



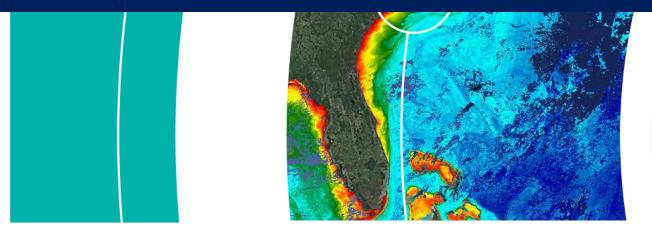
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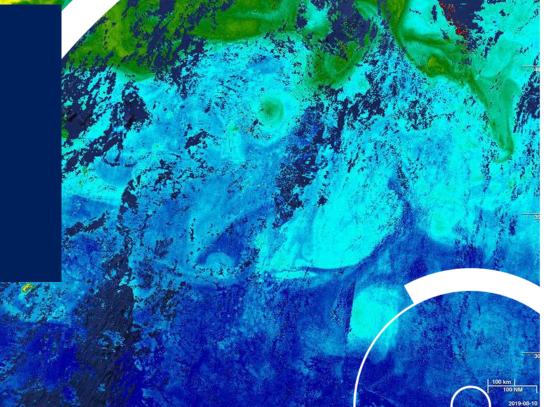


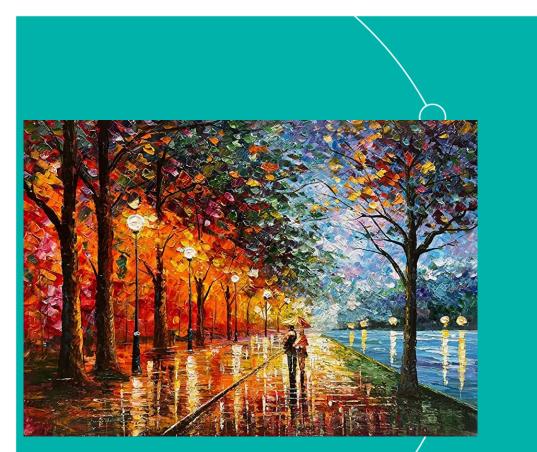
ThoMaS – a Tool to generate Matchups of OC products with Sentinel-3/OLCI

Juan Ignacio Gossn *EUMETSAT*

EUMETSAT series of short courses







Please interrupt me at any time! This presentation will be available and most material already available in ThoMaS repository

- 1. What's ThoMaS? Scope
- 2. Usage
- 3. Some background
- 4. Pre-requisites
- 5. Getting the code
- 6. Setting the environment
- 7. Set-up demo
- 8. Required inputs
- 9. Run the code
- 10. Run the code: demo
- 11. Short tour around ThoMaS



I. What's ThoMaS? Scope

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ThoMaS is a toolkit developed to create **matchups** of biogeophysical **insitu data** with **satellite ocean colour products** from **Sentinel-3 OLCI (S3/OLCI)**.

1. What's ThoMaS? Scope

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ThoMaS is a toolkit developed to create **matchups** of biogeophysical **insitu data (in SeaBASS/OCDB format)** with **satellite ocean colour products** from **Sentinel-3 OLCI (S3/OLCI) (also standard products from NASA's OBPG – l2gen – partially supported)**.

After running ThoMaS, you will get:

- → Insitu data transformed to spectrally match satellite (convolution, spectral matching).
- → Satellite data (L1B TOA radiance or L2 BOA water reflectance) from EUMETSAT Data Store (irresp. to whether it's reprocessed or operational) matching your insitu
- \rightarrow Extractions of satellite sata centred at lat/lon/time of insitu of user-defined size (3x3, 5x5..).
- → Statistics of extractions following EUMETSAT's or any user-defined matchup protocol.
- → Merging of simultaneous (spatially-temporally) insitu-satellite pairs, temporal interpolation, and statistics of matchups.

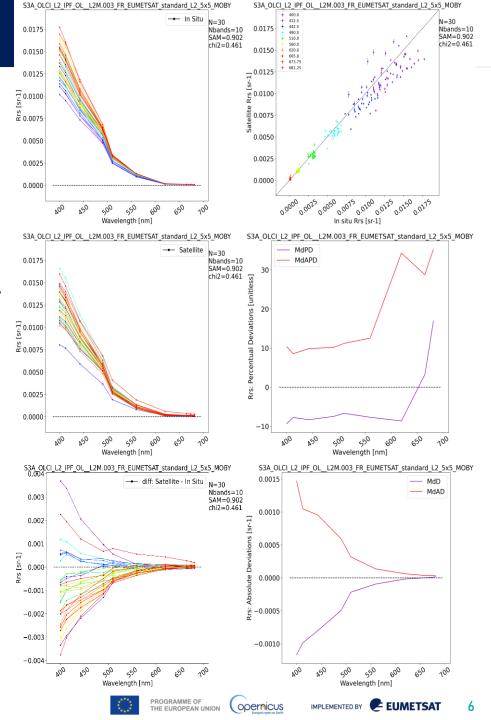
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\rightarrow Outputs:

- → NetCDF 4 files: SatData, minifiles, Extraction Data Base files, In situ Data Base file, Matchup Data Base files.
- \rightarrow CSV: summarizing satellite extraction statistics and matchup statistics.
- \rightarrow **PNG**: Standardised output plots.



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ThoMaS workflow is divided into **5** main steps:

The steps can be executed **sequentially** or **independently** in case the needed outputs of the previous steps are available.

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2. Usage

ThoMaS workflow is divided into **5** main steps:

The steps can be executed **sequentially** or **independently** in case the needed outputs of the previous steps are available.

1. Step insitu: Ingest insitu data from SeaBASS/OCDB input file and apply several transformations to make insitu comparable to satellite data (e.g. spectral matching with satellite, BRDF correction) and store them into standard IDB (In situ Data Base) netCDF4 file. This step can optionally include the acquisition of ancillary information from ECMWF at the lat-lon-times of your insitu measurements.

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4. Step **EDB**. Stack minifiles, apply transformations to SatData to make them comparable to in situ (e.g. **scale/unit conversion**, **BRDF** correction) and store into standard netCDF4 and CSV **EDB** (**Extraction Data Base**) files. This step includes calculating **statistics** over the extraction window following EUMETSAT's or any user-defined Matchup Protocol.

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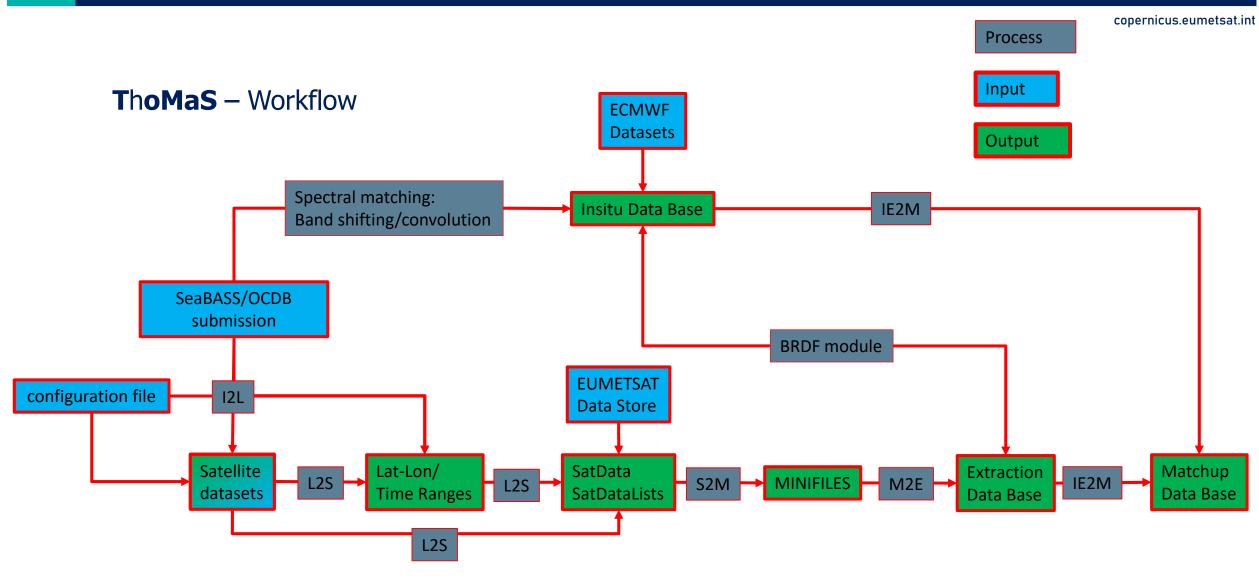
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5. Step MDB. Combine insitu (IDB) and satellite (EDB) information indexed into insitu-satellite matchup pairs, optionally apply time interpolation, calculate matchup statistics, and store into standard MDB (Matchup Data Base) netCDF4 and CSV files.

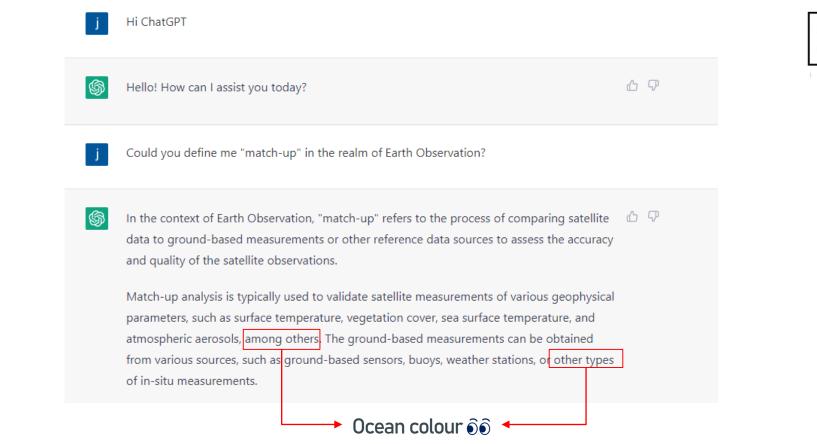




- IDB (In situ Data Base): a netCDF file containing all the information related to the inputted insitu data. + (if requested) ancillary information from ECMWF reanalysis datasets at the insitu geographic location and time stamp.
- SatData: an image file/directory. In the case of standard L1/L2 OLCI products, it is composed of a directory containing several netCDF files, each containing one/several products + a manifest.xml file.
- Minifile: A single netCDF file containing all the relevant L1/L2 products from a single SatData, but only at the required location (and with a predefined window size).
- EDB (Extraction Data Base): All the statistical information (pixel-by-pixel flagging, outlier removal, central and dispersion values before/after outlier/mask removal, etc., details of the extraction protocol) is stored for all the extractions in one single netCDF file per extraction set.
- MDB (Match-up Data Base): All the information from IDB and EDB combined and re-indexed according to matchup pairs + matchup statistics.

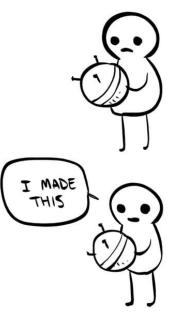
Find examples of all these files (except SatData) in the examples/example_files directory.

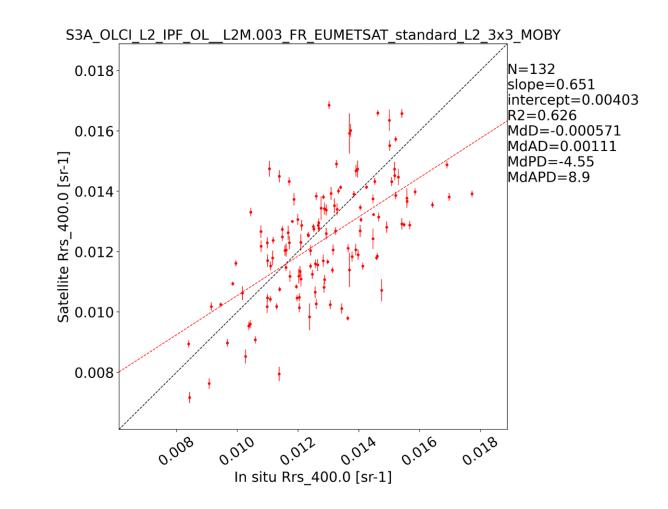
What is a match-up according to chatGPT?





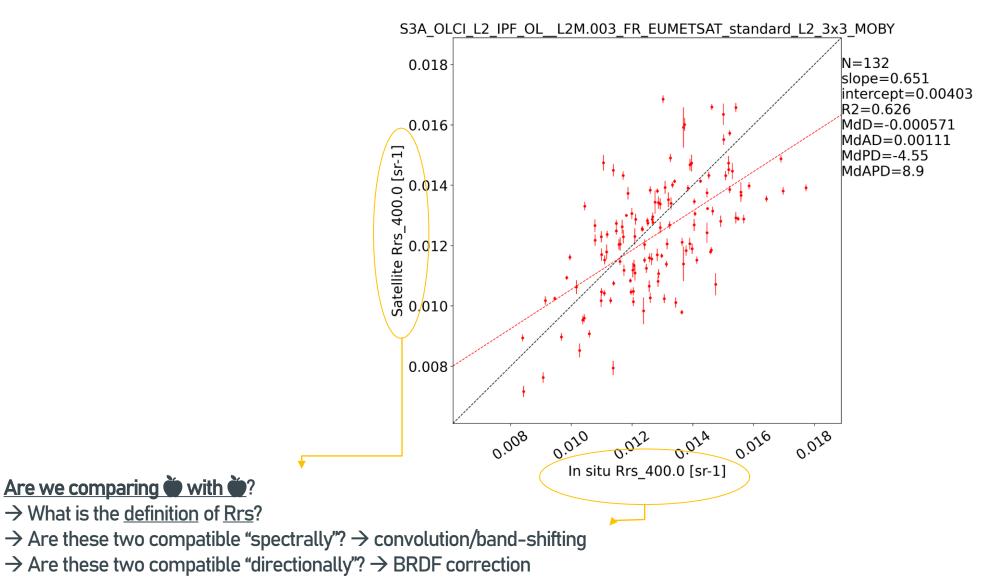






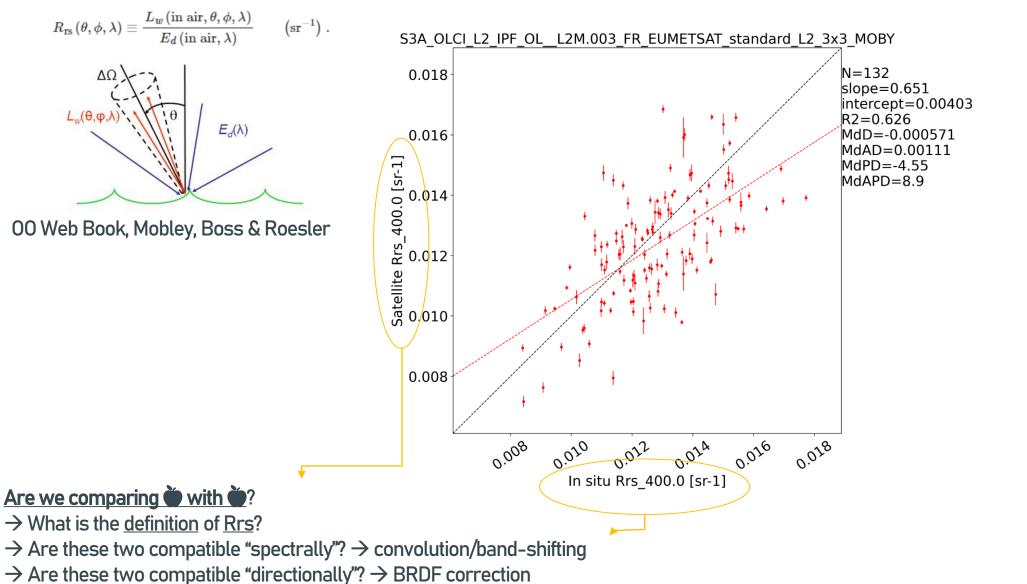
• Of course we have much more to define... and take care of...







Definition of Rrs





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copernicus.eumetsat.int **Definition of Rrs** $R_{
m rs}\left(heta,\phi,\lambda
ight)\equivrac{L_w\left({
m in\ air}, heta,\phi,\lambda
ight)}{E_d\left({
m in\ air},\lambda
ight)}$ (sr^{-1}) . S3A OLCI L2 IPF OL L2M.003 FR EUMETSAT standard L2 3x3 MOBY 0.018 N = 132slope=0.651 intercept=0.00403 $L_w(\theta, \phi)$ R2 = 0.626 $E_d(\lambda)$ 0.016 MdD=-0.000571 MdAD=0.00111 Rrs_400.0 [sr-1] MdPD=-4.55 MdAPD=8.9 00 Web Book, Mobley, Boss & Roesler Band-shifting (to pair multispectral to multispectral) Satellite $R_{RS}^{e}(\lambda_{i} \rightarrow \lambda_{t}) = R_{RS}^{f}(\lambda_{t}) \frac{R_{RS}(\lambda_{i})}{R_{RS}^{f}(\lambda_{i})}$ Melin & Sclep 2015 supported in ThoMaS 0.008 Spectral convolution 0.008 0.026 0.010 0.014 0.028 0.012 E_d In situ Rrs_400.0 [sr-1] Are we comparing **with ***? $R_{rs} \times S_B$ \rightarrow What is the <u>definition</u> of <u>Rrs</u>? $L_W \times S_B$ $E_d \times S_B$ S_B \rightarrow Are these two compatible "spectrally"? \rightarrow convolution/band-shifting \rightarrow Are these two compatible "directionally"? \rightarrow BRDF correction Burggraaff 2020

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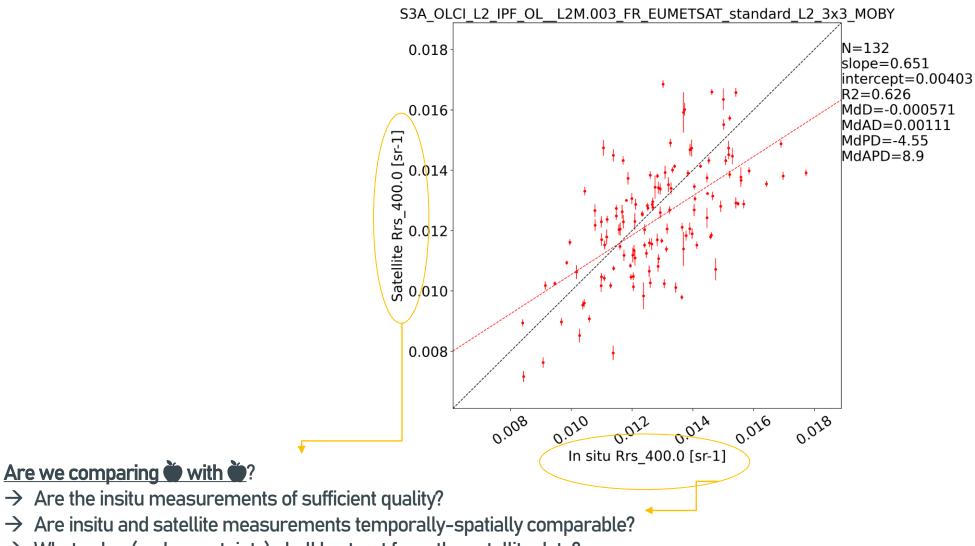
copernicus.eumetsat.int **Definition of Rrs** $R_{ ext{rs}}\left(heta,\phi,\lambda
ight)\equivrac{L_{w}\left(ext{in air}, heta,\phi,\lambda
ight)}{E_{d}\left(ext{in air},\lambda
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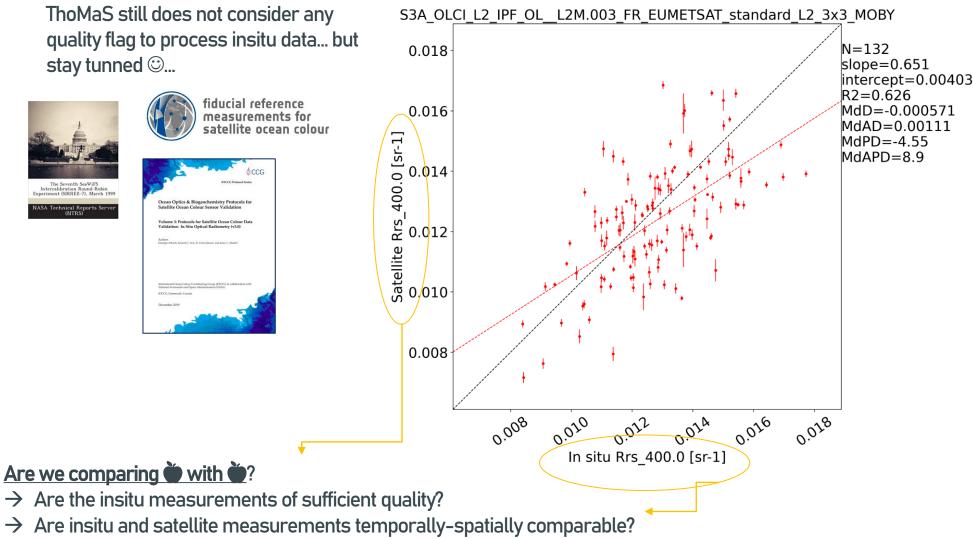
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ightarrow What value (and uncertainty) shall I extract from the satellite data?

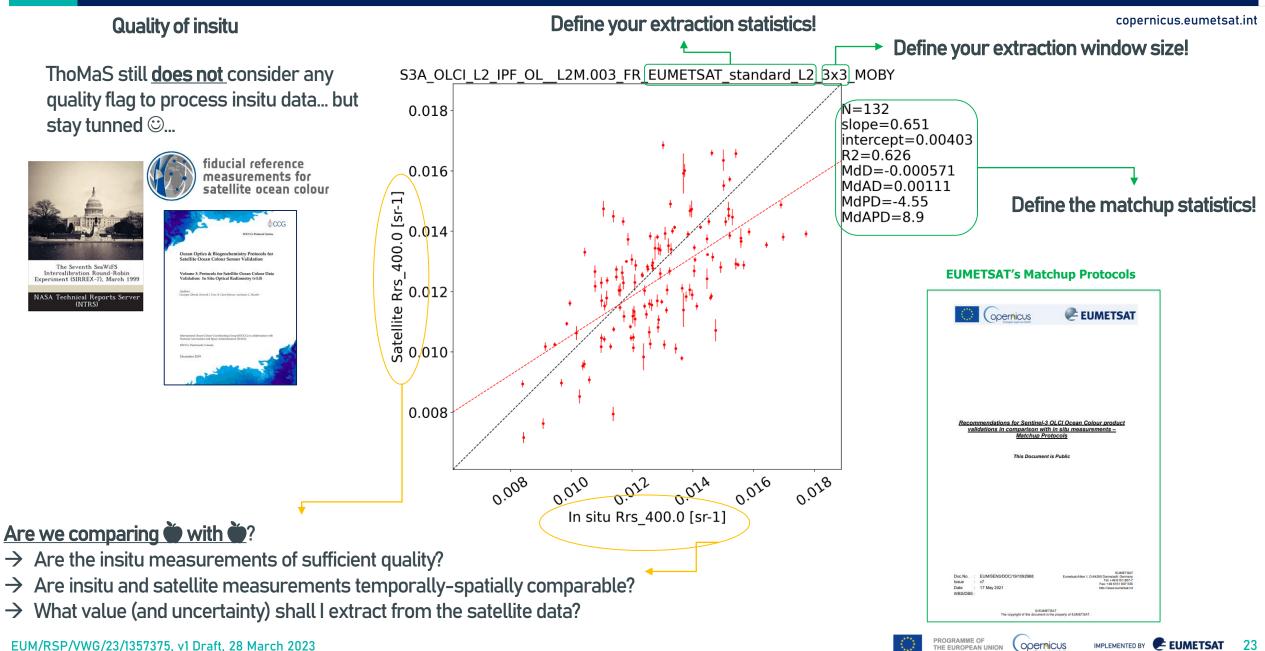
Quality of insitu

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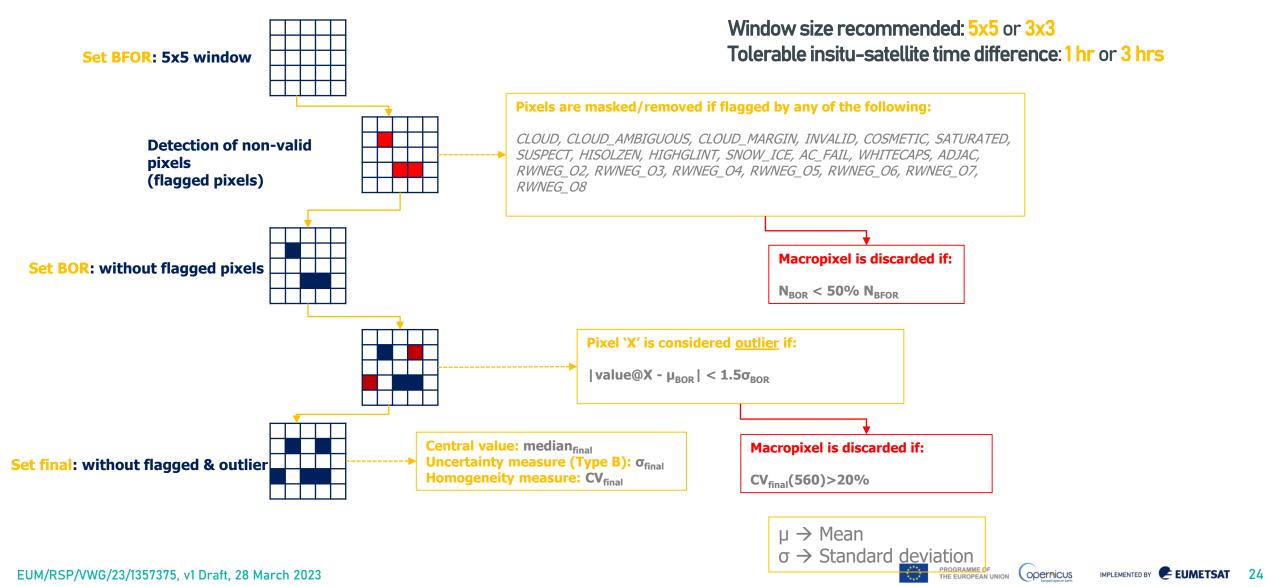




3. Some background: match-ups: EUMETSAT extraction protocol

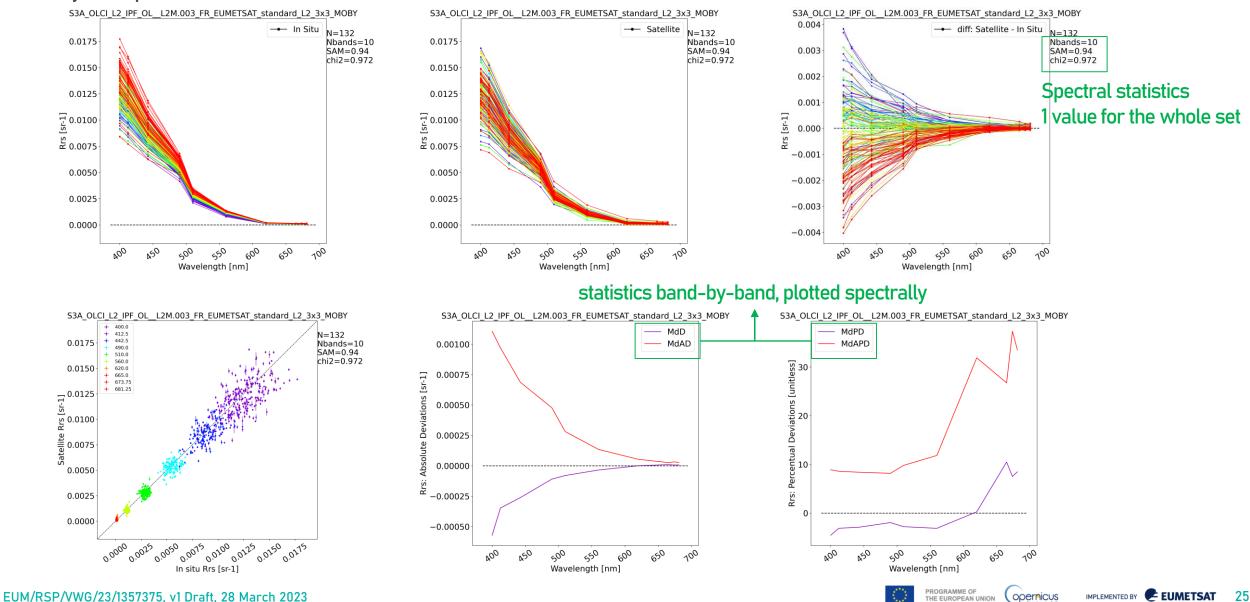
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EUMETSAT's Matchup Protocols: extraction of statistics at macropixel level



Band-by-band plots and statistics are often not sufficient...

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Band-by-band plots and statistics are often not sufficient...

Check recommended statistics and definitions at: **Spectral statistics EUMETSAT's Matchup Protocols** 1 value for the whole set **EUMETSAT** opernicus validations in comparison with in situ measurements statistics band-by-band, plotted spectrally Matchup Protocols This Document is Public ThoMaS: user can define it's own extraction statistics method window size time tolerance Doc.No. EUM/SEN3/DOC/19/1092968 Tet +49 6151 807-7 Fax: +49 6151 807 555 relevant statistics Issue ¥7 Date 17 May 2021 WBS/DBS CEUMETSAT The copyright of this document is the property of EUMETSA

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3. Some background: basic (Linux) terminal commands 2

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Command	Description
cd dir_name	Change directory to "dir_name"
cd ~	Change directory to home dir
mkdir dir_name	Make new directory "dir_name"
ls	List files in current directory
ls -a	List files including hidden ones
conda	Check conda is installed
conda env create _f env_file _n env_name	Create environment "env_name" from "env_file" file
conda activate env_name	Activate environment "env_name"
git	Check git is installed
git clone url .	Clone repository from URL to current directory
nano filename	Check/edit file "filename"
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🗲 4. Pre-requisites

- 1. Apart from that background knowledge...
- 2. Conda: Install the latest Anaconda Python distribution.
- 3. EUMETSAT Data Store: Create EO Portal user and get API consumer key and secret.
- 4. EUMETSAT Data Store: Save EO Portal API credentials under ~/.eumdac/credentials
- 5. ECMWF: Register to ADS/CDS and get url and key.
- ECMWF: store ADS/CDS url/keys under ~/.ecmwg_api_config

Dependencies

item	version	licence	package info
BeautifulSoup	4.6.0	MIT	https://anaconda.org/conda-forge/beautifulsoup4
cdsapi	0.1.6	Apache-2.0	https://anaconda.org/conda-forge/cdsapi
ephem	4.1.3	MIT	https://pypi.org/project/ephem/
eumdac	2.0.1	MIT	https://anaconda.org/eumetsat/eumdac
matplotlib	3.5.2	PSF-based	https://anaconda.org/conda-forge/matplotlib
netcdf4	1.5.8	MIT	https://anaconda.org/conda-forge/netcdf4
numpy	1.23.0	BSD-3-Clause	https://anaconda.org/conda-forge/numpy
pandas	1.4.3	BSD-3-Clause	https://anaconda.org/conda-forge/pandas
python	3.9	PSF	https://docs.python.org/3/license.html
scipy	1.8.1	BSD-3-Clause	https://anaconda.org/conda-forge/scipy
xarray	2022.3.0	Apache-2.0	https://anaconda.org/conda-forge/xarray

Conda will take care of this...

• Git way:

```
cd ~
mkdir ThoMaS
cd ThoMaS
ls
git clone https://gitlab.eumetsat.int/eumetlab/oceans/ocean-science-studies/ThoMaS .
```

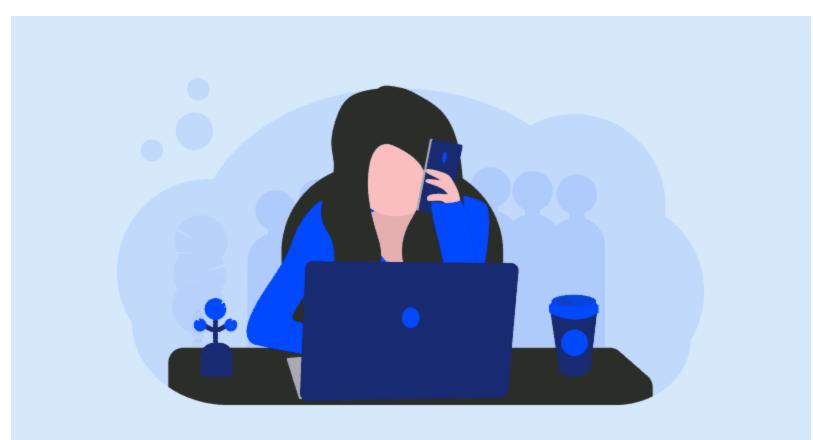
• Or direct download from

https://gitlab.eumetsat.int/eumetlab/oceans/ocean-science-studies/ThoMaS

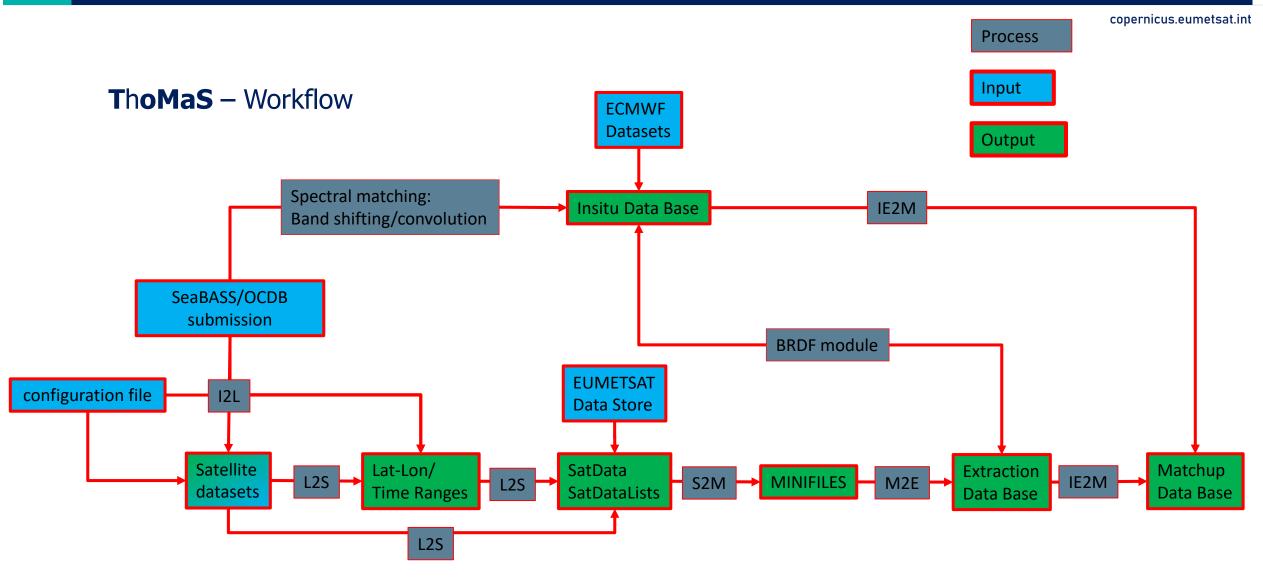
• Once conda and ThoMaS are installed:

```
conda
cd ~
cd ThoMaS
ls
nano environment.yml
conda env create -f environment.yml -n thomas
conda activate thomas
```









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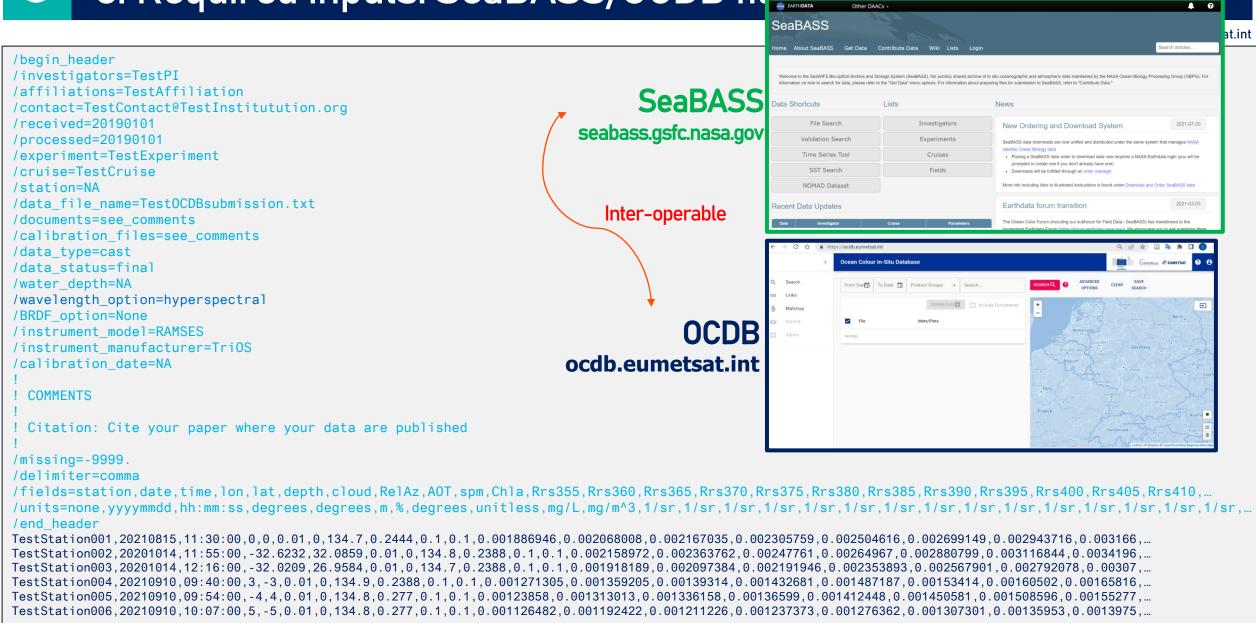
8. Required inputs: SeaBASS/OCDB file

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/begin header /investigators=TestPI /affiliations=TestAffiliation /contact=TestContact@TestInstitutution.org /received=20190101 /processed=20190101 /experiment=TestExperiment /cruise=TestCruise /station=NA /data file name=TestOCDBsubmission.txt /documents=see comments /calibration files=see comments /data type=cast /data status=final /water depth=NA /wavelength option=hyperspectral /BRDF option=None /instrument model=RAMSES /instrument manufacturer=TriOS /calibration date=NA ! COMMENTS ! Citation: Cite your paper where your data are published /missing=-9999. /delimiter=comma /fields=station,date,time,lon,lat,depth,cloud,RelAz,AOT,spm,Chla,Rrs355,Rrs360,Rrs365,Rrs370,Rrs375,Rrs380,Rrs385,Rrs390,Rrs395,Rrs400,Rrs405,Rrs410,... /end header TestStation001,20210815,11:30:00,0,0.0.01,0,134.7,0.2444,0.1,0.1,0.001886946,0.002068008,0.002167035,0.002305759,0.002504616,0.002699149,0.002943716,0.003166,... TestStation002,20201014,11:55:00,-32.6232,32.0859,0.01,0,134.8,0.2388,0.1,0.1,0.002158972,0.002363762,0.00247761,0.00264967,0.002880799,0.003116844,0.0034196,... TestStation003, 20201014, 12:16:00, -32.0209, 26.9584, 0.01, 0, 134.7, 0.2388, 0.1, 0.1, 0.001918189, 0.002097384, 0.002191946, 0.002353893, 0.002567901, 0.002792078, 0.00307, ... TestStation004,20210910,09:40:00,3,-3,0.01,0,134.9,0.2388,0.1,0.1,0.001271305,0.001359205,0.00139314,0.001432681,0.001487187,0.00153414,0.00160502,0.00165816,... TestStation005,20210910,09:54:00,-4,4,0.01,0,134.8,0.277,0.1,0.1,0.00123858,0.001313013,0.001336158,0.00136599,0.001412448,0.001450581,0.001508596,0.00155277,... TestStation006,20210910,10:07:00,5,-5,0.01,0,134.8,0.277,0.1,0.1,0.001126482,0.001192422,0.001211226,0.001237373,0.001276362,0.001307301,0.00135953,0.0013975,...



8. Required inputs: SeaBASS/OCDB file







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this format and links to all the necessary resources

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8. Required inputs: config_file.ini and satellite_datasets.csv

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Example 1:

1. I want to download Sen-3 data from the outer Gironde estuary at location (45.6N, 1.6W), where I deployed an in situ instrument measuring continuously during the first 5 days of September 2021.

2. I want data from both S3A and S3B, and L2 of the recent collection OL_L2M.003

3. Only full resolution (FR).

4. I just want to obtain the S3 files (SatData), minifiles and extractions, I have my own scripts to compute the statistics of the comparison with insitu.

5. In particular, I want to test EUMETSAT's standard protocol, but I want to test several window sizes: 3x3, 5x5, 7x7.

6. I want everything related to the run to be stored at ~/Gironde

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My config_file.ini should look like:

[global]

path_output: /tcenas/home/gossn/Gironde
SetID: Gironde

[workflow]
workflow: SatData, minifiles, EDB

[minifiles]
minifiles_winSize: 7

[EDB] EDB_protocols_L2: EUMETSAT_standard_L2 EDB_winSizes: 3, 5, 7

SetID	Region	Country	Lat	Lon	time_start	time_stop	Platform	Sensor	Level	Processor	Collection	Resolution	path_to_SatData
Gironde	Gironde	France	45.6	-1.6	2021-09-01T00:00:00	2021-09-05T23:59:59	S3A	OLCI	L2	IPF	OLL2M.003	FR	EUMETSATdataStore:~/Gironde/SatData
Gironde	Gironde	France	45.6	-1.6	2021-09-01T00:00:00	2021-09-05T23:59:59	S3B	OLCI	L2	IPF	OLL2M.003	FR	EUMETSATdataStore:~/Gironde/SatData

My satellite_datasets.csv should look like:



Example 2:

- 1. You have a prepared a set of hyperspectral Rrs insitu measurements from MOBY in SeaBASS format not corrected for BRDF effects.
- 2.You wish to get matchups between this MOBY subset and S3A/OLCI standard FR L2,
 •from the current collection OL__L2M.003
 •using the standard extraction protocol from EUMETSAT,
 •an extraction window of 3x3,
 •an insitu-satellite time difference threshold of 1 hour (3600 seconds).
- 3. You are not interested in getting ancillary data from ECMWF for to the insitu data.
- 4. You want to apply the Morel et al. 2002 BRDF correction to both satellite and insitu.
- 5.You may have several insitu measurements corresponding to one single SatData within the time window that you selected, but you wish to keep only the closest in time with the satellite overpass.
- 6.You wish:
 SatData to be stored at /home/myName/MOBY/SatData
 all the other outputs (IDB, minifiles, EDB, MDB, etc.) to be stored at /home/myName/MOBY



Example 2:

1. You have a prepared a set of hyperspectral Rrs insitu measurements from MOBY in SeaBASS format not corrected for BRDF effects.

2.You wish to get matchups between this MOBY subset and S3A/OLCI standard FR L2, •from the current collection OL_L2M.003

- •using the standard extraction protocol from EUMETSAT,
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6.You wish:
SatData to be stored at /home/myName/MOBY/SatData
all the other outputs (IDB, minifiles, EDB, MDB, etc.) to be stored at /home/myName/MOBY

In this case, **satellite_datasets.csv** will be generated automatically by ThoMaS and stored under path_output

[global]

path_output: /tcenas/home/gossn/MOBY
SetID: MOBY

[workflow]
workflow: insitu, SatData, minifiles, EDB, MDB

[insitu]

insitu_input: /tcenas/home/gossn/MOBY/MOBY_OCDB.csv insitu_satelliteTimeToleranceSeconds: 3600 insitu_getAncillary: False insitu_BRDF: M02

[satellite]

satellite_path-to-SatData: /tcenas/home/gossn/MOBY/SatData
satellite_source: EUMETSATdataStore
satellite_collections: OL__L2M.003
satellite_platforms: S3A
satellite_resolutions: FR
satellite_BRDF: M02

[minifiles]
minifiles_winSize: 5

[EDB]

EDB_protocols_L2: EUMETSAT_standard_L2 EDB_winSizes: 5

[MDB]

MDB_time-interpolation: insitu2satellite_NN MDB_stats_plots: True MDB_stats_protocol: EUMETSAT_standard_L2



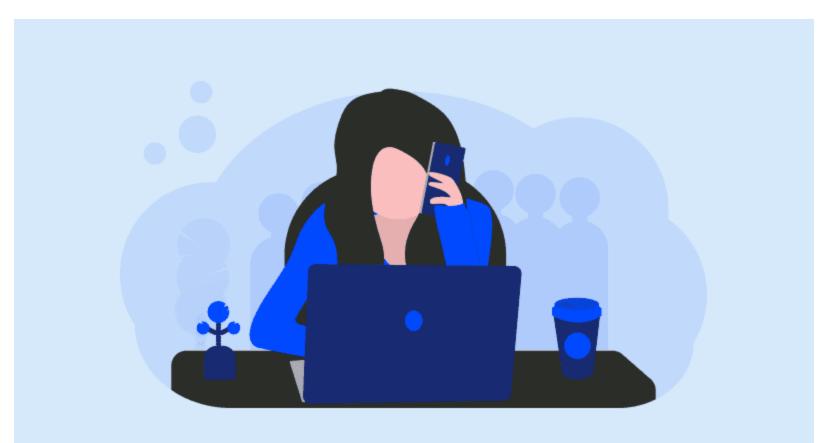
- 1. EUMETSAT Data Store credentials obtained and stored?
- 2. ECMWF ADS/CDS credentials obtained and stored?
- 3. ThoMaS code cloned?
- 4. thomas conda environment set up?
- 5. Required inputs in place? (config_file.ini, satellite_datasets.csv, SeaBASS/OCDB input file?

Then.. run by executing this command: **python /path/to/ThoMaS/main.py –cf /path/to/config_file.ini**



2 10. Run the code: Demo

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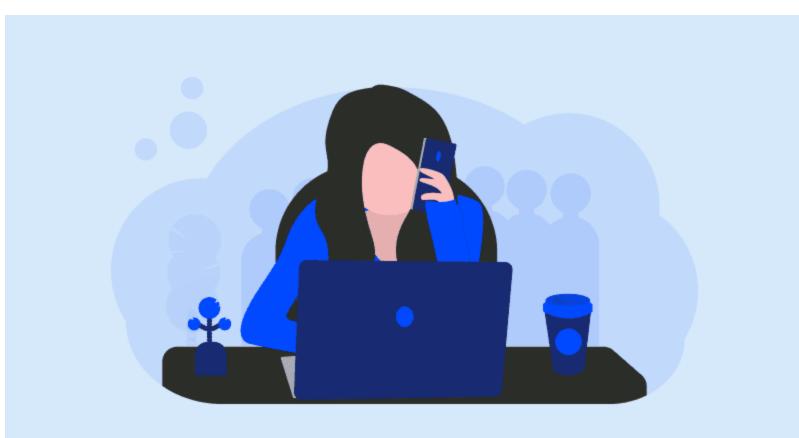




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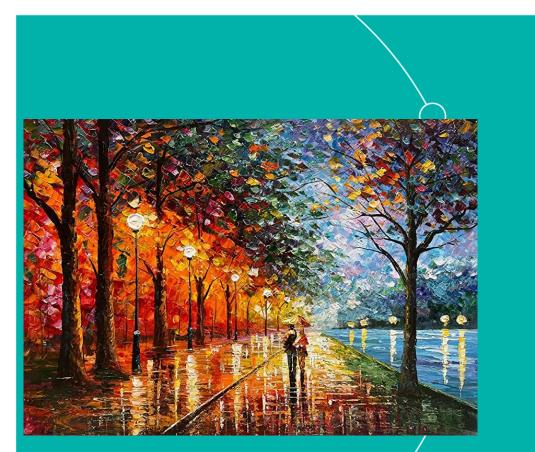
I1. Short tour around ThoMaS

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Hope you enjoyed it! Thank you! Questions are welcome.

- 1. What's ThoMaS? Scope
- 2. Usage
- 3. Some background
- 4. Pre-requisites
- 5. Getting the code
- 6. Setting the environment
- 7. Set-up demo
- 8. Required inputs
- 9. Run the code
- 10. Run the code: demo
- 11. Short tour around ThoMaS



opernicus

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