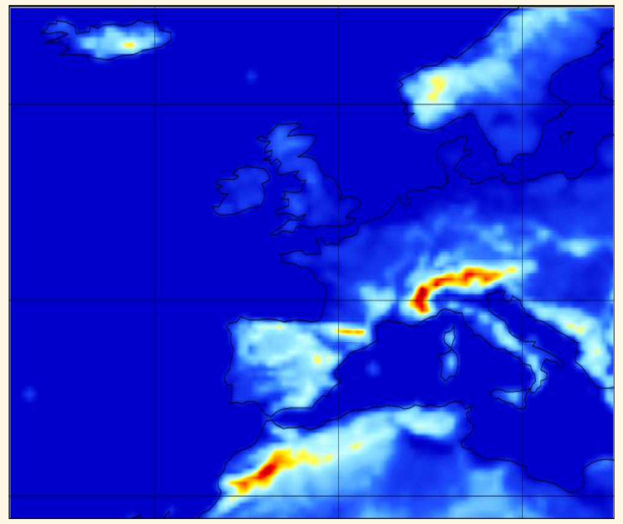


2. Implementation – WRF-CHEM (2/3)

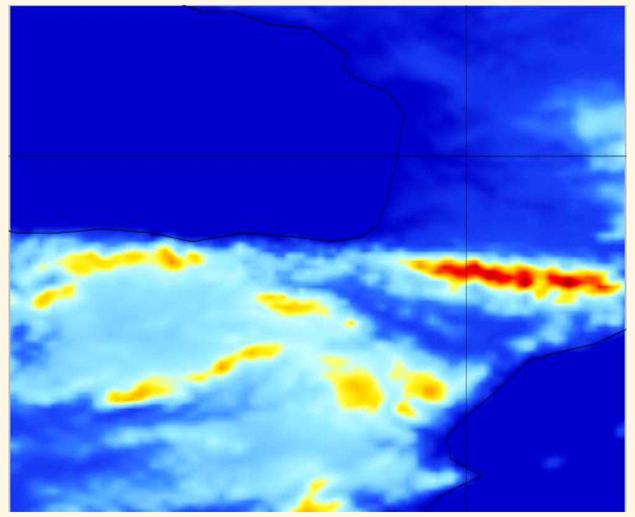
WRF-CHEM domains

Three nested domains are executed daily considering the GFS 1º outputs for 00h

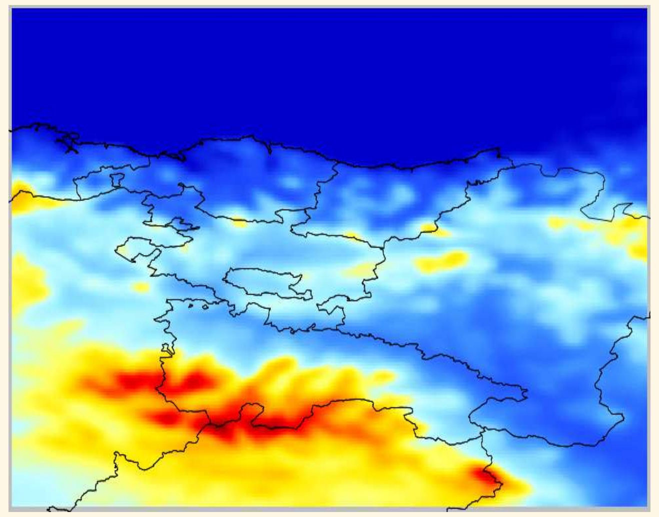
D1 ~ 44x44km



D2 ~ 11x11 km



D3 ~ 2.75 x 2.75 km



WRF-CHEM configuration

The mechanism used during the forecast is decided with the name list parameter chem_opt. It was selected selected 303 RADM2 Chemistry and GOCART aerosols with simple aerosol treatment.

The following options were selected,

- emiss_opt = 5, for GOCART RACM_KPP emissions, using RETRO/EDGAR emissions
- dmsemis_opt=1, it calculates biogenic emissions online using the Gunther scheme
- dust_opt=1 GOCART dust emissions were included
- seas_opt=1 for GOCART sea salt emissions
- bio_emiss_opt=1

2. Implementation – WRF-CHEM (3/3)

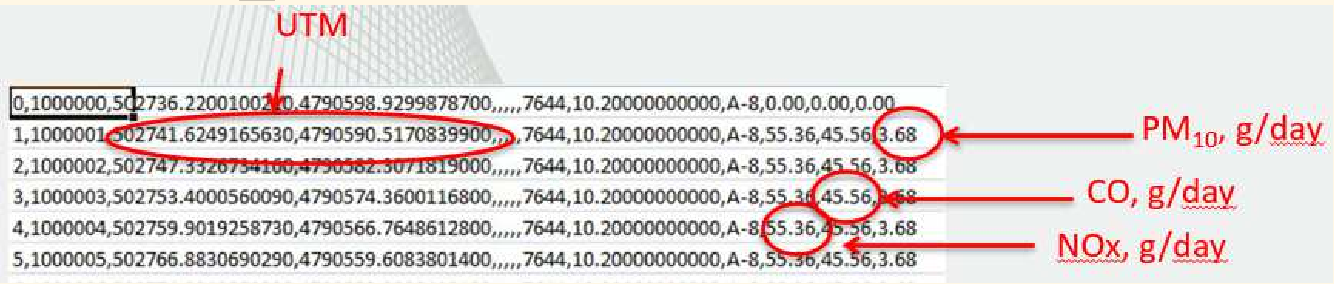
WRF-CHEM emissions

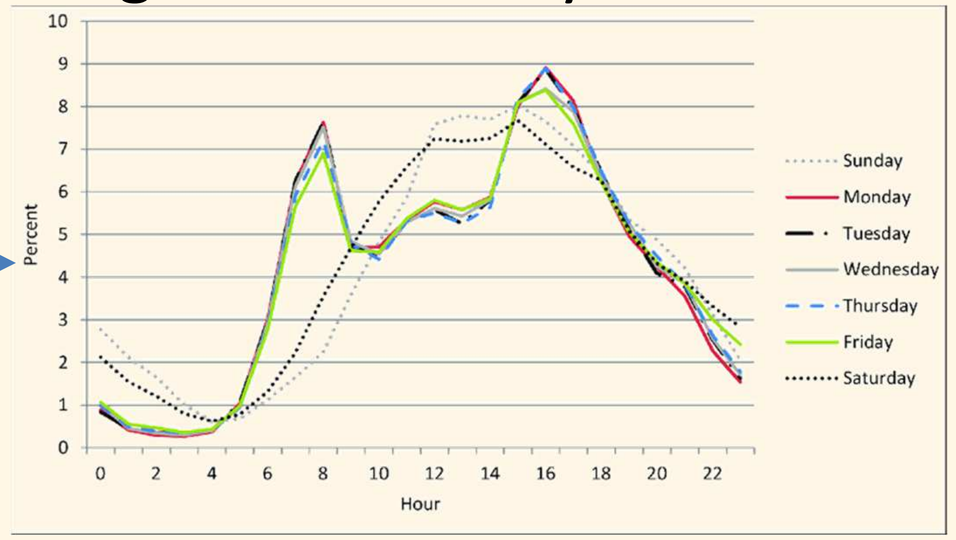
EDGAR/RETRO datasets is processed with prep_chem_sources.exe and with convert_emiss.exe

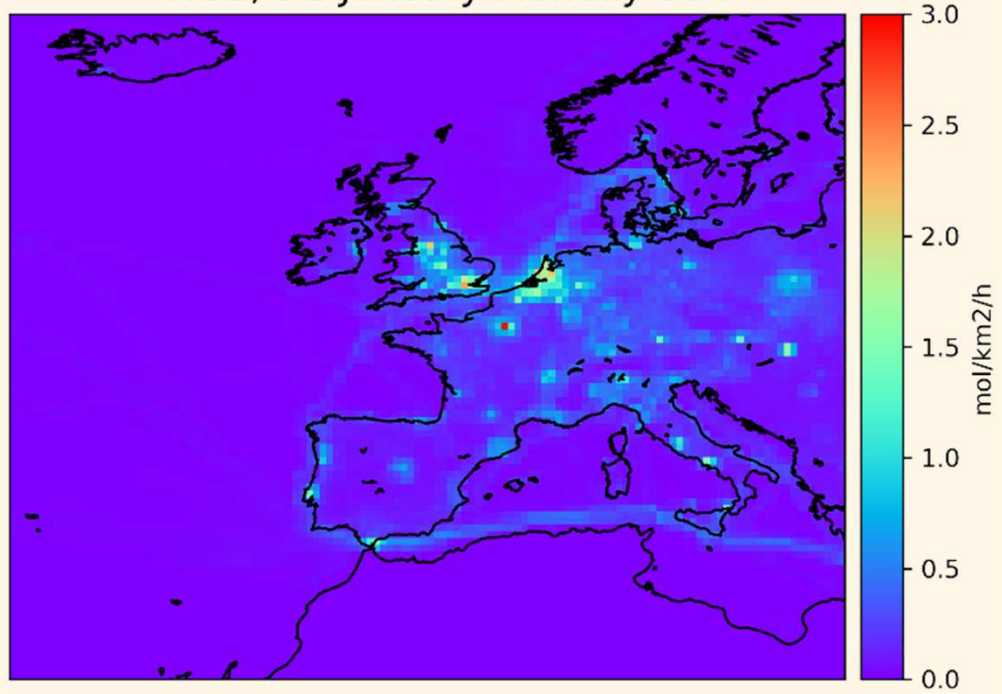
- matrixfire-T-2023-07-12-000000-g1.ctl
- matrixfire-T-2023-07-12-000000-g1.gra
- matrixfire-T-2023-07-12-000000-g1.vfm
- matrixfire-T-2023-07-12-000000-g1-ab.bin
- matrixfire-T-2023-07-12-000000-g1-bb.bin
- matrixfire-T-2023-07-12-000000-g1-gocartBG.bin

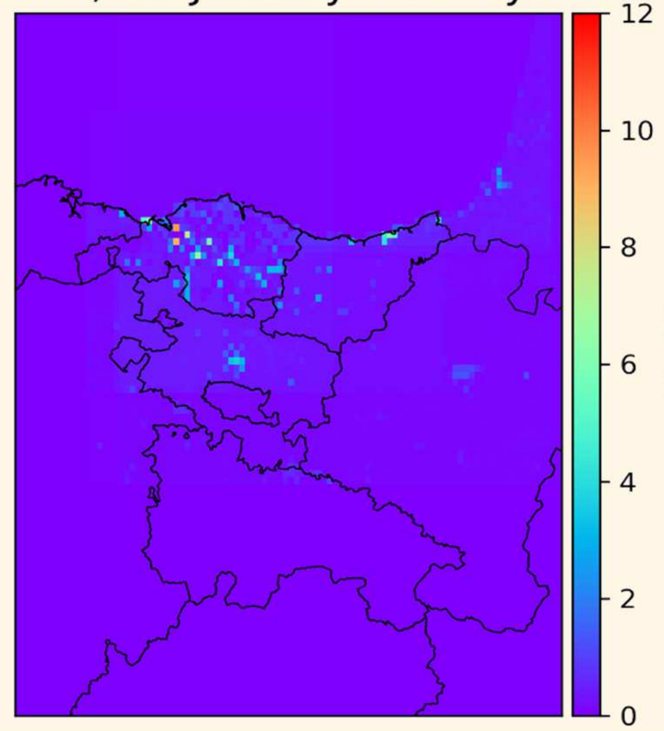
Local datasets are included in netcdfs generated by convert_emiss.exe

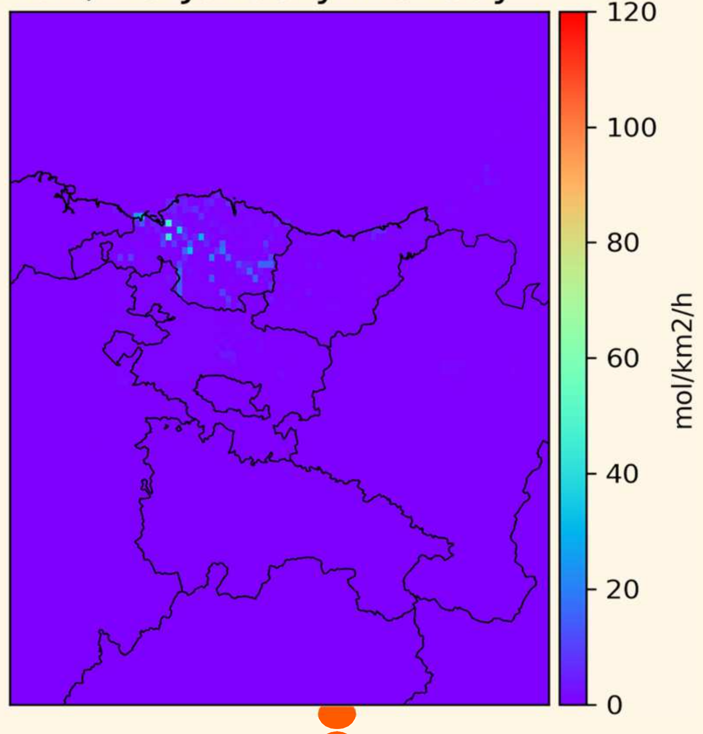
- wrfchemi_00z_d01
- wrfchemi_00z_d02
- wrfchemi_00z_d03
- wrfchemi_12z_d01
- wrfchemi_12z_d02
- wrfchemi_12z_d03
- wrfchemi_gocart_bg_d01
- wrfchemi_gocart_bg_d02
- wrfchemi_gocart_bg_d03











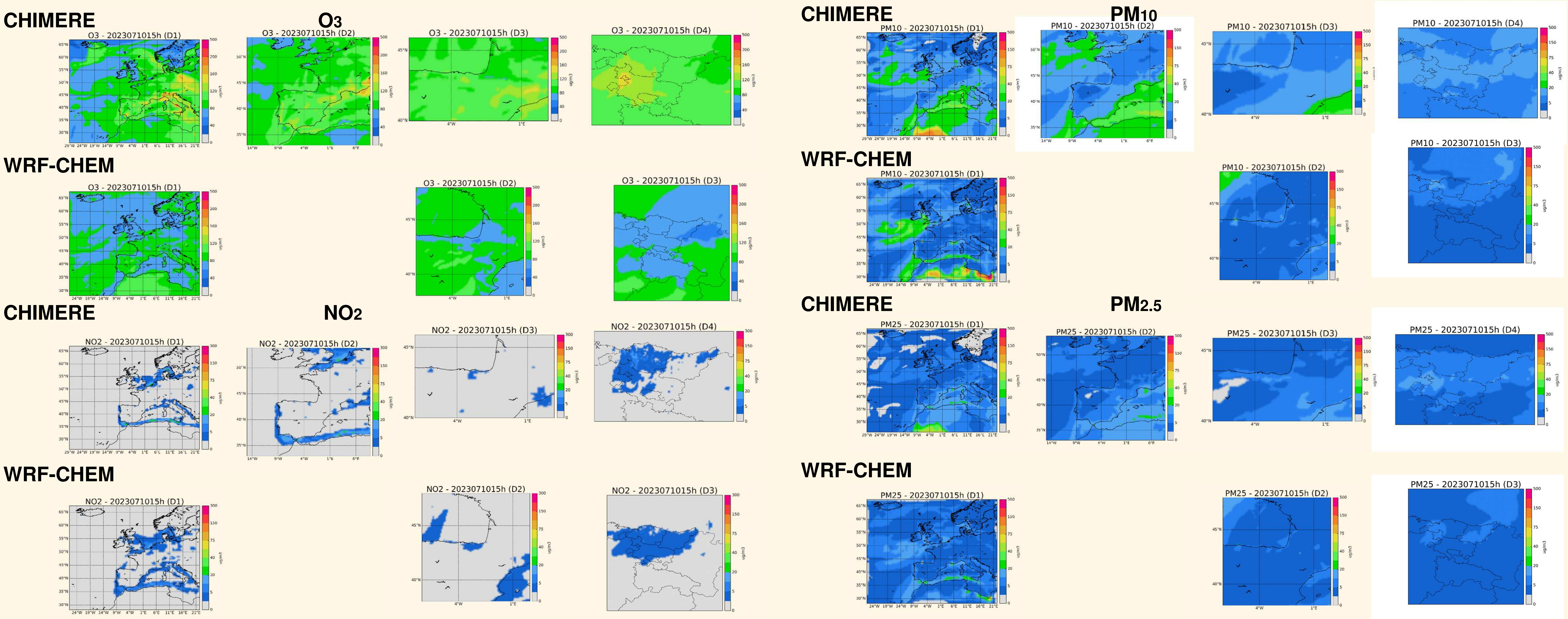
2. Implementation - Summary

- The air quality prediction multi-model system developed is based on two main modelization strategies, one using **CHIMERE** and another one based on **WRF-CHEM**.
- Both models are executed daily with a prediction horizon of up to **4 days** and with resolutions around **1 km**.
- In the case of the CHIMERE chemical transport model, **four nested domains** are considered, being the coarser domain Western Europe and the finer one the Autonomous Community of the Basque Country (CAE), **WRF** model meteorological fields are included **offline**.
- In the case of WRF-CHEM, three nested domains are implemented, the first one being Western Europe and the last one the CAE, in this case meteorology given by the **WRF** model and the pollutant transport module, are executed **online**.
- In both cases, model starts from the initial and boundary weather conditions given by the one-degree GFS global prediction model.
- The emissions are those given by the EMEP emissions inventory for the CHIMERE model and EDGAR for the anthropogenic emissions required by WRF-CHEM. A proprietary emissions inventory has been used for the domain of the Autonomous Community of the Basque Country.

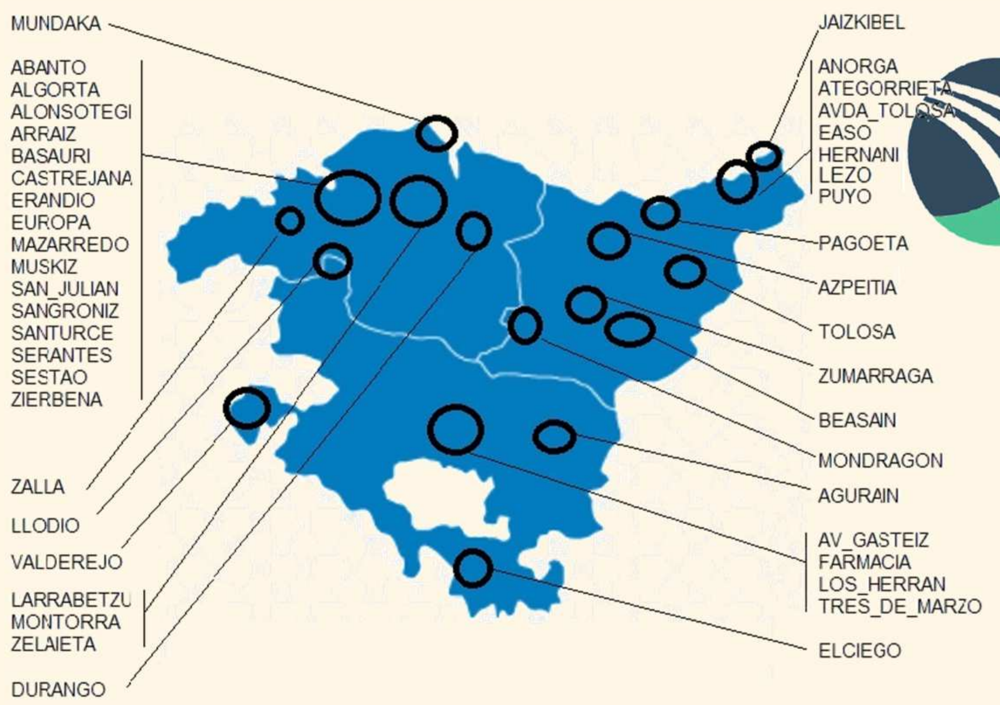
3. Post-processing (1/2)

- Native output fields are postprocessed through a set of python scripts in order to get different products (maps, graphs, tables, etc..) for operational exploitation.

Example of concentration maps on surface for different pollutants from CHIMERE and WRF-CHEM side.



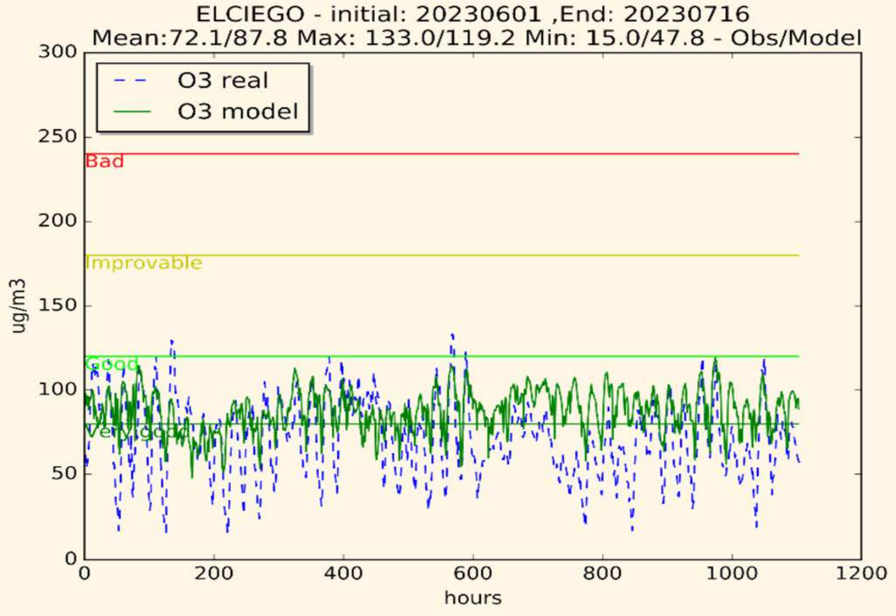
3. Post-processing (2/2)

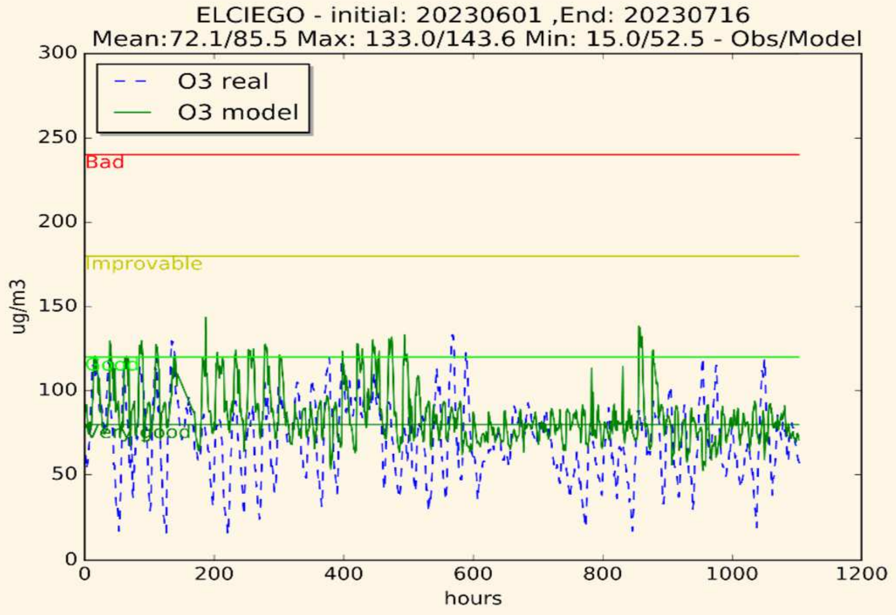


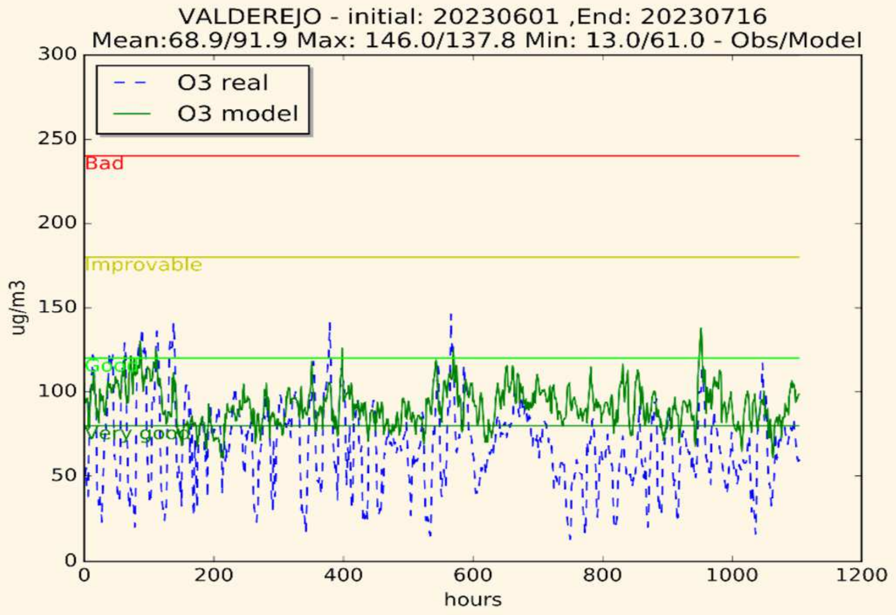
Example: Graphs with observations and model outputs for different air quality stations for a 45 days period from 2023/06/01 to 2023/07/12 (The levels to define the air quality very bad, bad, moderate, good and very good, depends on the european regulations)

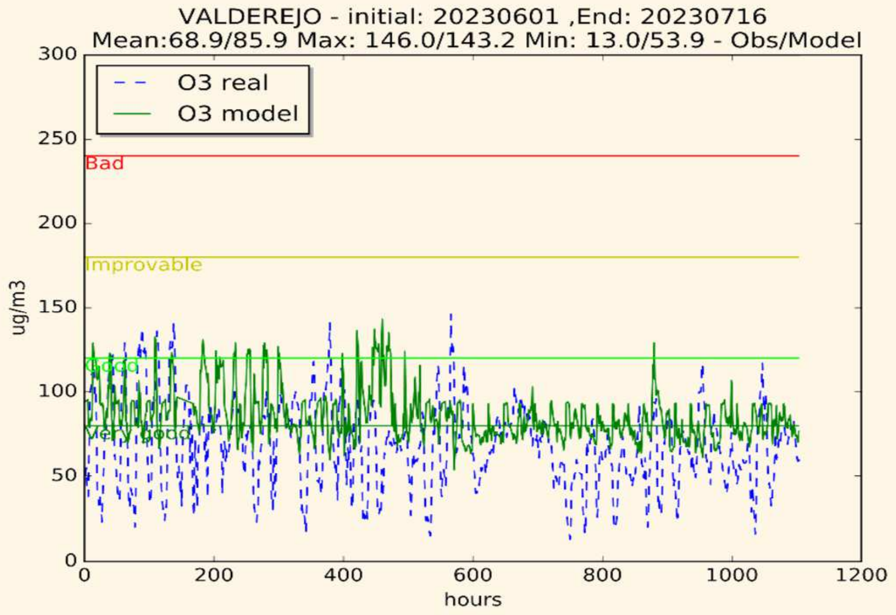
CHIMERE

WRF-CHEM



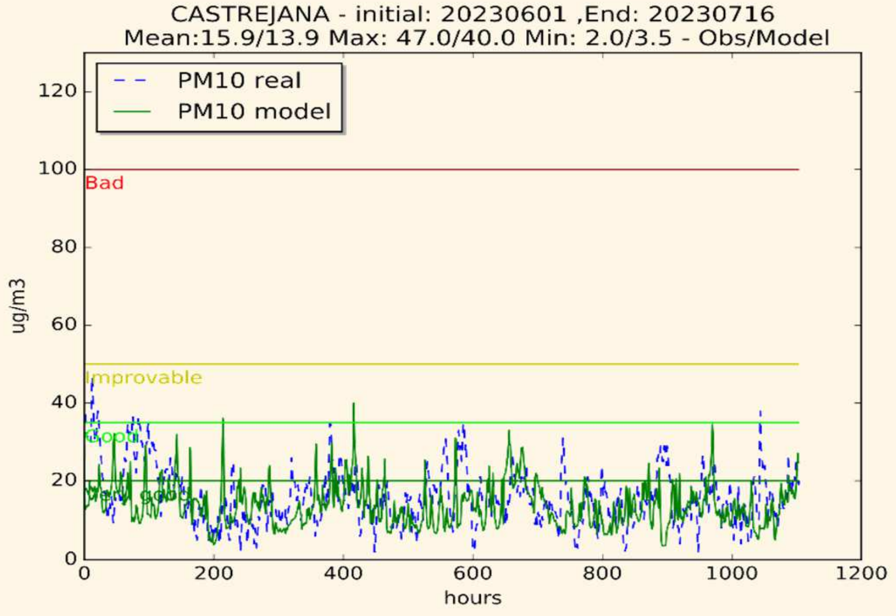


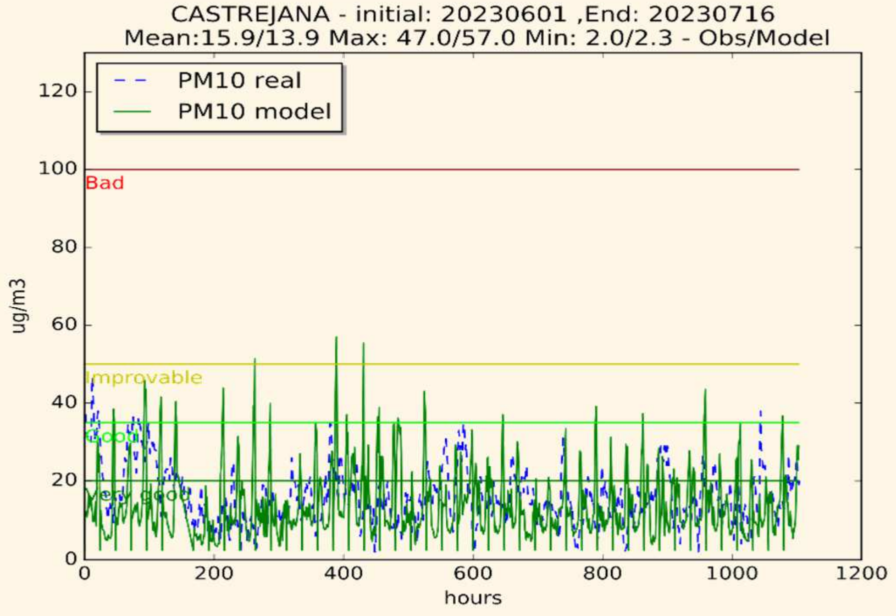


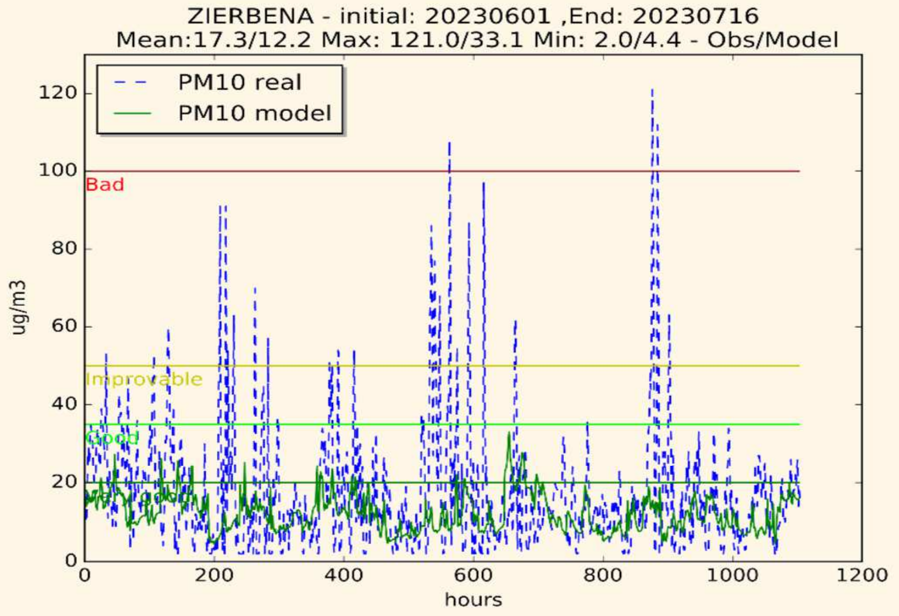


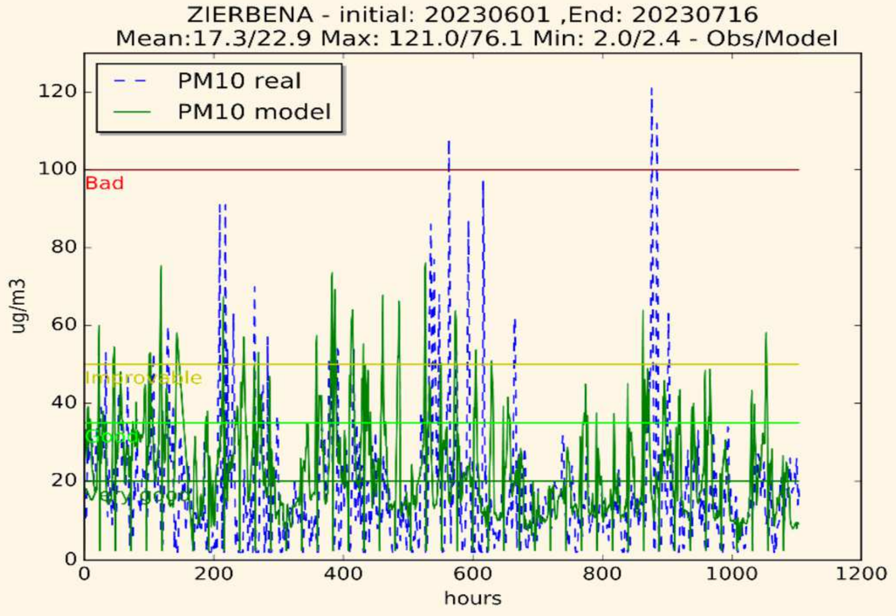
CHIMERE

WRF-CHEM









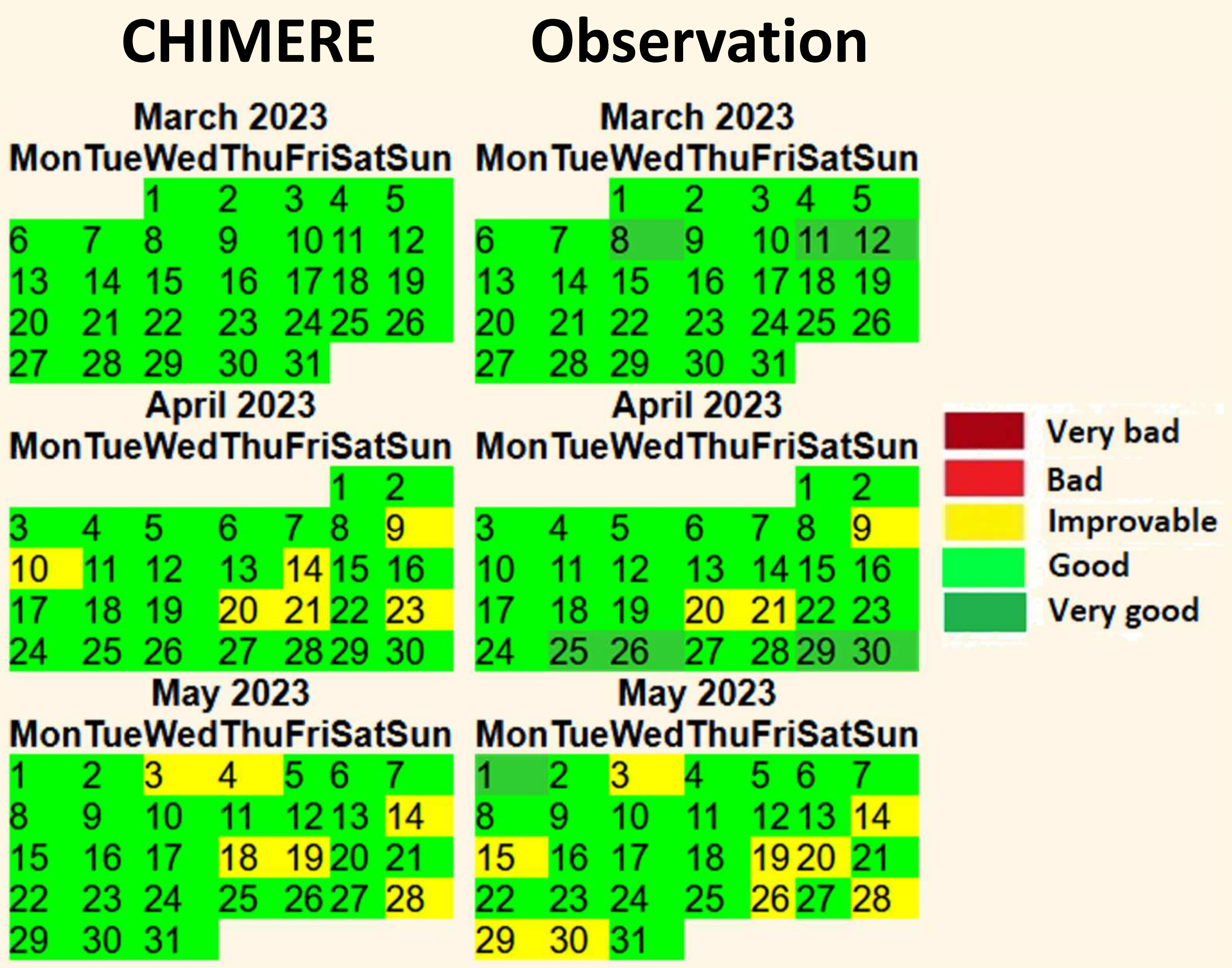
4. Validations (1/4)

- Validation has been set based on punctual forecasted-observed comparisons, per model, per pollutant, per categorical forecast accordingly with air quality thresholds.
- We include different metrics: Proportion Correct (PC) , Probability Of Detection (POD), False Alarm Ratio (FAR), Frequency Bias Index (BIAS), Critical Success Index (CSI) and Heidke Skill Score (HSS)
- Several contingency tables are prepared in order to compare different events in each category.

A change from one category to another is considered to occur when at least once a day the pollutant concentration value exceeds one of the levels marked by the following table.

Air quality	SO2 (µg/m3)	NO2 (µg/m3)	CO (mg/m3)	O3 (µg/m3)	PM10 (µg/m3)	PM2.5 (µg/m3)
Very good	0-100	0-40	0-5	0-80	0-20	0-10
Good	101-200	41-100	5-7	81-120	21-35	11-20
Moderate	201-350	101-200	7-10	121-180	36-50	21-25
Bad	351-500	201-400	10-20	181-240	51-100	26-50
Very bad	501-1250	401-1000	20-30	241-600	101-1200	51-800

Example of maximum daily concentration calendar for the Jaizkibel station (1 January to 25 July 2023)



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4. Validations (2/4)

(**Examples** for 1 January to 25 July 2023)

O3

ELCIEGO CHIMERE

	POD	FAR	BIAS	CSI
Very good	0.55	0.72	1.95	0.23
Good	0.79	0.13	0.9	0.71
Moderate	0.1	0.8	0.5	0.07
Bad				
Very bad				

PC=0.73
HSS=0.2

ELCIEGO WRF-CHEM

	POD	FAR	BIAS	CSI
Very good		1		0
Good	0.72	0.16	0.85	0.63
Moderate	0	1	0.2	0
Bad				
Very bad				

PC=0.63
HSS=-0.09

VALDEREJO CHIMERE

	POD	FAR	BIAS	CSI
Very good	0.2	0.92	2.5	0.06
Good	0.78	0.11	0.88	0.71
Moderate	0.59	0.52	1.23	0.36
Bad				
Very bad				

PC=0.73
HSS=0.25

VALDEREJO WRF-CHEM

	POD	FAR	BIAS	CSI
Very good		1		
Good	0.76	0.1	0.84	0.7
Moderate	0.25	0.78	1.13	0.13
Bad				
Very bad				

PC=0.70
HSS=-0.08

PM10

ZIERBANA CHIMERE

	POD	FAR	BIAS	CSI
Very good	0.32	0.16	0.38	0.3
Good	0.37	0.7	1.21	0.2
Moderate	0	1	22	0
Bad		1		
Very bad		1		

PC=0.33
HSS=0.06

ZIERBANA WRF-CHEM

	POD	FAR	BIAS	CSI
Very good	0.65	0.79	3.12	0.19
Good	0.36	0.71	1.25	0.19
Moderate	0.28	0.61	0.72	0.10
Bad	0.29	0.33	0.44	0.25
Very bad				

PC=0.34
HSS=0.13

CASTREJANA CHIMERE

	POD	FAR	BIAS	CSI
Very good	0.44	0.38	0.71	0.35
Good	0.43	0.64	1.2	0.24
Moderate	0	1	3.14	0
Bad	0	1	1.67	0
Very bad				

PC=0.42
HSS=0.01

CASTREJANA WRF-CHEM

	POD	FAR	BIAS	CSI
Very good	0.59	0.8	3	0.17
Good	0.48	0.41	0.82	0.36
Moderate	0.12	0.74	0.46	0.09
Bad	0	1	0.45	0
Very bad				

PC=0.38
HSS=0.06

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4. Validations (3/4)

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(**Examples** for 1 January to 25 July 2023)

NO_2

SANTURCE CHIMERE

	POD	FAR	BIAS	CSI
Very good	0.66	0.26	0.89	0.54
Good	0.58	0.56	1.3	0.33
Moderate	0		0	0
Bad				
Very bad				

PC=0.61
HSS=0.21

SANTURCE WRF-CHEM

	POD	FAR	BIAS	CSI
Very good	0.57	0	0.57	0.57
Good		1		0
Moderate				
Bad				
Very bad				

PC=0.57
HSS=-0.0

MUSKIZ CHIMERE

	POD	FAR	BIAS	CSI
Very good	0.95	0.35	1.46	0.63
Good	0.05	0.67	0.15	0.04
Moderate	0		0	0
Bad				
Very bad				

PC=0.64
HSS=0.0

MUSKIZ WRF-CHEM

	POD	FAR	BIAS	CSI
Very good	0.96	0.96	0	0.97
Good		1		0
Moderate				
Bad				
Very bad				

PC=0.96
HSS=-0.0

PM2.5

EUROPA WRF-CHEM

	POD	FAR	BIAS	CSI
Very good	0.25	0.86	1.79	0.1
Good	0.5	0.47	0.94	0.34
Moderate	0.14	0.78	0.63	0.09
Bad	0.31	0.71	1.08	0.17
Very bad		1		

PC=0.36
HSS=0.04

MUNDAKA WRF-CHEM

	POD	FAR	BIAS	CSI
Very good	0.43	0.89	3.86	0.1
Good	0.56	0.68	1.76	0.25
Moderate	0.12	0.79	0.55	0.08
Bad	0.32	0.28	0.44	0.28
Very bad		1		

PC=0.34
HSS=0.1

SO_2

ABANTO WRF-CHEM

	POD	FAR	BIAS	CSI
Very good	1	0	1	1
Good				
Moderate				
Bad				
Very bad				

PC=1

CO

ALGORTA CHIMERE

	POD	FAR	BIAS	CSI
Very good	1	0	1	1
Good				
Moderate				
Bad				
Very bad				

PC=1

4. Validations (4/4)

Preliminary results:

- In the case of particulate material better results are found with the WRF-CHEM model that the CHIMERE model.
- In general, the forecasted ozone concentrations are higher with CHIMERE model that with the WRF-CHEM model, in both cases lows concentrations are not well forecasted.
- In the case of nitrogen oxides both models are not able to forecast the maximum concentrations.

5. Conclusions and future work

Conclusions

- ✓ An air quality forecasting system has been implemented for Basque Country. Based on CHIMERE and WRF-CHEM proving that operational air quality local forecast based on community models and public data is a plausible task.
- ✓ The WRF-CHIMERE and WRF-CHEM models were configured and validated to simulate concentrations of main pollutants (CO, NO2, PM10, PM2.5, O3 and SO2) including global and local datasets of emissions.
- ✓ The present work represents a first step in the use of numerical models for atmospheric chemistry simulations in Euskalmet.

5. Conclusions and future work

Future work

- ➢ A better and more complete representation of local emission sources (temporal evolution, emissions ratios, …) are going to be introduced in order to improve results, particularly discrepancies observed in the hourly trends of modelled pollutants.
- ➢ A dedicated intranet is going to be implemented in order to full exploitation of results from the multi-model air quality system.
- ➢ Further work is needed in order to obtain a full operational system (four executions daily, improve final products usefulness, blending , resolution, bias correction, etc …)
- ➢ New strategies based on AI and ML approach are planned exploiting air quality and weather available data at different spatial and temporal resolutions.

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WRF — WRF-Chem — python — Chimere

Thank you for your attention : QUESTIONS ?