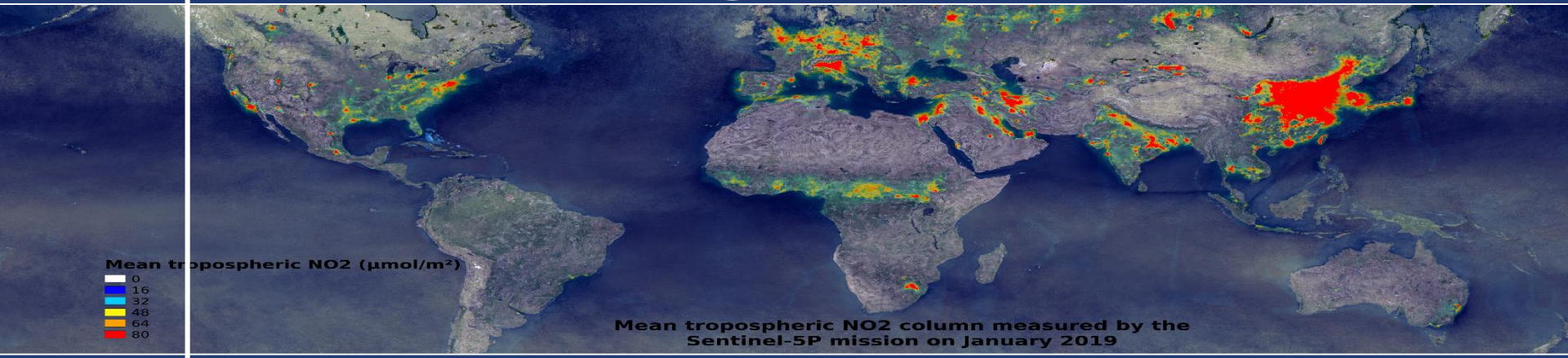
RUS Copernicus

European Commission

esa



TRAINING KIT

Monitoring tropospheric NO2 with Sentinel-5P

Part 1

S. BOITARD - NOVELTIS| simon.boitard@noveltis.fr

RUS Online| 22nd September 2021

NOVELTIS serco ALONG-TRACK ROMANIA

Outline

- Sentinel-5P
- The Sentinel 5P products
- Focus on NO2
- The Atmospheric Toolbox
- Exercises

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Outline

- **Sentinel-5P**
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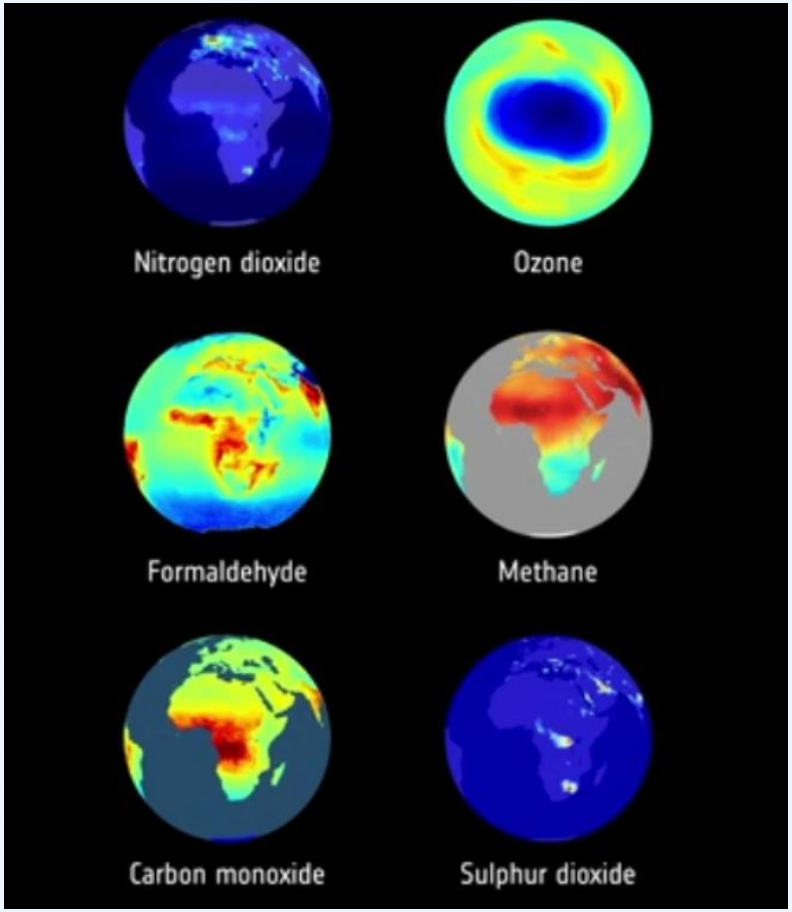
Sentinel-5P | Mission objectives

- Poor air quality results in 400,000 premature deaths in Europe (EEA) per year
- 1 in 8 deaths in Europe is linked to air pollution
- Mapping atmospheric gases, the Sentinel-5P mission arms decision-makers with the information they need to implement appropriate strategies to reduce air pollution, which in turn will help save lives



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Sentinel-5P | Mission objectives

MISSION OBJECTIVE

Provide global information on a multitude of atmospheric trace gases, aerosols and cloud distributions affecting air quality and climate.

- Air Quality
- Ozone Layer
- Climate change
- Input data to CAMS

Measurement continuity between previous (ENVISAT, AURA) and future (S5) missions

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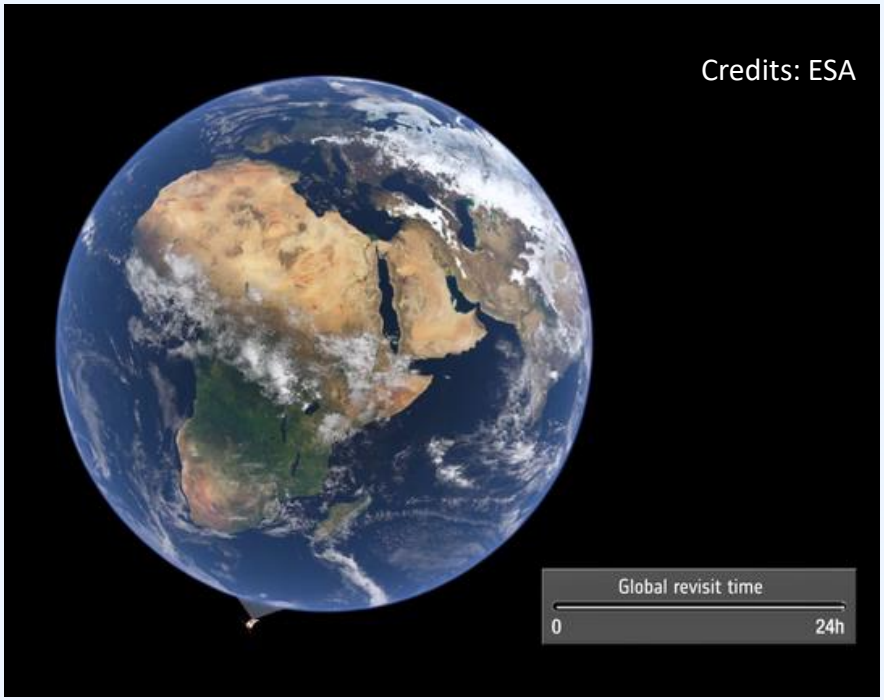
Sentinel-5P | Characteristics

- European Earth Observation satellite
- Single satellite mission carrying a single payload (TROPOMI)
- Swath: **2600 km,** allowing the whole planet to be mapped every 24 hours.
- Revisit time: **Daily** global coverage
- Spatial resampling: **5.5** km x **3.5** km
- **Orbit:** Polar, Sun-synchronous at an altitude of 824 km



Launch: 2017

Operational phase: early 2019

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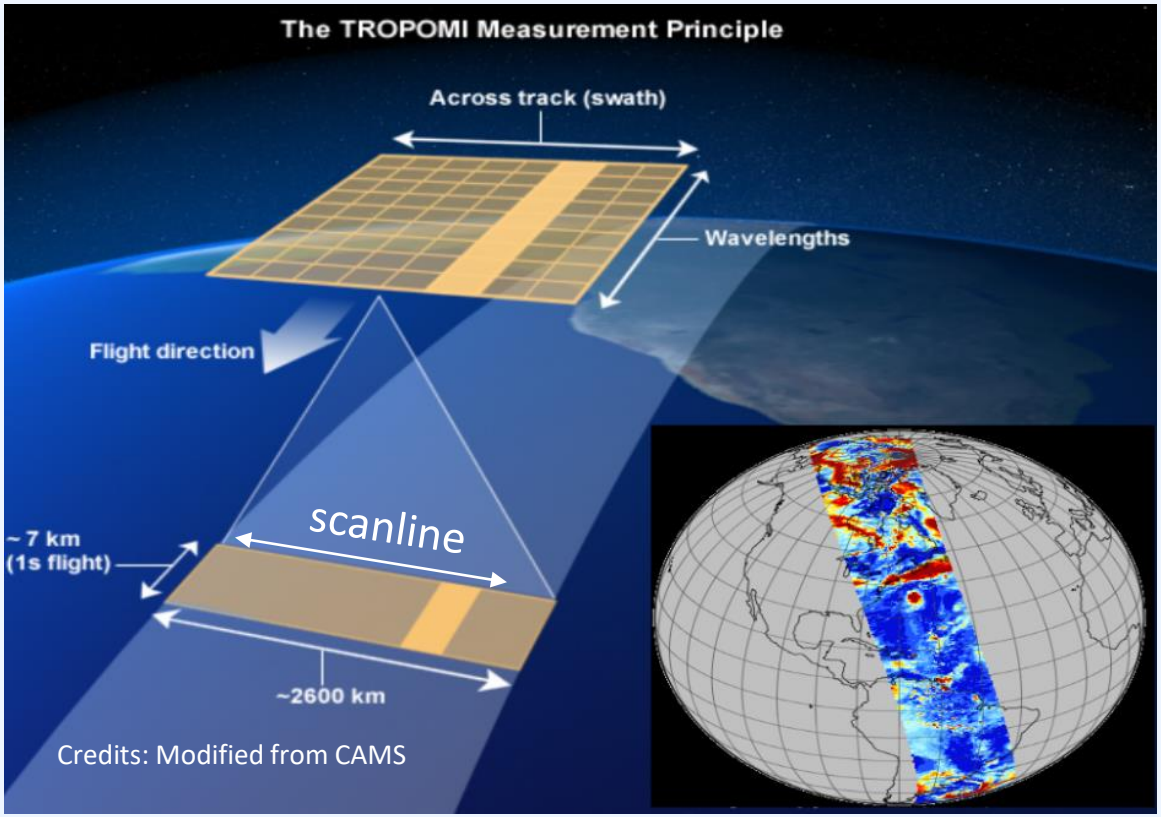
Sentinel-5P | Terminology



- A 1-second swath is called a scanline
- Each scanline is divided into 450 ground pixels
- We will find these terms as dimensions in native Sentinel-5P Level-2 products

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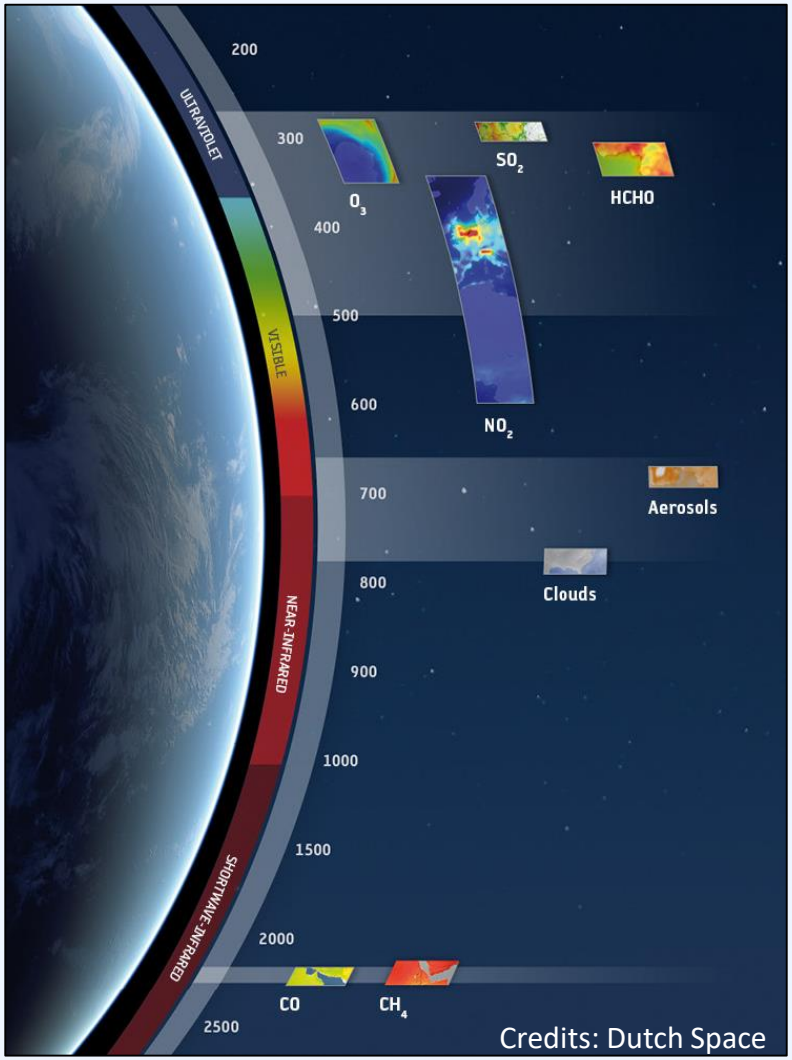
Sentinel-5P | TROPOMI

- **Instrument:** Tropospheric Monitoring Instrument (Tropomi)
- Passive sun backscatter imaging spectrometer
- Collects parts of the solar spectrum reflected back by the Earth
- Large spectral range for a large number of trace gas species detection
- 8 different spectral bands
  - 2 in ultraviolet (270 – 320 nm)
  - 2 in visible (320 – 500 nm)
  - 2 in NIR (675 – 775 nm)
  - 2 in SWIR (2305 – 2385 nm)



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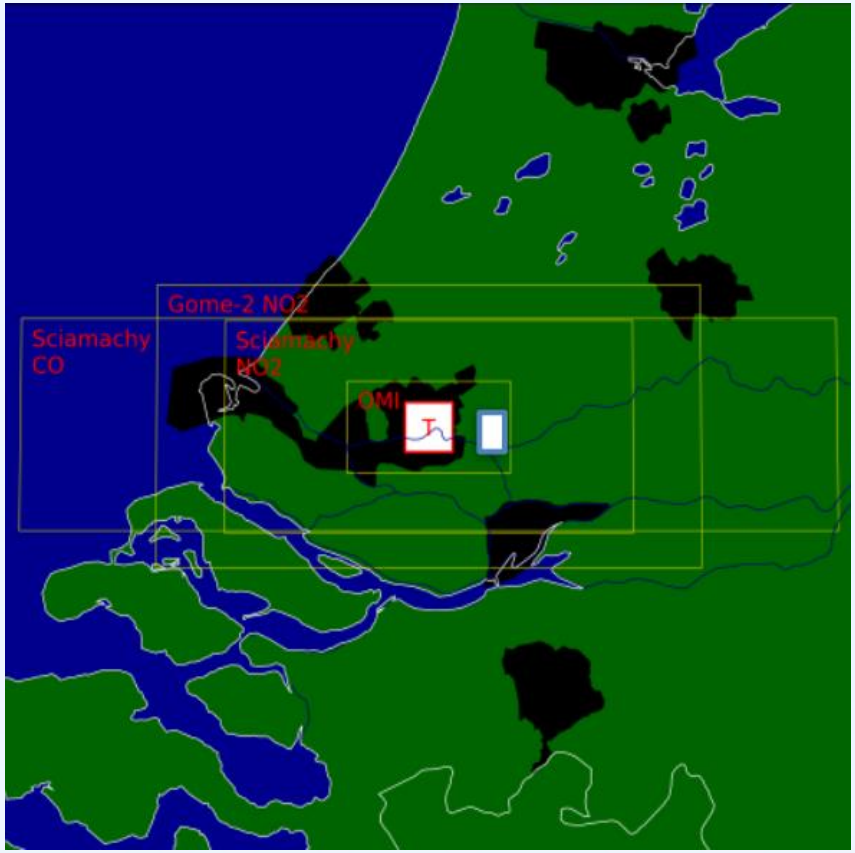
Sentinel-5P | TROPOMI

TROPOspheric Monitoring Instrument

Daily global coverage

High spatial resolution 3.5x5.5 km²



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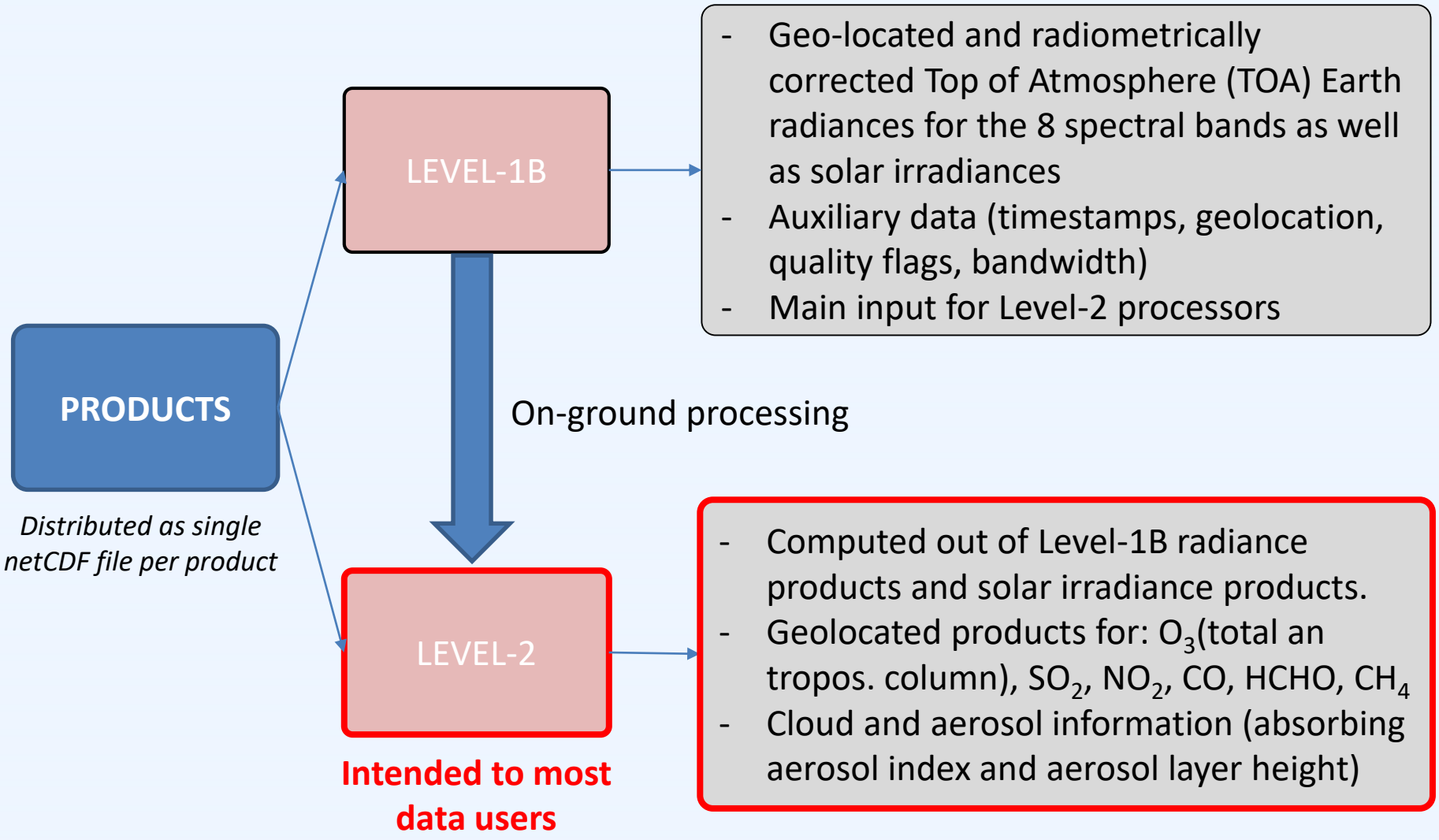
S5P Products



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S5P Products| L1B

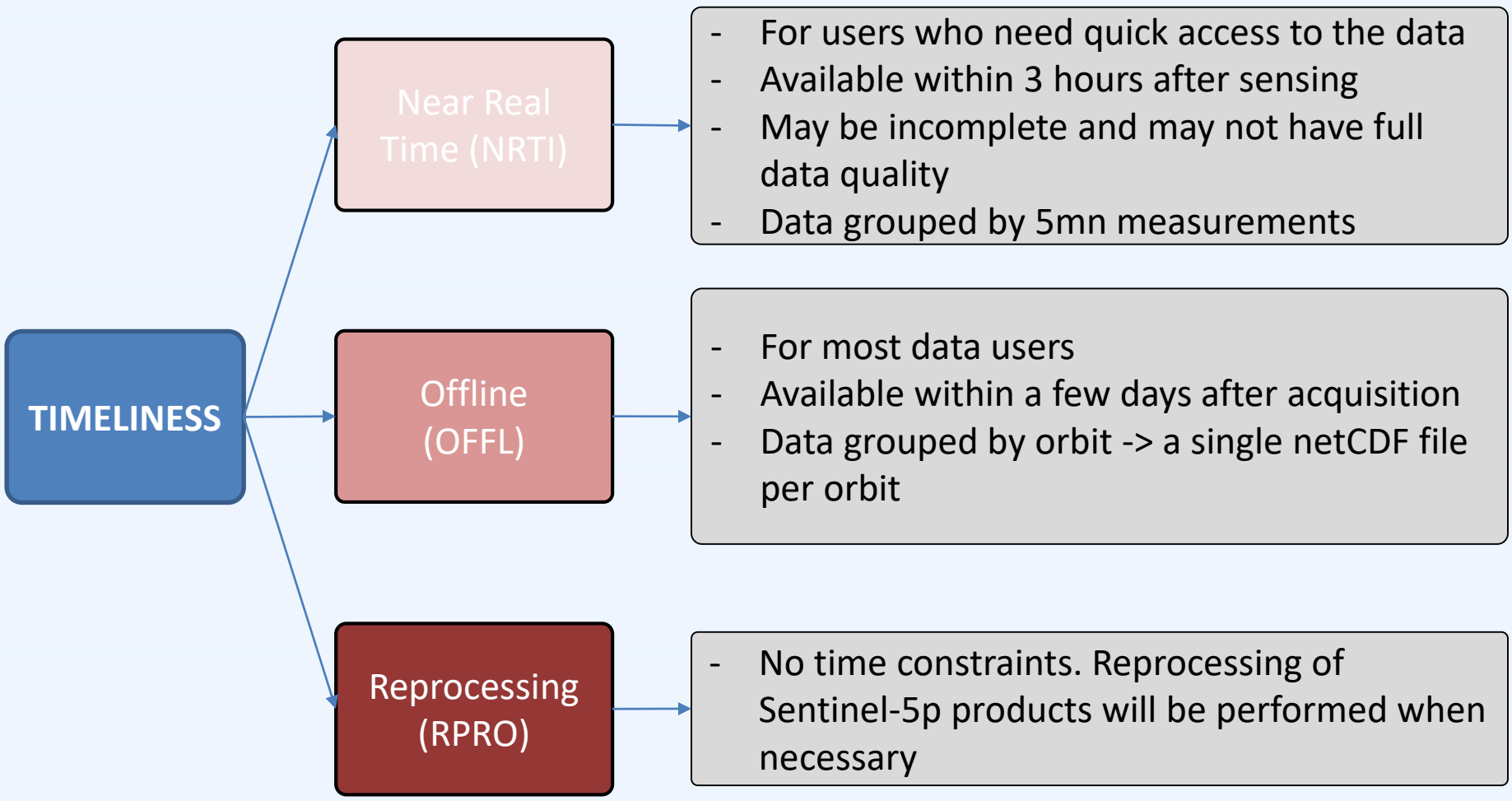
File type	Spectrometer	Spectral range [nm]	Comment
L1B_RA_BD1	UV	270 - 300	Radiance product band 1
L1B_RA_BD2		300 - 320	Radiance product band 2
L1B_RA_BD3	UVIS	320 - 405	Radiance product band 3
L1B_RA_BD4		405 - 500	Radiance product band 4
L1B_RA_BD5	NIR	675 - 725	Radiance product band 5
L1B_RA_BD6		725 - 775	Radiance product band 6
L1B_RA_BD7	SWIR	2305-2345	Radiance product band 7
L1B_RA_BD8		2345-2385	Radiance product band 8

TROPOMI Level 1B radiance products (Credit: S5P technical guide, ESA)

S5P Products| L2

PRODUCT TYPE	PARAMETER
L2__O3____	Ozone (O_3) total column
L2__O3_TCL	O_3 tropospheric column
L2__NO2___	Nitrogen Dioxide (NO_2) total and tropospheric columns
L2__SO2___	Sulfur Dioxide (SO_2) total column
L2__CO____	Carbon monoxide (CO) total column
L2__CH4___	Methane (CH_4) total column
L2__HCHO__	Formaldehyde (HCHO) total column
L2__CLOUD_	Cloud fraction, albedo, cloud height (pressure)
L2__AER_AI	UV Aerosol Index
L2__AER_LH	Aerosol Layer Height (mid-level pressure)

S5P Products | Timeliness



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S5P Products | Naming

S5P_OFFL_L2__O3____20200406T120948_20200406T121448_12855

Mission name, always S5P

Processing stream: Near Real Time **(NRTI),** Offline **(OFFL),** Reprocessing **(RPRO)**

Processing level: Level-1B **(L1B)**, Level-2 **(L2)**

Product identifier (Level-2): Cloud **(CLOUD),** HCHO **(HCHO),** SO_2 **(SO2),** O_3 Total Column **(O3)** O_3 Tropospheric Column **(O3_TCL**), Aerosol layer height **(AER_LH),** Ultra violet aerosol index **(AER_AI)** O_3 Full profile **(O3_PR),** NO_2 **(NO2),** CO **(CO),** CH_4 **(CH4),** NPP-VIIRS Clouds **(NO_BDx)**

Start and end of the granule in UTC (YYYYMMDDTHHMMSS) where T is a fixed character

Orbit number

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S5P Products | NetCDF format

netCDF File

Stores multidimensional scientific data (variables) such as temperature, humidity, pressure, wind speed, and direction

Self-describing → A netCDF file includes information about the data it contains, such as when data elements were captured and what units of measurement were used.

Portable → A netCDF file created on one type of operating system can often be read by software on another type of operating system.

Scalable → A small subset of a large netCDF file can be accessed efficiently without reading the entire file.

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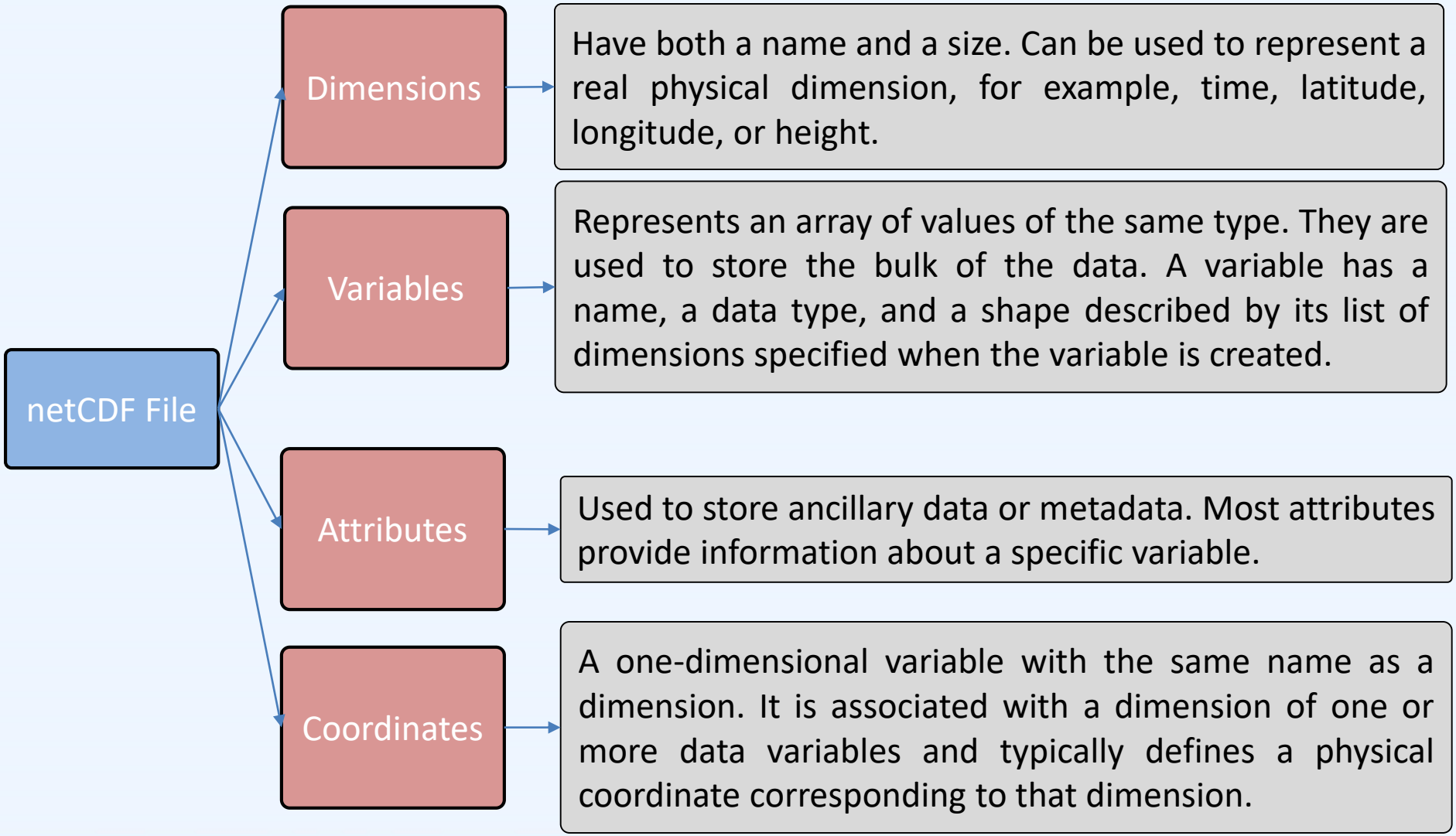
S5P Products | NetCDF format



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S5P products | Download

Where to find Sentinel-5P data ?

- **S5P data products are** provided by ESA
  - Copernicus Open Access Hub: https://scihub.copernicus.eu/
- More information on S5P products can be found at:
  - http://www.tropomi.eu
  - https://earth.esa.int/web/sentinel/technical-guides/sentinel-5p/products-algorithms
  - Contact: EOSupport@Copernicus.esa.int for any questions related to S5P data

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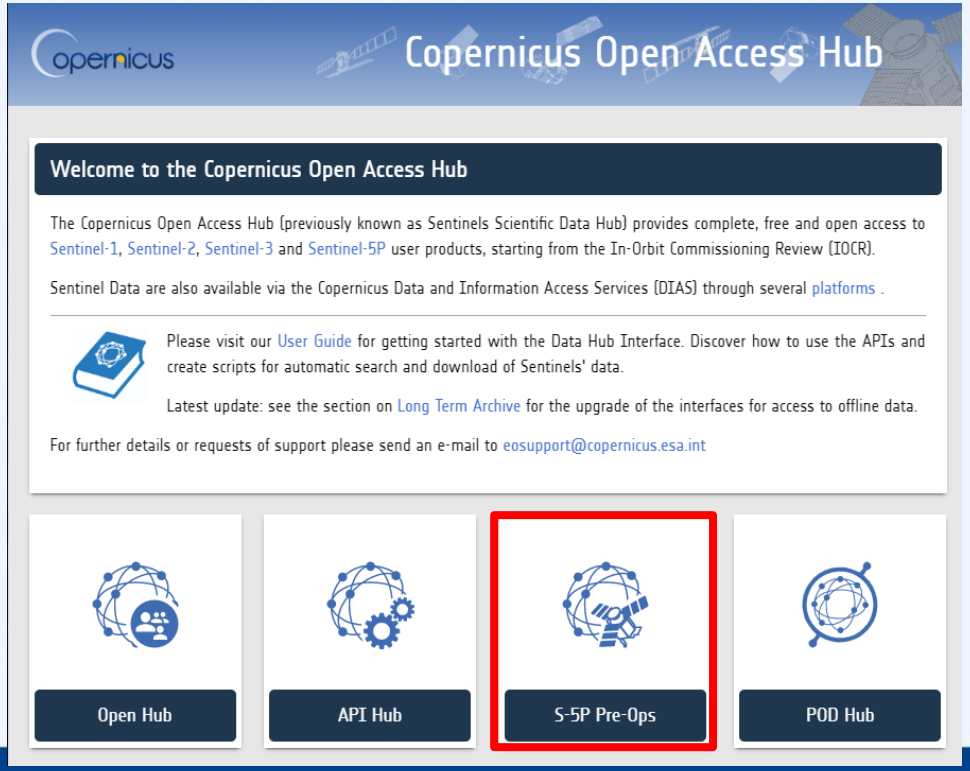
S5P products | Download

- **S5P products are** provided by ESA
  - Copernicus Open Access Hub: https://scihub.copernicus.eu/
  - S5P dedicated hub: **S-5P Pre-Obs**



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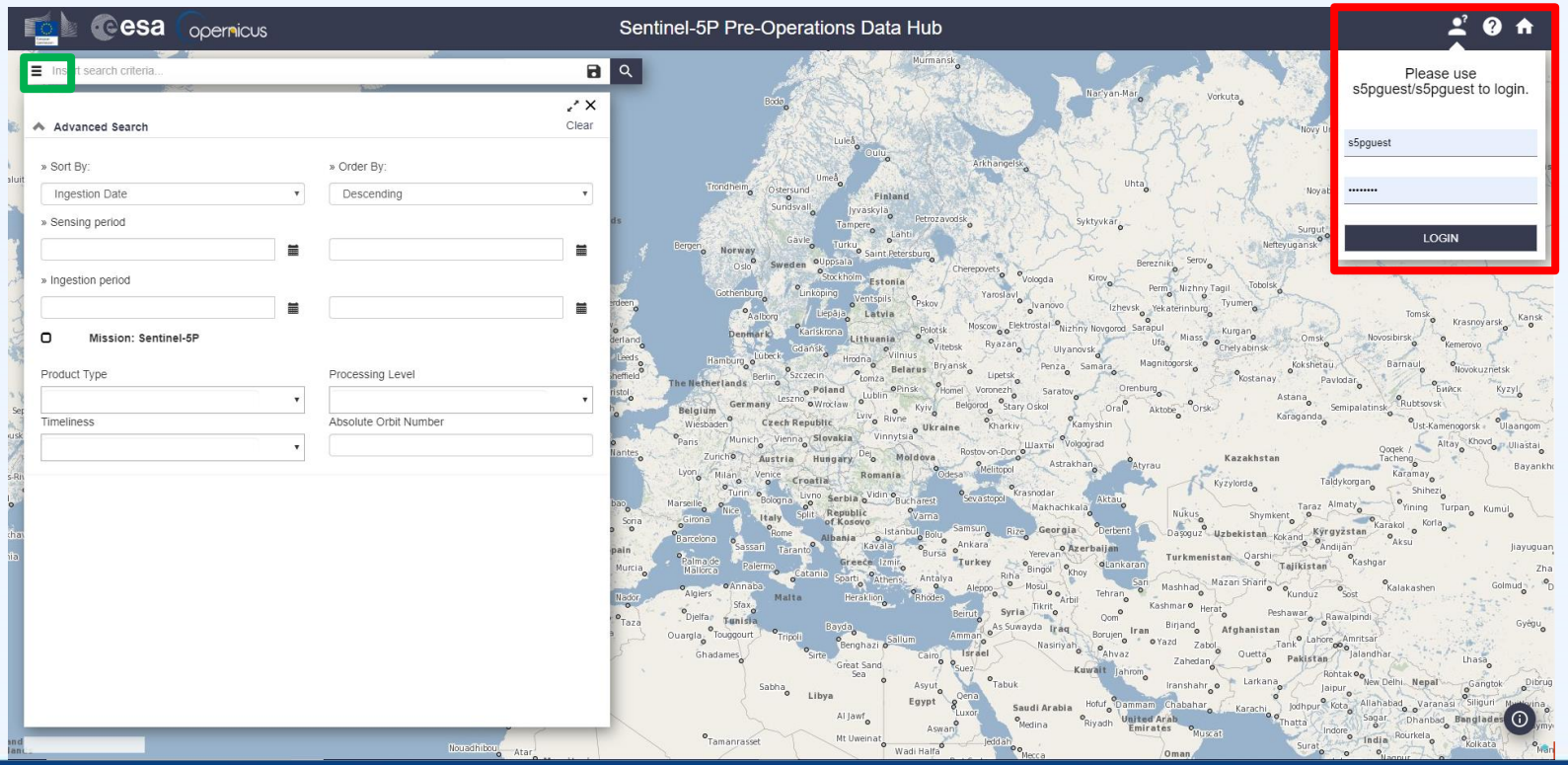
S5P products | Download

- **S-5P Pre-Obs Interface**
  - **Login/Password: s5pguest/s5pguest**
  - Open the product searching tool by clicking on the **top-left button**



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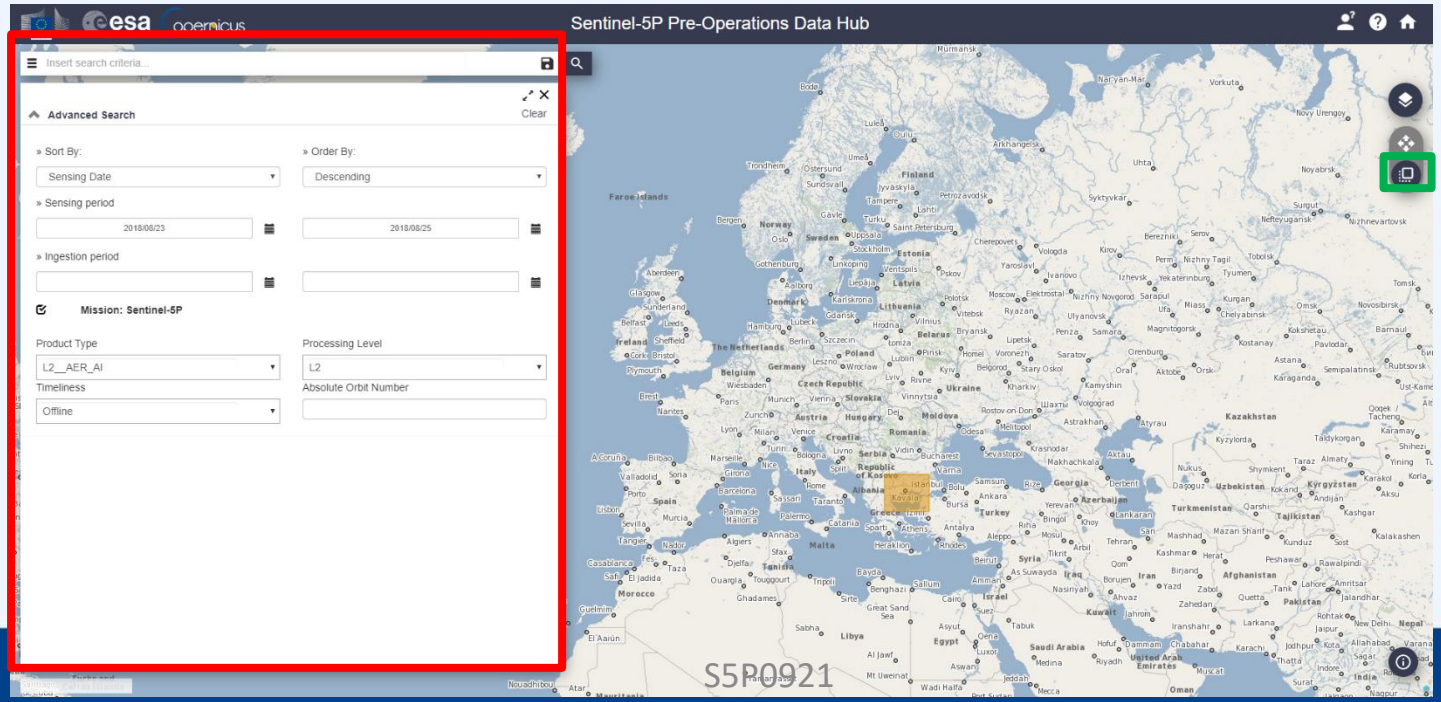
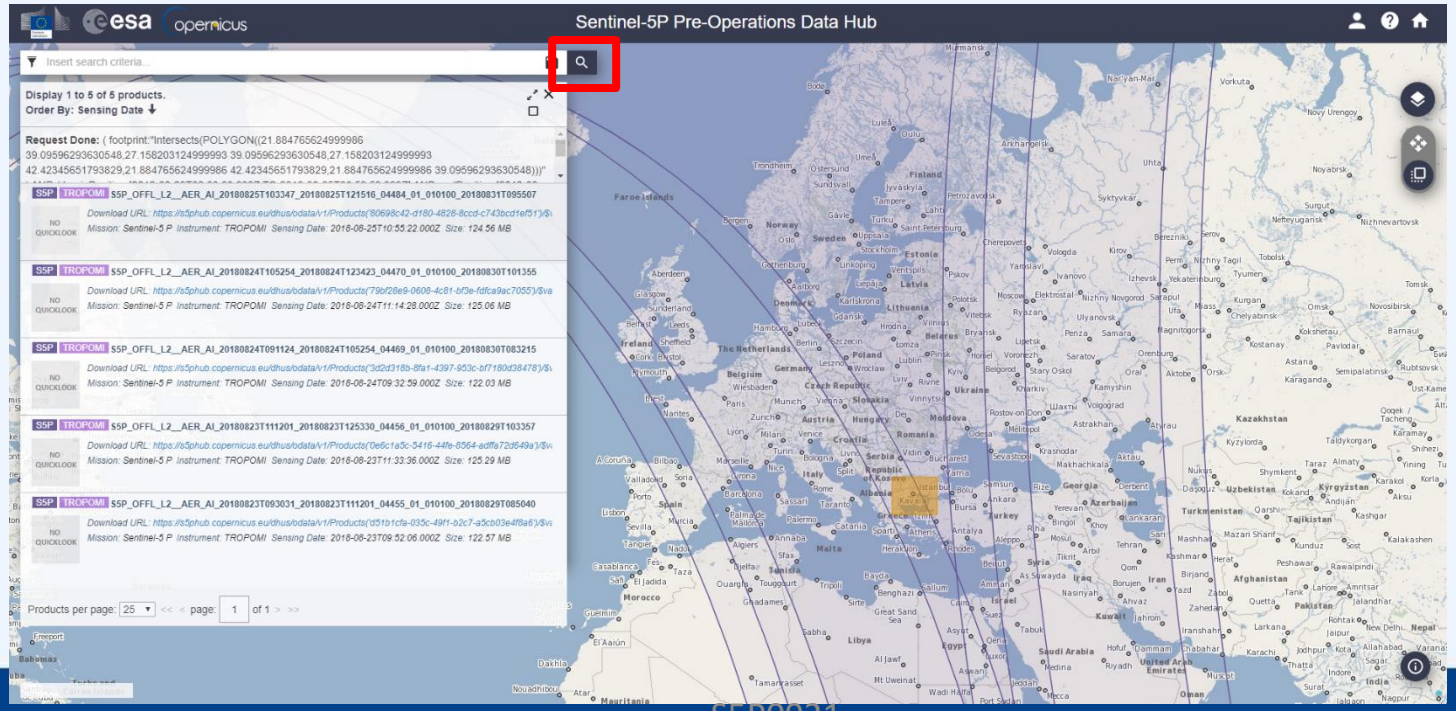
S5P products | Download

- **S-5P Pre-Obs Interface**
  - Use the **left pannel** to define your search criteria (date of interest, product type, Timeliness, processing level)
  - Hit the **double square button** on the right, to draw your area of interest



S5P products | Download

- **S-5P Pre-Obs Interface**
  - Hit the **search button**!
  - The purple contours show the geographical hold of each product
  - You can then download any product you want



S5P0921

Outline

- Sentinel-5P
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- **Focus on NO2**
- The Atmospheric Toolbox
- Exercises

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NO2 | Background

- Nitrogen Dioxide is an important trace gas in the Earth's atmosphere
- Brown gas responsible for the colour of photochemical smog
- Most of the NO_2 is in the troposphere
- Enters the atmosphere as a result of:
  - Anthropogenic activities (traffic, industrial fossil fuel combustion, biomass burning, ships)
  - Natural processes (wildfires, lightning)
- Irritating gaz -> Increases the intensity and frequency of asthma attacks

NO2 | Background

- NO_2 has a short lifetime in the atmosphere: from a few hours up to a half day
- NO2 concentrations are indicators on changes in economic slowdowns
- Remains relatively close to its source -> NO2 sources well detectable from space.
- Measures still need to be completed by ground-based measurements
- NO2 concentrations in the atmosphere vary widely from day to day (emissions and weather conditions variations)
- To identify longer-term variations, two-week averages are computed

NO2 | Background

- More information on NO2 effects and the computation method for TROPOMI can be found here
- If you are more interested in NO2 retrieval processes from satellite measurements, visit the EUMETSAT second Joint school on Atmospheric Composition.
  - Presentation on NO2 column computation from S5P measurement
  - Associated YouTube video
- S5P L2 NO2 Product User Manual
- Easily check NO2 concentrations maps on the Copernicus S5P Mapping Portal

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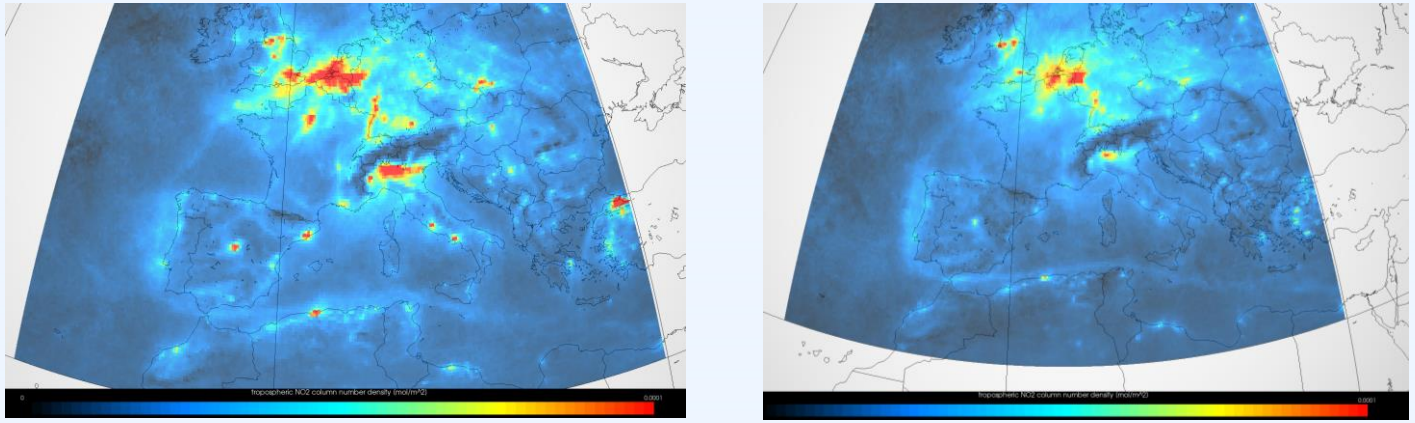
NO2 | S5P Products

- Available quantities in the product:
  - **Tropospheric** vertical column of NO_2 (mol/m² or molec/cm²): for a ground pixel, integrated amount of NO_2 in the **troposphere** (lower layer of the atmosphere)
  - **Stratospheric** vertical column of NO_2 (mol/m² or molec/cm²): for a ground pixel, integrated amount of NO_2 in the **stratosphere** (upper layer of the atmosphere)
  - **Total** vertical column of NO_2 (mol/m² or molec/cm²) in the **atmosphere**



TROPOMI averaged tropospheric NO2 column over Europe in March 2019 (left) & March 2020 (right)

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Outline

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The Atmospheric Toolbox

- **Atmospheric Toolbox**
  - Open source software for ingesting, processing and analyzing atmospheric remote sensing data
  - Developed, designed and maintained under ESA contracts
  - Support several instruments: TROPOMI, GOME-2 and IASI, OMI, TES and MLS, MIPAS and SCIAMACHY
  - Help can be found at: https://atmosphericatoolbox.org/
    Extremely useful forum for questions : https://forum.atmosphericatoolbox.org/

The Atmospheric Toolbox

- **3 components:**
  - **HARP:**
    - Toolset for ingesting and processing atmospheric data
    - Set of command line tools, a library of analysis functions and direct import/export interfaces for Python, IDL and MATLAB
  - **VISAN:**
    - Visualization and analysis application for atmospheric data.
    - Commands provided through Python
    - 2D plots and worldplots
  - **CODA:**
    - Direct reading access to product data thanks to a C library
    - Other interfaces are allowed e.g.: Fortran, IDL, MATLAB & Python

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  - **Introduction**
  - Starting with the RUS environment
  - Starting with Panoply
  - Creation of NO2 gridded product
  - Jupyter Notebook exercises

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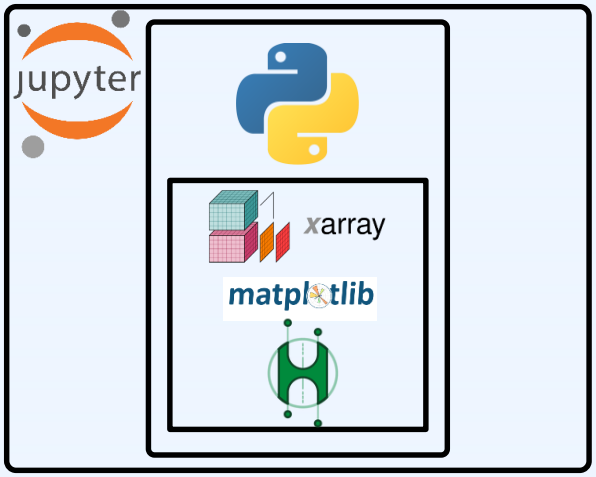
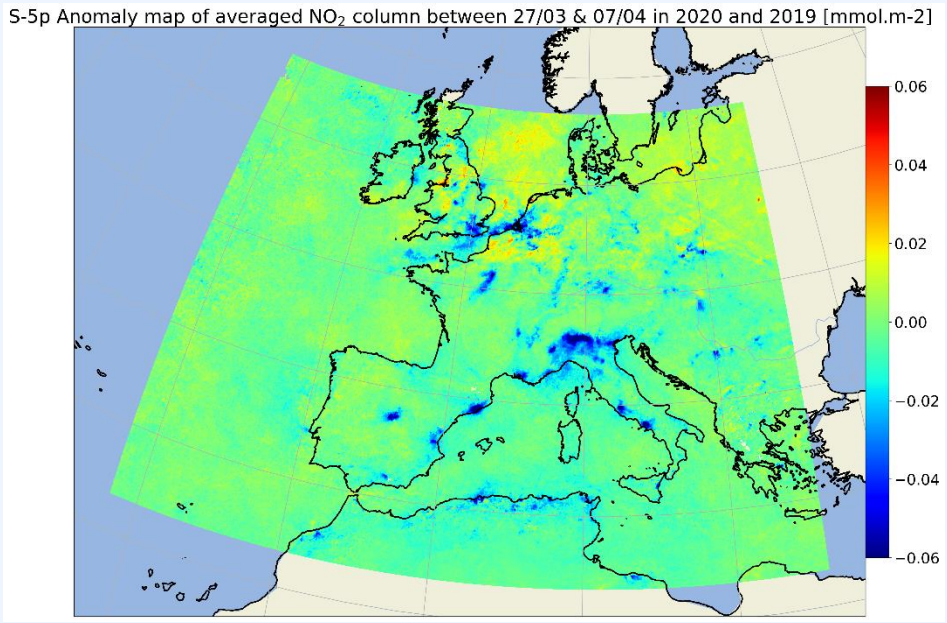
Exercise | Introduction

OBJECTIVE

Monitor the tropospheric NO2 in the atmosphere and assess the impact of anthropogenic activities on air quality.

TOOLS

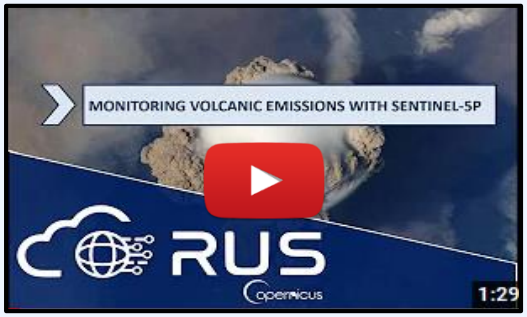




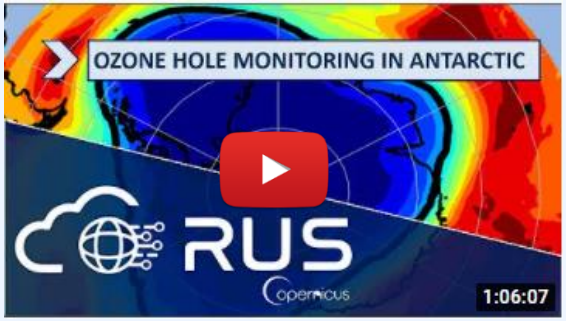
Exercise | Introduction

ATMO01 Available in YouTube
https://bit.ly/2Vcz7eP

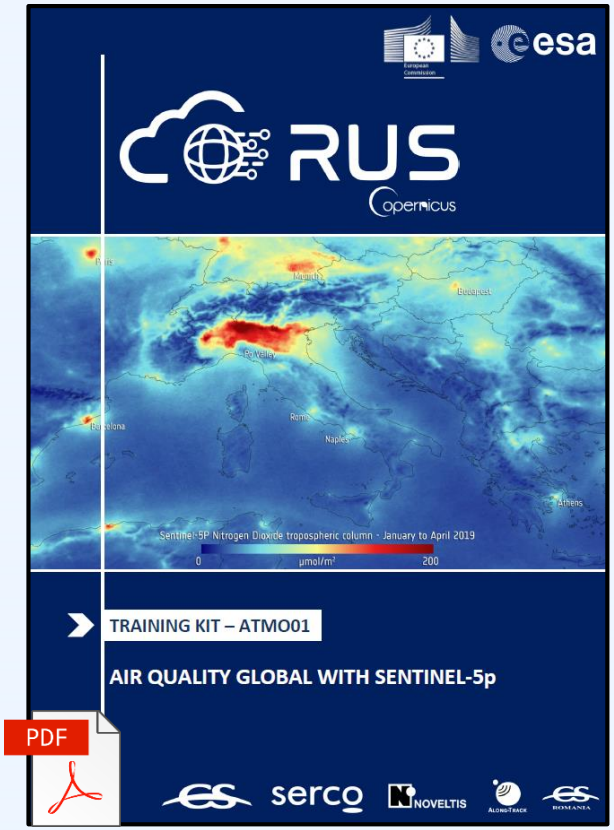
ATMO02 Available in YouTube
https://bit.ly/2TgMX37



ATMO03 Available in YouTube
https://bit.ly/3x9p4ZR



ATMO04 Available in YouTube
https://bit.ly/3BSuhHt



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  - Jupyter Notebook exercises

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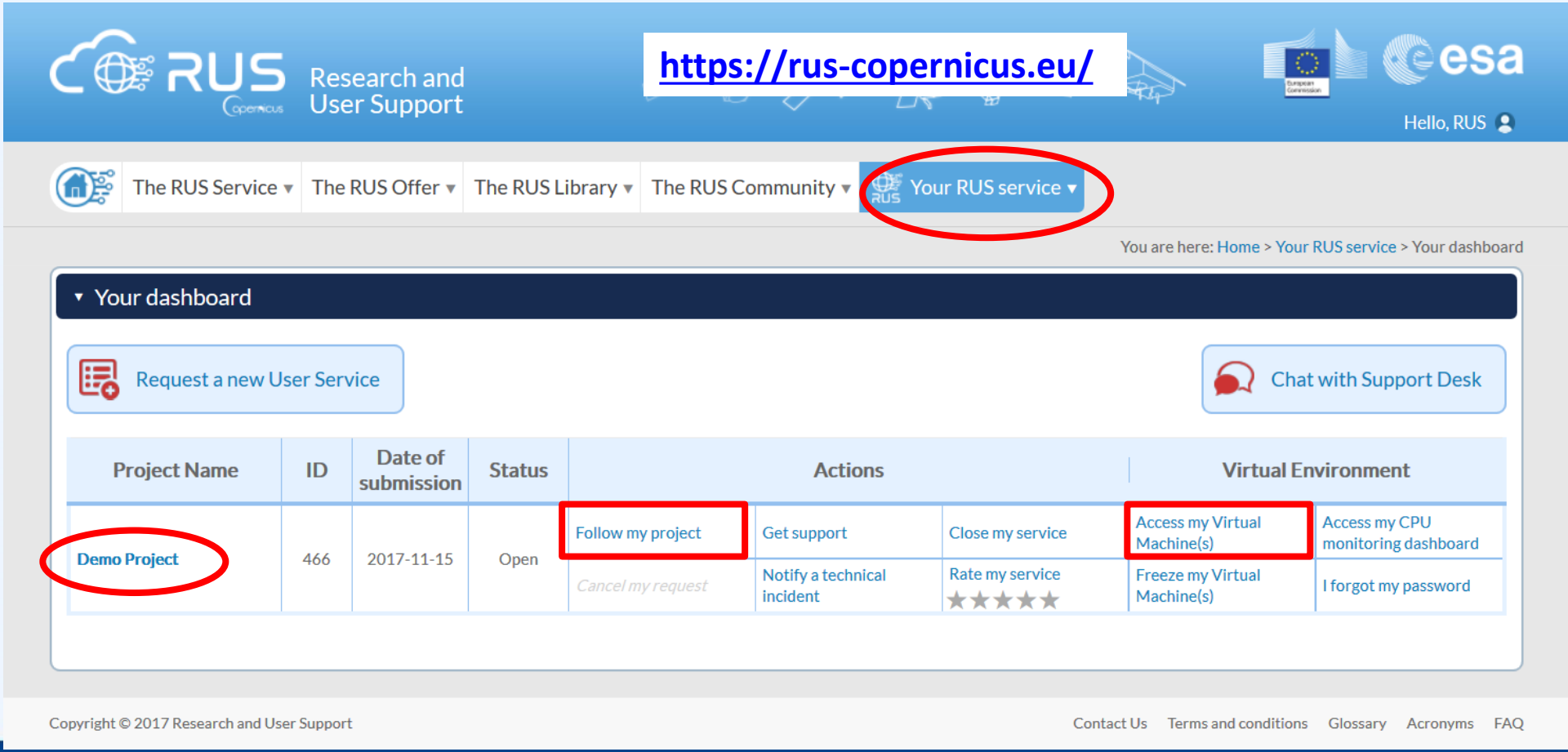
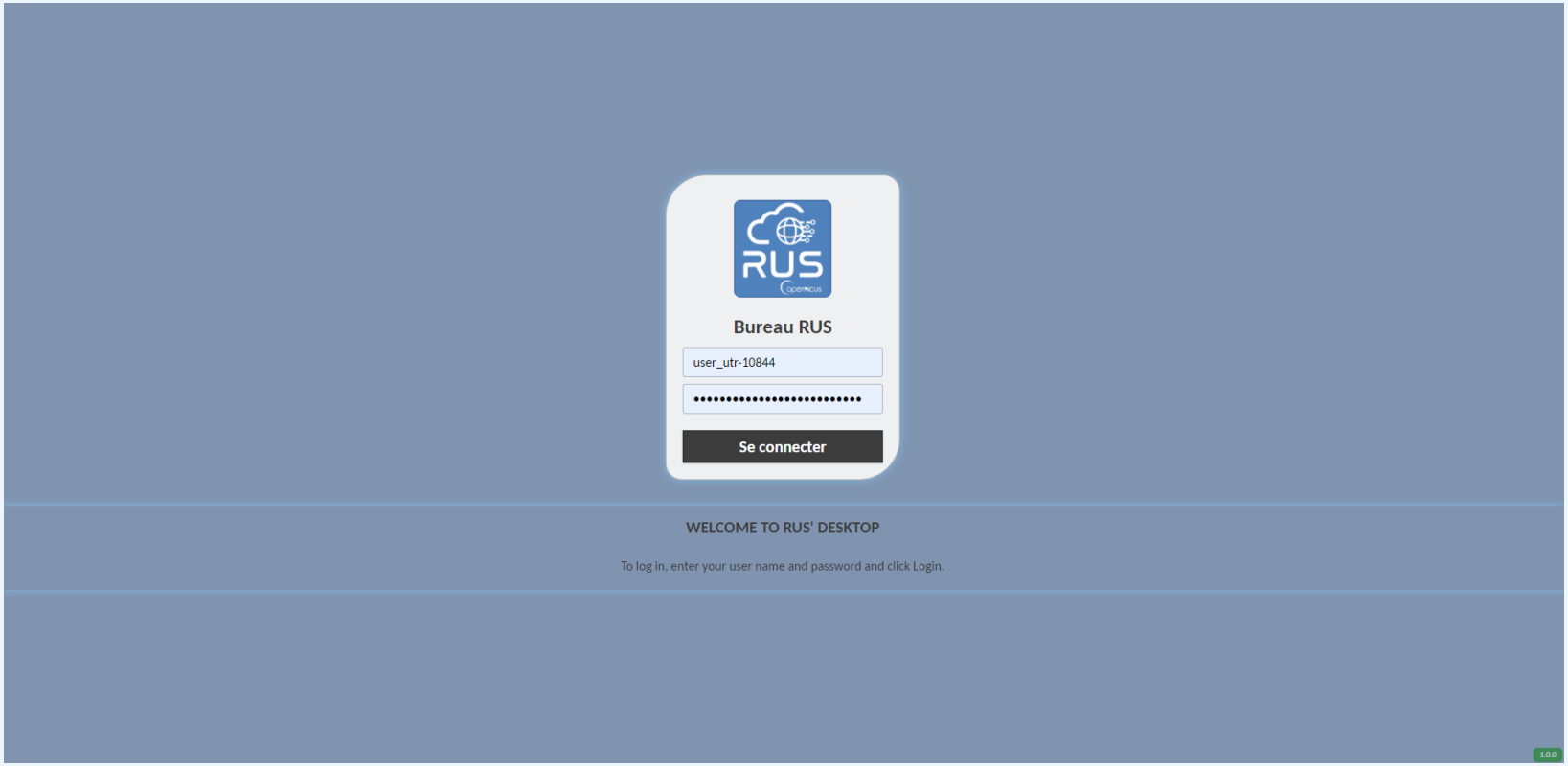
The RUS virtual machine

- **How to connect to your RUS virtual machine**
  - Go to your Virtual Machine (VM) from your RUS dashboard or using the direct URL you received by email in a web browser



The RUS virtual machine

- **How to connect to your RUS virtual machine**
  - Authorize the access certificate
  - Log in with your **RUS VM identifiers** (in the Follow my project tab of your dashboard)



The RUS virtual machine

- **Exploring the desktop of your Virtual Machine**

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The RUS virtual machine

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The RUS virtual machine

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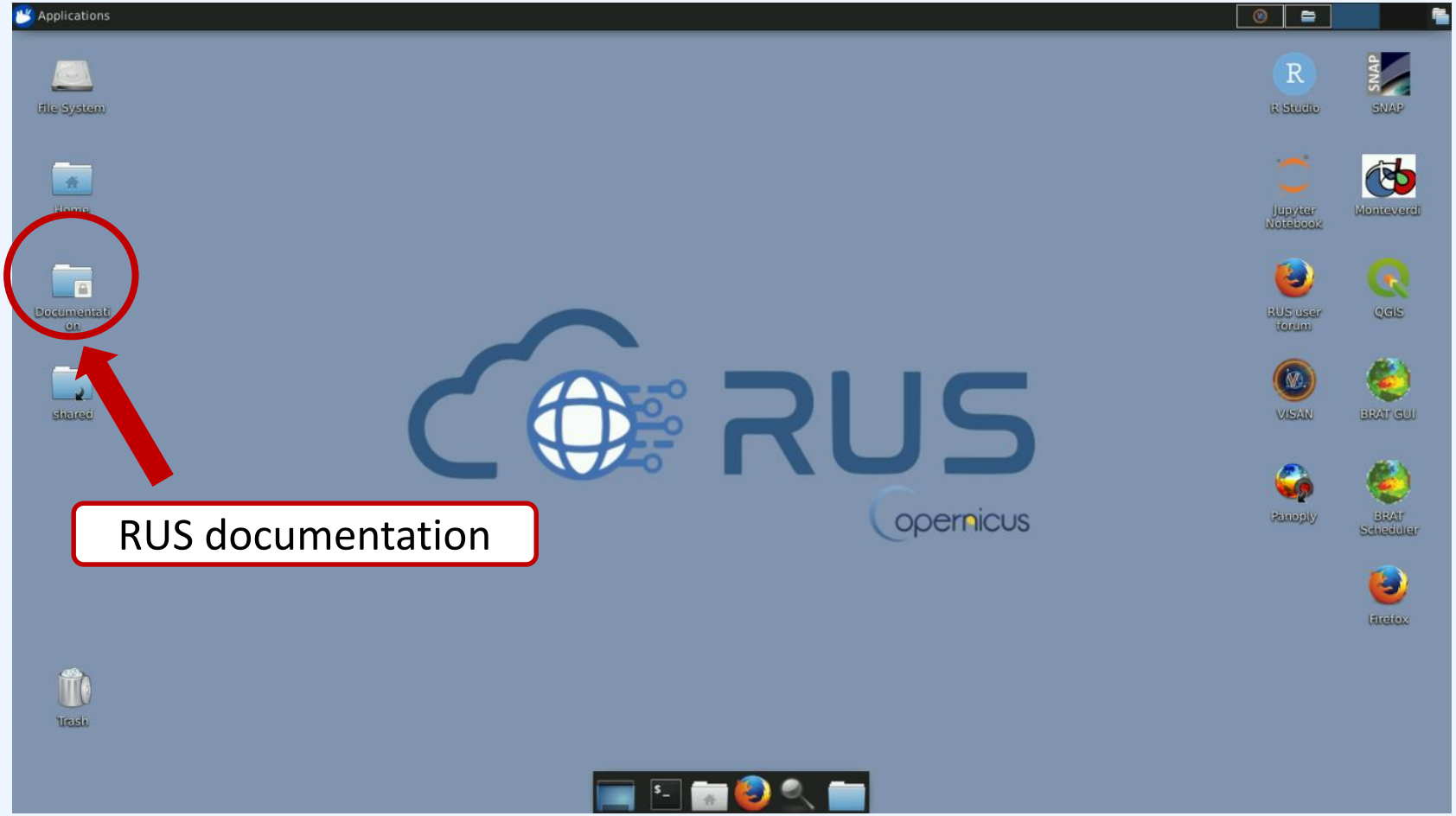

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The RUS virtual machine

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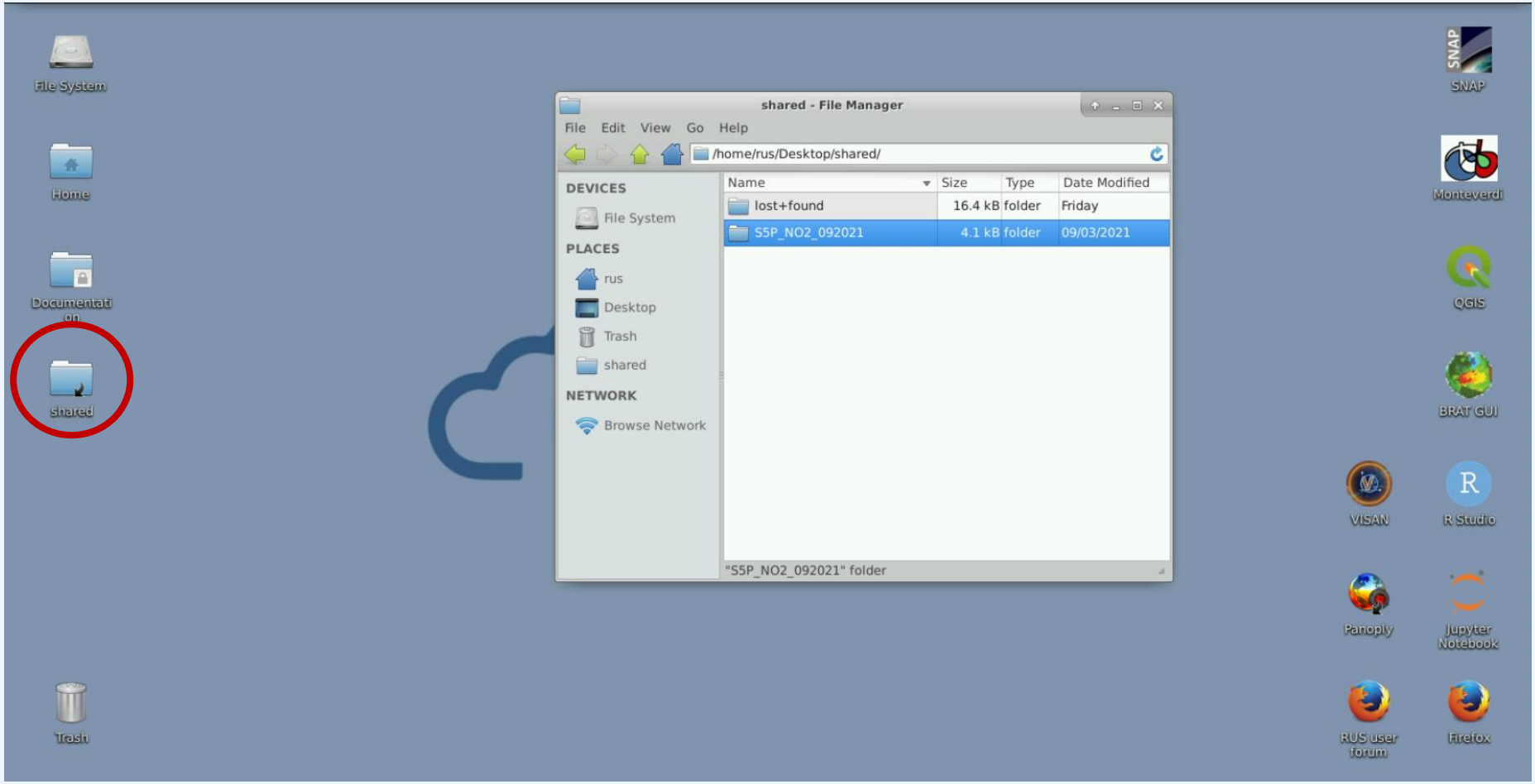

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The RUS virtual machine

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  - **Starting with Panoply**
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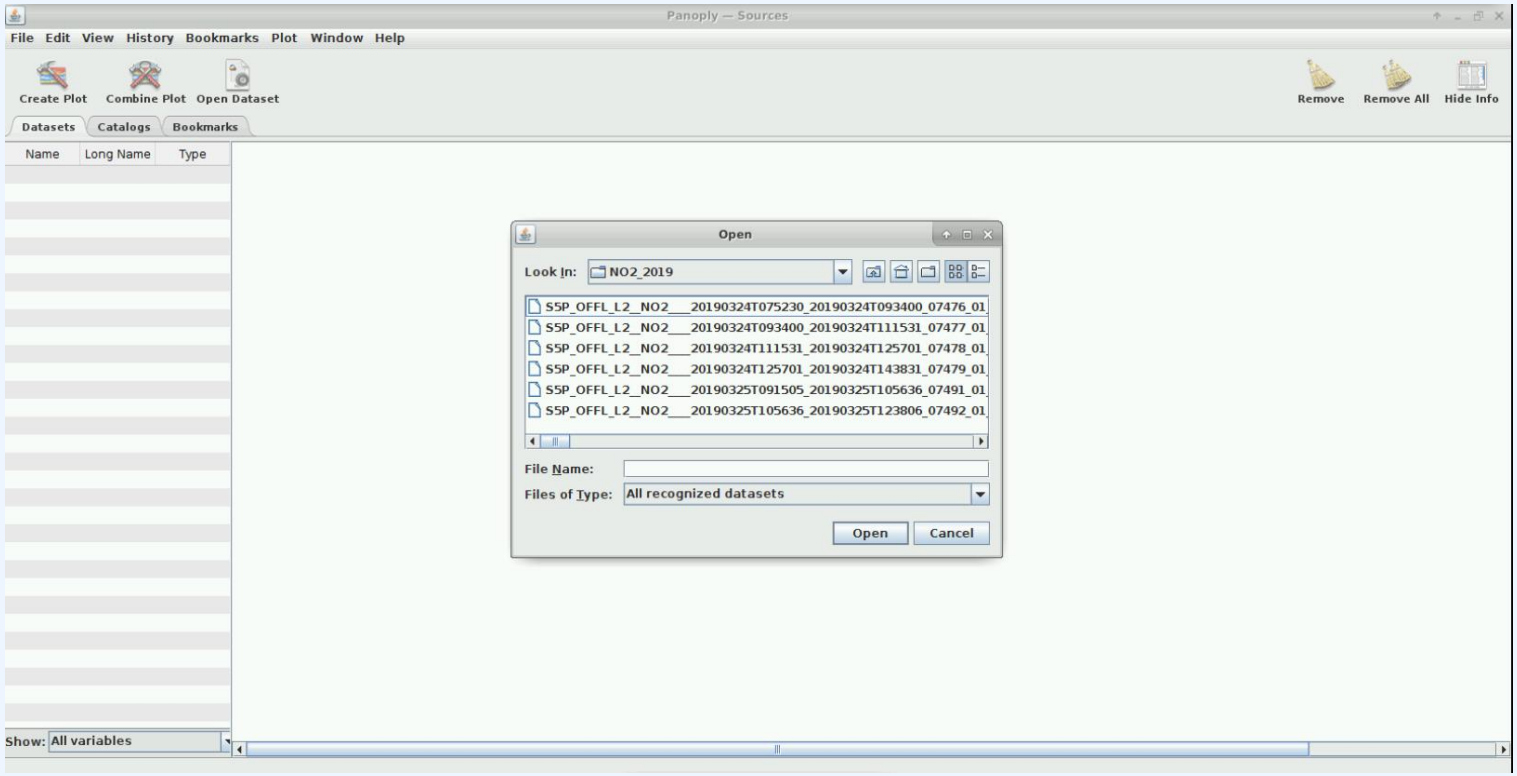
About Panoply

- Panoply plots geo-referenced and other arrays from netCDF, HDF, GRIB and other datasets
- It is a cross-platform application that runs on Macintosh, Windows, Linux and other desktop computers.
- Link to panoply website: https://www.giss.nasa.gov/tools/panoply/
- Download panoply

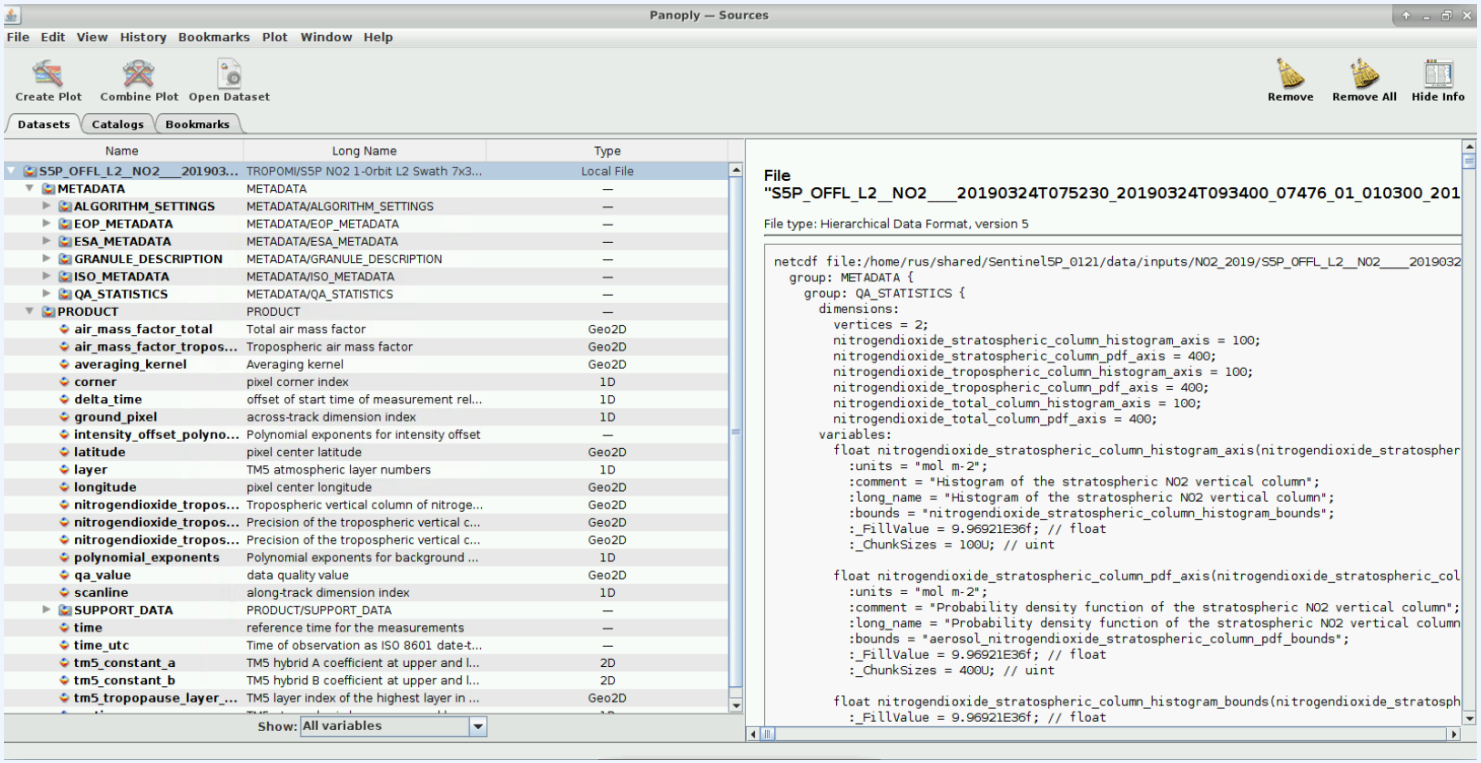
Exploring a product

- Let's start exploring a S5P L2 product!
- Open a product from /shared/S5P_NO2_092021/training_NO2_22092021/Original/NO2_24032019



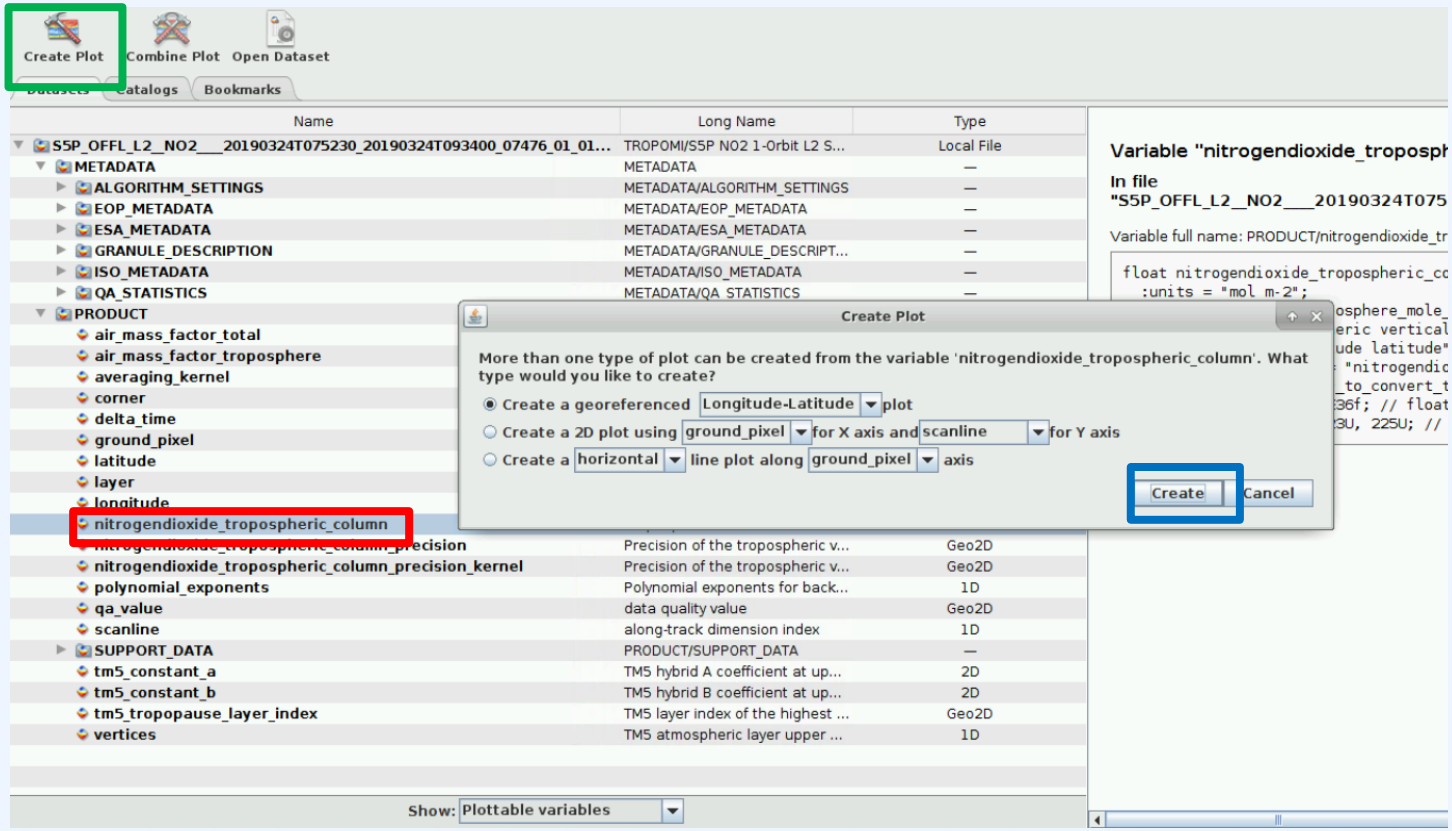
Exploring a product

- There are two groups in each Sentinel-5P netCDF file
  - **METADATA:** This is a group to collect metadata items (facilitate dataset discovery)
  - **PRODUCT:** This group stores the main fields (latitude, longitude, main variables)



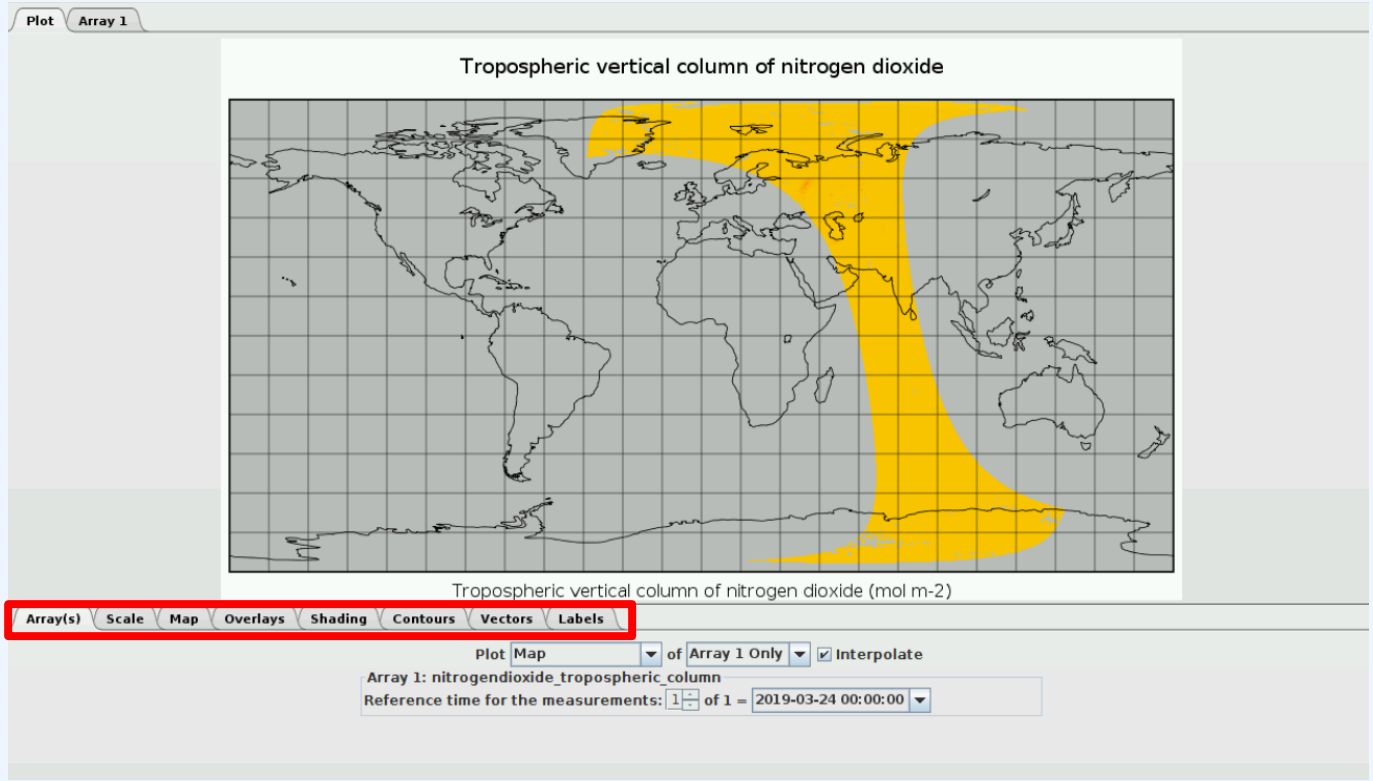
Exploring a product

- Plotting an imported product in Panoply
  - Select the **nitrogendioxide_tropospheric_column** and hit **Create plot**
  - Finally click on **"Create"**



Exploring a product

- The plot of the variable opens
- All the **tabs down the plots** are very useful to set up the plot options



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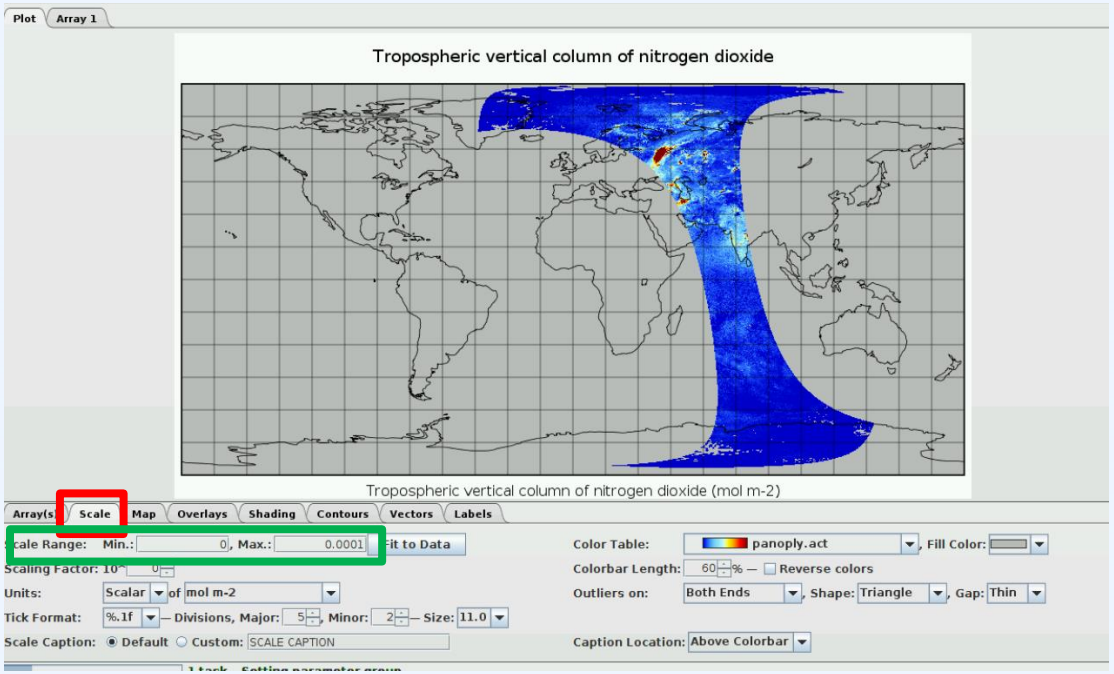
Exploring a product

- Plotting an imported product in Panoply
  - Select **Scale** and change the Scale Range :
    - **Min : 0,0000 mol.m-2**
    - **Max : 0.0001 mol.m-2**
  - Some NO2 tropospheric column values are negative
  - This is expected when the NO2 tropos. Column value is low and the error is high
  - As the error is random, some values end up being below 0.



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L3 NO2 gridded product

Creation of L3 gridded products

- 1 S5P file per orbit. What if we want to map a whole day over a user defined area?
- Original S5P data is binned by time, not by latitude/longitude
- Before merging several L2 products having different spatial grids, we need to convert them to L3 products and create a common regular grid for all orbits

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L3 NO2 gridded product

The HARP bin_spatial() operation: practical use

- **bin_spatial(lat_edge_length, lat_edge_offset, lat_edge_step, lon_edge_length, lon_edge_offset, lon_edge_step):** for all variables in a product, map all time samples onto a regular spatial lat/lon grid
  - Example: bin_spatial(**120**,**-90**,**0.5**,**720**,**-180**,**0.5**) bins all samples into a regular 0.5*0.5 lat/lon grid where:
    - Lat min=**-90**
    - Lat max=**-90**+**120***0.5=-30
    - Lon min=**-180**
    - Lon max= **-180**+**720***0.5=180
  - The choice of the **spatial resolution (lat/lon_edge_step)** and the boundaries (**lat/lon_edge_offset**, **lat/lon_edge_length**) are up to the user
  - A better resolution and a larger area of interest increase the computing time
  - A 0.5*0.5° resolution is sufficient for this example but you can increase it later on to practice.

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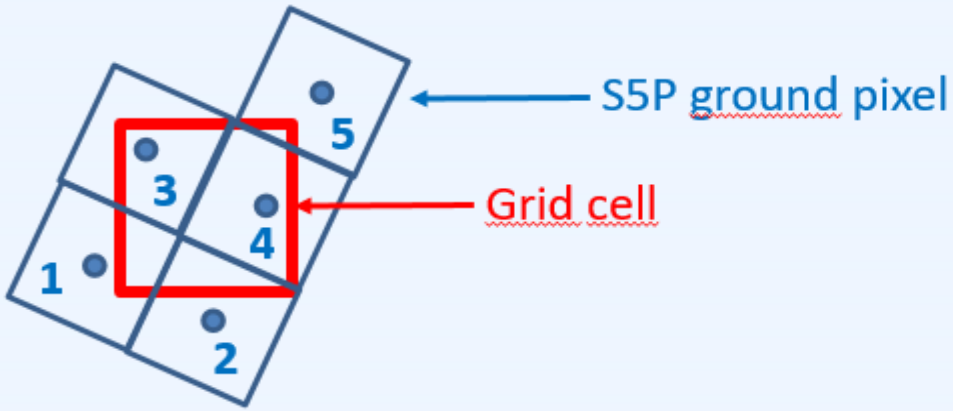
L3 NO2 gridded product

How does bin_spatial() operate?

- If only lat/lon center coordinates of gound pixels in the products: **bin_spatial()** performs an average of all values whose center point falls in the grid cell: Case 1
- S5P products provide with lat/lon_bounds variables: **bin_spatial()** proceeds to an area weighted average based on ground pixel areas and grid cell intersection (a_i): Case 2



$$\text{Value}=\frac{Pixel_3+Pixel_4}{2}$$

$$\text{Value}=\frac{\sum_{i=1}^{5} a_i * Pixel_i}{\sum_{i=1}^{5} a_i}$$

L3 NO gridded product

The HARP derive() operation: practical use

- When spatially binning a product with **bin_spatial(),** only the lat/lon_bounds of the grid cells will be saved in the output product.
- Most software and GIS tools will expect the lat/lon center coord. of the pixels to plot the NO2 column.
- To write the lat/lon center coord. of the spatial grid in the output use:
  - Derive(variable {dimension})
  - Example: ‘derive(longitude {longitude});derive(latitude {latitude})’

L3 NO2 gridded product

The HARP comparison filter operation: practical use

- Filter a dimension for all variables in the product such that items for which the value of the provided variable does not match the expression get excluded
- Example: ‘longitude>0 [degree_east]; ’
- To filter by variable, use the keep() operation
  Example keep(latitude,longitude, tropospheric_NO2_column_number_density) if you wish to only keep these three variables
- Restricting the output product to your variable of interest will greatly enhance the computing time.

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L3 NO2 gridded product

HARPCONVERT Command line tool: practical use

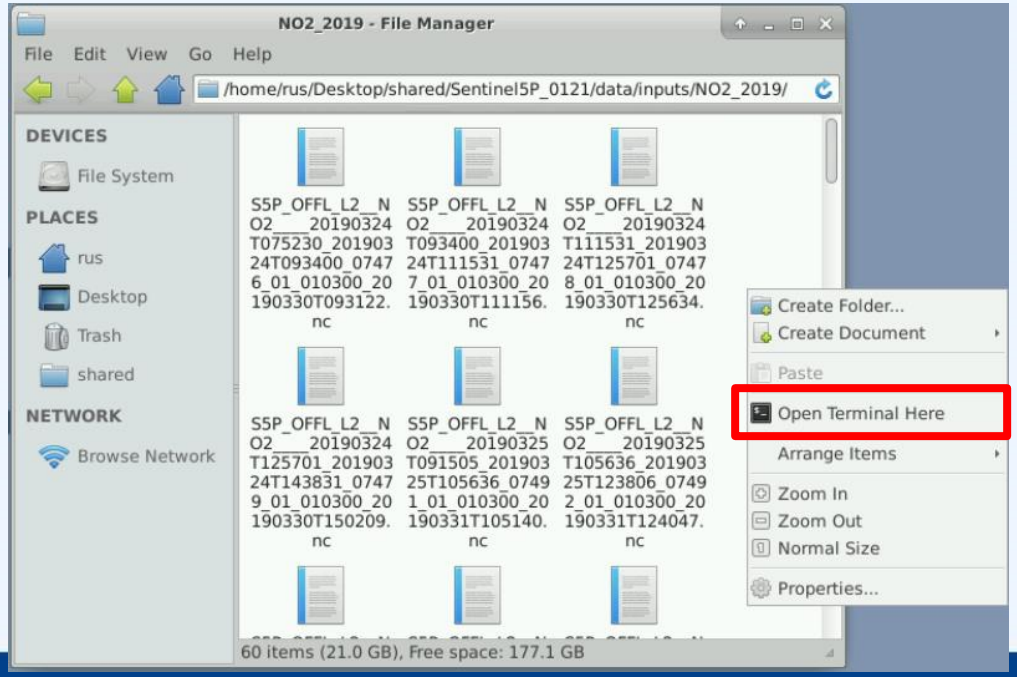
- Allows to define a list of operations to apply to each product : **-a 'operation_list()'**
  - Example: **-a 'bin_spatial(…); derive(…)'**
- Allows to define ingestion options: **-o 'ingestion_option'**
- Allows to define the output format: **-f 'format'**
  - The default NETCDF format will be kept during the exercise
  - HDF4 and HDF5 are supported too
- When ingesting products, HARP will rename the product variables. The HARP variable mapping for S5P products is available here.

L3 NO2 gridded product

HARPCONVERT Command line tool: practical use

- In a file browser, from the working directory, go to **/shared/S5P_NO2_092021/training_NO2_22092021/Original/NO2_24032019/**
- In this directory, all S5P NO2 products on March 24th have been downloaded ahead of this training session

- Hit the right button of your mouse and **Open Terminal Here**



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L3 NO2 gridded product

HARPCONVERT Command line tool: practical use

- **harpconvert –a 'operations_list' –o 'ingestion_option' input_file output_Directory/output_file**
- Grid cell area is fixed at 0.5*0.5 to avoid long processing time
- No ingestion option

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L3 NO2 gridded product

HARPCONVERT Command line tool: practical use

- *Right click on the NO2_command_line.sh file in the AuxData/bash/ folder and select Open with -> Open with « Mousepad »*
- In Mousepad select View -> Color Scheme -> Classic
- Copy/Paste the following command line in the open terminal and press Enter
- **harpconvert -a 'latitude > -50 [degree_east]; latitude < 50 [degree_east]; bin_spatial(200,-50,0.5,360,0,0.5); derive(latitude {latitude}); derive(longitude {longitude}); keep(latitude,longitude,tropospheric_NO2_column_number_density)' /shared/S5P_NO2_092021/training_NO2_22092021/Original/NO2_24032019/S5P_OFFL_L2__NO2____20190324T075230_20190324T093400_07476_01_010300_20190330T093122.nc /shared/S5P_NO2_092021/training_NO2_22092021/Processing/pre_processed_files/one_file/S5P_converted_onefile.nc**

L3 NO2 gridded product

HARPCONVERT Command line tool: Visualizing the output

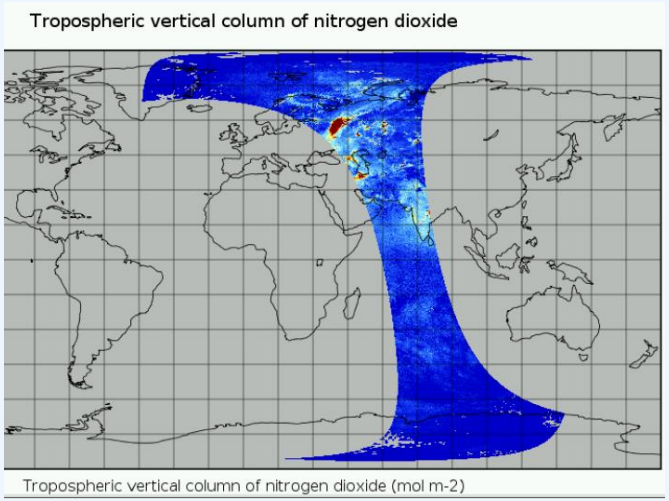
- Import the **S5P_converted_onefile.nc** product in Panoply (File -> Open…)
- File Path **/shared/S5P_NO2_092021/training_NO2_22092021/Processing/pre_processed_files/one_file/**
- All groups have disappeared, and only the *longitude, latitude and tropospheric_NO2_column_number_density* variables are present as requested by the *keep()* operation
- Double click on the **tropospheric_NO2_column_number_density** variable and hit « Create »

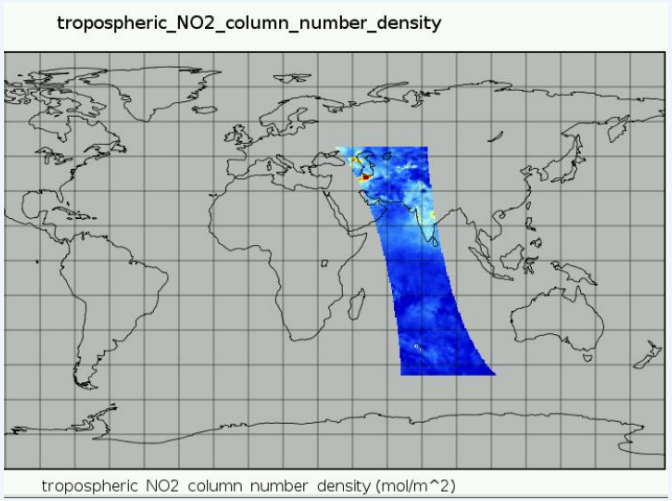
L3 NO2 gridded product

HARPCONVERT Command line tool: Visualizing the output

- The product has been regridded into a lower resolution
- Later, you can try to regrid it into a higher resolution!
- Data above 50°N and below 50°S have been discarded thanks to a filter on latitude
- Set the Min/Max of the colorbar to 0.0/0.0001

L2 NO2 product





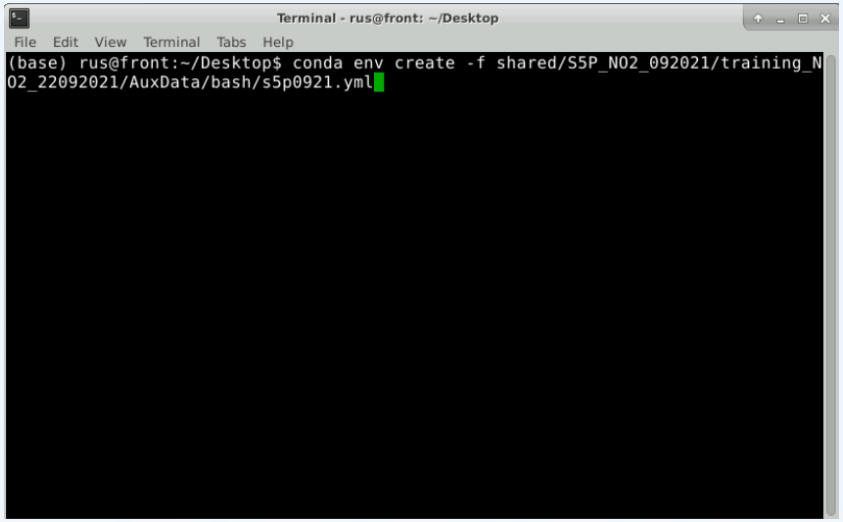
L3 NO2 product

Outline

- The Sentinel-5P mission
- The Sentinel 5P products
- The Atmospheric Toolbox
- **Exercises**
  - Introduction
  - Starting with the RUS environment
  - Starting with VISAN
  - Creation of NO2 gridded product
  - **Jupyter Notebook exercises**
    - Discovery of Python in the Jupyter Notebook environment
    - Creation of daily averages of tropospheric NO_2 column products out of single orbit files

Jupyter Notebook

- Second part of the training will be performed using Python code in JupyterLab (Anaconda Distribution)
- We will open JupyterLab by launching it from a specific conda environment (named **s5p0921**) that is provided to you
- Open a Terminal in your RUS virtual machine and copy paste the following line:
- conda env create -f shared/S5P_NO2_092021/training_NO2_22092021/AuxData/bash/s5p0921.yml

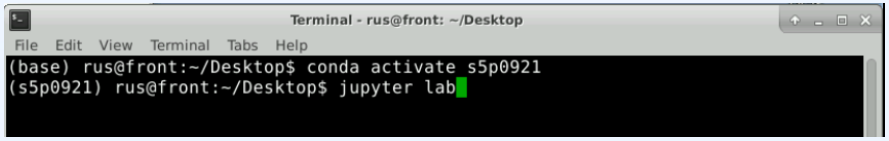


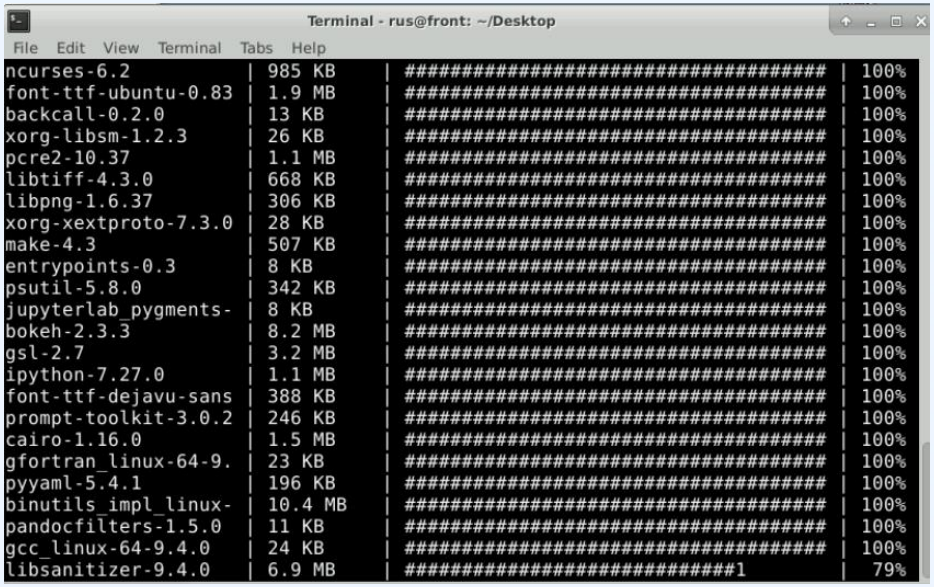
Jupyter Notebook

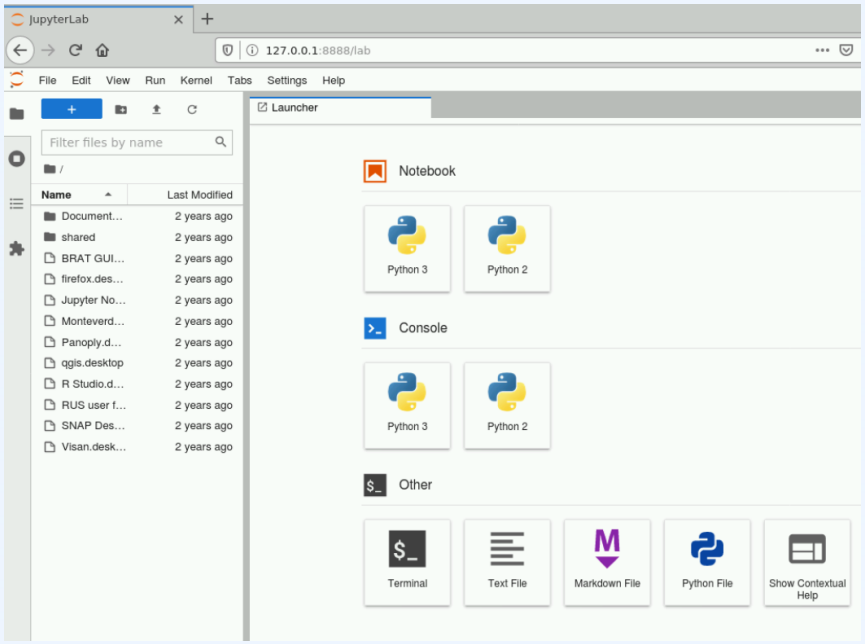
- It may take a few minutes to download and install all librairies
- In the meantime… A few words about Anaconda
  - Free & open source distribution of Python & R
  - For scientific computing
  - Simplifies package management (conda) and deployment
  - More info at https://www.anaconda.com/distribution/
- And Jupyter
  - Notebooks contain both computer code & rich text elements
- More info at https://www.jupyter.org

Jupyter Notebook

- Once the processing is finished, simply write
  - conda activate s5p0921
  - jupyter lab
- A JupyterLab instance opens

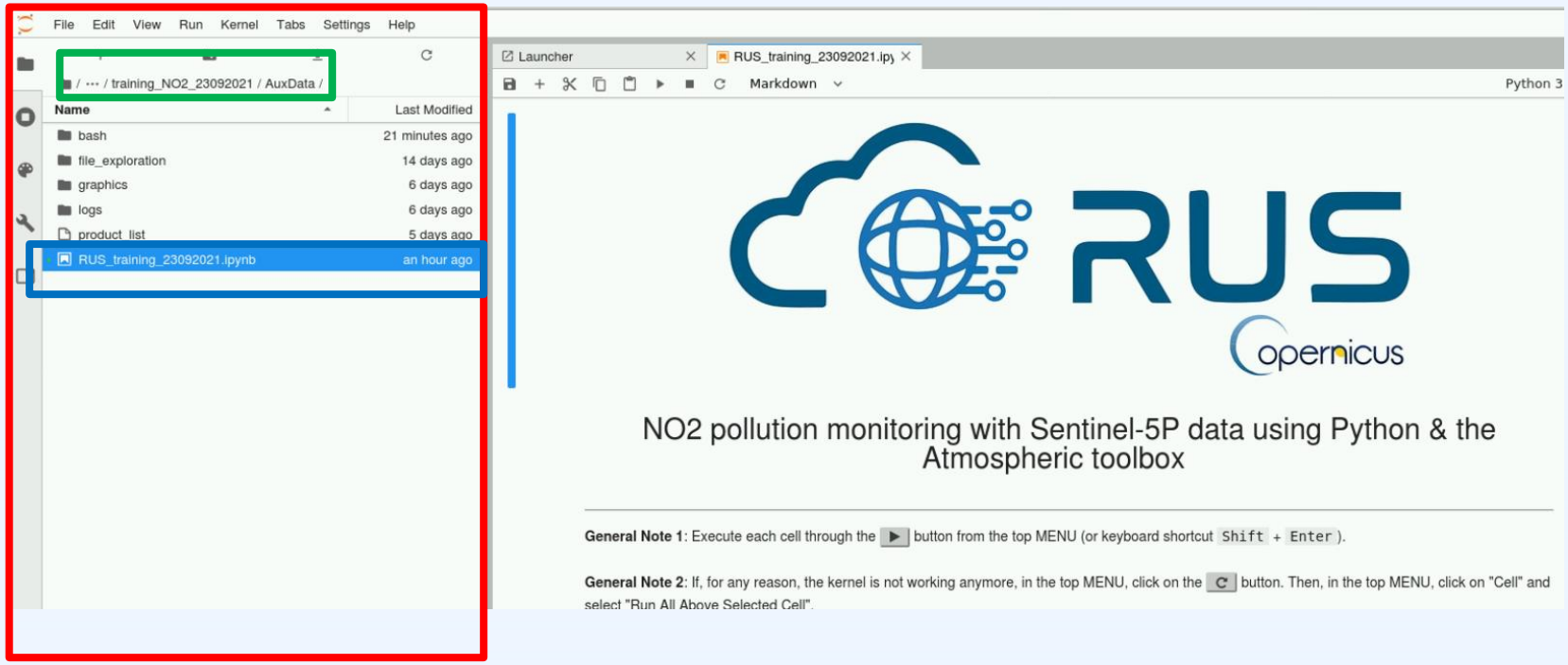






Jupyter Notebook

- From the **left panel**, navigate to
  /shared/S5P_NO2_092021/training_NO2_22092021/AuxData/
  Open *RUS_training_22092021.ipynb*



Jupyter Notebook

From now on, let’s follow the exercises on the Notebook!

Combining multiple products

Combining multiple products: HARPMERGE Command line/function

- Combines multiple products from files or directories by appending them accross the time dimension and storing the result into a single output file
- Defines a list of operations to apply to each product before it is appended:
  -a 'operation1(); operation2(); operationN();'
  - *Performs the same processing as the HARPCONVERT command line tool*
- Defines a list of operations to apply to the merged product:
  -ap 'operation1(); operation2(); operationN();'
  - *Operations to properly concatenate the inputs and export the merged product*
- Define ingestion options: **-o 'ingestion_option'**
- Define the output format: **-f 'format'**
  - The default NETCDF format will be kept during the exercise
  - HDF4 and HDF5 are supported too

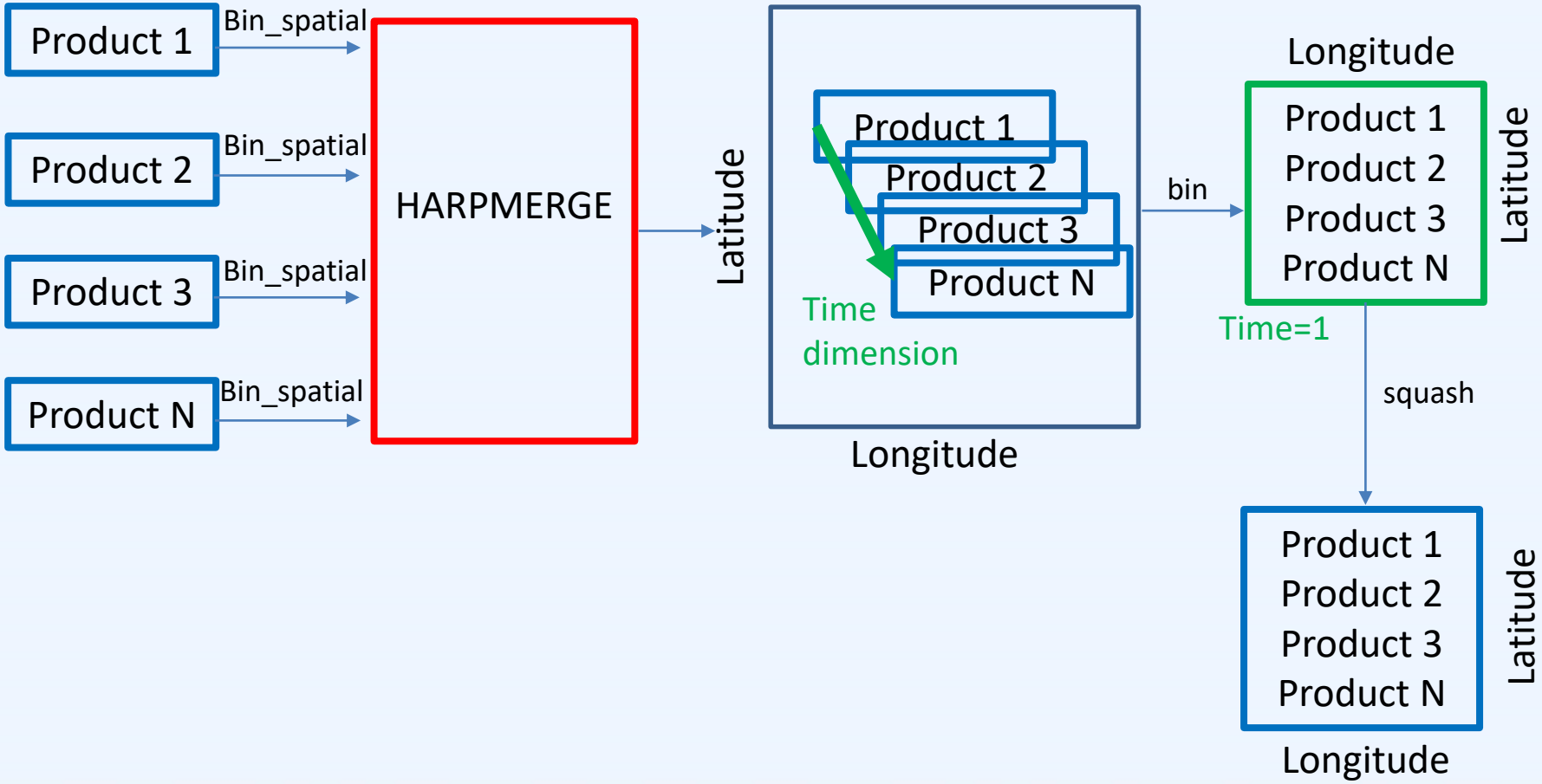
Combining multiple products

HARPMERGE Command line tool: practical use

- **Harpmerge –ap 'operations_list' –a 'operations_list' –o 'ingestion_option' input_files output_Directory/output_file**
- bin_spatial creates a regular lat/lon grid per product (dimension {lat,lon})
- Merging multiple products with the same lat/lon grid will produce {time,lat,lon} elements (time = number of merged products)
- In the **–ap** argument we will use:
  - **Bin()** operation: **average each of the lat/lon grid cells over time** so that we have {1,lat,lon} elements
  - **squash**(time, (latitude,longitude)): **remove the artificial time=1 dimension** created by the **bin()** operation from lat/lon variables to have proper **Georeferenced products for further use in other sofwares** (e.g: QGIS, Panoply…)
  - **Keep**(latitude, longitude, tropospheric_NO2_column_number_density,weight) : All variables marked for inclusion will be kept in the ingested product, all other variables will be excluded.

Combines multiple products

HARPMERGE Command line tool: Merging several products



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Combines multiple products

HARPMERGE Command line tool:

- "qa_value" parameter summarizes the processing flags into a continuous value, giving a quality percentage: 100 % is the most optimal value, 0 % is a processing failure
- Pixels can be filtered out by applying a quality filter when executing the HARPMERGE command line tool
  - **tropospheric_NO2_column_number_density_validity>75 (0: worst quality and 100: full quality, 75 is the recommended value)**
- From the notebook run the line:

```
#Starting time of the cell
t0= time.time()

#harpmerge in command line
!harpmerge -ap 'bin(); squash(time, (latitude,longitude,tropospheric_NO2_column_number_density))' \
-a 'tropospheric_NO2_column_number_density_validity>75; \
bin_spatial(1800,-90,0.1,3600,-180,0.1); \
derive(longitude {longitude});derive(latitude {latitude}); \
keep(latitude,longitude,tropospheric_NO2_column_number_density,weight)' \
/shared/S5P_NO2_092021/training_NO2_22092021/Original/NO2_24032019/S5P_OFFL_L2__NO2____20190*.nc \
/shared/S5P_NO2_092021/training_NO2_22092021/Processing/merged_files/command_line/converted_NO2_command_line.nc

#End time for command line
t1 = time.time()

command_line_time = t1-t0

print("Command line time: {} seconds".format(command_line_time))
```

Thank you !

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