

Work Package 3: Atmospheric research services

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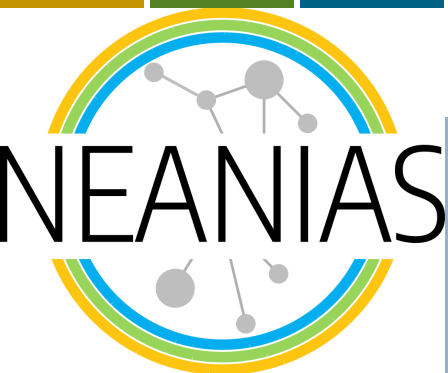
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Novel EOSC Services for Emerging
Atmosphere, Underwater & Space
Challenges

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Atmospheric Work package Goal

- › Develop and integrate at EOSC three innovative cross-cutting atmospheric services.
- › To allow tackling operationally atmospheric-related studies and engineering tasks
- › Towards engaging several user communities linked to the atmosphere, including:
 - › meteorologists, industrial air pollutant emitters, ecologists, rural urban planners and air quality authorities, geohazards, civil protection, insurance, health agencies.

Work package 3 Services

- › T3.2: **Service A1 (ATMO-FLUD)** – Greenhouse gases flux density monitoring service implementation
- › T3.3: **Service A2 (ATMO-STRESS and ATMO-SEISM)** – Monitoring atmospheric perturbations and components in active tectonic regions service implementation
- › T3.4: **Service A3 (ATMO-4CAST)** – Air quality estimation, monitoring and forecasting service implementation

Results so far

- › Requirements collected, updated, and published
- › Software for all 3 services deployed, operational, published at EOSC for public consumption
- › Three validation rounds already done
- › All above results are reported at the corresponding project deliverables

T3.2 – Service A1 (ATMO-FLUD) Overview

- › Calculating Flux Densities of momentum, energy and scalars, using two methods:
 - › Eddy covariance
 - › Gradient method
- › Started with existing proven algorithms:
 - › implemented in Matlab
 - › at TRL6

T3.2 – Service A1 (ATMO-FLUD) Overview

- › Developed and deployed a web service that produces the following outputs:
 - › A series of graphs
 - › A text file with results
 - › A pdf report with all graphs and a scientific background preamble, that is ready for publication.
- › Already published at EOSC
- › Integrated with NEANIAS Core Services: AAI, Logging, Accounting, Data Sharing, Monitoring
- › More technical details [here](#)

Eddy-Covariance method

- › This method determines the **co variation** of turbulent vertical motion of air and the vertical turbulent motion of energy, or momentum, or mass.

Reynold's deconvolution principle:

$$w(t) = \bar{w}(t) + w'(t)$$

$$c(t) = \bar{c}(t) + c'(t)$$

$$\overline{wc} = \overline{\bar{w}\bar{c}} + \overline{\bar{w}c'} + \overline{w'\bar{c}} + \overline{w'c'} \quad \overline{wc} = \overline{\bar{w}\bar{c}} + \overline{w'c'} \quad \bar{w} \rightarrow 0$$

$$F = \overline{w'c'}$$

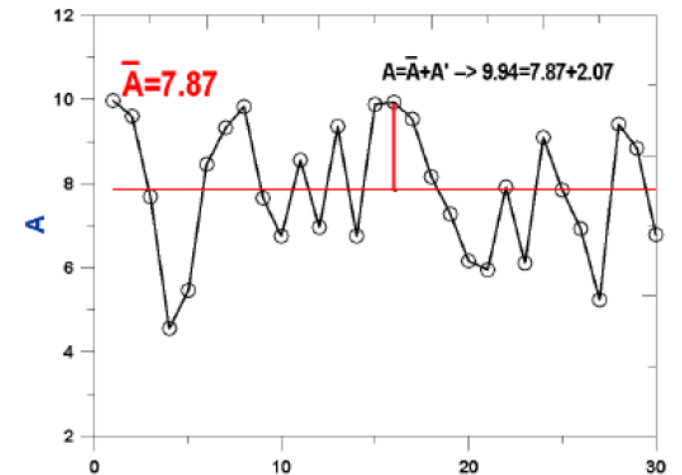
$$u = \bar{u} + u'$$

$$v = \bar{v} + v'$$

$$w = \bar{w} + w'$$

$$\theta = \bar{\theta} + \theta'$$

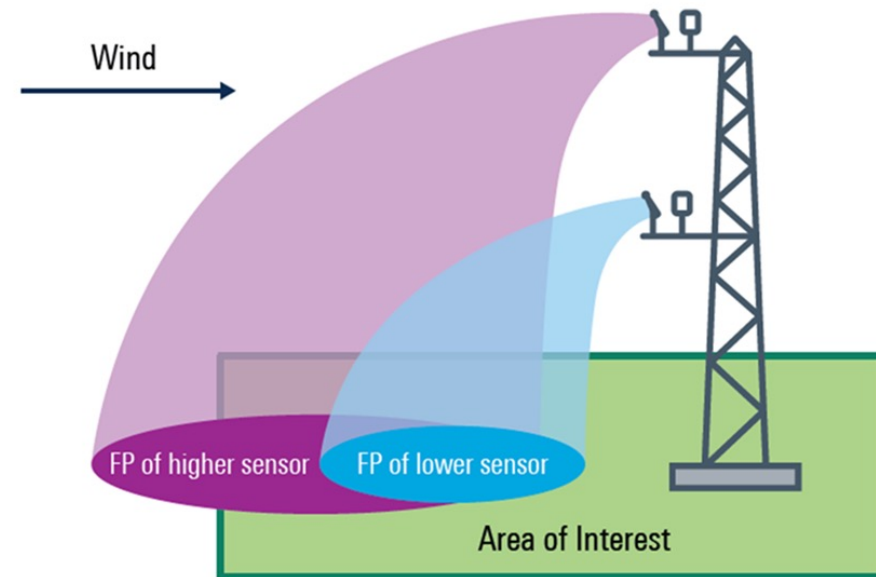
$$c = \bar{c} + c'$$



- Flux of CO₂ above a surface = mean of the variation of the vertical wind velocity in meters per second times the mean variation of the concentration of CO₂, in mg per cubic meter, resulting in a flux density of mg. m⁻².s⁻¹

Basic assumptions

- › Measurements at a point can represent an upwind area
- › Flux is fully turbulent
- › Terrain is horizontal and uniform
- › Instruments can detect very small changes at a very high frequency (>10 Hz)
- › Measurements are done inside the boundary layer of interest and inside the constant flux layer
- › Fetch and footprint are assumed adequate



Dynamic Gradient Method

- › The gradient method can be used to calculate the momentum, energy and scalar flux densities. The method depends upon measurement of vertical gradients of concentration, temperature and wind speed above the surface.

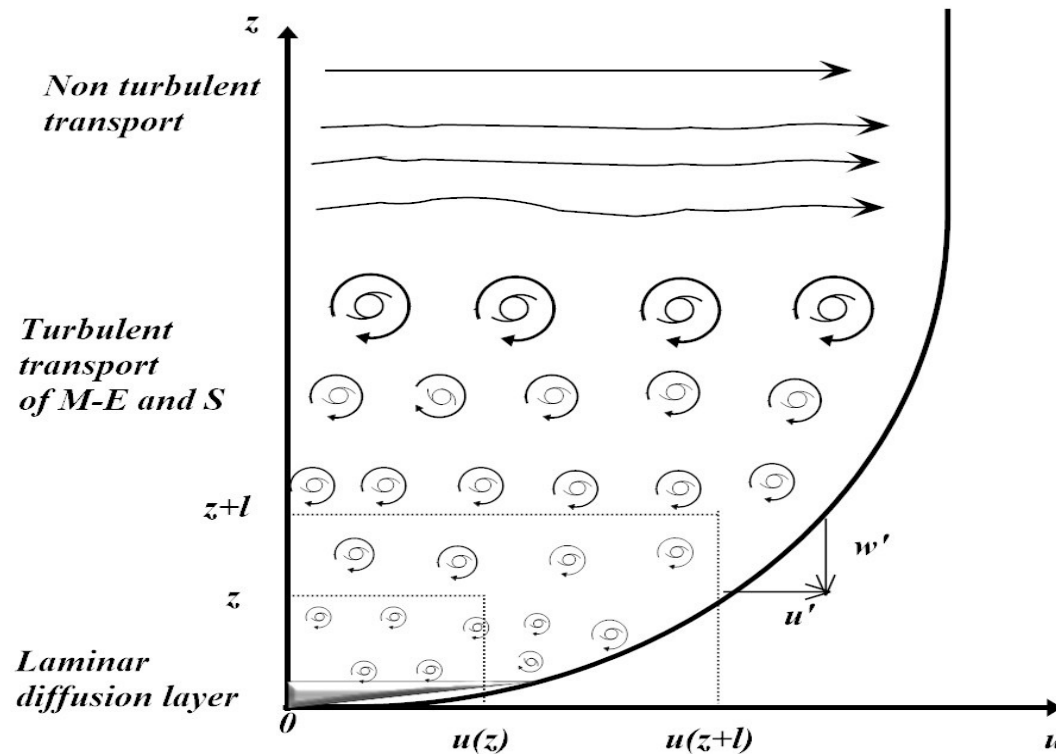
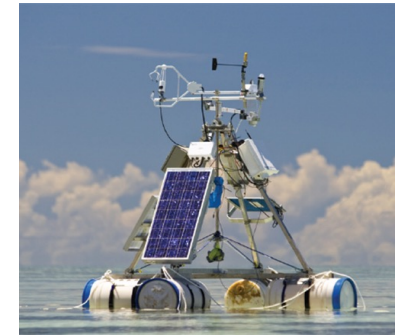


Figure 1. Idealized turbulent, flow over a smooth surface and transport of M=momentum, E= Energy and S= scalars. Where, u = horizontal wind speed, z = height and l indicates a height from which we may consider the downward turbulent transport of M, E or S.

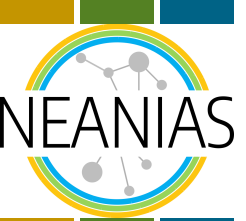
Applications

- › Scientific applications (e.g. climate change research, oceanography)
- › Regulatory applications (e.g. landfill monitoring, municipal emissions)
- › Commercial applications (e.g. leak detection, agricultural carbon sequestration, irrigation and water use efficiency)



Data pretreatment and post-calculation corrections

- › Despiking (>3.5 *standard deviation)
- › Filtering (only high frequencies)
- › Block averaging (mean values)
- › Ogives representation (usually 30 min)
- › Planar rotation (leveling of sonic anemometer)
- › Footprint analysis (area sampled by instrumentation)



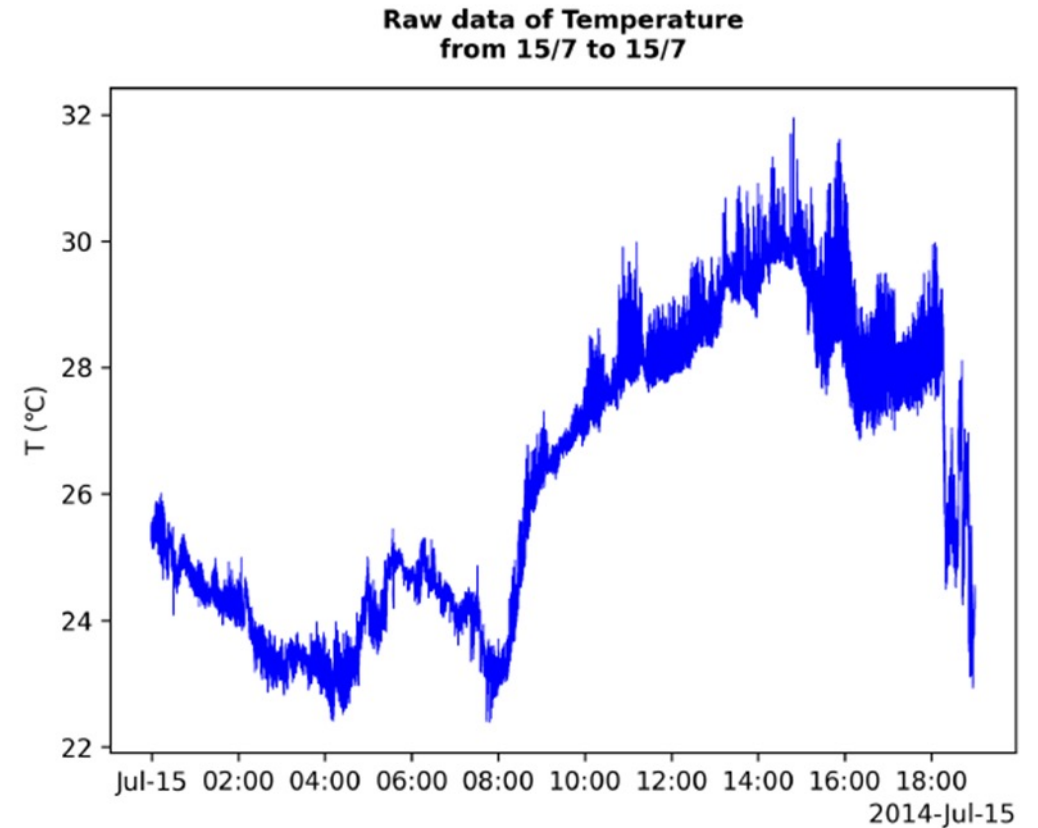
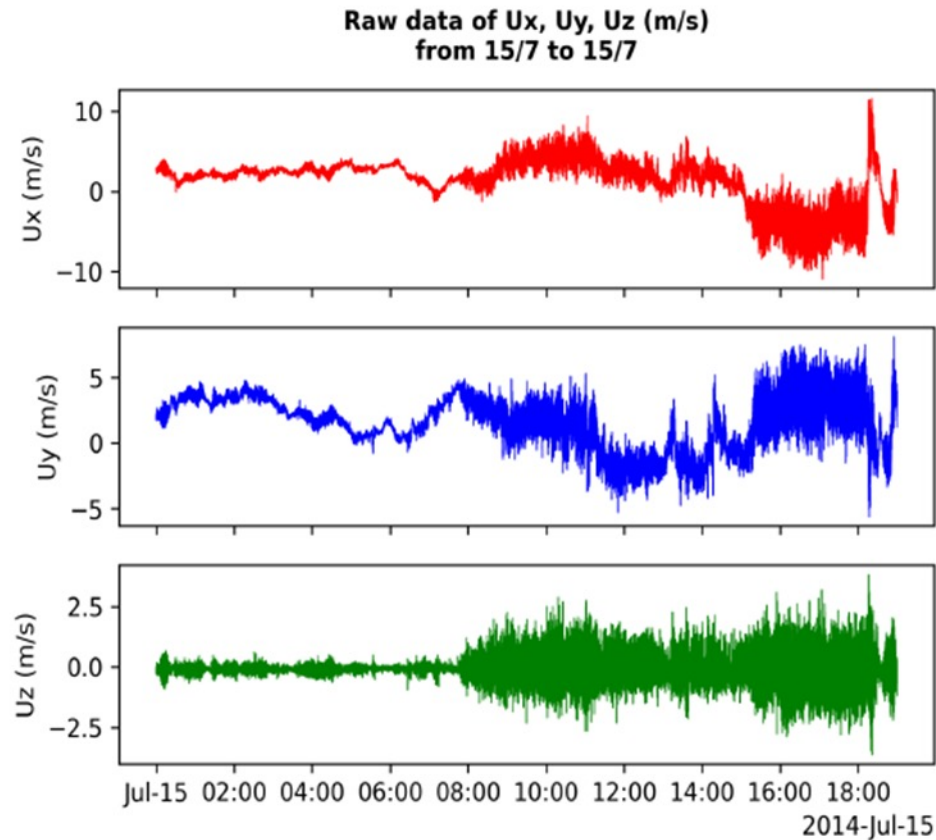
Video presentation for ATMO-FLUD - [link](#)

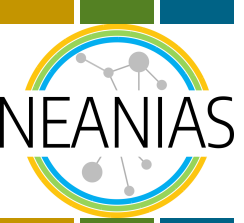


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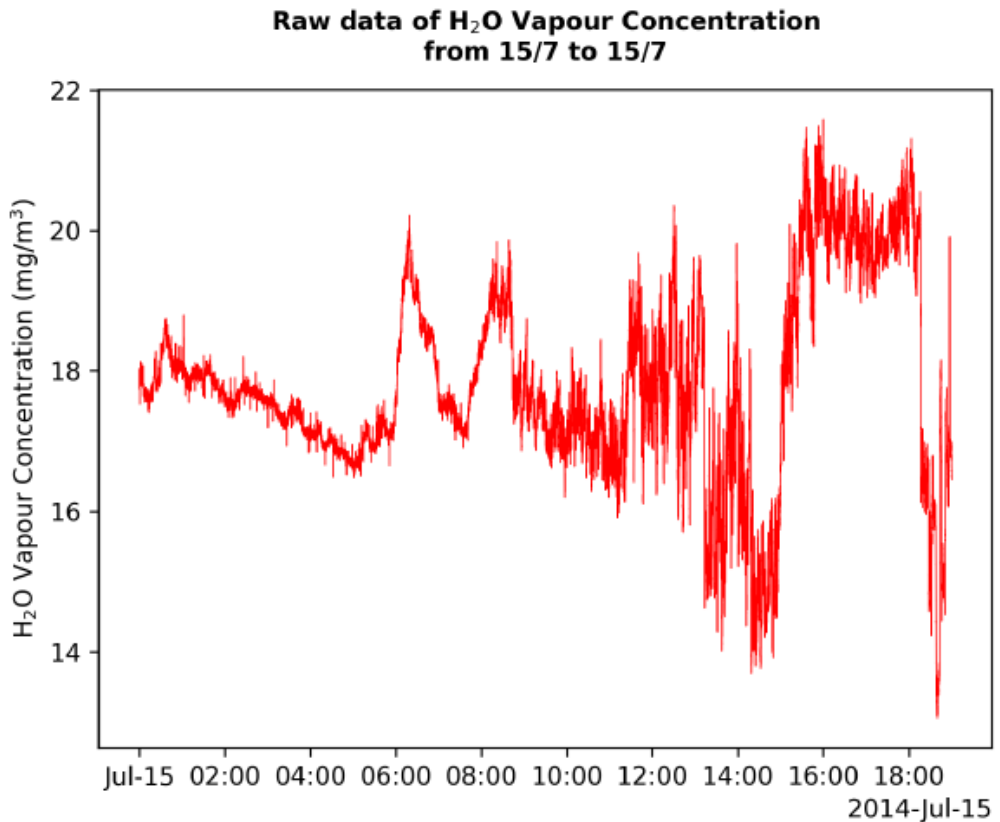
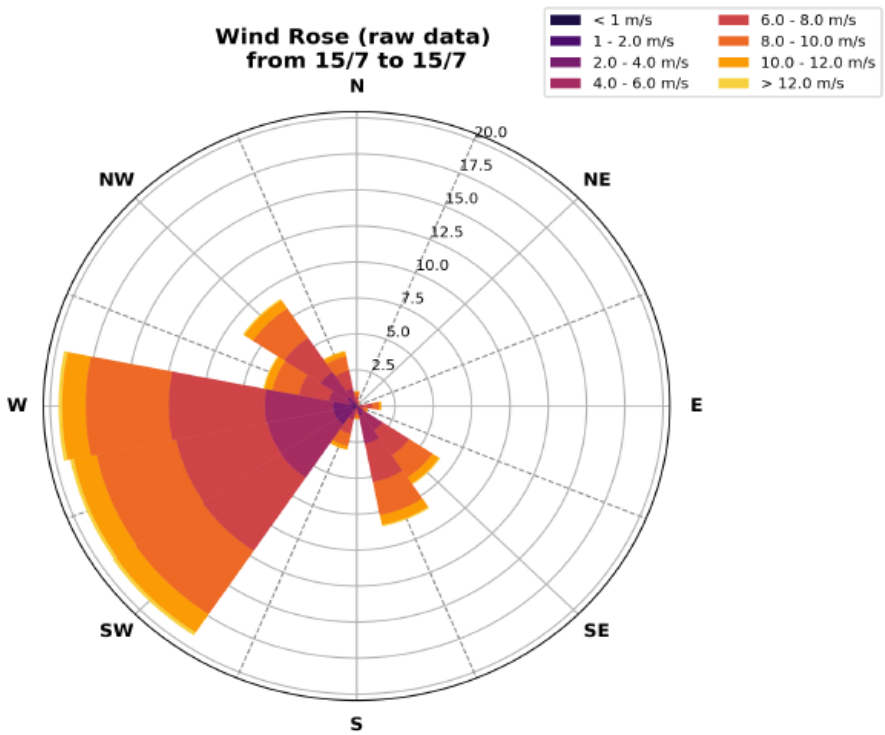
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Service Results for Eddy-Covariance



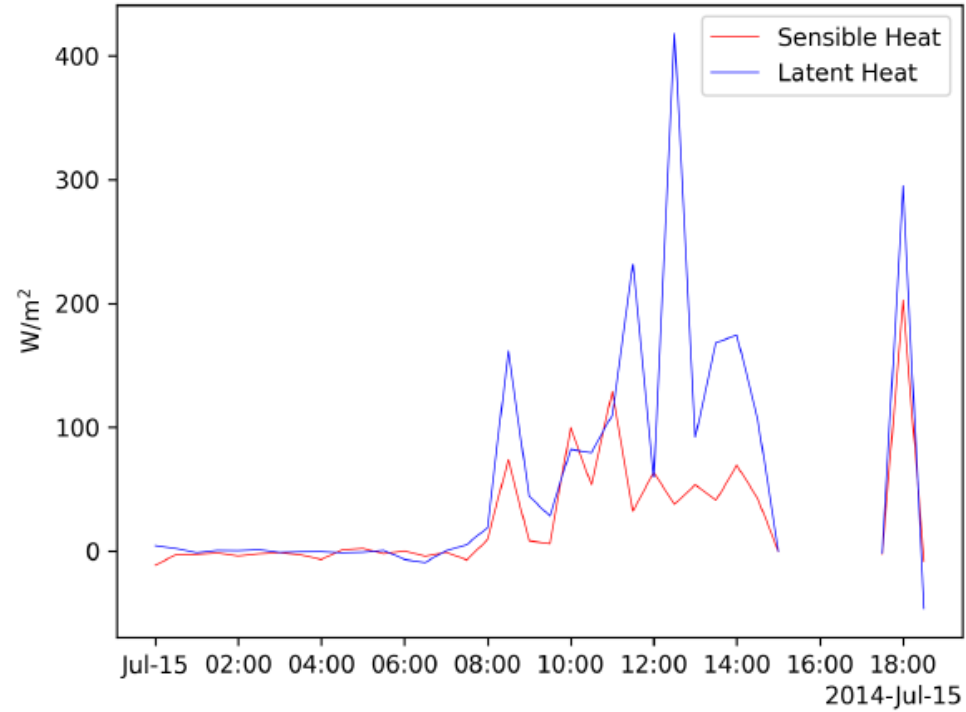


Service Results for Eddy-Covariance



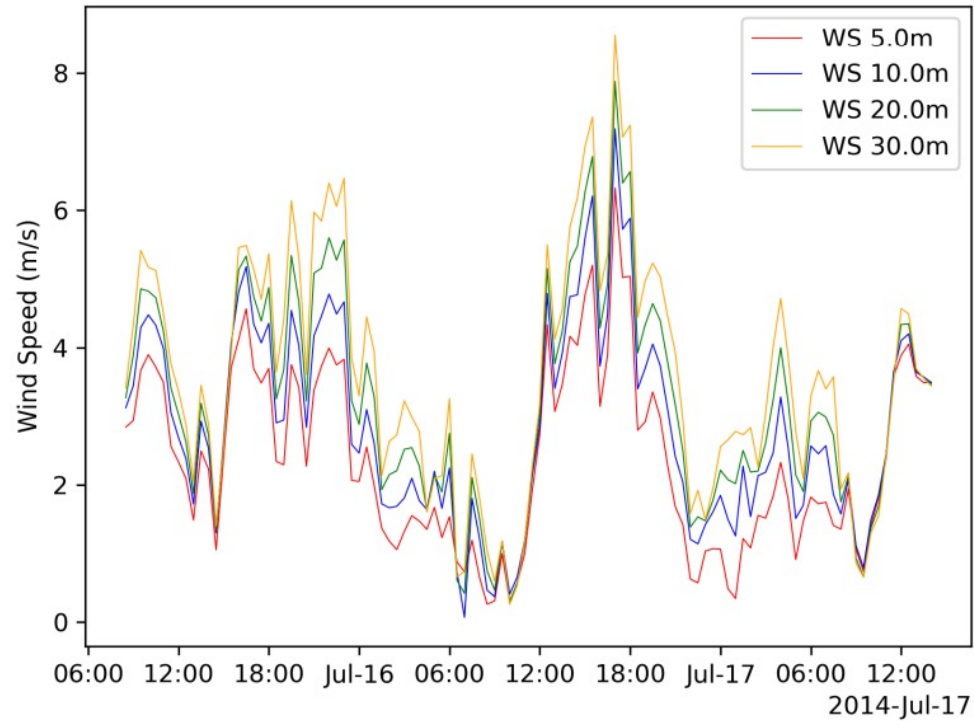
Service Results for Eddy-Covariance

Comparison of QH block averaged and QE block averaged for period=18000 and limit=3.5 from 15/7 to 15/7

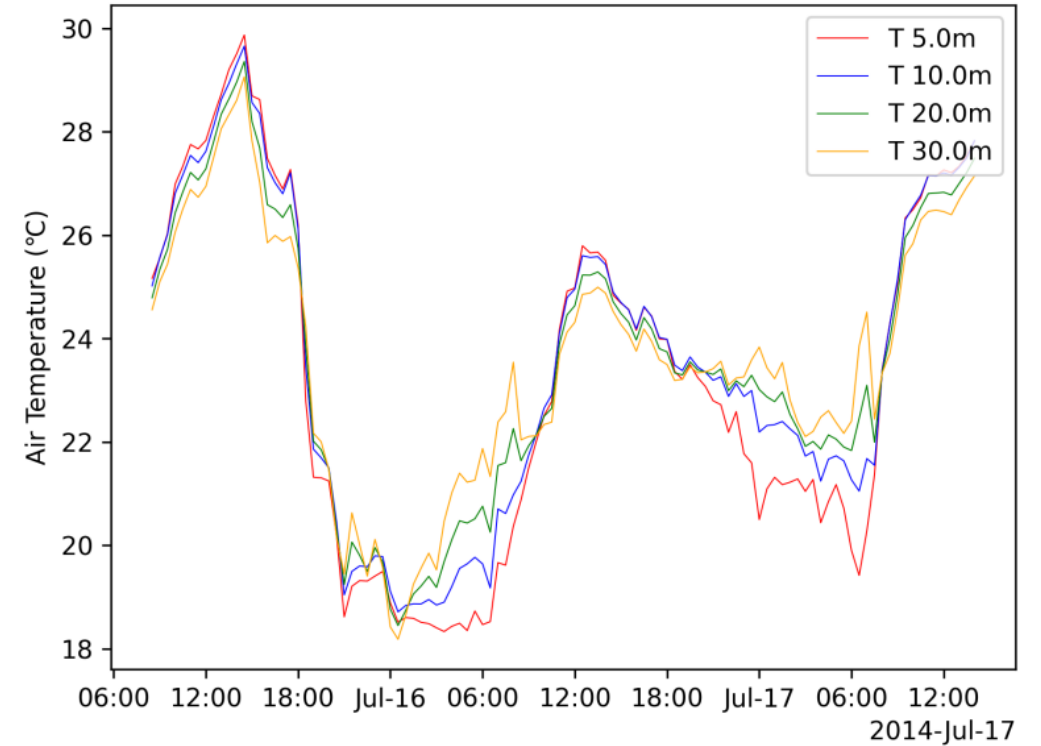


Service Results for the Gradient Method

**Blocked average data of Wind Speed
from 15/7 to 17/7**

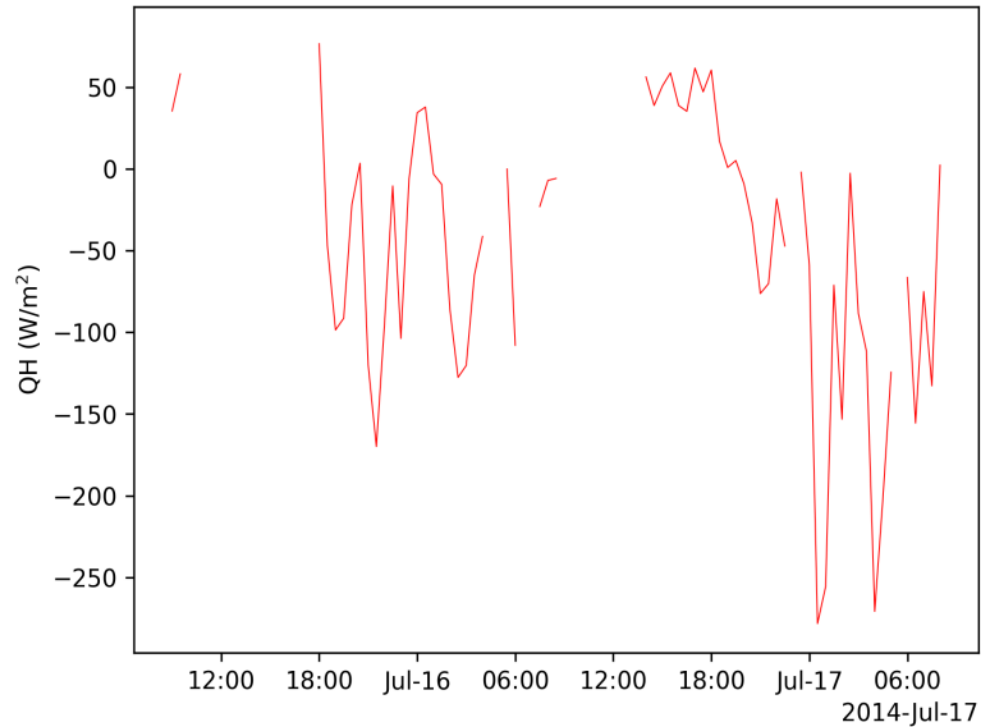


**Blocked average data of Air Temperature
from 15/7 to 17/7**

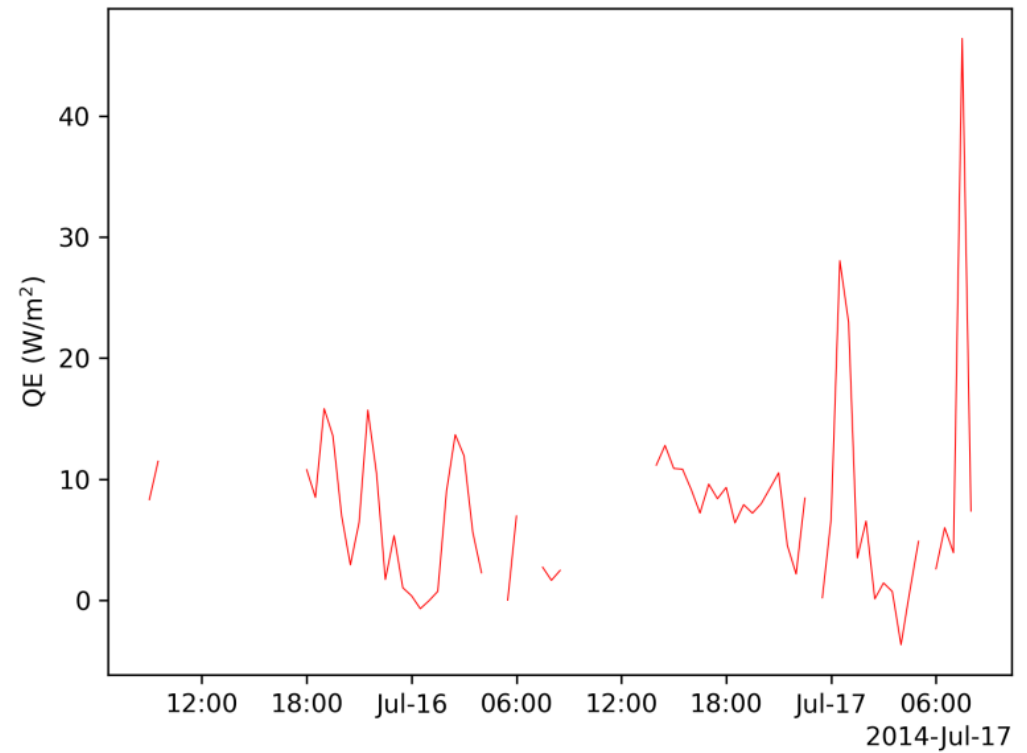


Service Results for the Gradient Method

Blocked average data of Sensible Heat
from 15/7 to 17/7

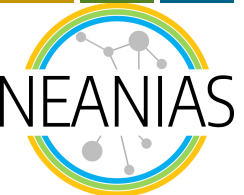


Blocked average data of Latent Heat
from 15/7 to 17/7

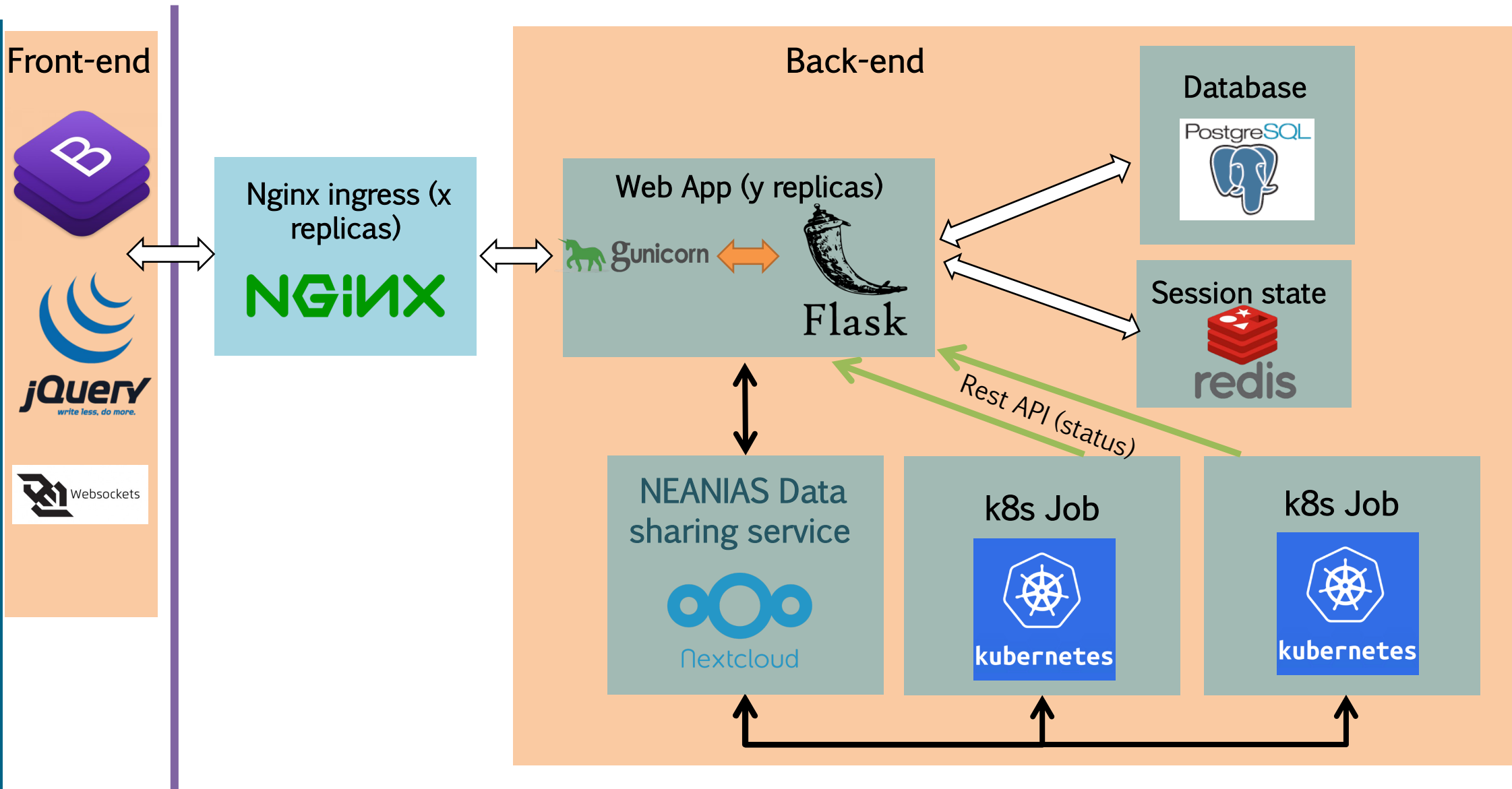


ATMO-FLUD Service Reusability, Scalability, and Quality Assurance

- › Besides the U/I, a REST API is also provided that allows other services to invoke new studies, monitor them, and obtain the results.
- › Service is deployed at the NEANIAS production Kubernetes cluster, and studies are queued there
- › Quality assurance measures include:
 - Service is replicated for fault-tolerance
 - Data is backed-up off-site daily
 - Use of CI/CD pipelines for automatic deployment in three environments (development, staging, production)
 - automated unit/integration tests, including Selenium for web U/I



Internal Architecture



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A2 Services: Overview

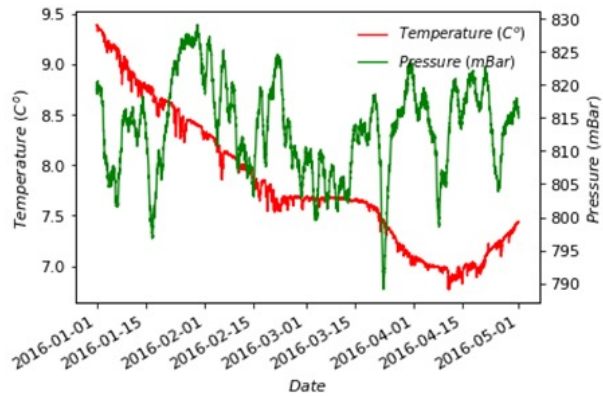
- › The purpose is to monitor atmospheric perturbations and components in active tectonic regions by
 1. Correlating gas emissions with earthquakes and atmospheric conditions using **ATMO-SEISM** service
 2. Computing regional stress field of a study area using the **ATMO-STRESS** service
- › Developed and deployed as a cloud service:
 - hosted on GARR Kubernetes cluster
 - currently at TRL 7
- › Integration with essential core services (AAI, logging, accounting, data sharing, and monitoring)

ATMO-SEISM: Targets and technology

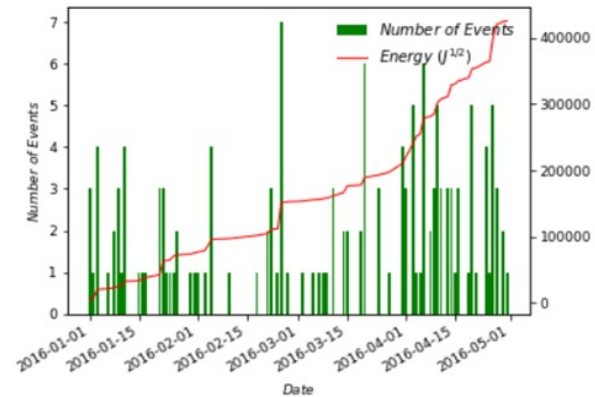
- › Rationale and scientific motivation
 - Comprehension of the interplay between tectonic activity, volcanic eruptions and gas release through faults (e.g. radon, CO₂, SO₂ etc.).
 - Special concern is linked to the diffusion of gas radon, because it could be used to estimate volcanic and seismic hazard, and for its dangerousness for human health.
- › Targets and possible users:
 - Civil Protection agencies, which can use it to monitor the gas emission in tectonic and volcanic active areas, especially radon.
 - Researchers and volcanologists, who can monitor the state of stress of an active volcano measuring gas emission in the atmosphere
- › Technology
 - Based on work from Neri *et al.*, 2016, but it allows to **automatically** correlate gas emission, atmospheric conditions, and earthquake parameters
 - Developed as a Jupyter Notebook service hosted in a dedicated JupyterHub deployment

ATMO-SEISM: service and output

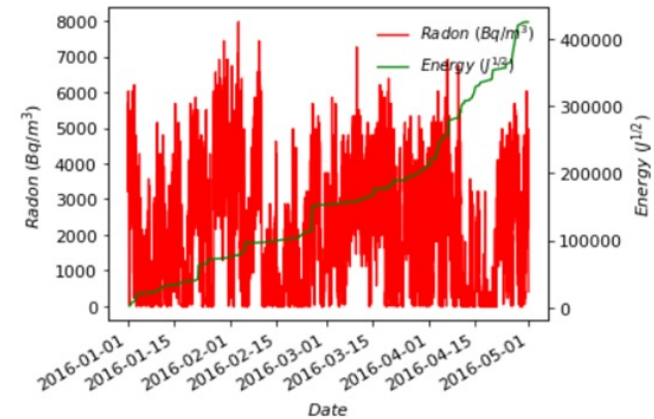
- › The input files accepted by the service are .csv and Excel files (both .xls and .xlsx).
- › Two input datasets: the first including information about gas and atmospheric conditions; the second including information about earthquakes.
- › The service relates all the inserted parameters, returning several graphs as outputs. Some examples are shown:



Data vs temperature and pressure



Released energy and number of seismic events



Released energy and radon emissions

ATMO-STRESS service: Targets and type of users

- › Tectonic area: calculate and reconstruct the stress field trajectories

Type of Users:

- Scientific community
- Public and private institutions for the prevention and management of natural hazards
- European citizens who are not members of the scientific community

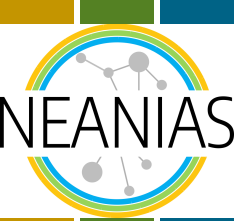


- › Volcanic areas: to identify the possible uprising pathway of the magma and/or gases components

Type of Users:

- › Oil and gas/petroleum and geothermal industries





A2 Services: Video - [link](#)



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ATMO-STRESS service: service operation

- › Input files provided by the user: excel or text file format
- › Analysis of input data and automatic evaluation of parameters
- › Georeferenced maps as outputs: grid and trajectories

Select file to upload

Please select a file for classification:

Atmo-STRESS_Demo_Dataset.txt

Please select data fields:

Longitude / X Latitude / Y Azimuth Angular Error

Lon Lat Azimuth

Reference System:

Geographic WGS'84/UTM Local

N S

Interpolation method: Order:

Distance Weighted Global

Parameters:

k p R

 Auto Auto

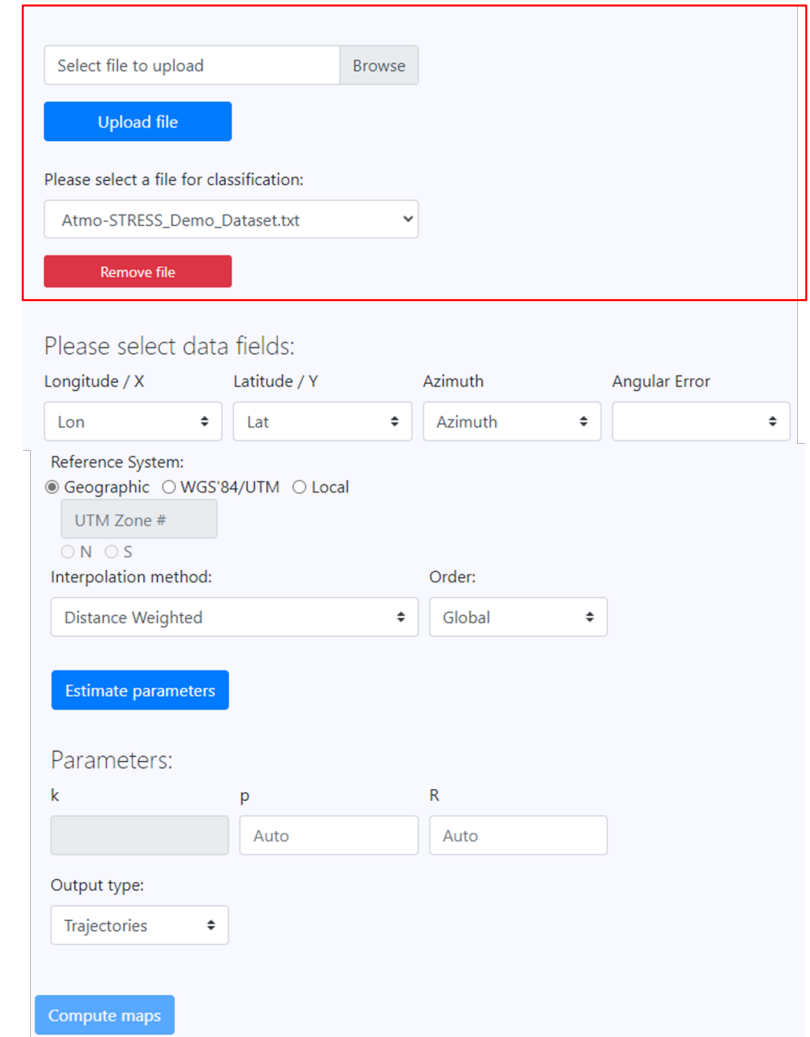
Output type:

Trajectories

ATMO-STRESS service: workflow

› It is possible to upload several type of input data collected in excel file with .xls extension

- Data collecting on the field: σ_{hmax} or σ_{hmin}
- Focal mechanism solutions arising from seismic events
- In situ Geotechnical measurements

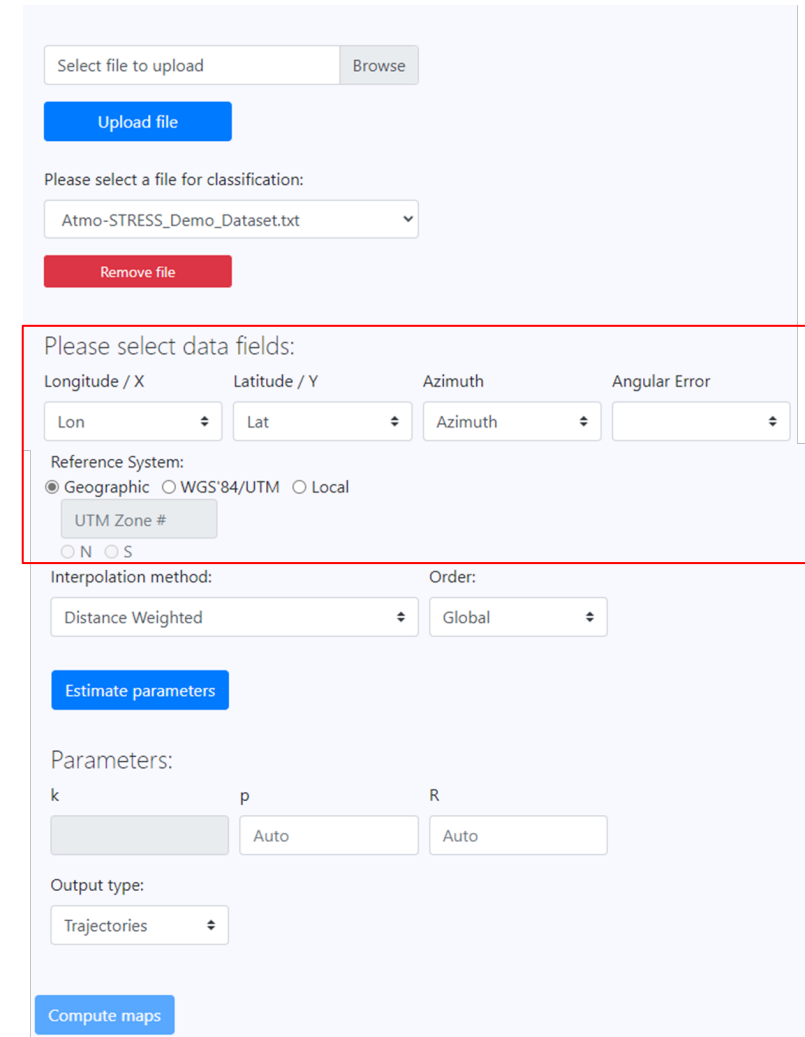


The screenshot shows the ATMO-STRESS service workflow interface. It includes a file upload section with a 'Select file to upload' input and a 'Browse' button. Below this is an 'Upload file' button. A section for file classification shows a dropdown menu with 'Atmo-STRESS_Demo_Dataset.txt' selected and a 'Remove file' button. The 'Please select data fields:' section contains dropdown menus for 'Longitude / X' (set to 'Lon'), 'Latitude / Y' (set to 'Lat'), 'Azimuth' (set to 'Azimuth'), and 'Angular Error'. The 'Reference System:' section has radio buttons for 'Geographic' (selected), 'WGS'84/UTM', and 'Local', with a 'UTM Zone #' input field and radio buttons for 'N' and 'S'. The 'Interpolation method:' section has a dropdown set to 'Distance Weighted' and an 'Order:' dropdown set to 'Global'. An 'Estimate parameters' button is located below these sections. The 'Parameters:' section has input fields for 'k', 'p' (set to 'Auto'), and 'R' (set to 'Auto'). The 'Output type:' section has a dropdown set to 'Trajectories'. A 'Compute maps' button is at the bottom.

ATMO-STRESS service: workflow

› Data selection

- **Coordinates:** define the geographic position of the data
- Reference **coordinate system:** the user can choose between
 - Geographic: coordinates must be written in lat/long
 - WGS 84: metric coordinates expressed by X and Y
- **Azimuth** or direction of the stress value (0-360°)
- **Error** evaluated during the calculation of the stress



The screenshot shows the ATMO-STRESS service workflow interface. It includes a file upload section with a 'Select file to upload' input and a 'Browse' button. Below this is an 'Upload file' button. A section for file classification shows a dropdown menu with 'Atmo-STRESS_Demo_Dataset.txt' selected and a 'Remove file' button. A red box highlights the 'Please select data fields:' section, which contains dropdown menus for 'Longitude / X' (set to 'Lon'), 'Latitude / Y' (set to 'Lat'), 'Azimuth' (set to 'Azimuth'), and 'Angular Error'. Below this is the 'Reference System' section with radio buttons for 'Geographic' (selected), 'WGS'84/UTM', and 'Local'. There is also a 'UTM Zone #' input field and radio buttons for 'N' and 'S'. The 'Interpolation method' is set to 'Distance Weighted' and the 'Order' is set to 'Global'. An 'Estimate parameters' button is present. The 'Parameters' section has input fields for 'k', 'p' (set to 'Auto'), and 'R' (set to 'Auto'). The 'Output type' is set to 'Trajectories'. A 'Compute maps' button is at the bottom.

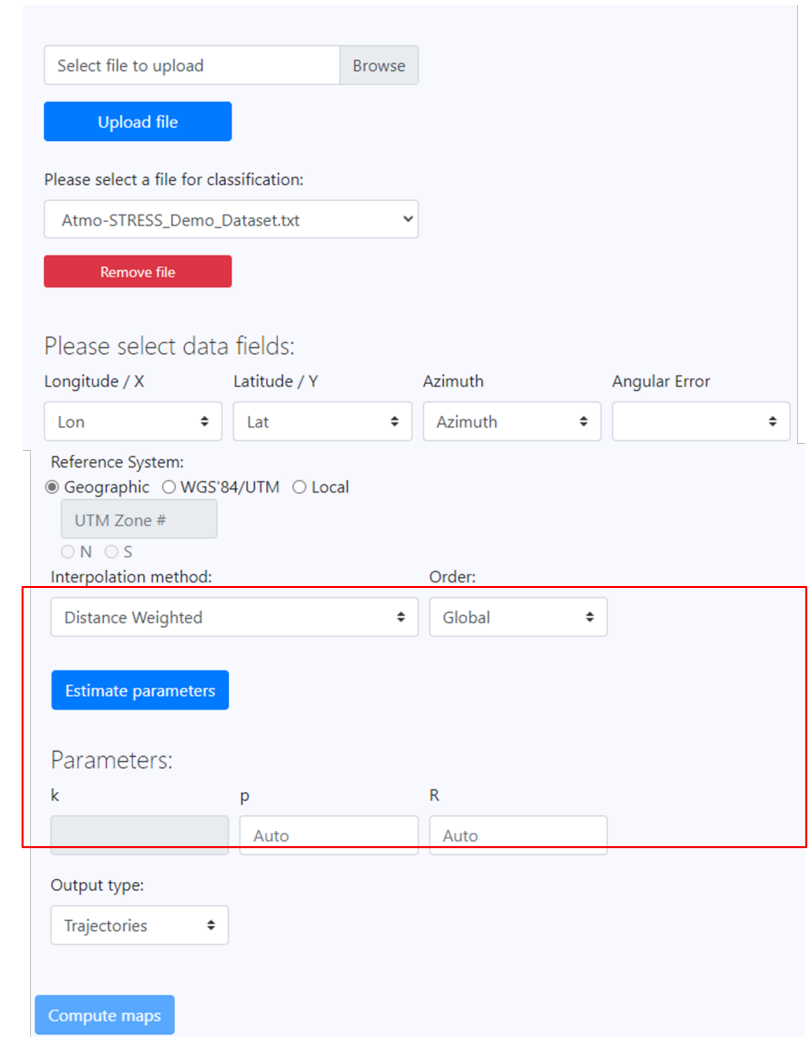
ATMO-STRESS service: workflow

> Interpolation method

- **Polynomial:** a linear function is introduced to fit smooth directional field and a bivariate polynomial function for 2-D data in the x - y plane is used
- **Distance waiting:** Use an inverse distance-weighting averaging technique as an interpolation method

> Order: defines the dimensions of the study area

- Global (P value =0)
- Medium (P value =2)
- Local (P value =10)



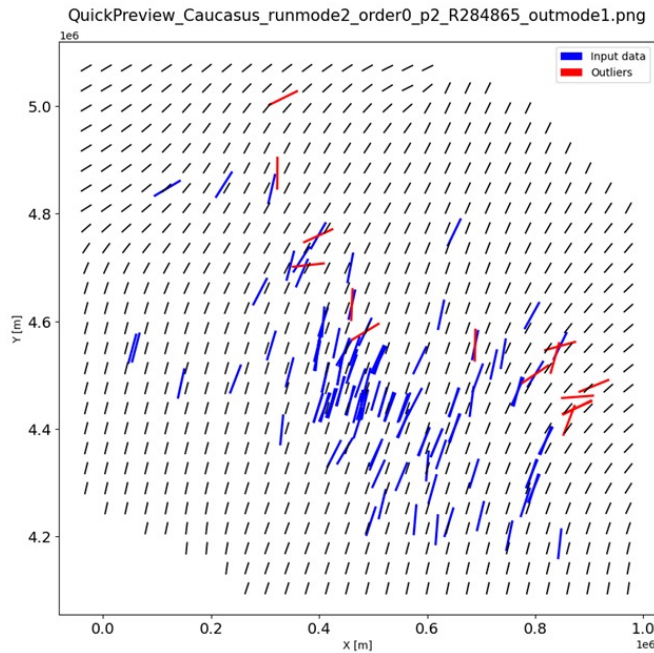
The screenshot shows the ATMO-STRESS service workflow interface. The interface includes a file upload section with a 'Select file to upload' input and a 'Browse' button. Below this is an 'Upload file' button. A section for file classification shows a dropdown menu with 'Atmo-STRESS_Demo_Dataset.txt' selected and a 'Remove file' button. The 'Please select data fields:' section has four dropdown menus: 'Longitude / X' (Lon), 'Latitude / Y' (Lat), 'Azimuth' (Azimuth), and 'Angular Error'. The 'Reference System:' section has radio buttons for 'Geographic' (selected), 'WGS'84/UTM', and 'Local', along with a 'UTM Zone #' input and radio buttons for 'N' and 'S'. The 'Interpolation method:' section has a dropdown menu with 'Distance Weighted' selected. The 'Order:' section has a dropdown menu with 'Global' selected. Below these is an 'Estimate parameters' button. The 'Parameters:' section has input fields for 'k', 'p' (Auto), and 'R' (Auto). The 'Output type:' section has a dropdown menu with 'Trajectories' selected. At the bottom is a 'Compute maps' button.

ATMO-STRESS service: workflow

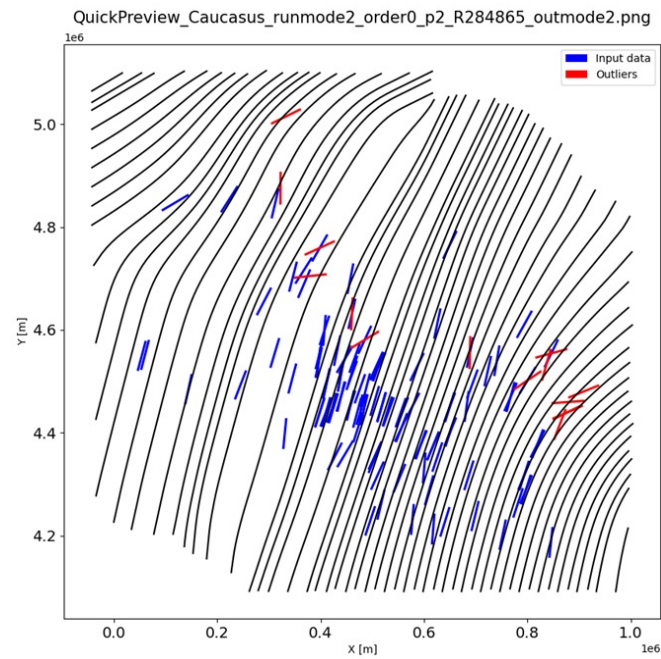
› Output type

- Both results are generated in different formats (.json, .kml, .shp and .png)

- Grid



- Trajectories



Select file to upload

Please select a file for classification:

Atmo-STRESS_Demo_Dataset.txt

Please select data fields:

Longitude / X	Latitude / Y	Azimuth	Angular Error
Lon <input type="button" value="↕"/>	Lat <input type="button" value="↕"/>	Azimuth <input type="button" value="↕"/>	<input type="button" value="↕"/>

Reference System:

Geographic WGS'84/UTM Local

UTM Zone #

N S

Interpolation method:

Order:

Parameters:

k <input type="text"/>	p <input type="text" value="Auto"/>	R <input type="text" value="Auto"/>
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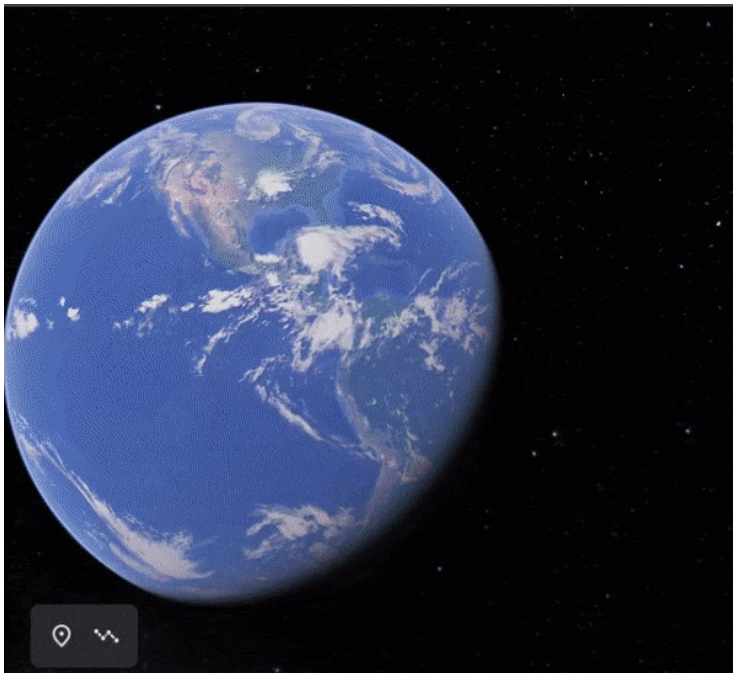
Output type:

Trajectories

Service results for different case study

CASE STUDY N°1: ICELAND

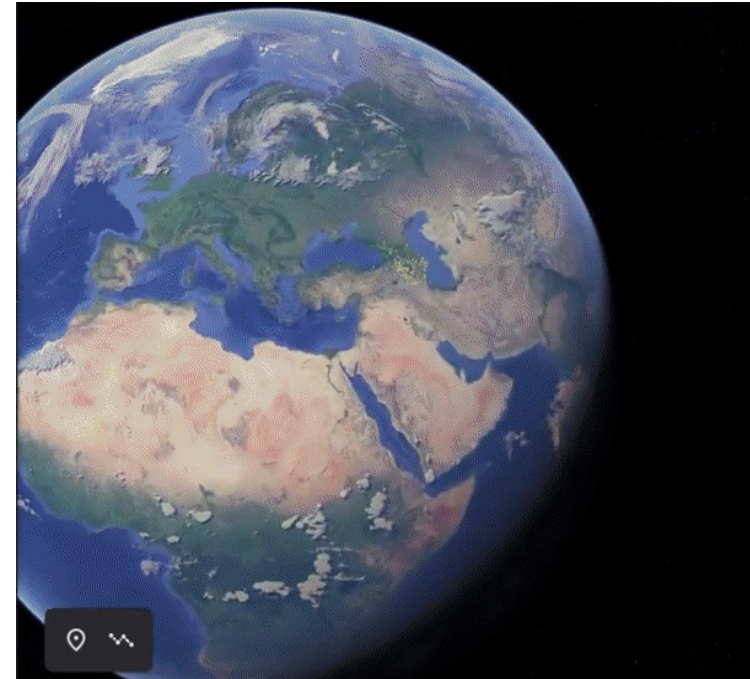
- Geological setting: **Divergence** between the North American and Eurasian plates.
- Type of data: data collecting on the field



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CASE STUDY N°2: CAUCASUS

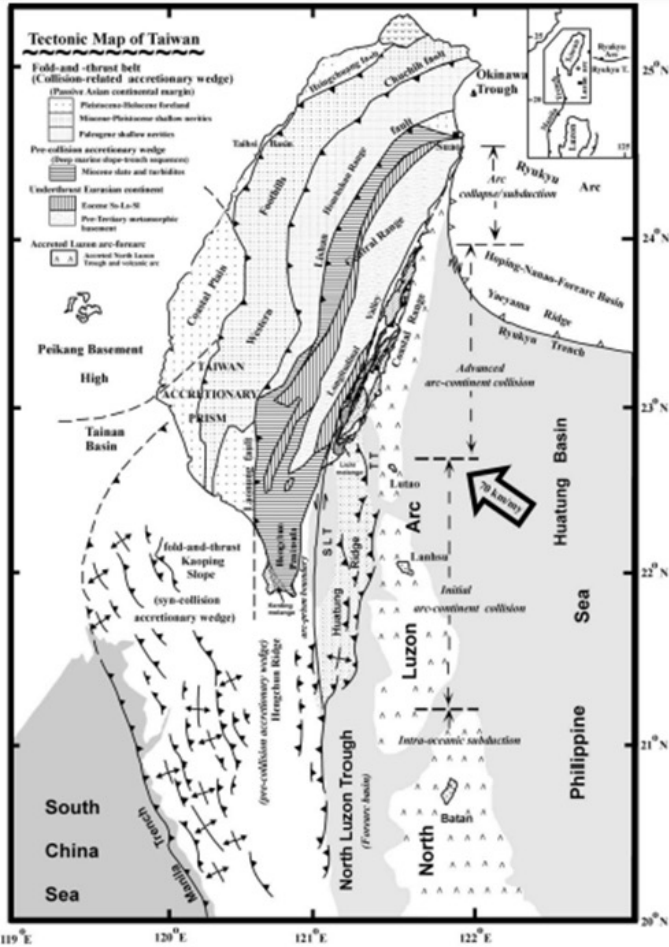
- Geological setting: The Caucasus belt is the result of the **convergence** between the Arabian and Eurasian plates.
- Type of data: GPS data



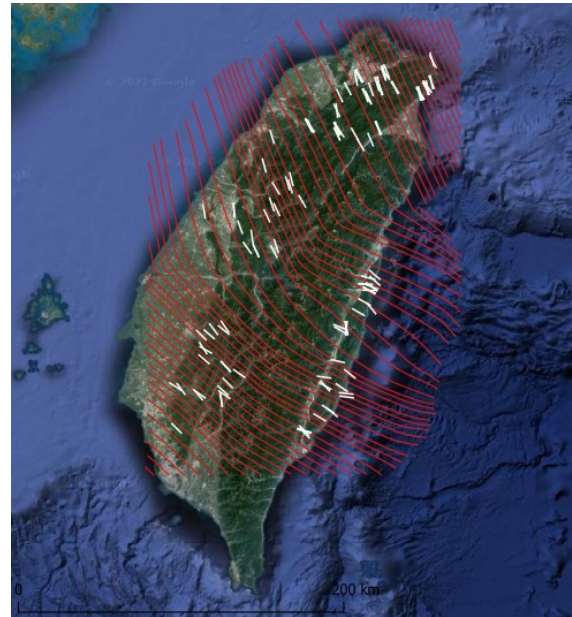
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Service results for different case study

CASE STUDY N°3: TAIWAN

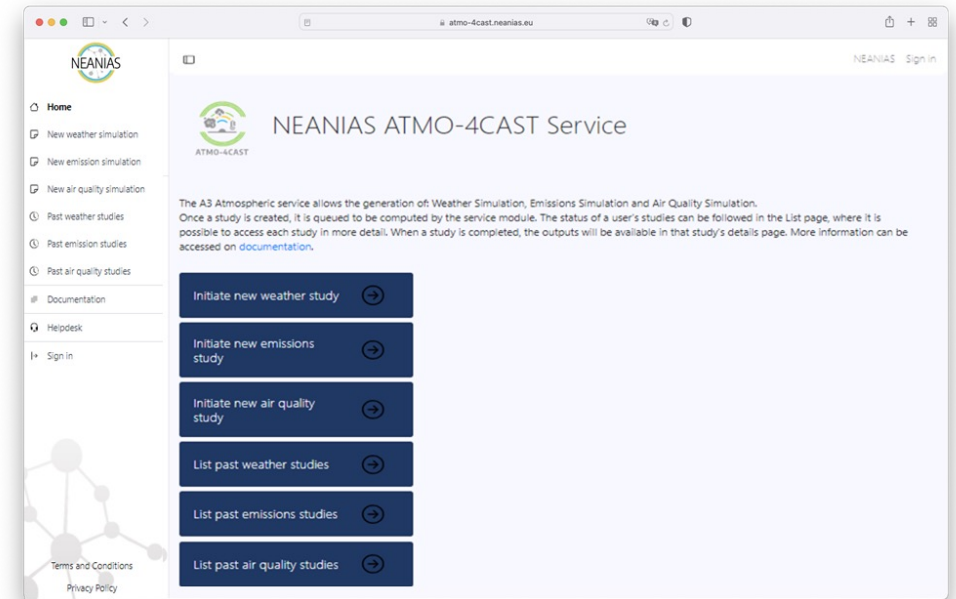


- **Convergence** between the Philippine Sea plate relatively to the Eurasian one. Relative velocity of about 7 cm/yr in a WNW-ESE direction (300°N).
- The direction of the maximum compressive stress (σ_1) varies from 320°N in northwestern Taiwan to 285°N in the southern island.



A3 service ATMO-4CAST: Purpose

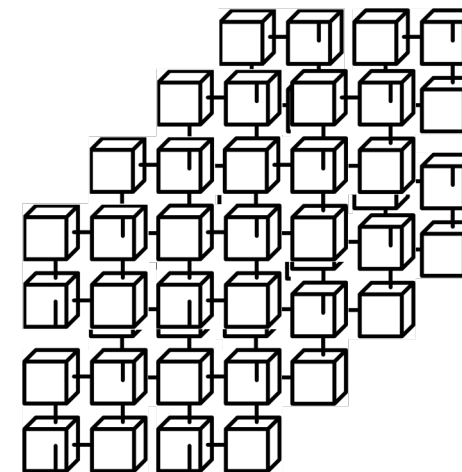
- › Weather and Air quality estimation, monitoring and forecasting



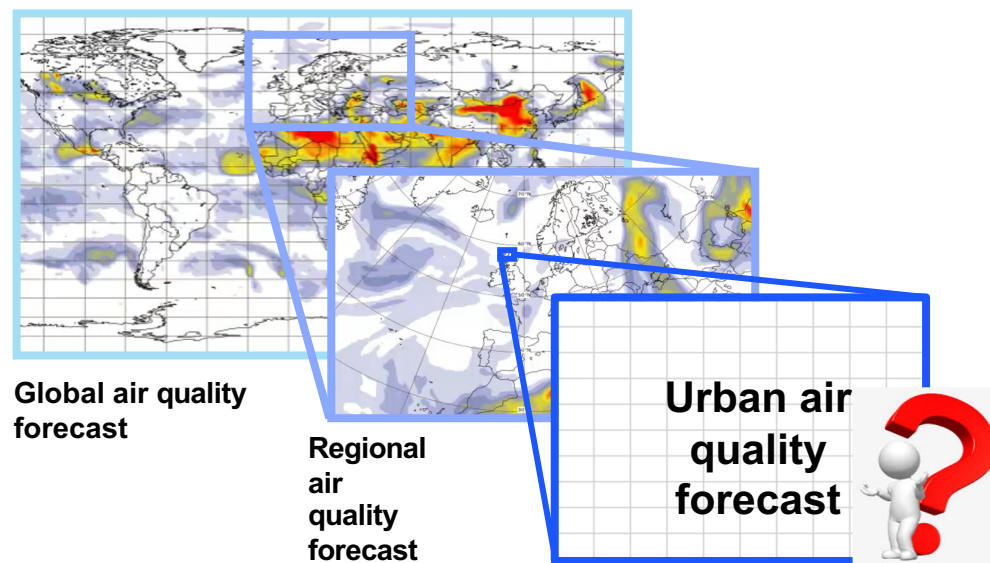
<https://atmo-4cast.neanias.eu/>

A3 service ATMO-4CAST: Why?

- Forecasting is **focused on predictive models**
- **Complex models** that involve physical and chemical transformations
- **Complex to understand** and **initiate** a simulation
- Different **dependencies**



State-of-the-art



A3 service ATMO-4CAST: Solution

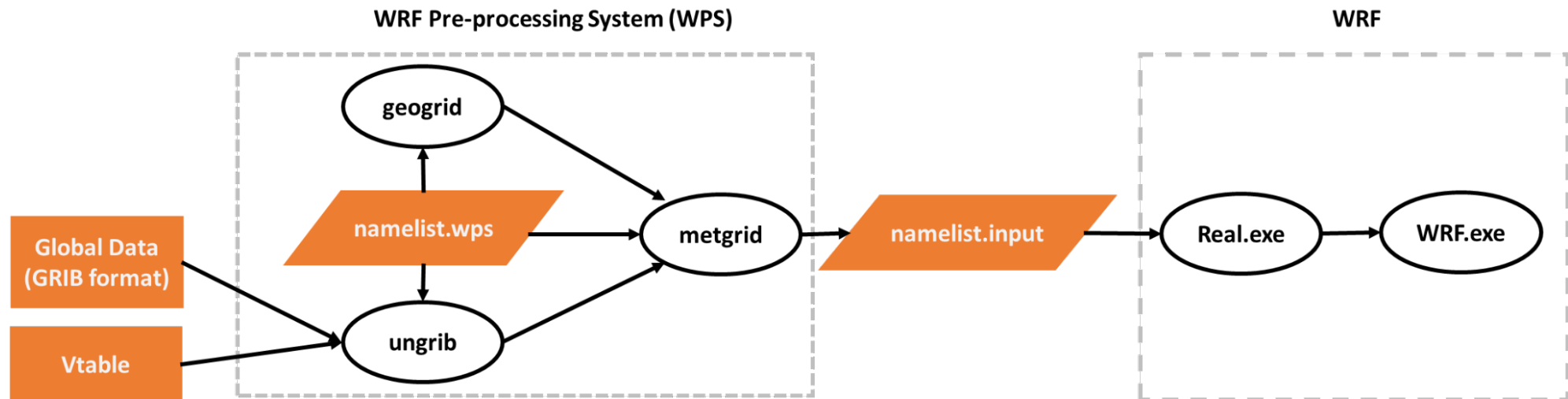
- › Composed by 3 different modules (air quality, emission and weather simulations)

- › Based on well established core models:
 - Janicke, U. (2014). AUSTAL2000, Program Documentation of Version 2.6. 2014-02-24. Janicke Consulting, Dunum (Germany).
 - Dias D., Antunes A. P., Tchepel O., 2019. Modelling of emissions and energy use from biofuel fuelled vehicles at urban scale. Sustainability, 11(10), 2902.
 - UCAR (2019). Weather Research & Forecasting Model, Version 4 Modeling System User's Guide. https://www2.mmm.ucar.edu/wrf/users/docs/user_guide_v4/

A3 service ATMO-4CAST: Solution

Weather Module

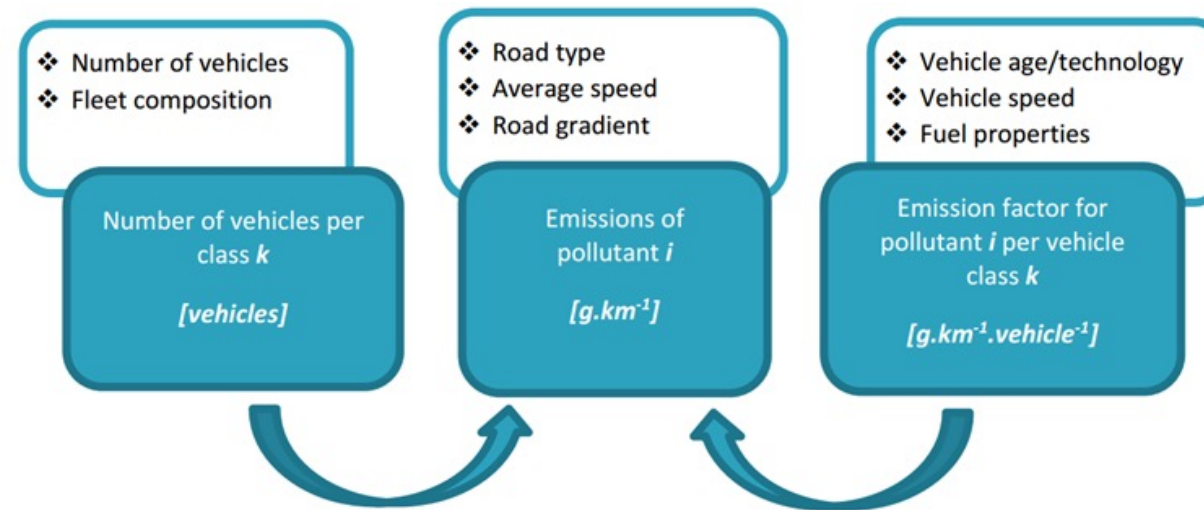
- › Based on WRF model
- › From UCAR
- › Different input data (GRIB and JSON format)



A3 service ATMO-4CAST: Solution

Emission Module

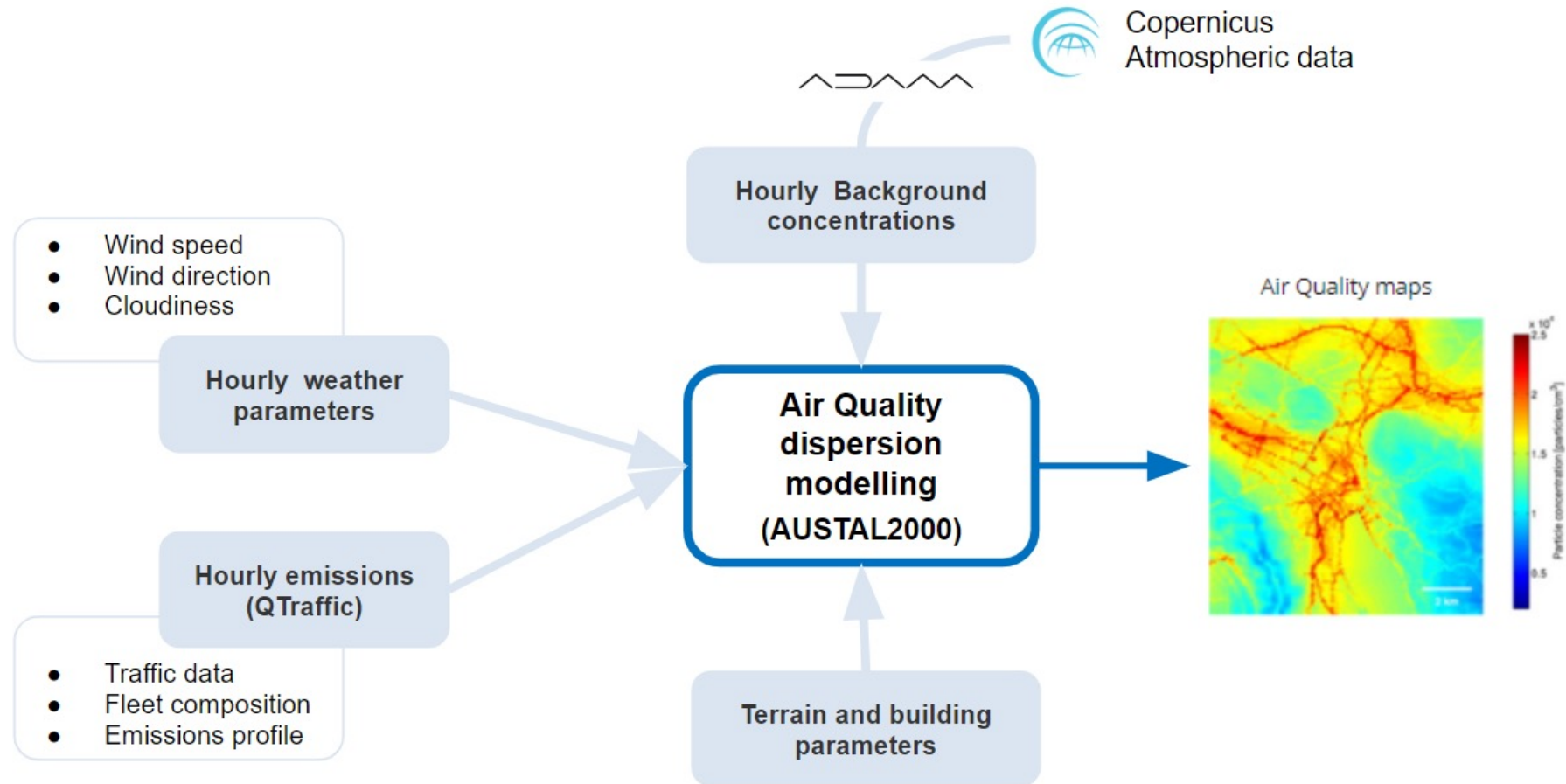
- › Based on QTraffic model (developed in the University of Coimbra)
- › Provides the emissions calculation at road segment level
- › Road traffic emissions (ozone precursors; Greenhouse gases; Acidifying substances; Particulate matter; Carcinogenic species)



Dias et al. (2015)

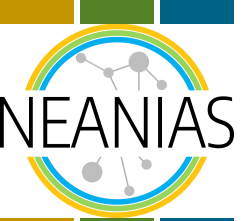
A3 service ATMO-4CAST: Solution

Air Quality Module



A3 service ATMO-4CAST: Workflow

- › Input files:
 - Weather(global data; Vtables and configuration files)
 - Emissions (traffic fleet and activity data)
 - Air Quality (local weather parameters; emission rates and profile; terrain and building parameters; hourly background concentrations -opt. from ADAM Platform - CAMS)
- › Core models process the data
- › Visualize and download outputs (grid maps or table data; format - .json; .txt; .dmna; .netcdf)



A3 service ATMO-4CAST: Video - [link](#)



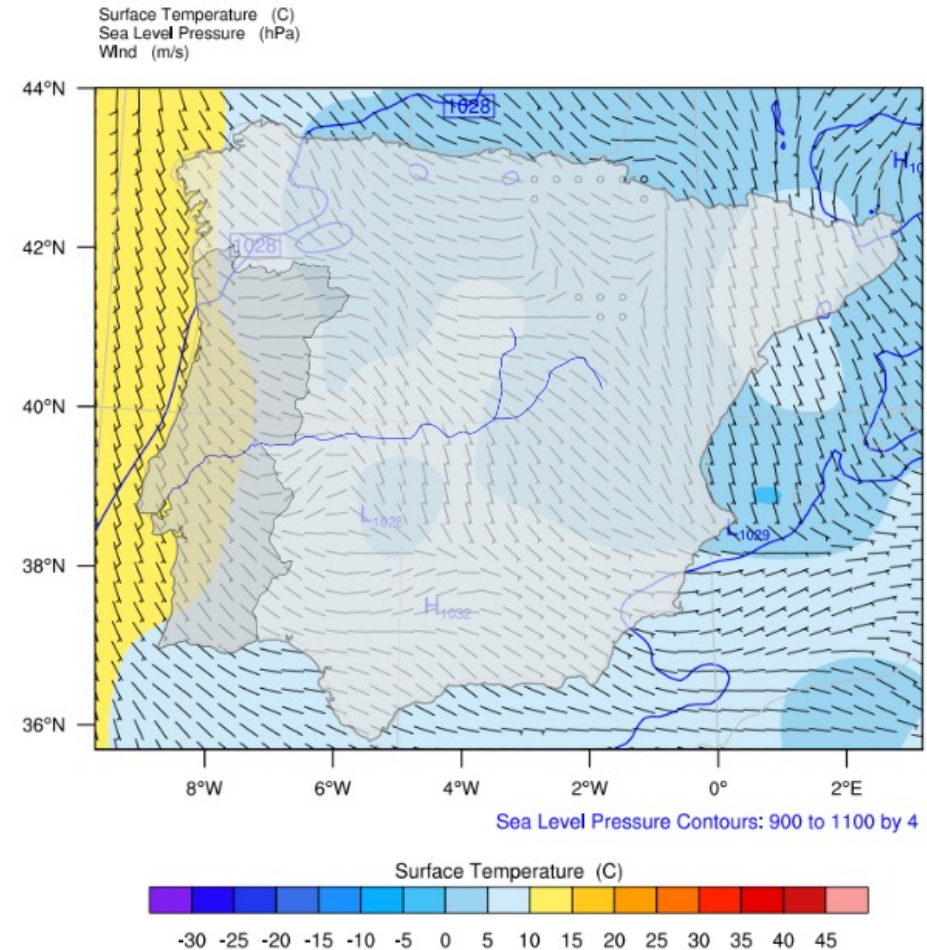
A3 service ATMO-4CAST: Use case (Iberian Peninsula)

Weather Module

Worldwide coverage (regional to urban scale)
 Input in GRIB or JSON format (see samples)

Output:

- Several meteorological parameters (e.g. surface temperature; pressure; wind speed and direction; precipitation)
- Plots generated in different formats (netCDF and JSON) and also visualised in the webpage



A3 service ATMO-4CAST: Use case (Stavanger city)

Emission Module

Domain area: 11 km²

Main roads (81 line sources)

Real traffic counting

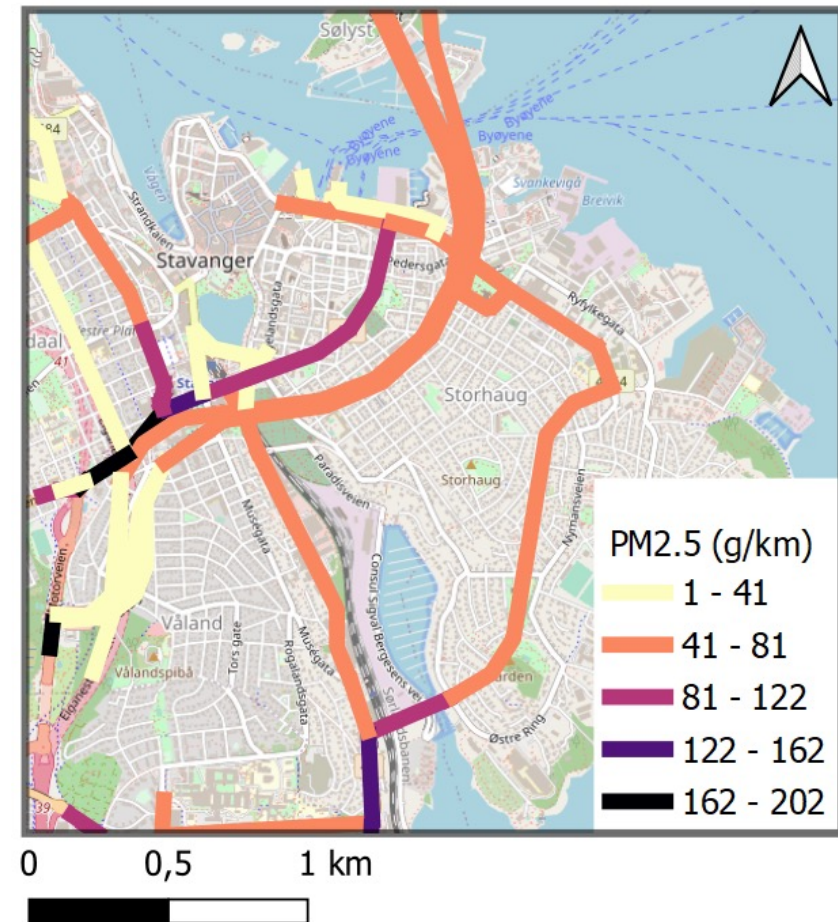
Updated statistical information from UNECE database

Duration: seconds to complete

Outputs:

- Several pollutants (air quality and GHG gases); Fuel consumption
- Plots generated in different formats (csv; shapefile; geojson)

PM2.5 daily emissions



A3 service ATMO-4CAST: Use case (Stavanger city)

Air quality module

Domain area: 11 km²

Traffic emissions input (same from Emission module)

Background concentrations from CAMS (ADAM api)

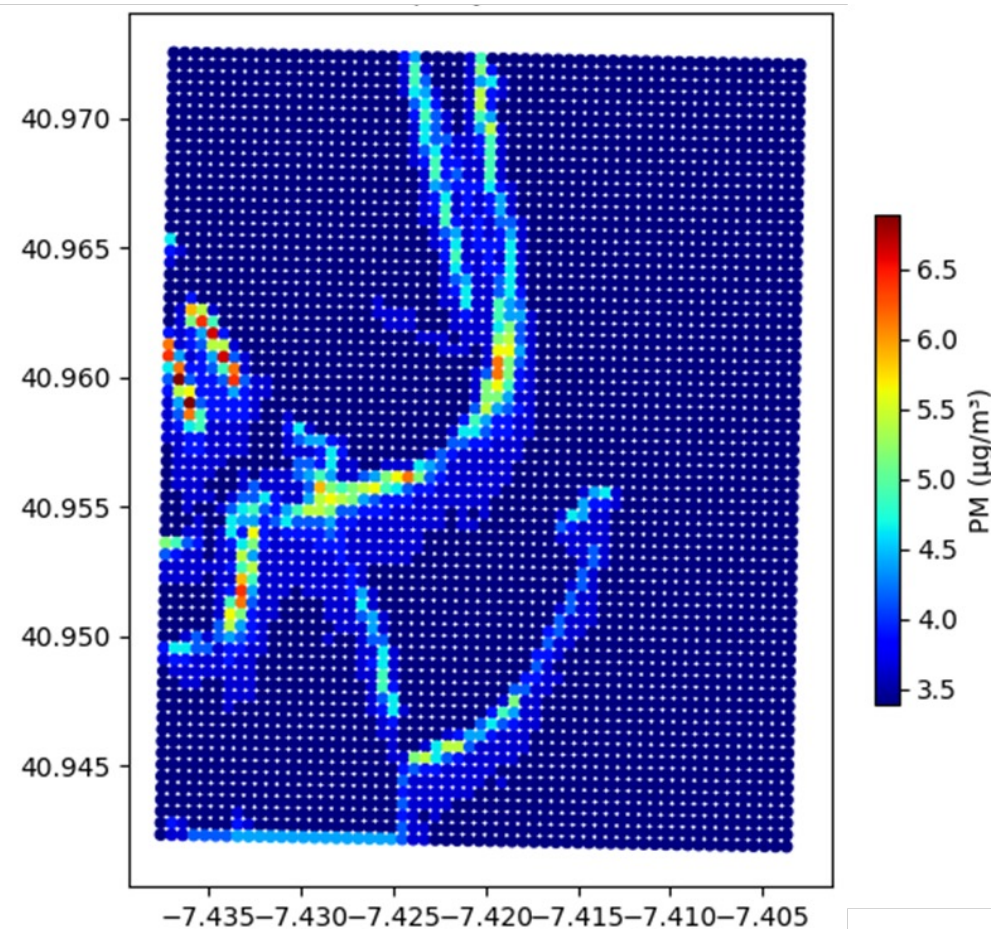
Local weather obtained from local forecasts

Duration: 4 min to complete

Outputs:

- Plots generated for every single hour in different formats (csv; png; tiff; geojson) and visualized on the webpage

PM2.5 daily concentrations



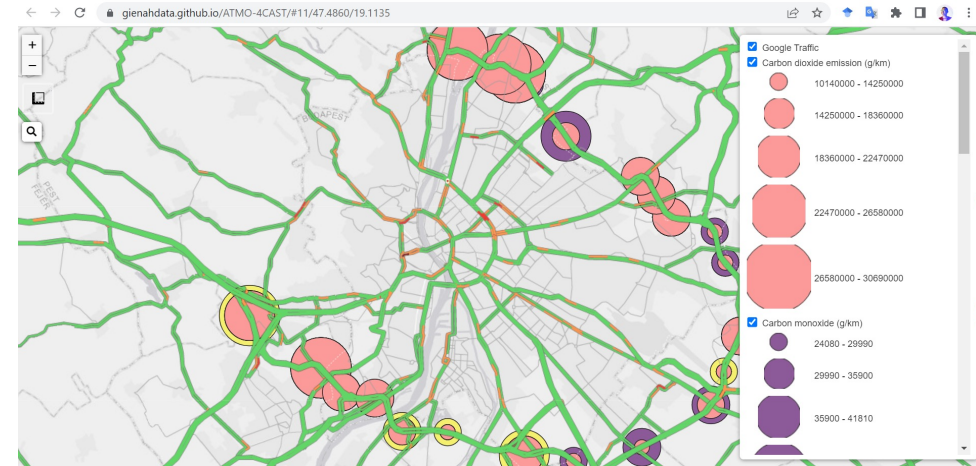
A3 service ATMO-4CAST: Overview

- › Implemented in Python, usable through frontend UI and API
- › Service already on EOSC
- › Supports different data formats (e.g. GRIB, JSON, txt, dmna files)
- › Example use cases are available
- › Outputs (2D maps) are generated in different formats (png; geojson; tiff; shapefile; csv)

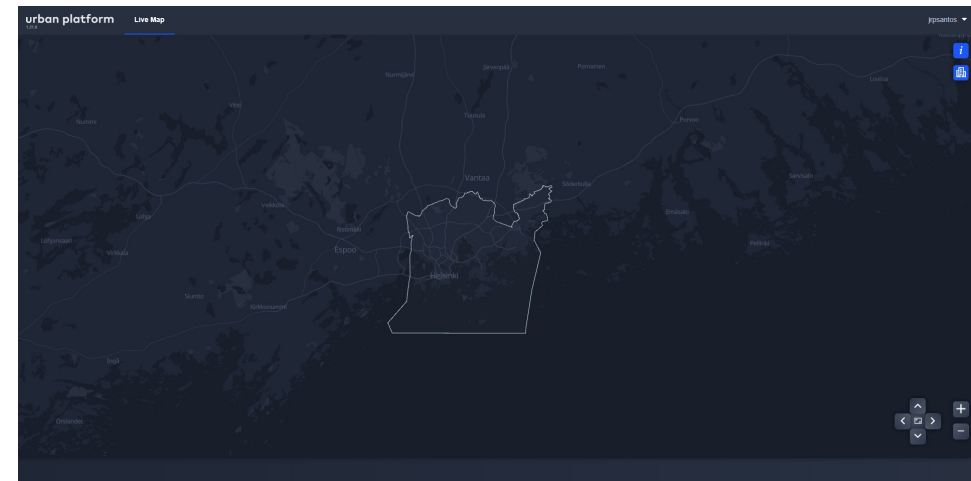
A3 service ATMO-4CAST: Target Users and Reusability

› Target users:

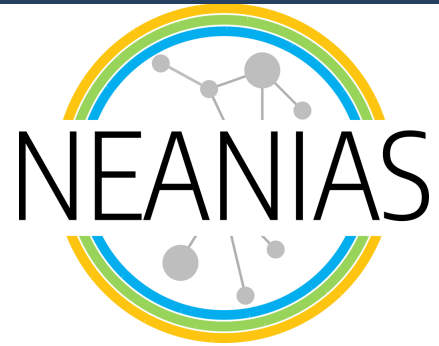
- Research groups and community focused on weather/air quality domains
- Urban authorities and decision-makers
- **Business companies** focused on air quality issues



GeoInsight (Budapeste)



Ubiwhere (Helsinki)



Novel EOSC Services for
Emerging Atmosphere,
Underwater & Space
Challenges



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Thank you! Questions?

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Nikos Chondros (NKUA)

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