



**Barcelona
Supercomputing
Center**
Centro Nacional de Supercomputación



EXCELENCIA
SEVERO
OCHOA

Adaptación de inventarios para modelización de la calidad del aire

M. Guevara, Tena, C., Jorba, O., Pérez García-Pando, C.

13/06/2019

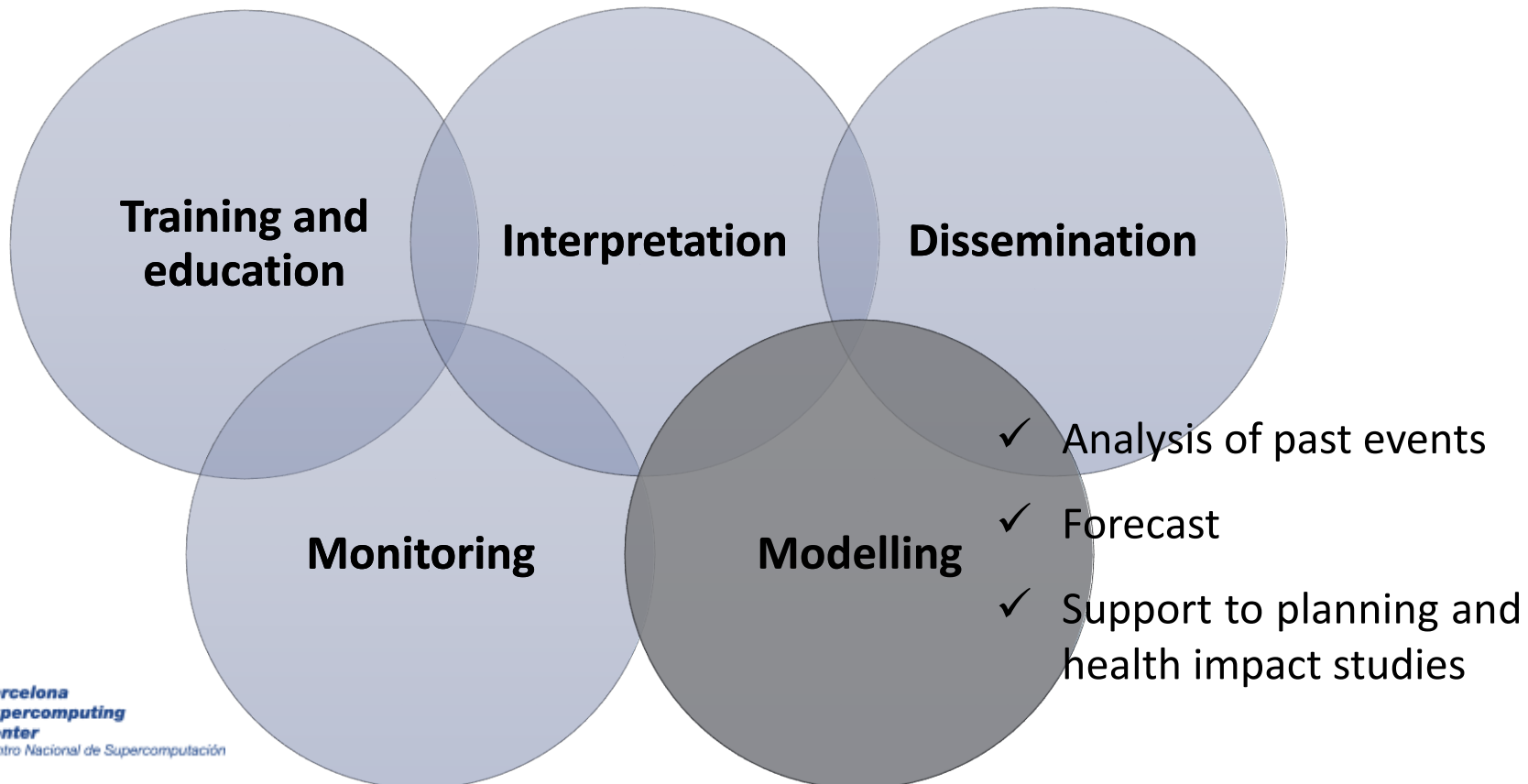
Foro tecnológico. Bases científico técnicas para la mejora de la calidad del aire en España. Valencia, 11-13 Junio 2019

Five steps to improve air-quality forecasts

A worldwide monitoring and modelling network would reduce the dramatic toll of air pollution on health and food production, urge Rajesh Kumar and colleagues.

<https://www.nature.com/articles/d41586-018-06150-5>

Rajesh Kumar , Vincent-Henri Peuch, James H. Crawford & Guy Brasseur

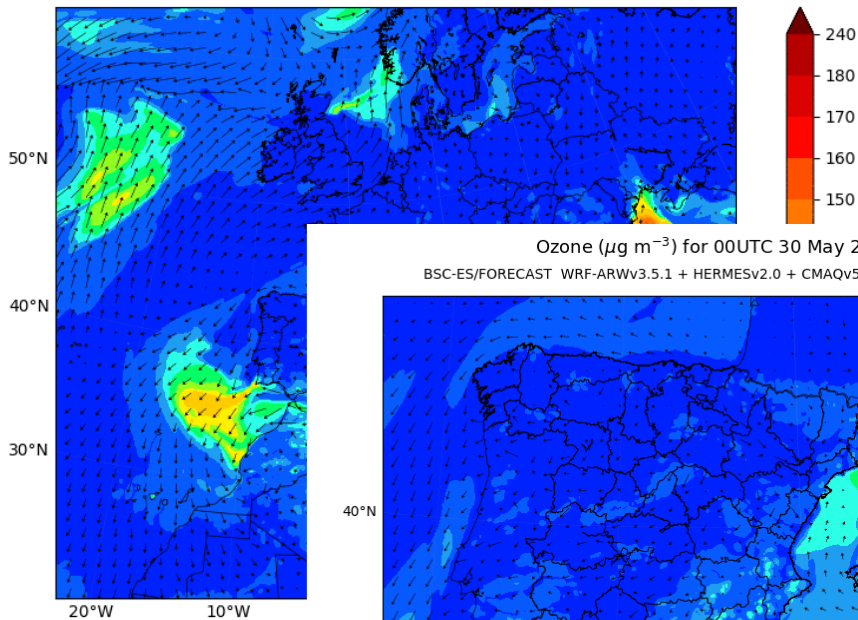


CALIOPE air quality system

Provides air quality information for the coming days and for the application of short term action plans for air quality managers.

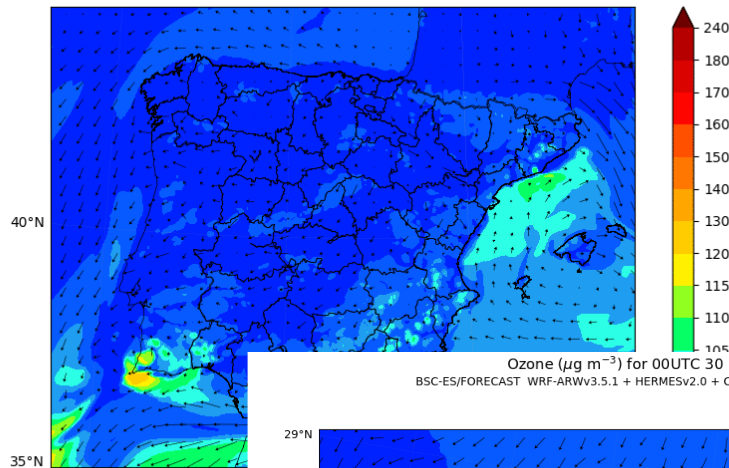
Ozone ($\mu\text{g m}^{-3}$) for 00UTC 30 May 2019

BSC-ES/FORECAST WRF-ARWv3.5.1 + HERMESv2.0 + CMAQv5.0.2 - Resolution: 12x12



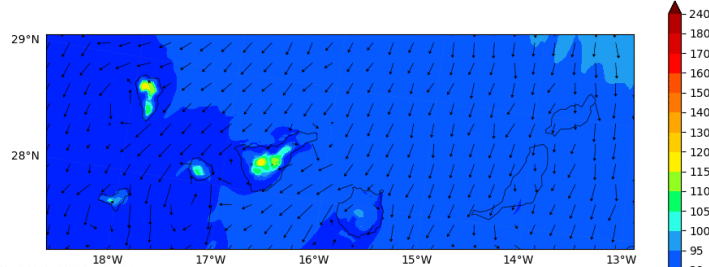
Ozone ($\mu\text{g m}^{-3}$) for 00UTC 30 May 2019

BSC-ES/FORECAST WRF-ARWv3.5.1 + HERMESv2.0 + CMAQv5.0.2 - Resolution: 4x4



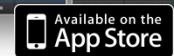
Ozone ($\mu\text{g m}^{-3}$) for 00UTC 30 May 2019

BSC-ES/FORECAST WRF-ARWv3.5.1 + HERMESv2.0 + CMAQv5.0.2 - Resolution: 2x2



Information is delivered using both online or custom applications:

www.bsc.es/caliope

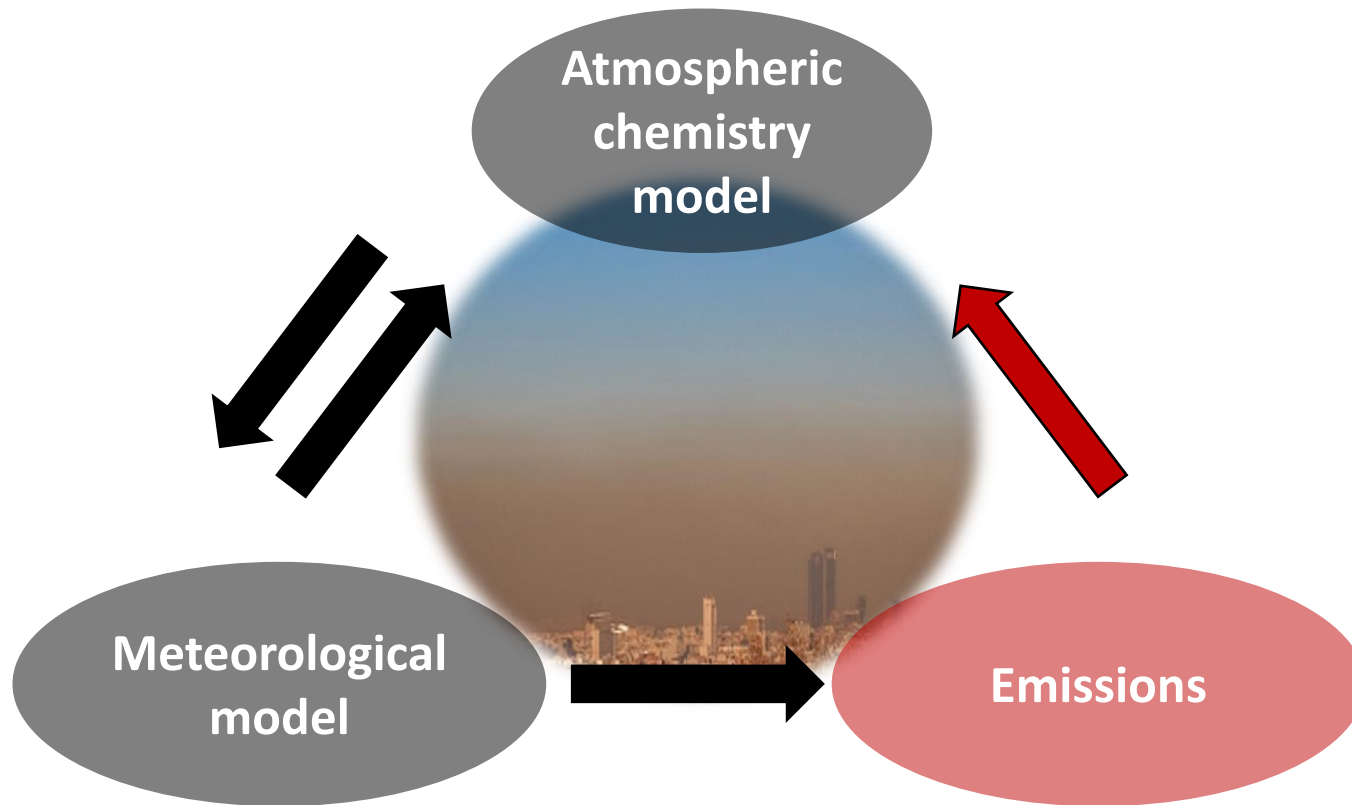


Smart city platform



20 ms^{-1}

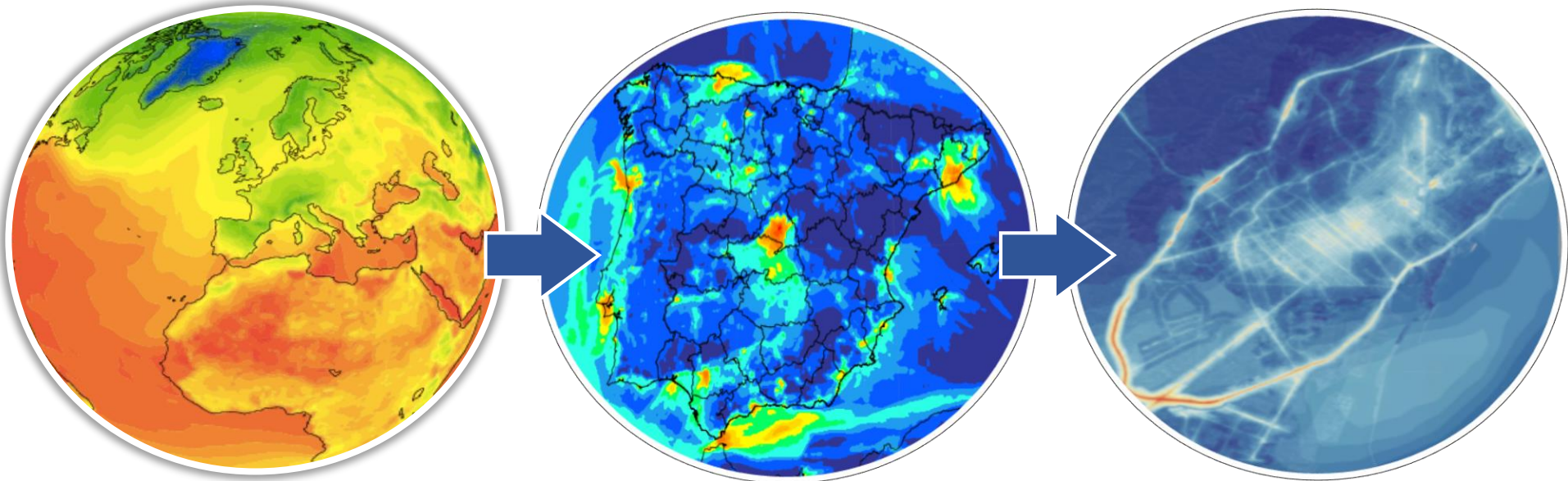
Air quality modelling chain



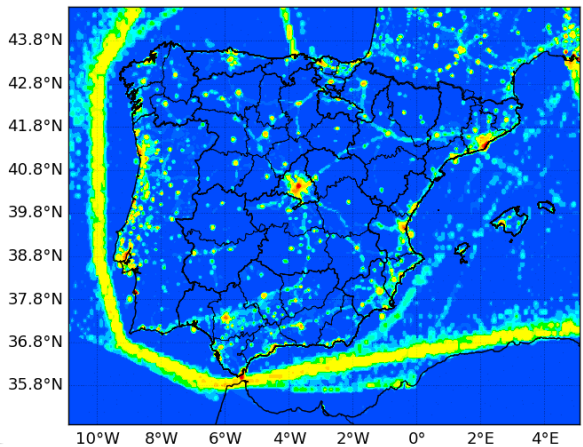
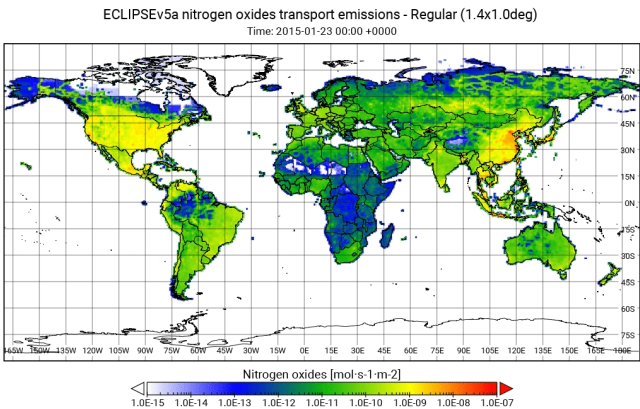
Emissions requirements:

- Spatially distributed over a gridded domain
- Temporally resolved with (typically) an hourly resolution
- Mapped to the species defined in the atmospheric chemistry model (e.g. VOC, NO_x)

From global to local scales

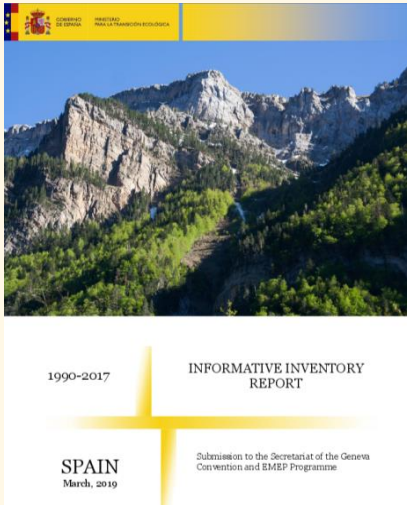


EMISSIONS: DIFFERENT NEEDS FOR DIFFERENT SCALES

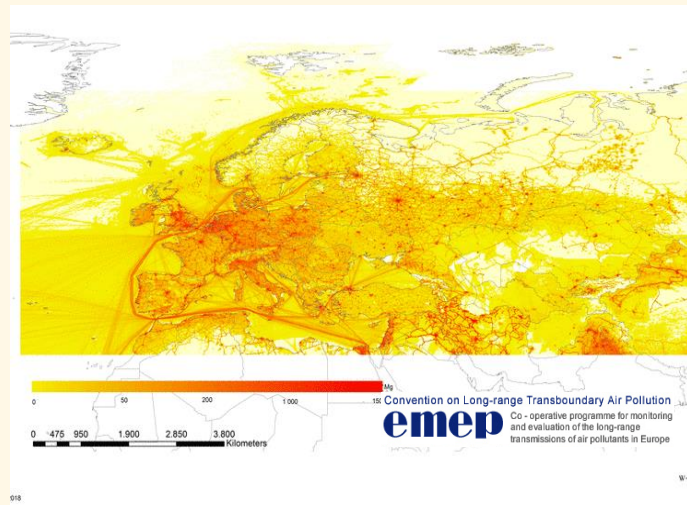


Emission inputs

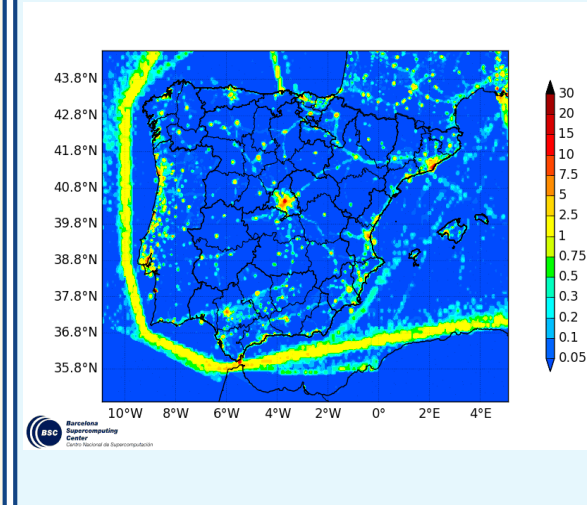
National emission inventories



Gridded emission inventories



Modelled emissions



X Not gridded (total national)

✓ Gridded (fixed grid)

X Not hourly (annual)

X Not hourly (annual, monthly)

X Not speciated

X Not speciated

✓ Gridded (any grid)

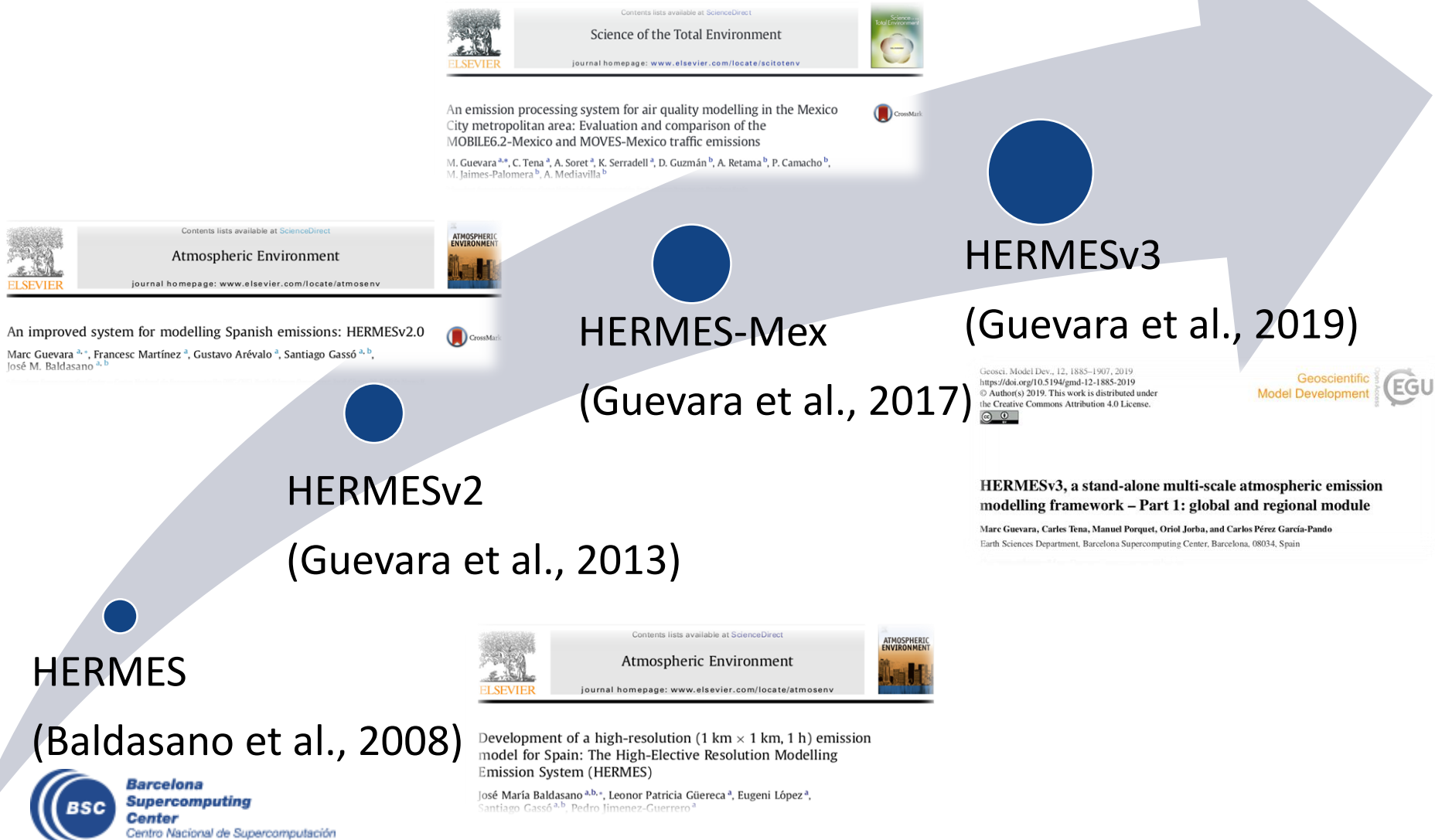
✓ Hourly

✓ Speciated

**Emission processing systems:
Adapt the emission data to the
air quality model's requirement**

**Emission models:
Combine activity and
emission factors to estimate
hourly, gridded emissions**

HERMES: The high-Elective Resolution Modelling Emissions System



Contents lists available at ScienceDirect
Science of the Total Environment
journal homepage: www.elsevier.com/locate/scitotenv

An emission processing system for air quality modelling in the Mexico City metropolitan area: Evaluation and comparison of the MOBILE6.2-Mexico and MOVES-Mexico traffic emissions

M. Guevara^{a,*}, C. Tena^a, A. Soret^a, K. Serradell^a, D. Guzmán^b, A. Retama^b, P. Camacho^b, M. Jaimes-Palomera^b, A. Mediavilla^b



Contents lists available at ScienceDirect
Atmospheric Environment
journal homepage: www.elsevier.com/locate/atmosenv

An improved system for modelling Spanish emissions: HERMESv2.0

Marc Guevara^{a,*}, Francesc Martínez^a, Gustavo Arévalo^a, Santiago Gassó^{a,b}, José M. Baldasano^{a,b}



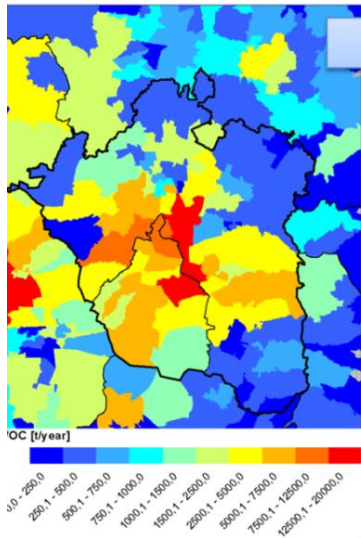
Contents lists available at ScienceDirect
Atmospheric Environment
journal homepage: www.elsevier.com/locate/atmosenv

Development of a high-resolution (1 km × 1 km, 1 h) emission model for Spain: The High-Elective Resolution Modelling Emission System (HERMES)

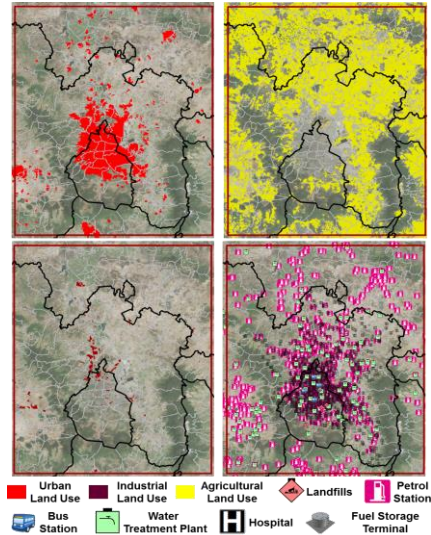
José María Baldasano^{a,b,*}, Leonor Patricia Güereca^a, Eugeni López^a, Santiago Gassó^{a,b}, Pedro Jimenez-Guerrero^a

HERMES-Mex: An emission processing tool for Mexico

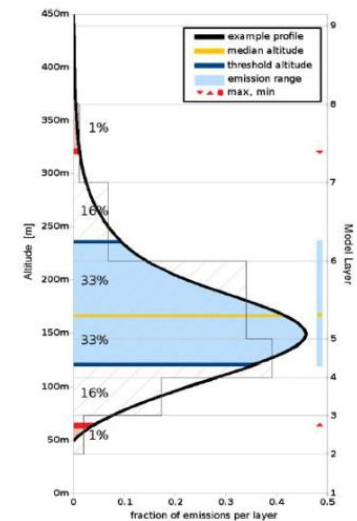
Official Emission Dataset



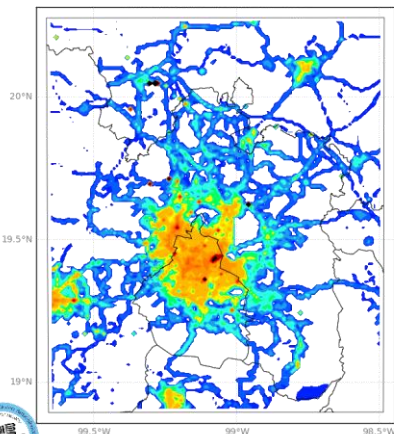
Spatial Allocation



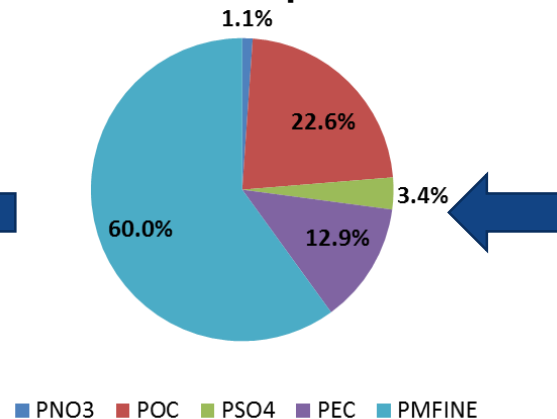
Vertical Allocation



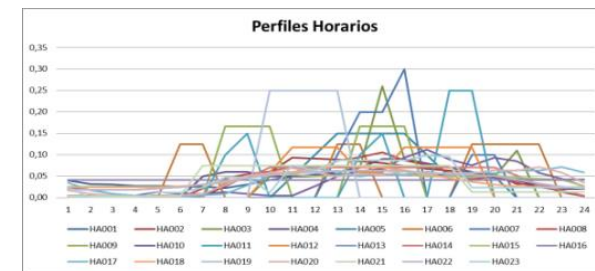
CMAQ ready emission data



Chemical Speciation

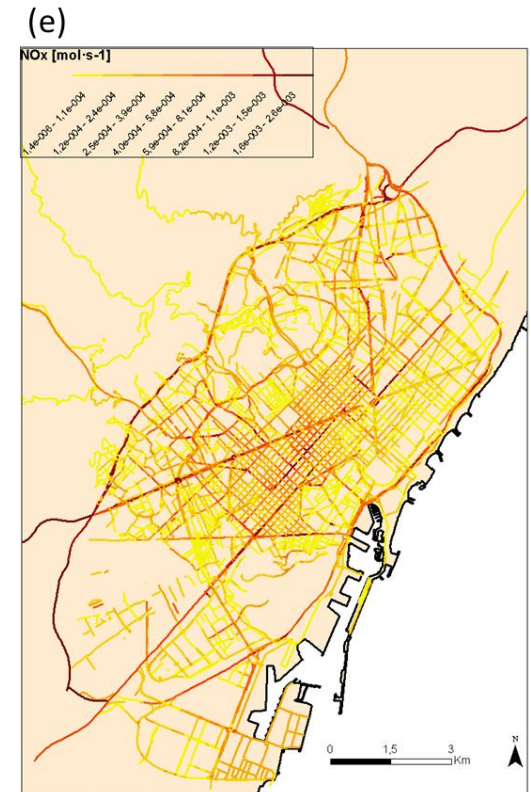
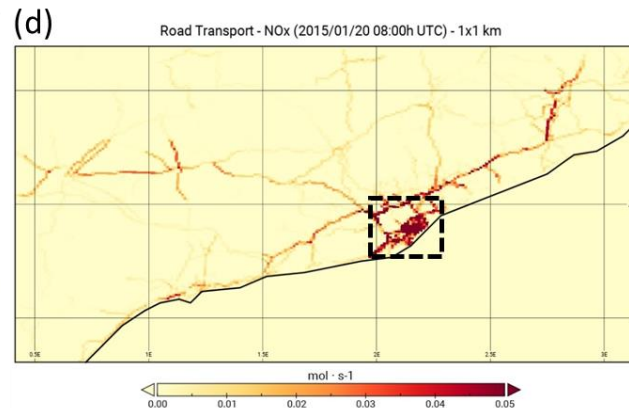
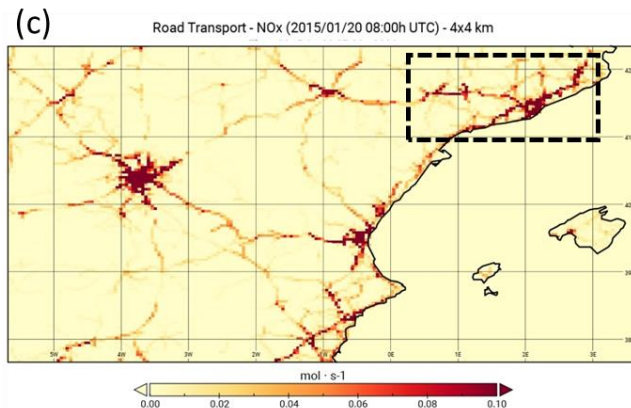
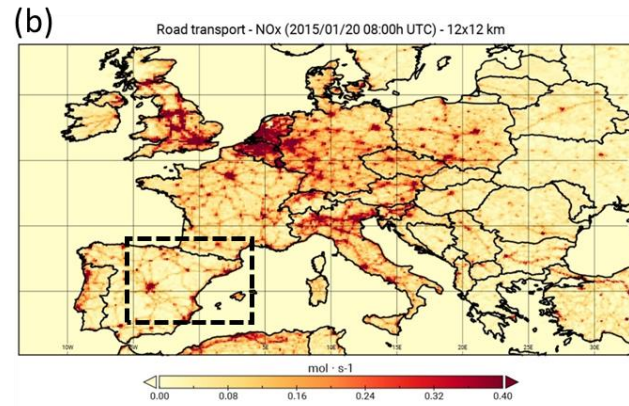
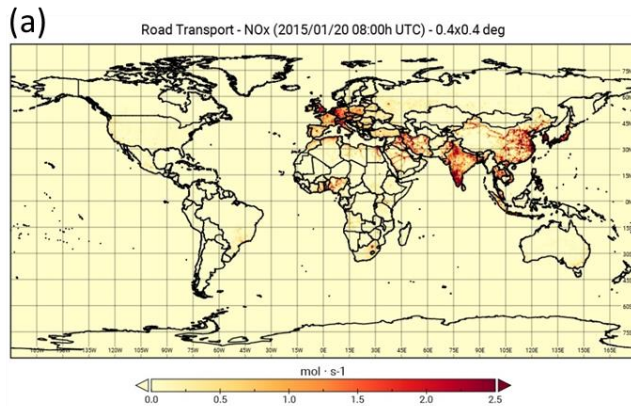


Temporal Allocation



HERMESv3

A **python-based, open source and multiscale** emission modelling framework that **processes and estimates gas and aerosol emissions** for use in atmospheric chemistry models.



HERMESv3

A **python-based, open source and multiscale** emission modelling framework that **processes and estimates gas and aerosol emissions** for use in atmospheric chemistry models.



global-regional module
(HERMESv3_GR)

A **processing system** to calculate emissions through an automatic **combination of existing inventories** and user defined vertical, temporal and speciation profiles

Guevara et al. (2019a, GMD)

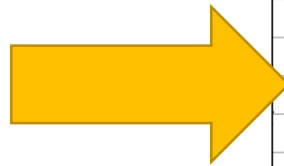
bottom-up module
(HERMESv3_BU)

An **emission model** to estimate emissions at the source level (e.g. road link) combining state-of-the-art **bottom-up methods** with **local activity and emission factors**

Guevara et al. (2019b, in preparation)

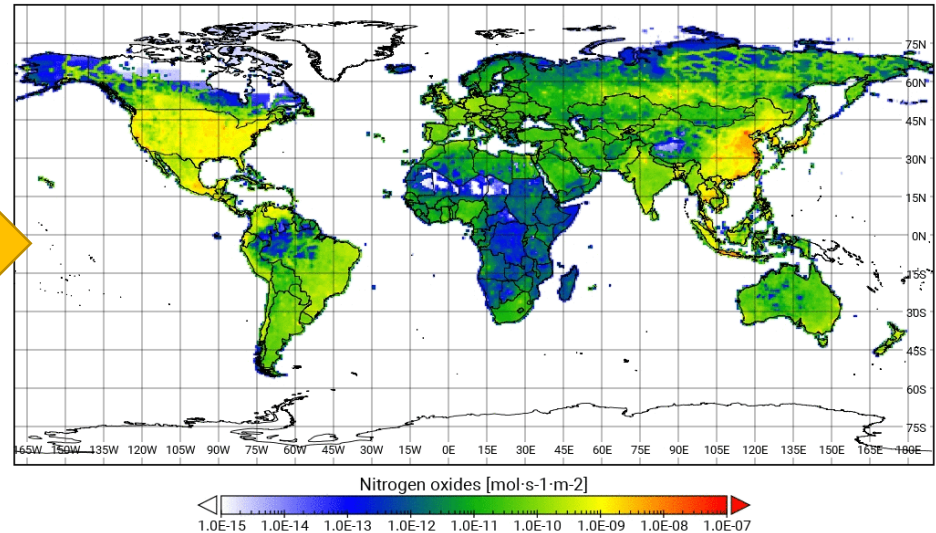
HERMESv3_GR: global-regional module

Emission data library



HERMESv3_GR output

ECLIPSEv5a nitrogen oxides transport emissions - Regular (1.4x1.0deg)
Time: 2015-01-23 00:00 +0000

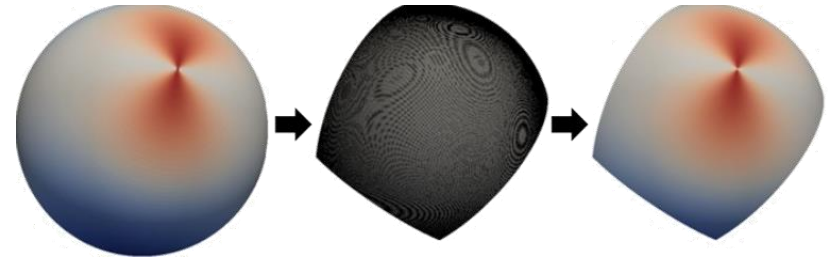


- Combination of multiple up-to-date gridded emission inventories
- User defined destination working domain (multiple projections)
- Application of country-specific scaling and masking factors
- Temporal profiles per sector and pollutant
- Speciation profiles for multiple chemical mechanisms (CB05, RADM2, AERO5, AERO6)
- Outputs for multiple atmospheric chemistry models (CMAQ, WRF-Chem, MONARCH)
- Available at the BSC git repository: https://earth.bsc.es/gitlab/es/hermesv3_gr

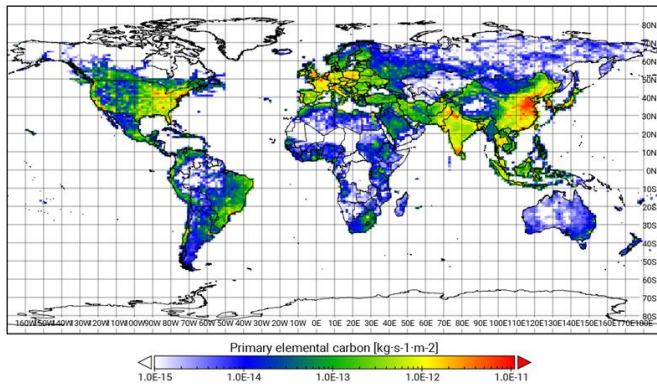
HERMESv3_GR: Spatial remapping

User defined destination working domain:

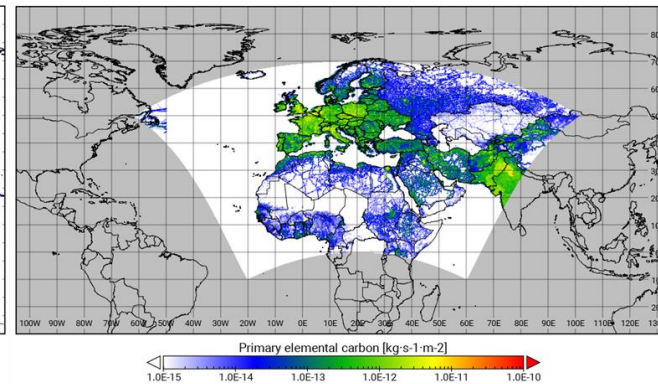
- Conservative remapping (ESMF)
- Multiple spatial resolutions
- Multiple projections: regular lat-lon, rotated lat-lon, mercator, lambert conformal conic



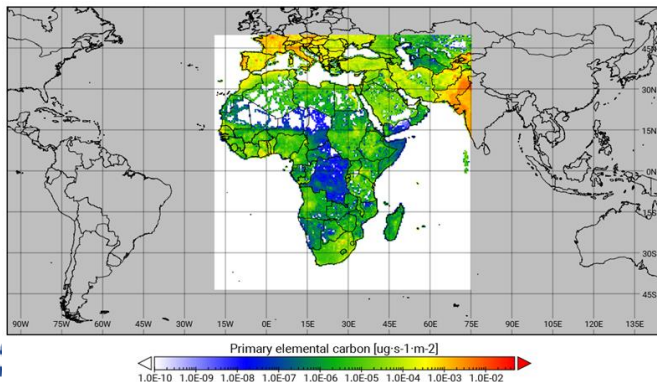
Regular lat-lon
(1.4*1.0 deg)



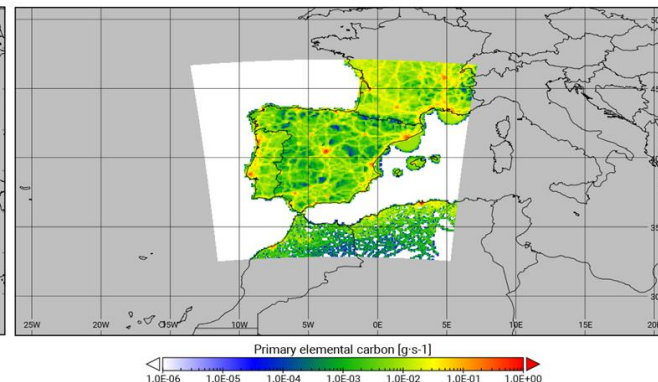
Rotated lat-lon
(0.1*0.1 deg)



Mercator
(50kmx50km)



Lambert conformal conic
(4kmx4km)

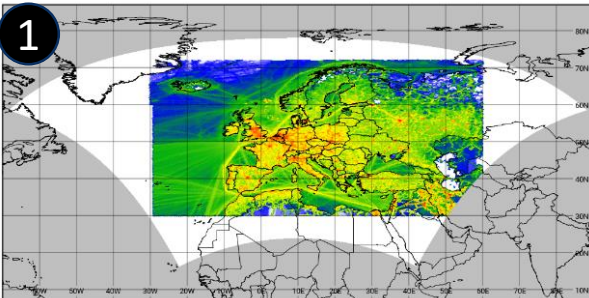


HERMESv3_GR: Designing your experiment

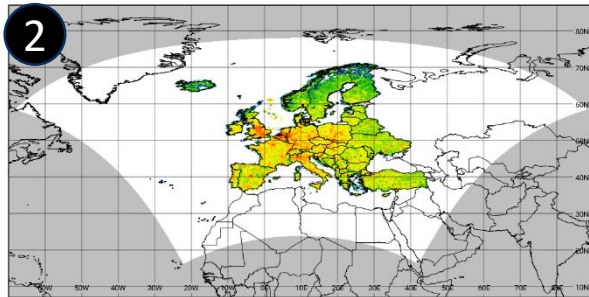
- Combination of multiple emission inventories
- Application of country-specific scaling factors/masks



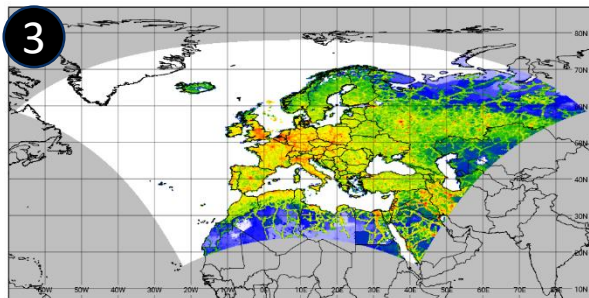
NO2 hourly emissions - 2015/01/01 08:00hUTC (0.2x0.2 deg)



NO2 hourly emissions - 2015/01/01 08:00hUTC (0.2x0.2 deg)

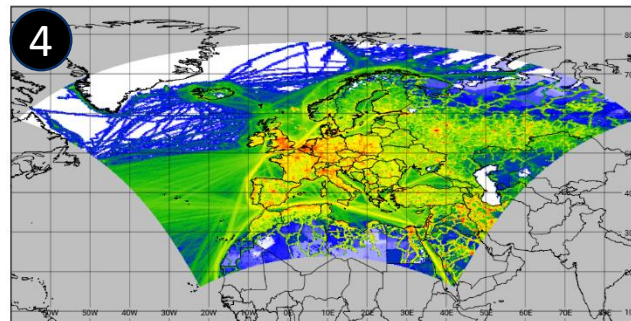


NO2 hourly emissions - 2015/01/01 08:00hUTC (0.2x0.2 deg)

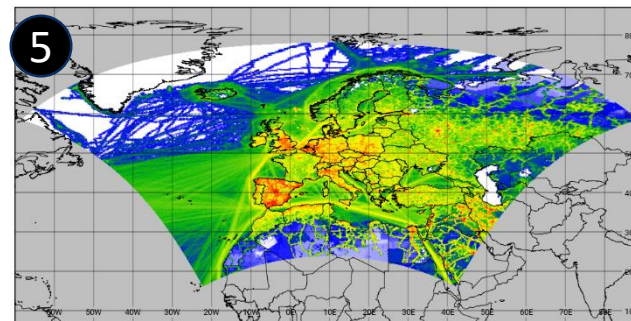


NO2 [mol·m⁻²·s⁻¹]
1.0E-15 1.0E-14 1.0E-13 1.0E-12 1.0E-11 1.0E-10 1.0E-09 1.0E-08

NO2 hourly emissions - 2015/01/01 08:00hUTC (0.2x0.2 deg)



NO2 hourly emissions - 2015/01/01 08:00h UTC (0.2x0.2 deg)



NO2 [mol·m⁻²·s⁻¹]
1.0E-15 1.0E-14 1.0E-13 1.0E-12 1.0E-11 1.0E-10 1.0E-09 1.0E-08

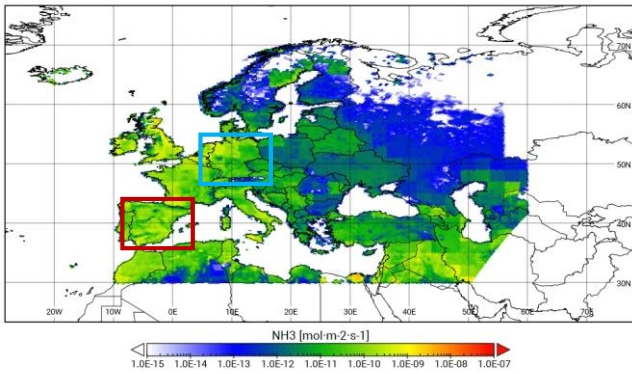
- 1 CAMS_REG_APv2.2.1
- 2 CAMS_REG_APv2.2.1 (EU)
- 3 CAMS_REG_APv2.2.1 (EU) + CAMS_GLOB_ANTv2.1 (rest)
- 4 CAMS_REG_APv2.2.1 (EU) + CAMS_GLOB_ANTv2.1 (rest) + CAMS_GLOB_SHIPv1.1
- 5 CAMS_REG_APv2.2.1 (ESP*10, FRA*0.1) + CAMS_GLOB_ANTv2.1 + CAMS_GLOB_SHIPv1.1

HERMESv3_GR: Temporal distribution

- Specific monthly, weekly and diurnal profiles per sector and pollutant
- Use of gridded profiles (variation not uniform across the space)

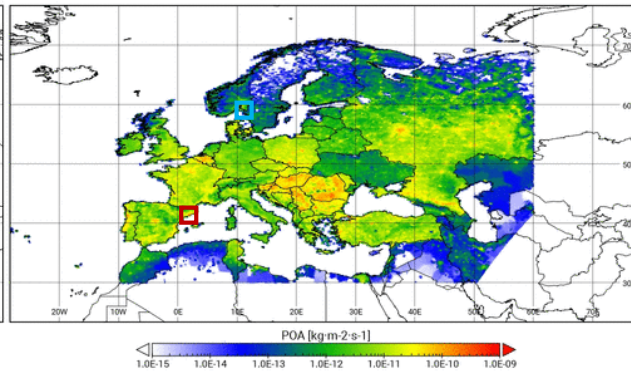
Monthly – NH₃ fertilizers

NH₃ fertilizer emissions (0.2x0.2 deg)
Time: 2015-01-01 00:00 +0000



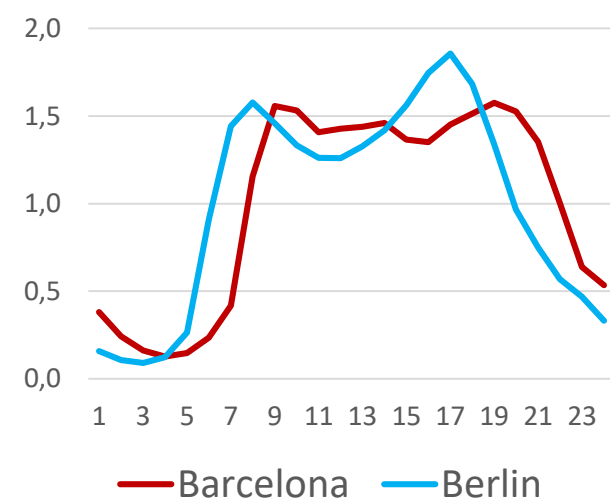
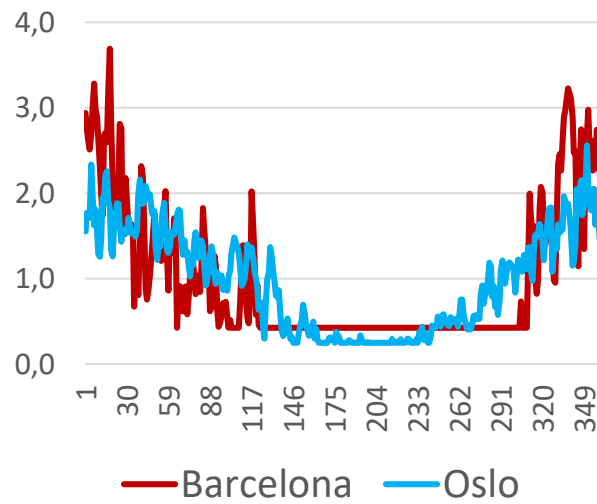
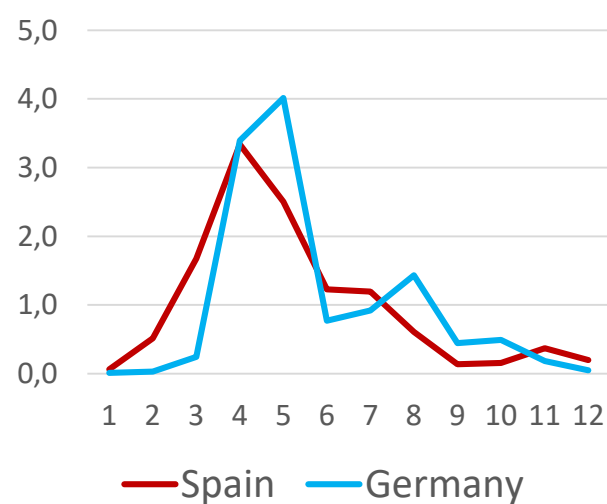
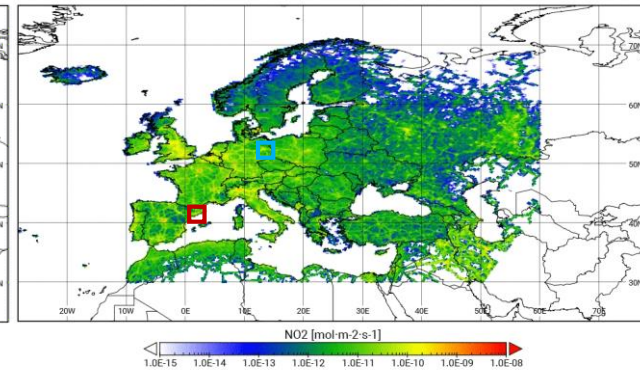
Daily – PM_{2.5} residential

POA Other Stationary Combustion emissions (0.2x0.2 deg)
Time: 2017-01-01 00:00 +0000

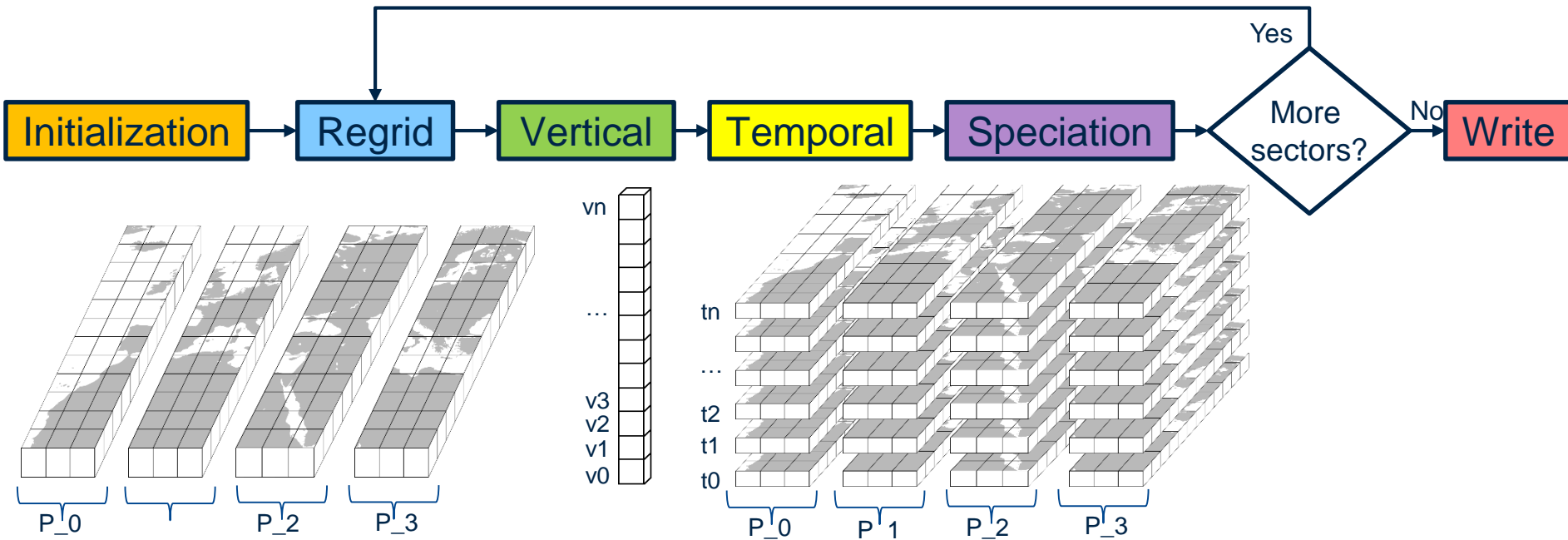


Hourly – NO₂ traffic

NO₂ Road Transport emissions (0.2x0.2 deg)
Time: 2015-01-07 00:00 +0000

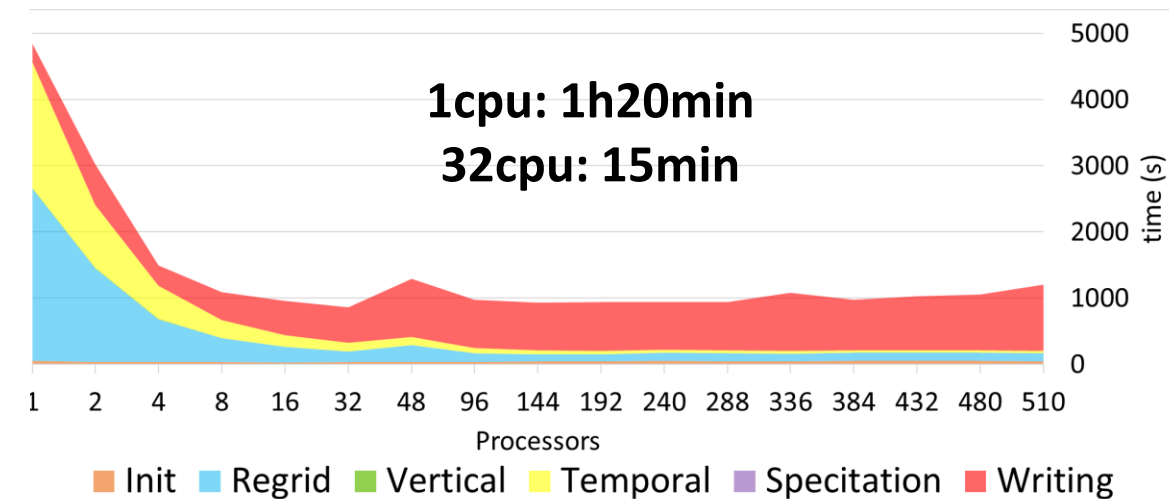


HERMESv3_GR: Technical Implementation



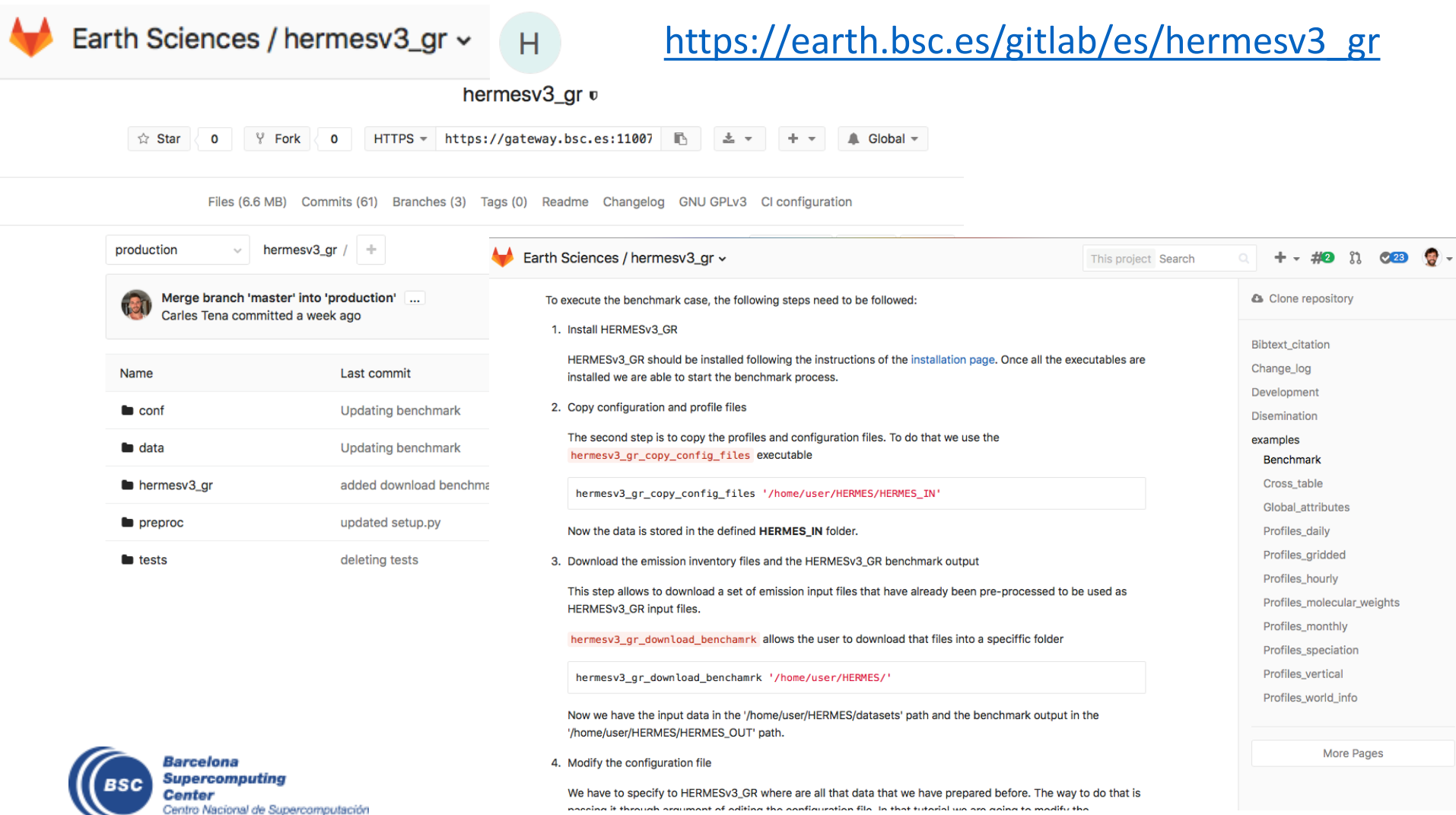
Test case:

- **Domain:** Europe-North Africa-Middle East (1021 x 721 cells)
- **Spatial resolution:** 0.1x0.1deg
- **Vertical resolution:** 48 layer
- **Emissions:** TNO_MACC-iii (EU) + HTAPv2 (others)
- 24-h simulation



HERMESv3_GR: Code Availability

HERMESv3_GR code, test case and user guide available at BSC gitlab repository



The screenshot shows the GitLab repository page for 'hermesv3_gr' under the 'Earth Sciences' organization. The page includes a navigation bar with the repository name, a search bar, and various icons for cloning and notifications. Below the navigation bar, there are statistics for stars (0), forks (0), and HTTPS links. The main content area is divided into three sections: a left sidebar with a file tree, a central main content area with instructions, and a right sidebar with a list of repository files.

Earth Sciences / hermesv3_gr

https://earth.bsc.es/gitlab/es/hermesv3_gr

hermesv3_gr

☆ Star 0 🍴 Fork 0 HTTPS https://gateway.bsc.es:11007

Files (6.6 MB) Commits (61) Branches (3) Tags (0) Readme Changelog GNU GPLv3 CI configuration

production hermesv3_gr /

Merge branch 'master' into 'production'
Carles Tena committed a week ago

Name	Last commit
conf	Updating benchmark
data	Updating benchmark
hermesv3_gr	added download benchm
preproc	updated setup.py
tests	deleting tests

Earth Sciences / hermesv3_gr

To execute the benchmark case, the following steps need to be followed:

1. Install HERMESv3_GR
HERMESv3_GR should be installed following the instructions of the [installation page](#). Once all the executables are installed we are able to start the benchmark process.
2. Copy configuration and profile files
The second step is to copy the profiles and configuration files. To do that we use the `hermesv3_gr_copy_config_files` executable

```
hermesv3_gr_copy_config_files '/home/user/HERMES/HERMES_IN'
```


Now the data is stored in the defined **HERMES_IN** folder.
3. Download the emission inventory files and the HERMESv3_GR benchmark output
This step allows to download a set of emission input files that have already been pre-processed to be used as HERMESv3_GR input files.
`hermesv3_gr_download_benchmark` allows the user to download that files into a specific folder


```
hermesv3_gr_download_benchmark '/home/user/HERMES/'
```


Now we have the input data in the `'/home/user/HERMES/datasets'` path and the benchmark output in the `'/home/user/HERMES/HERMES_OUT'` path.
4. Modify the configuration file
We have to specify to HERMESv3_GR where are all that data that we have prepared before. The way to do that is passing it through argument of editing the configuration file. In that tutorial we are going to modify the

Clone repository

Bibtex_citation
Change_log
Development
Disemination
examples
 Benchmark
 Cross_table
 Global_attributes
 Profiles_daily
 Profiles_gridded
 Profiles_hourly
 Profiles_molecular_weights
 Profiles_monthly
 Profiles_speciation
 Profiles_vertical
 Profiles_world_info

More Pages

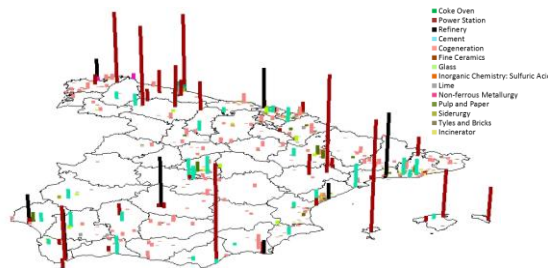


HERMESv3_BU: Bottom-up module



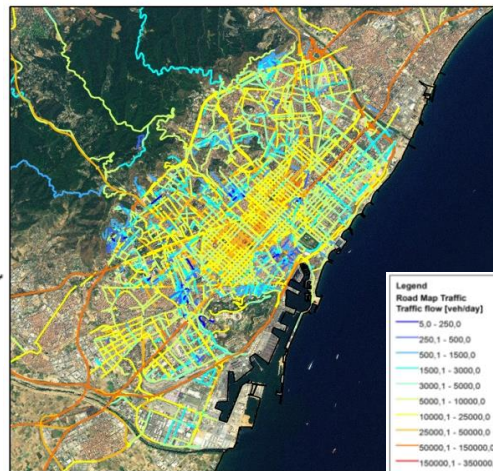
Point Source

P
●
 (x, y)



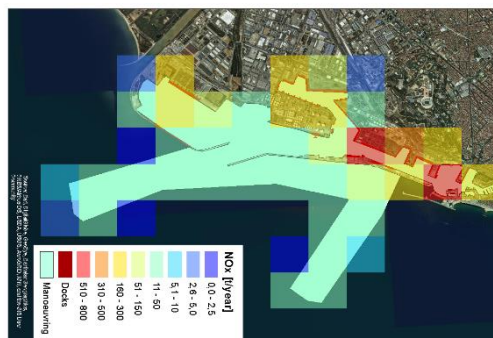
Line Source

S
 a
 $\{P_1, \dots, P_n\}$

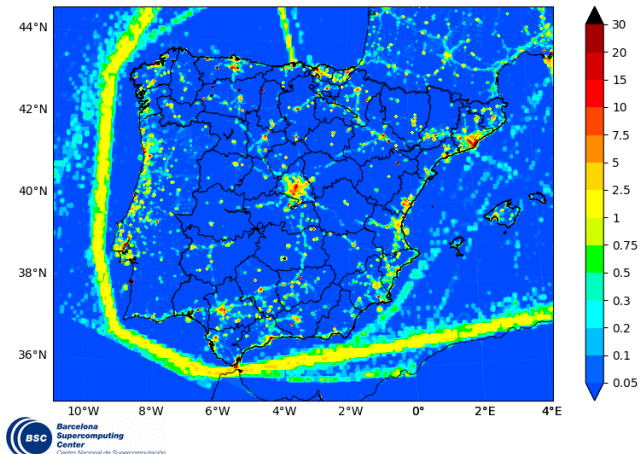


Area Source

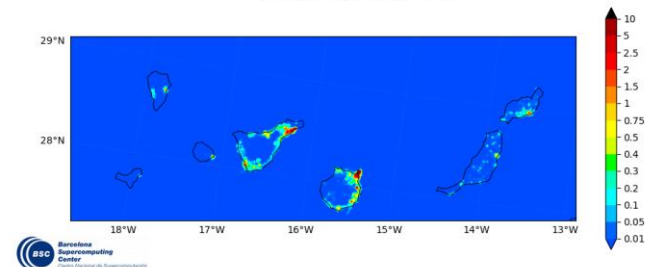
F
 A
 $\{S_1, \dots, S_n\}$



NO₂ Emissions (kg h⁻¹) for 00UTC 29 May 2019
BSC-ES/HERMESv2.0 - Resolution 4x4 km



NO₂ Emissions (kg h⁻¹) for 00UTC 29 May 2019
BSC-ES/HERMESv2.0 - Resolution 2x2 km



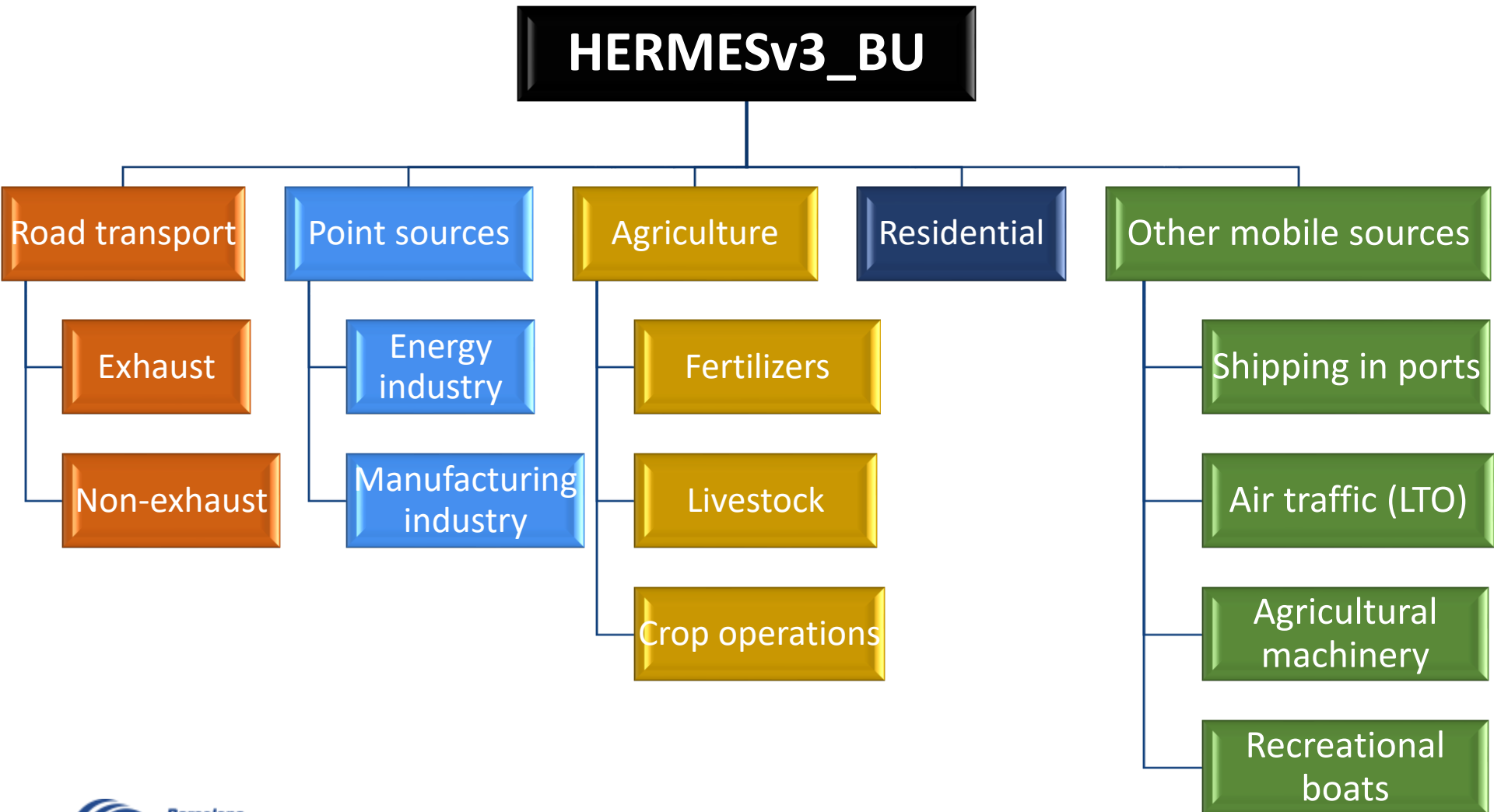
Criteria pollutants:

NO_x, CO, SO₂, NMVOC, NH₃,
PM₁₀, PM_{2.5}

Greenhouse gases:

CO₂, CH₄

HERMESv3_BU: Bottom-up module



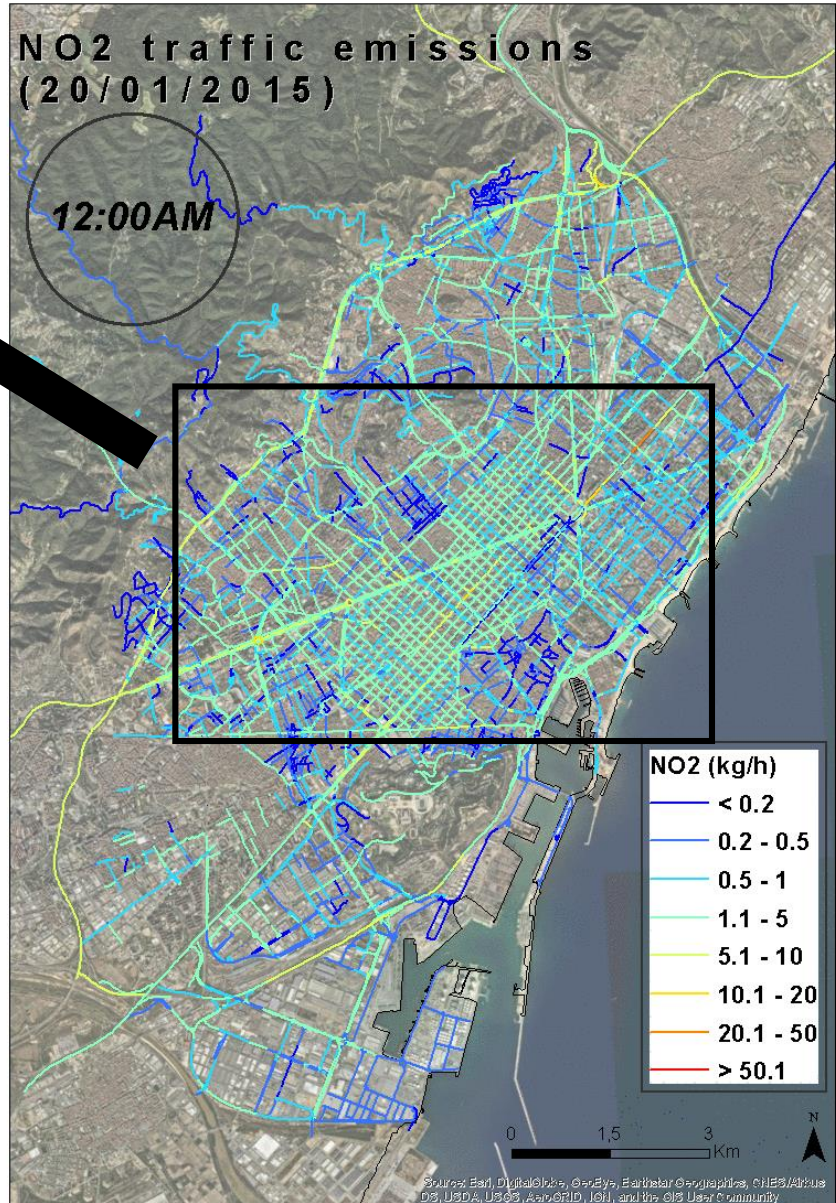
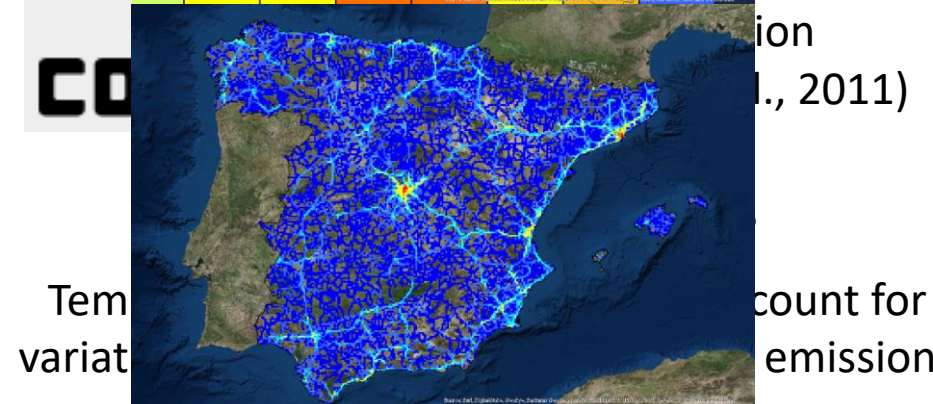
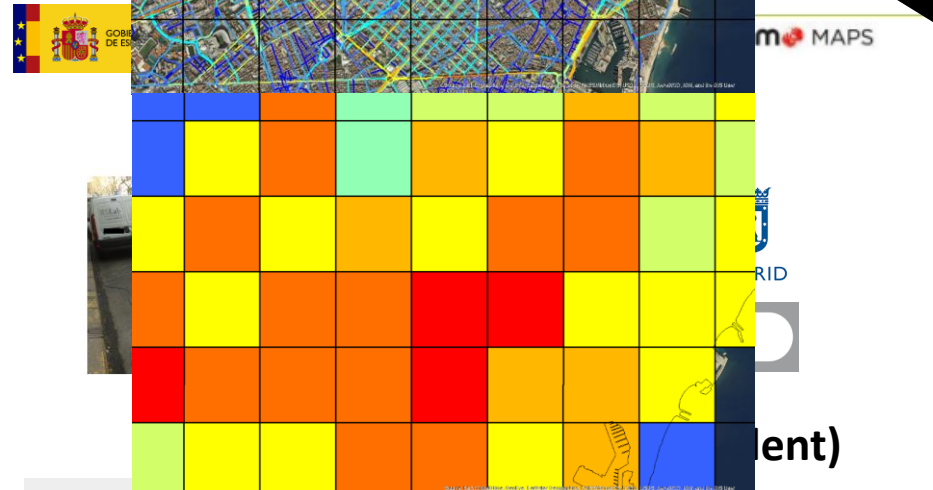
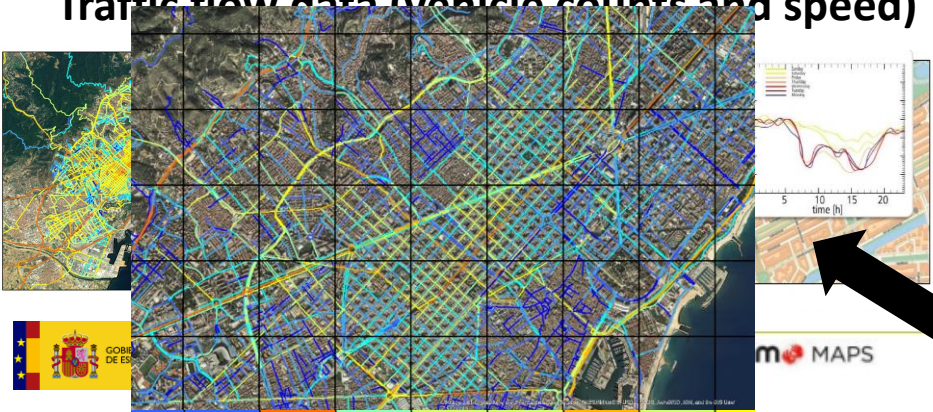
HERMESv3_BU: Input data

More than 75% of the time spent building up an emission inventory is devoted to compile and homogenise all the input data.
There is a need to centralise all this information.



HERMESv3_BU: Road transport

Traffic flow data (vehicle counts and speed)



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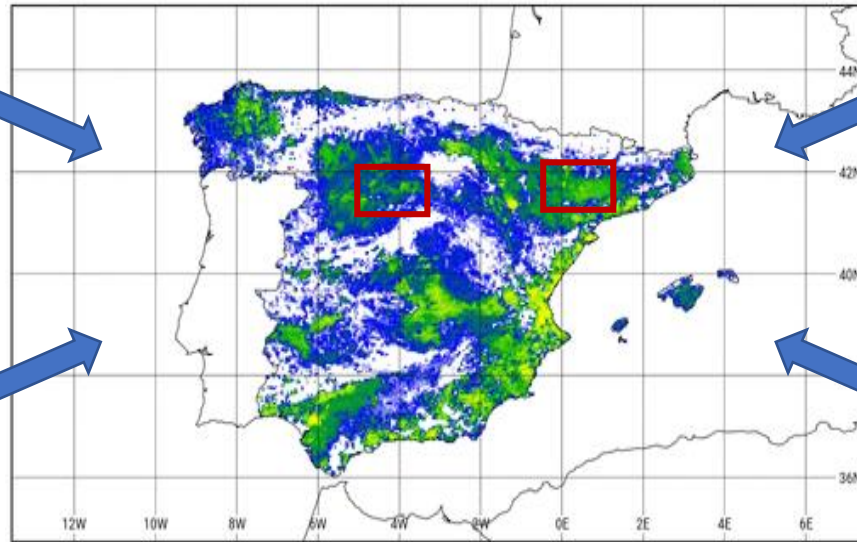
ent)
ion
(, 2011)
count for
emissions

HERMESv3_BU: Fertilizers



Daily NH3 emissions from fertilizers (Spain, 2016)

Time: 2016-01-01



General information

- Crop hectares
- Land uses

Cultural techniques

- N application rate
- Crop calendars
- Type of fertilizers
- Type of application

Meteorology

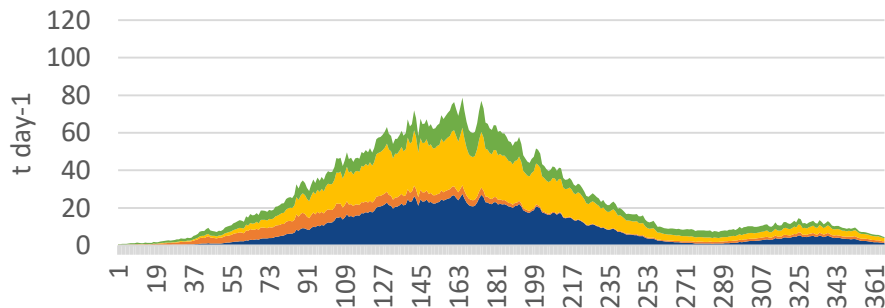
- Temperature
- Wind speed
- Growing Degree Days

Soil properties

- PH
- CEC

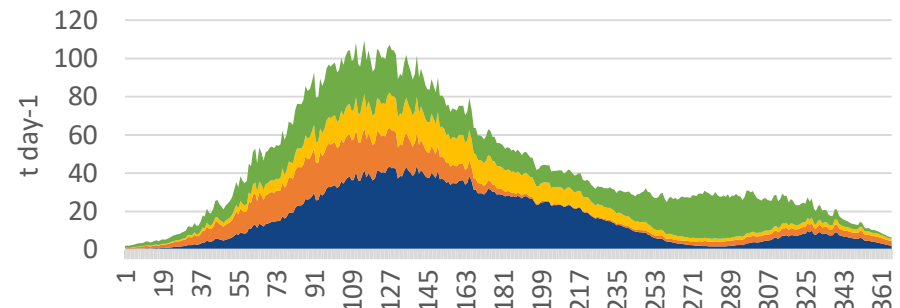


South of Castilla Leon



■ Barley ■ Maize ■ Wheat ■ Others

Lleida



■ Barley ■ Maize ■ Wheat ■ Others

HERMESv3_BU: Livestock



General information

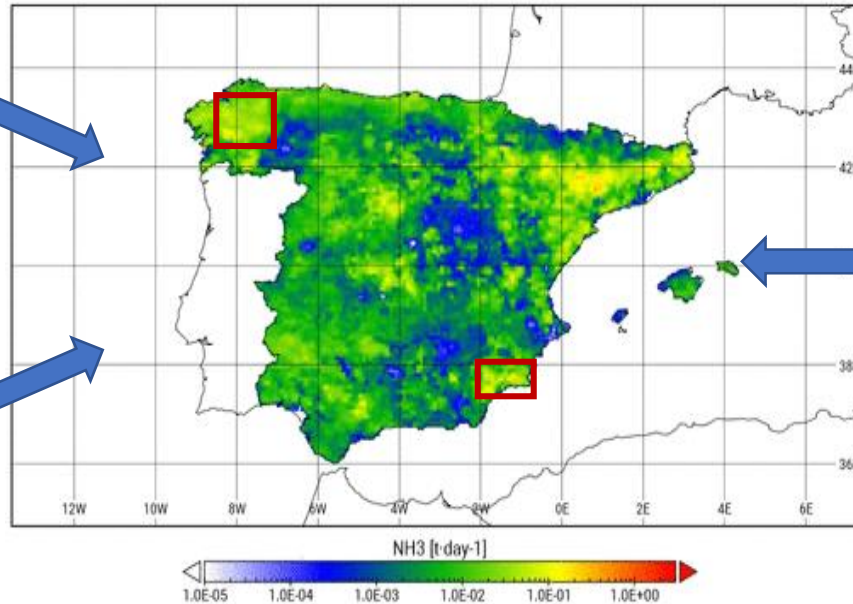
- Number of animals

Cultural techniques

- N excreta rate
- TAN
- Barn type
- Storage type

Daily NH₃ emissions from livestock (Spain, 2016)

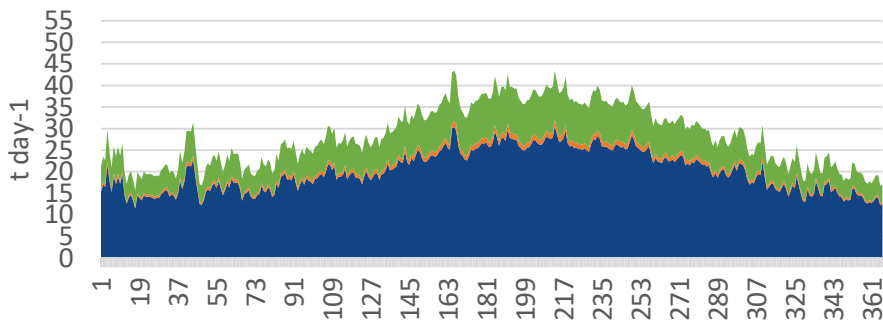
Time: 2016-01-01



Meteorology

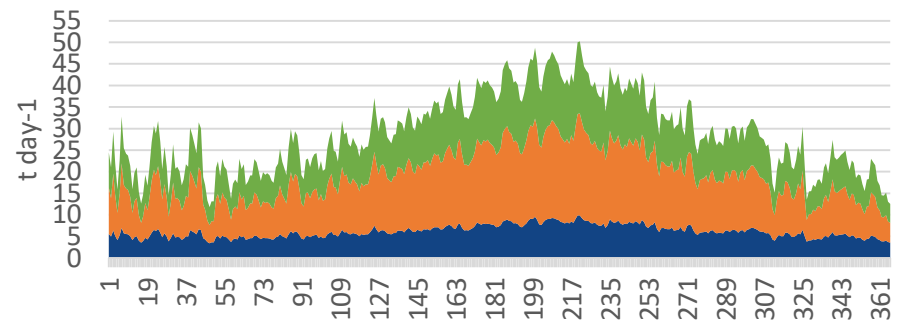
- Temperature
- Wind speed

Murcia



■ Pigs ■ Cattle ■ Others

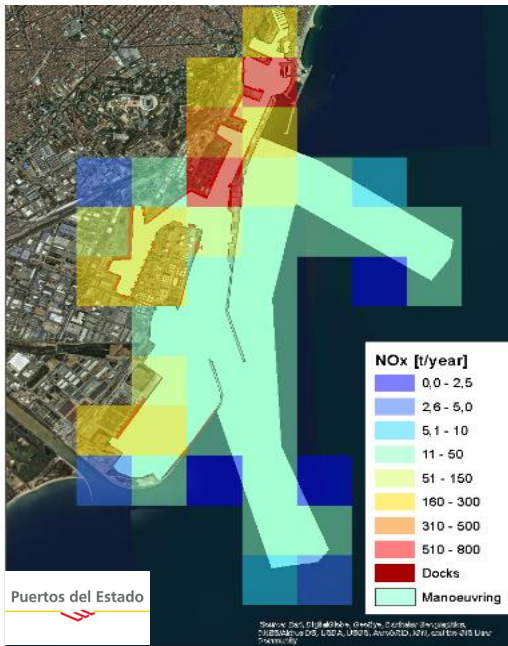
Galicia



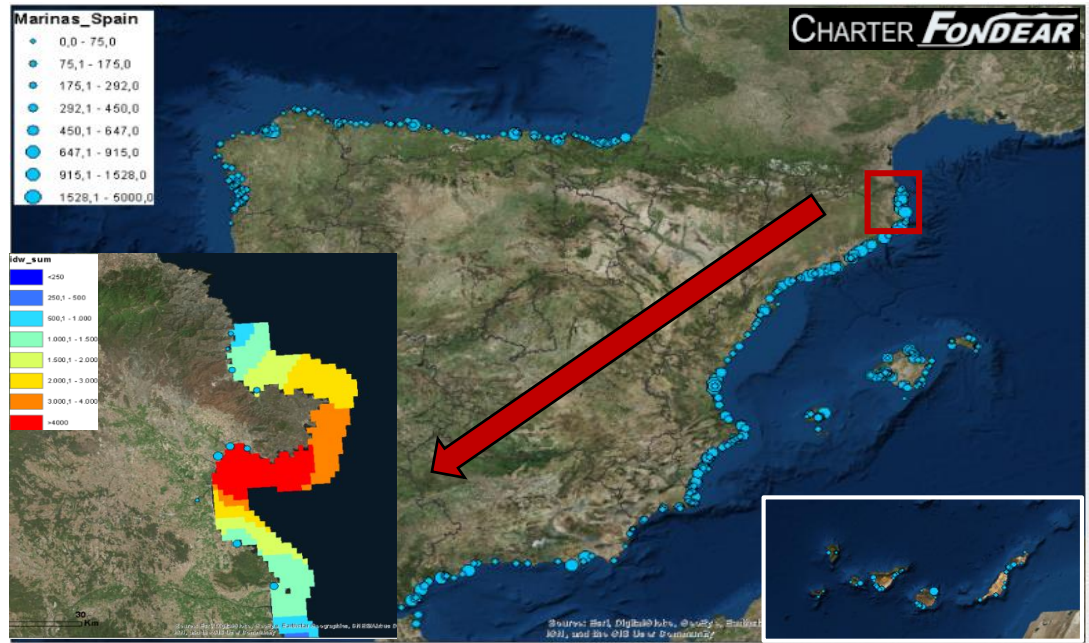
■ Pigs ■ Cattle ■ Others

HERMESv3_BU: Other mobile sources

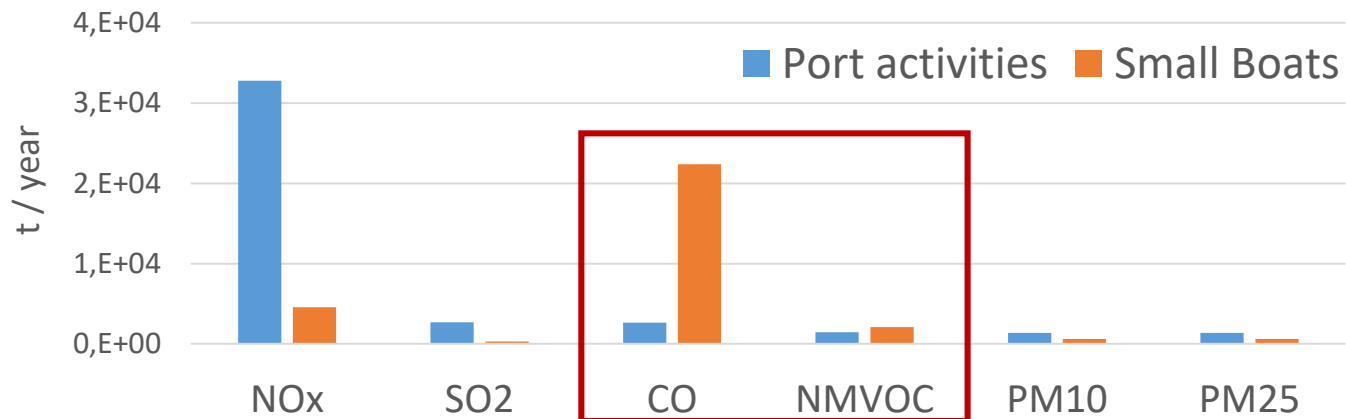
Shipping activities in ports



Recreational boats in marinas



Total annual emissions



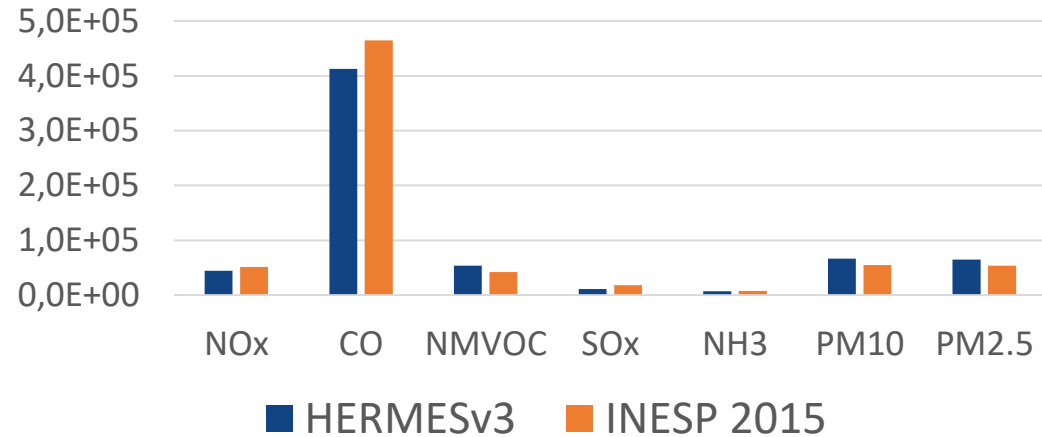
HERMESv3_BU: Inter-comparisons



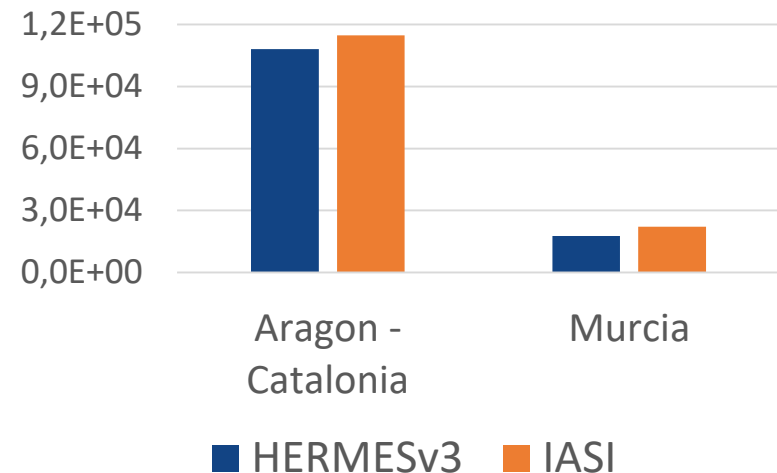
1990-2017
INFORMATIVE INVENTORY REPORT
SPAIN
March, 2019
Submission to the Secretariat of the Geneva Convention and EMEP Programme



Other stationary combustion [t/year]



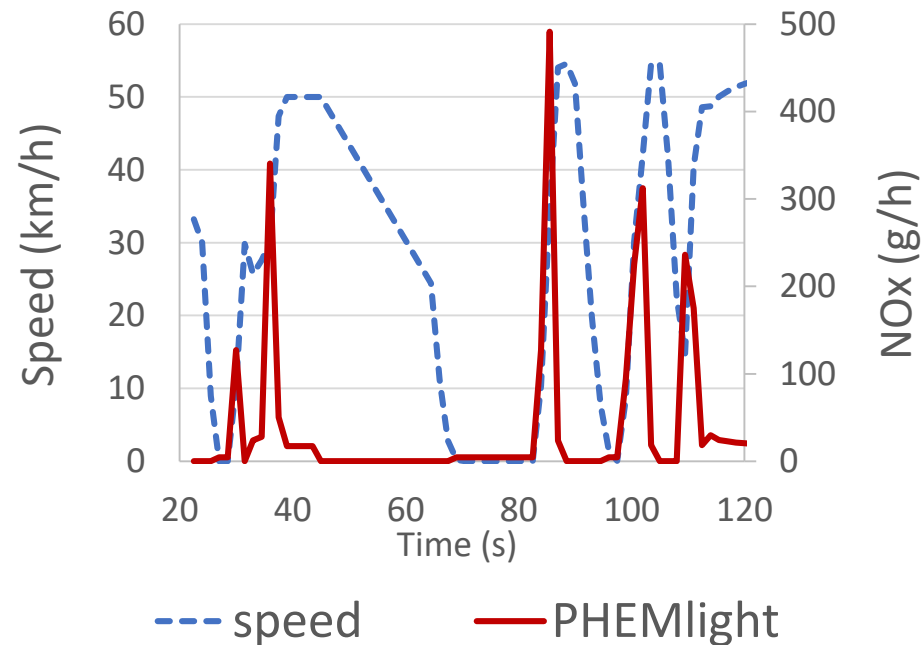
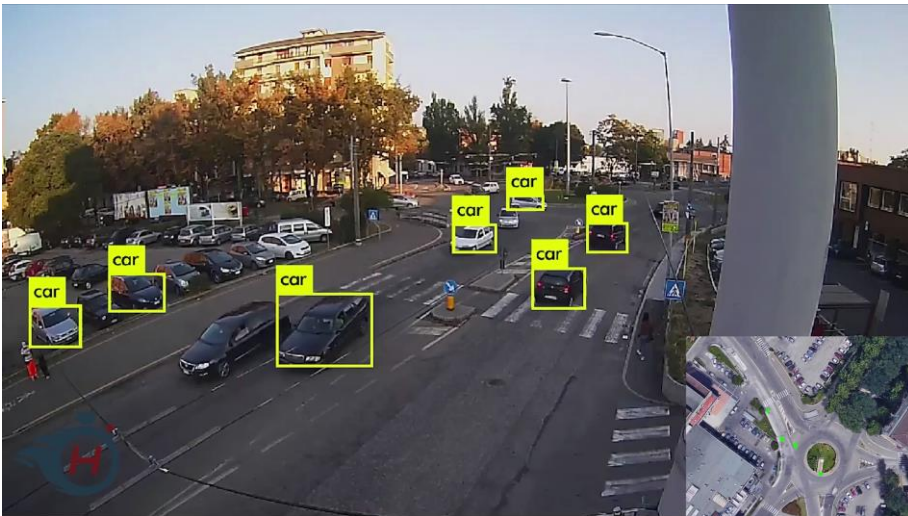
Total NH3 [t/year]



Van Damme et al. (2018, Nature)

Beyond the state-of-the-art

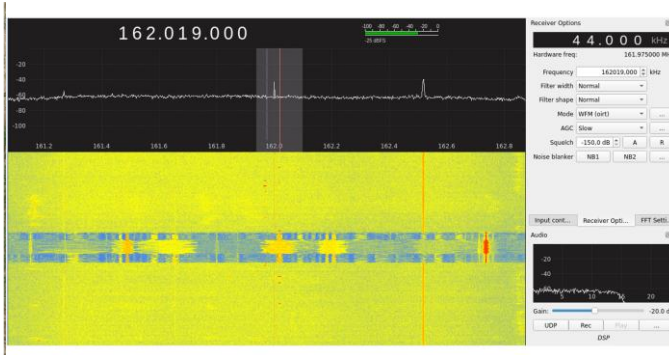
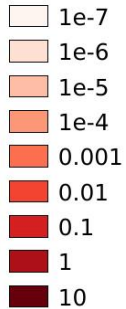
Use of **artificial intelligence** to combine high resolution **video-based traffic data** with **instantaneous emission models**



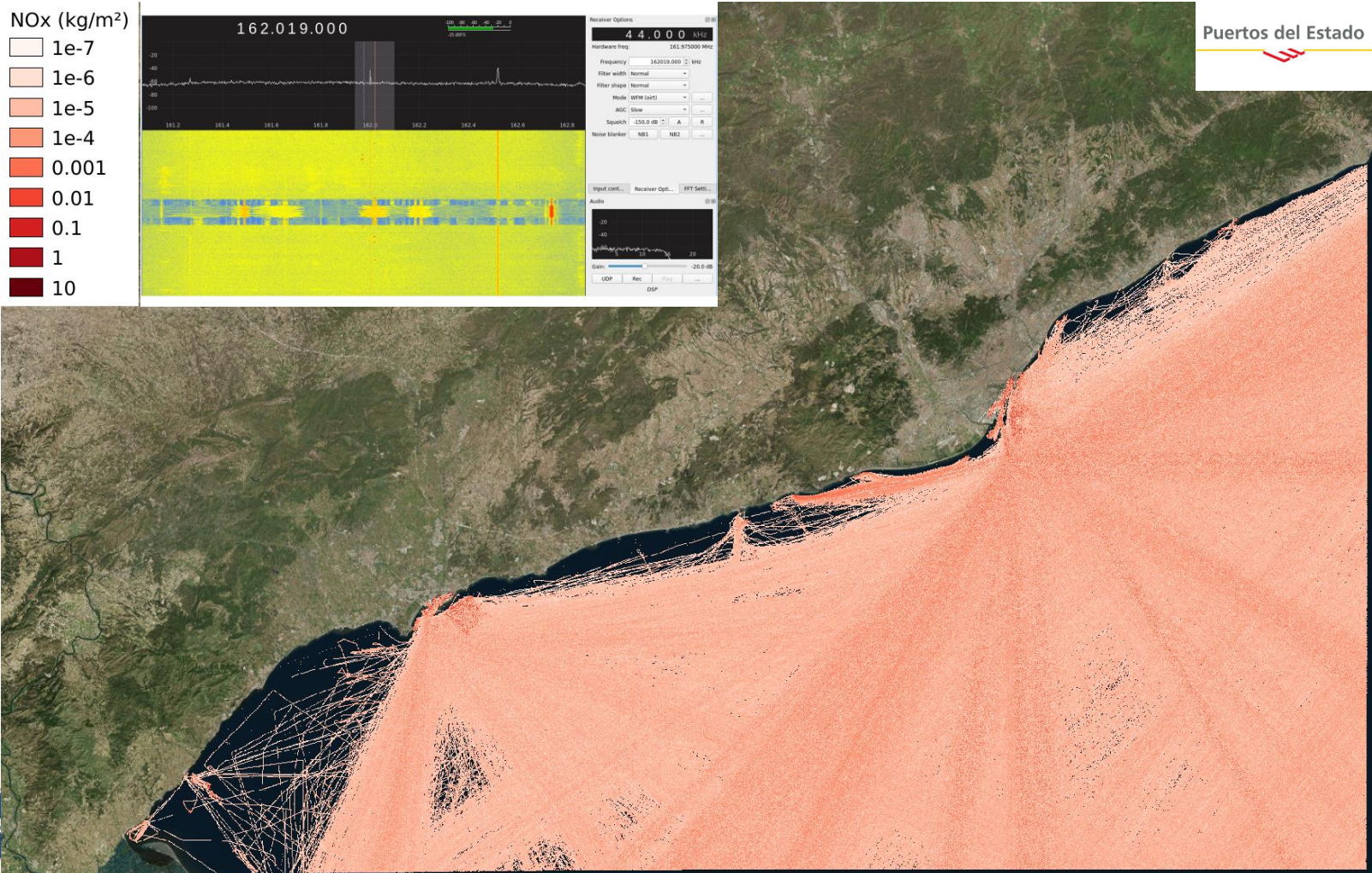
Beyond the state-of-the-art

Use of **GPS data from ships** and **data mining and machine learning** techniques to assess very high resolution shipping emissions

NOx (kg/m²)



Puertos del Estado





**Barcelona
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Center**
Centro Nacional de Supercomputación



EXCELENCIA
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OCHOA

HERMESv3 represents an effort to facilitate the use of emission inventories within the air quality modelling community

Next step: Engage and collaborate with key actors to develop a national emission tool that fulfils the needs of researchers, operational services, administrations and companies

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