EUMETSAT

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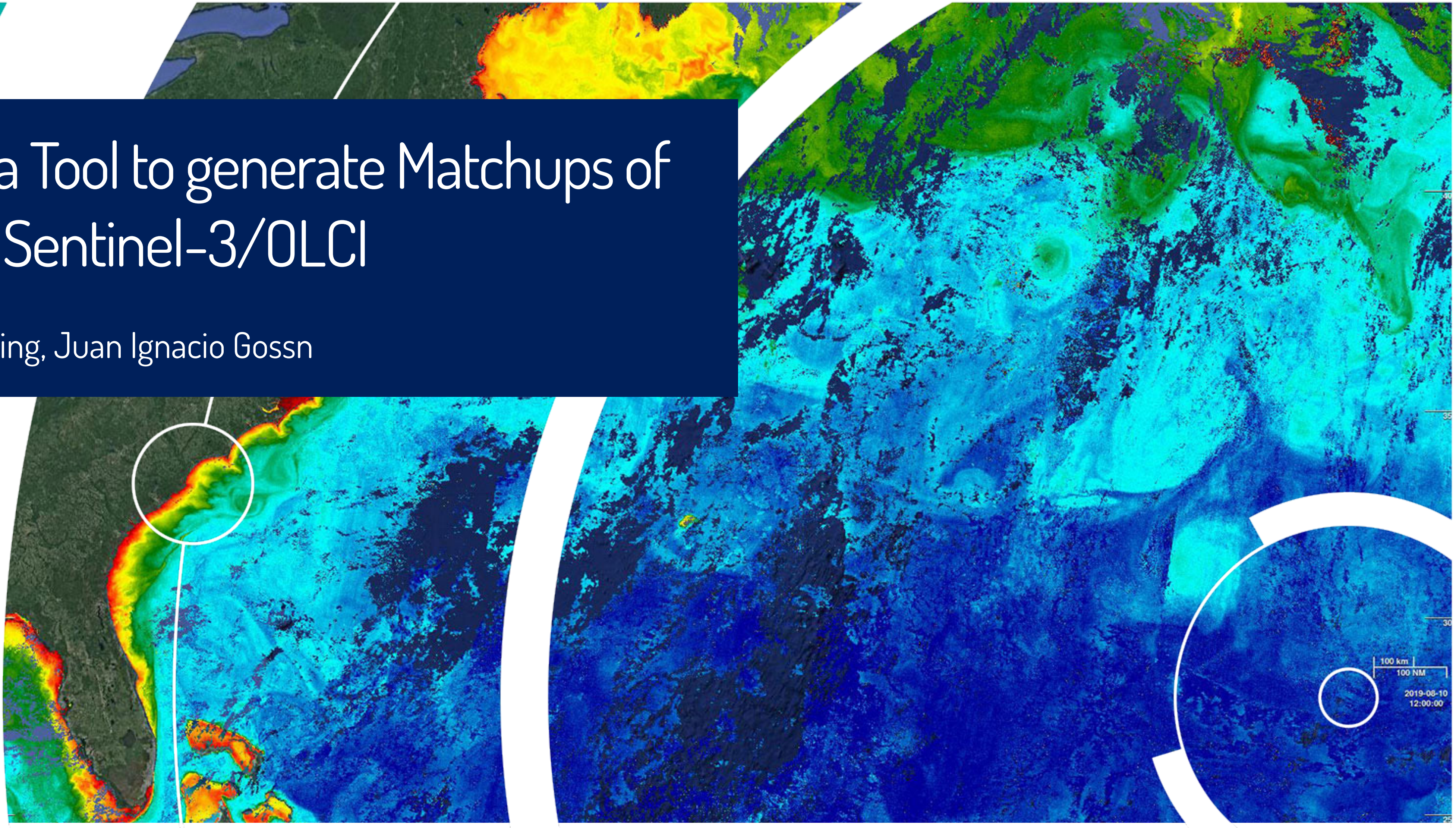
Europe's eyes on Earth

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

Ben Loveday, Hayley Evers-King, Juan Ignacio Gossn



Today's tour with ThoMaS – a Tool to perform Matchups with S3-OLCI

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

1. Some background...Why do we care about matchups?

- How do we know that the instruments on our satellites are recording signals accurately over time?
- How do we relate these signals to actual geophysical quantities of the ocean?

→ Validation!

1. Some background: match-ups

- What is a match-up according to **chatGPT**?

j Hi ChatGPT

Hello! How can I assist you today?

j Could you define me "match-up" in the realm of Earth Observation?

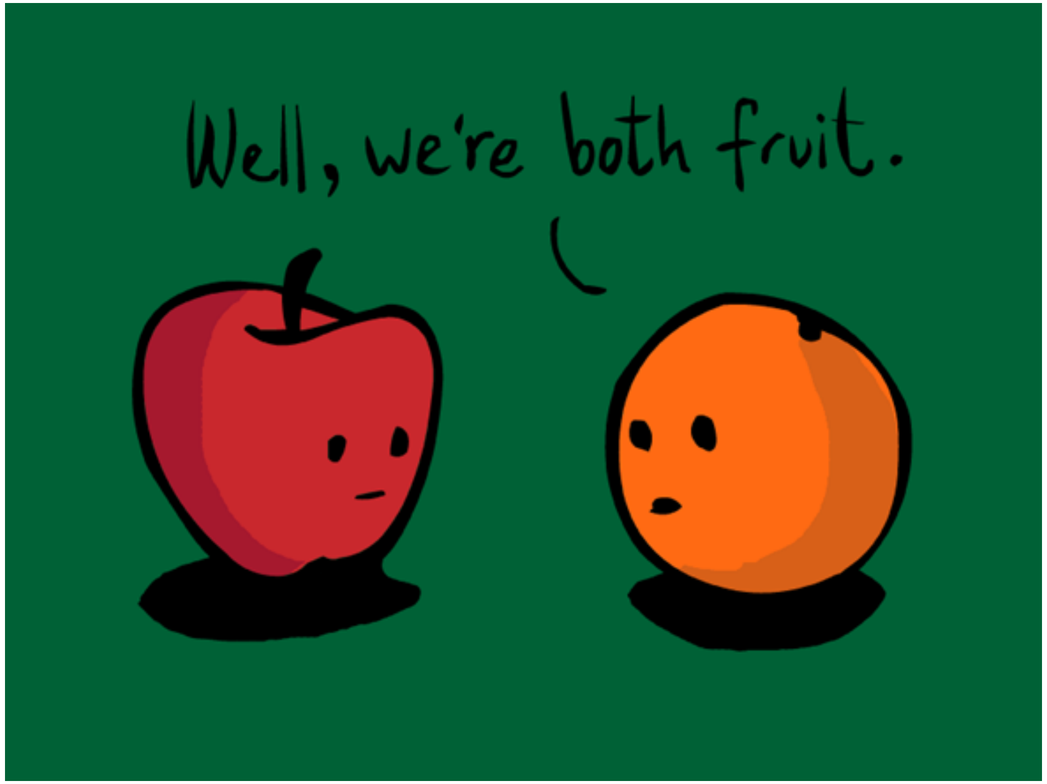
In the context of Earth Observation, "match-up" refers to the process of comparing satellite data to ground-based measurements or other reference data sources to assess the accuracy and quality of the satellite observations.

Match-up analysis is typically used to validate satellite measurements of various geophysical parameters, such as surface temperature, vegetation cover, sea surface temperature, and atmospheric aerosols, among others. The ground-based measurements can be obtained from various sources, such as ground-based sensors, buoys, weather stations, or other types of in-situ measurements.

→ Ocean colour 👀 ←

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

1. Some background…what makes a good matchup?



- We have to consider a lot of things:
  - How closely does the in situ measurement represent a satellite pixel in space/time?
  - Is the in situ data processed in a way that's as similar to the satellite out as possible?
  - What about uncertainties (in both data sets?)
  - How does my validation compare to someone else's?

1. Some background…motivation for having ThoMaS

1. Well documented, suited for a first approach to the matchup exercise for those who are new to the intricacies of the matchup steps.
2. Versatile: new types of satellite products can be easily added via configuration files (depending on mission, processor and processing baseline).

   → Currently supports Sentinel-3 (standard) L1B, L2, MODIS L2 (standard), VIIRS L2 (standard).

3. Versatile: new matchup protocols can be easily added via configuration files.

   → e.g. of existing ones: Bailey & Werdell 2006, EUMETSAT's standard, Copernicus SVC_VIS

4. It's published and open to scrutiny: it serves for the purpose of converging to a standard matchup practice.

2. What's ThoMaS? Scope

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

in SeaBASS format

Standard products from NASA's OBPG also supported
Others easily configurable, if netCDF or series of netCDFs

2. What's ThoMaS? Scope

After running **ThoMaS**, you will get:

→ **Insitu** data "transformed" to **match satellite** (spectral **convolution**, **band-shifting, BRDF…**).

→ **Satellite** data (L1B – TOA radiance - or L2 – BOA water reflectance) from **EUMETSAT Data Store** (reprocessed/operational) matching spatially/temporally your insitu.

→ **Extractions** of satellite data centred at lat/lon of insitu of user-defined size (3x3, 5x5..).

→ **Statistics of extractions** following EUMETSAT's or any user-defined **matchup protocol**.

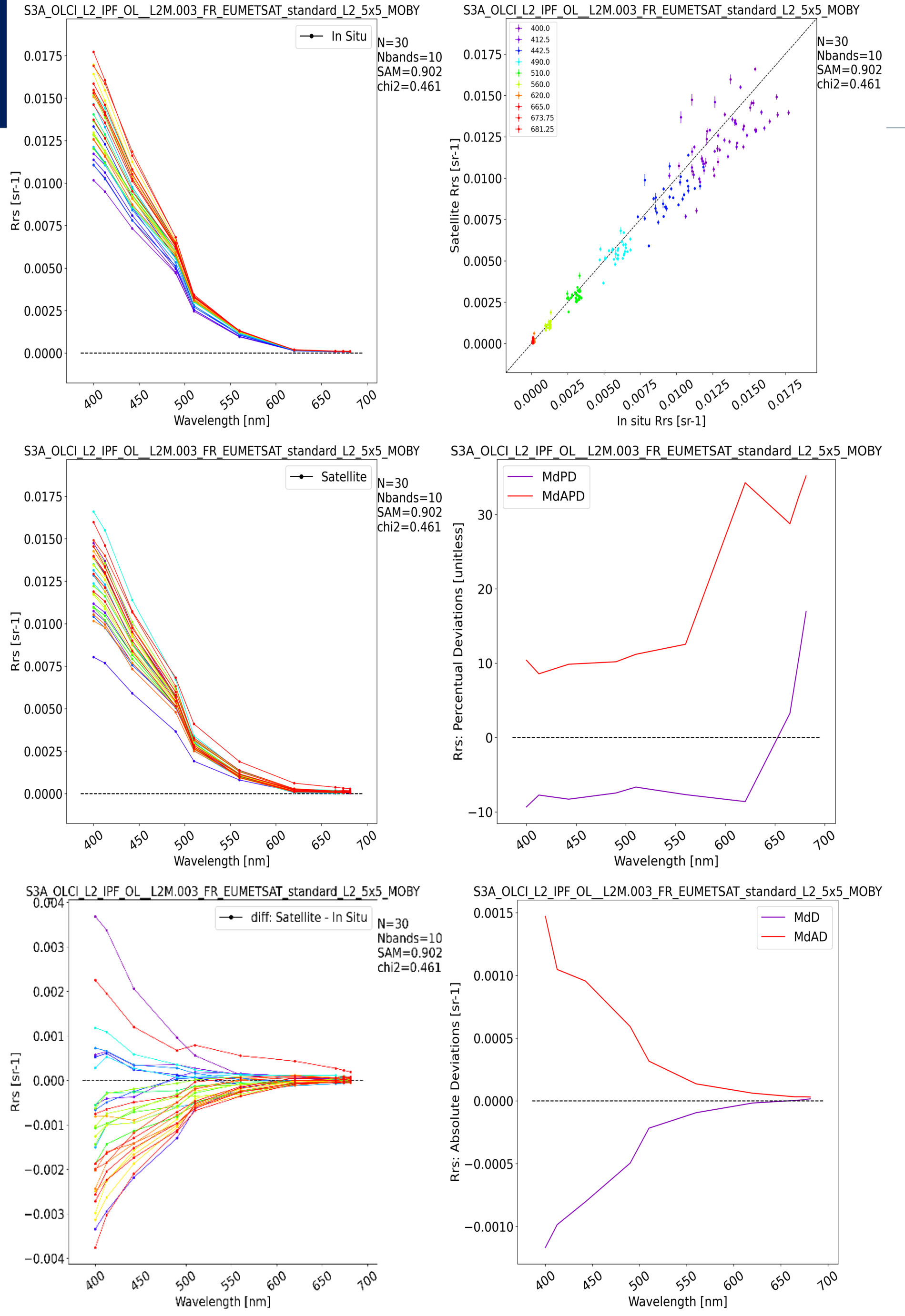
→ **Merging of simultaneous** (spatially-temporally) **insitu-satellite pairs**, **temporal interpolation**, and **statistics of matchups**.

→ **Outputs:**

→ **NetCDF 4** files: SatData, minifiles, Extraction Data Base files, In situ Data Base file, Matchup Data Base files.

→ **CSV**: summarizing satellite extraction statistics and matchup statistics.

→ **PNG**: Standardised output plots.



3. 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**
    1. Ingest insitu data from **SeaBASS** input file
    2. Apply several transformations to make **insitu comparable to satellite** data (e.g. **spectral matching** with satellite, **BRDF** correction)
    3. 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.

2. Step **SatData**: Download and list the **satellite products (L1B and/or L2)** matching spatially-temporally your insitu data.

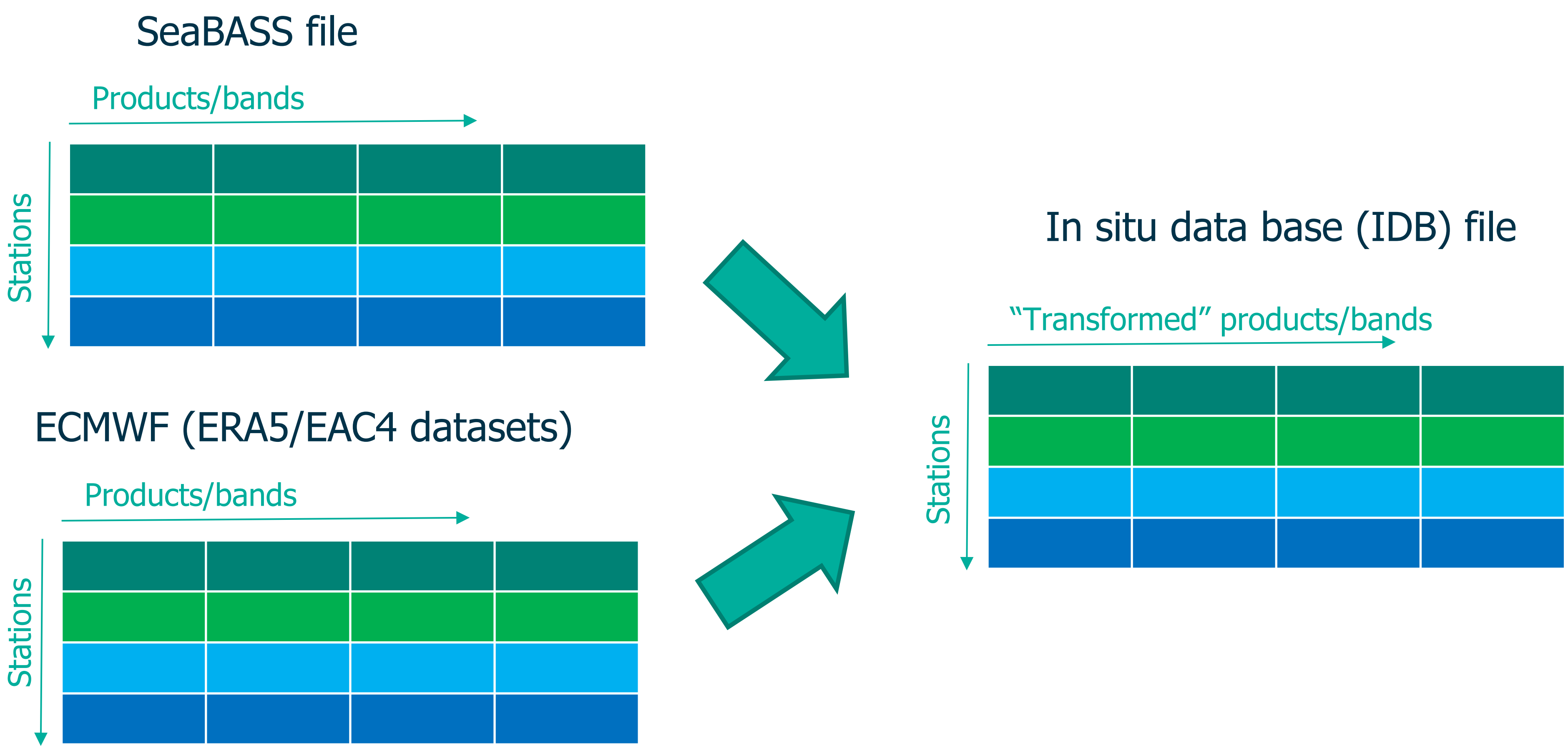
    → Download only for products available in EUMETSAT data store.

3. Step **minifiles**: SatData are grouped/unnested into single netCDF4 file, sliced in horizontal dimensions, centred at the desired (in situ) location.

4. Step **EDB**.
    1. Stack minifiles into single netCDF
    2. Apply transformations to SatData to make them comparable to in situ (e.g. **scale/unit conversion**, **BRDF** correction)
    3. Calculate extraction **statistics** over the extraction window following EUMETSAT's or any user-defined Matchup Protocol.
    4. Store into standard **EDB** (**Extraction Data Base**) netCDF4 and CSV files.

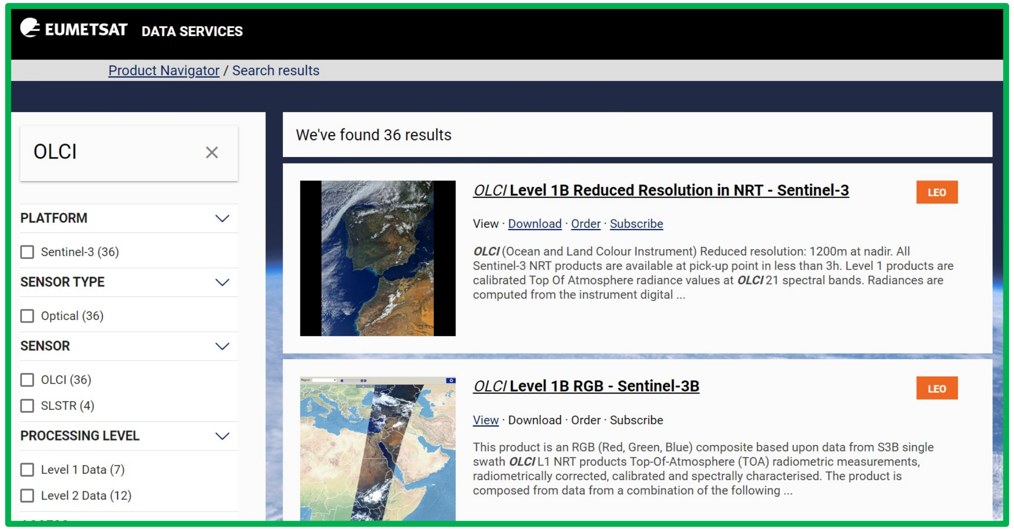
5. Step **MDB**.
    1. Combine insitu (**IDB**) and satellite (**EDB**) information indexed into insitu-satellite **matchup pairs**
    2. **Optionally apply time interpolation**
    3. Calculate **matchup statistics**
    4. Store into standard **MDB** (**Matchup Data Base**) netCDF4 and CSV files.

3. Usage: Step insitu

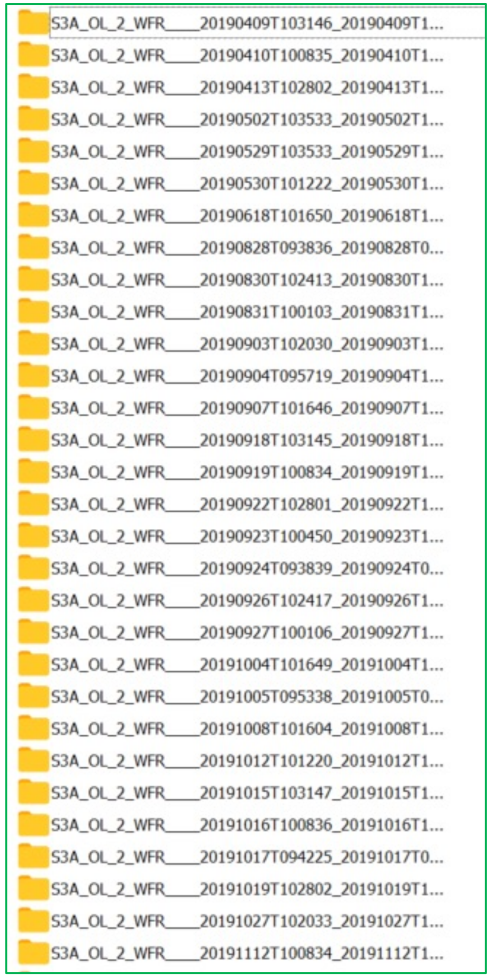


3. Usage. Step SatData

EUMETSAT Data Store



Your local system



NASA's OBPG L2 standard products

. . .

. . .

+ SatData Lists matching in situ

3. Usage: Step minifiles

- S3A_OL_2_WFR____20190409T103146_20190409T1...
- S3A_OL_2_WFR____20190410T100835_20190410T1...
- S3A_OL_2_WFR____20190413T102802_20190413T1...
- S3A_OL_2_WFR____20190502T103533_20190502T1...
- S3A_OL_2_WFR____20190529T103533_20190529T1...
- S3A_OL_2_WFR____20190530T101222_20190530T1...
- S3A_OL_2_WFR____20190618T101650_20190618T1...
- S3A_OL_2_WFR____20190828T093836_20190828T0...
- S3A_OL_2_WFR____20190830T102413_20190830T1...
- S3A_OL_2_WFR____20190831T100103_20190831T1...
- S3A_OL_2_WFR____20190903T102030_20190903T1...
- S3A_OL_2_WFR____20190904T095719_20190904T1...
- S3A_OL_2_WFR____20190907T101646_20190907T1...
- S3A_OL_2_WFR____20190918T103145_20190918T1...
- S3A_OL_2_WFR____20190919T100834_20190919T1...
- S3A_OL_2_WFR____20190922T102801_20190922T1...
- S3A_OL_2_WFR____20190923T100450_20190923T1...
- S3A_OL_2_WFR____20190924T093839_20190924T0...
- S3A_OL_2_WFR____20190926T102417_20190926T1...
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- S3A_OL_2_WFR____20191004T101649_20191004T1...
- S3A_OL_2_WFR____20191005T095338_20191005T0...
- S3A_OL_2_WFR____20191008T101604_20191008T1...
- S3A_OL_2_WFR____20191012T101220_20191012T1...
- S3A_OL_2_WFR____20191015T103147_20191015T1...
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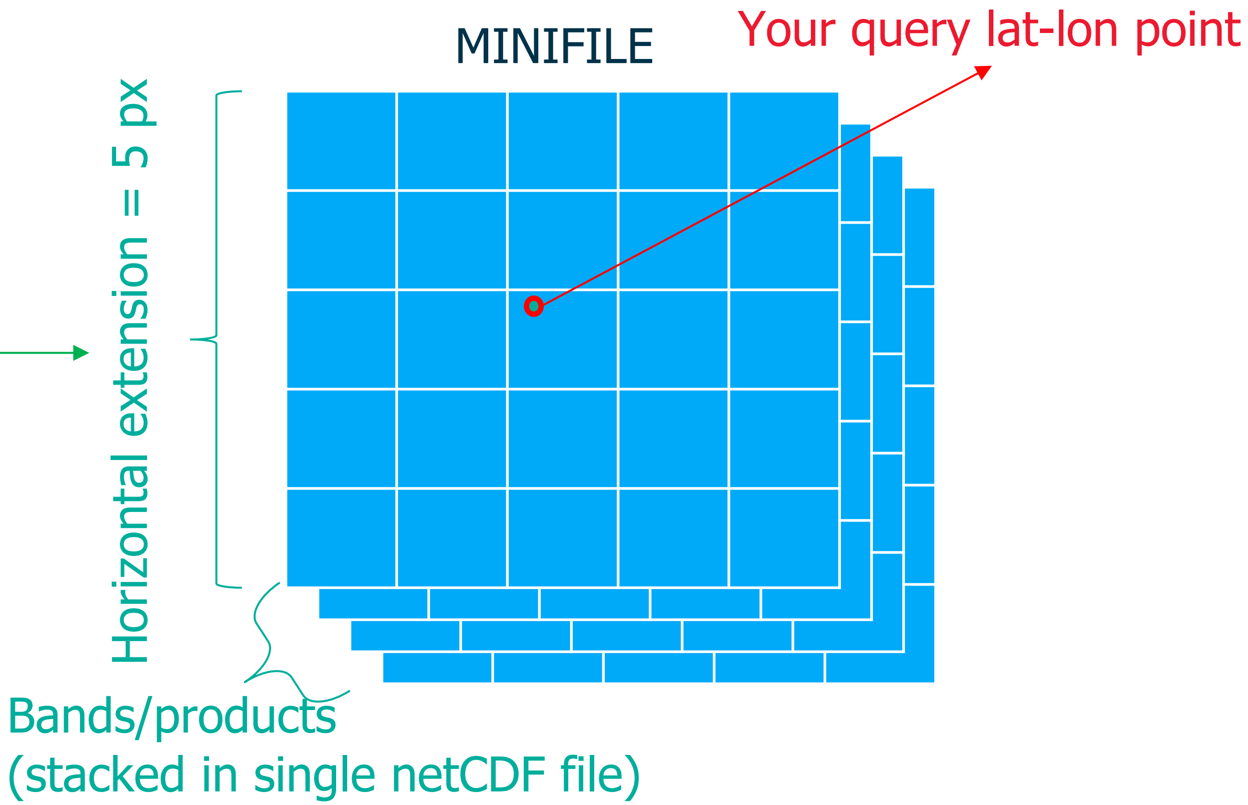
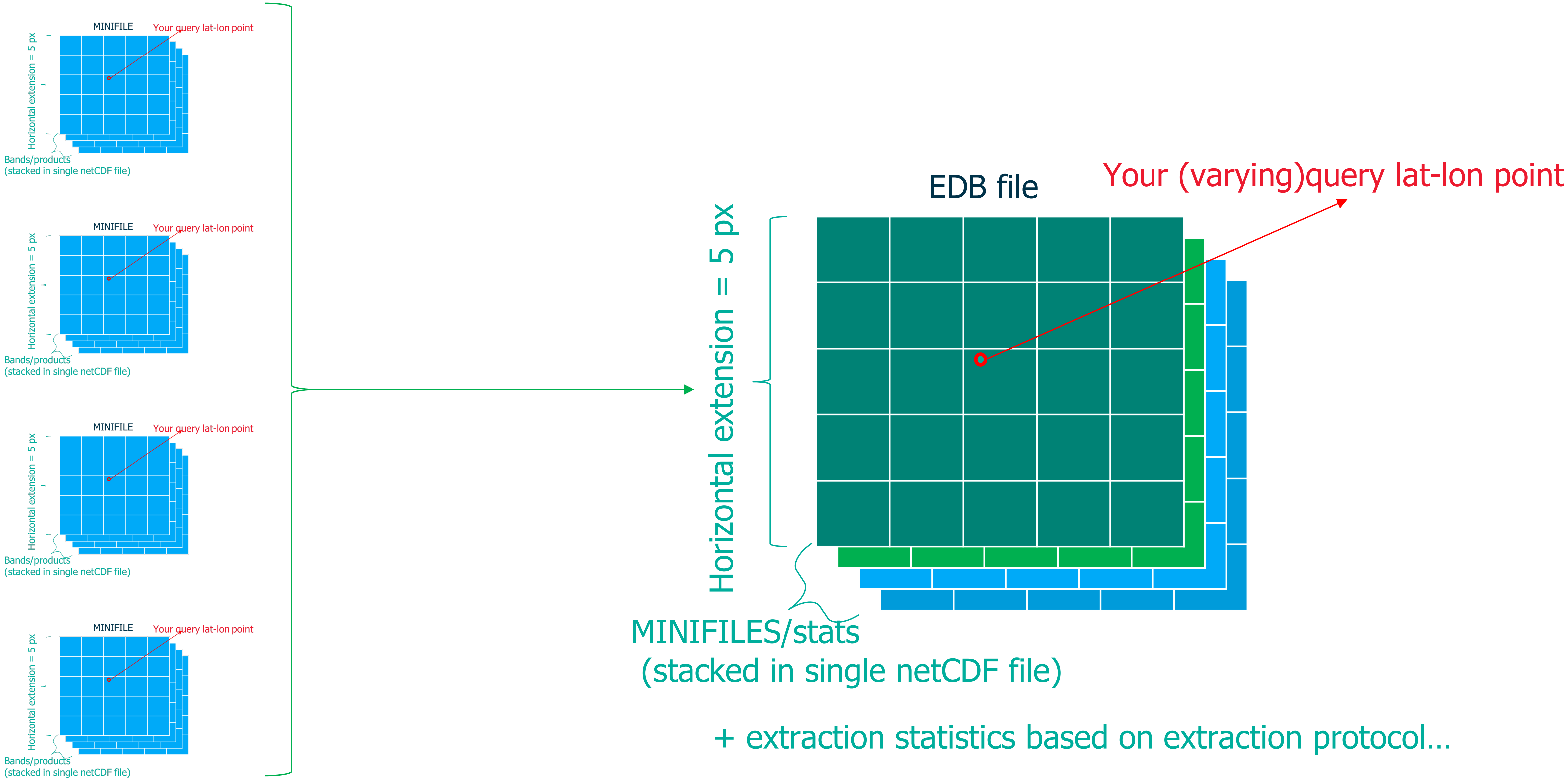
- S3A_OL_2_WFR____20191112T100834_20191112T1...



3. Usage: Step EDB

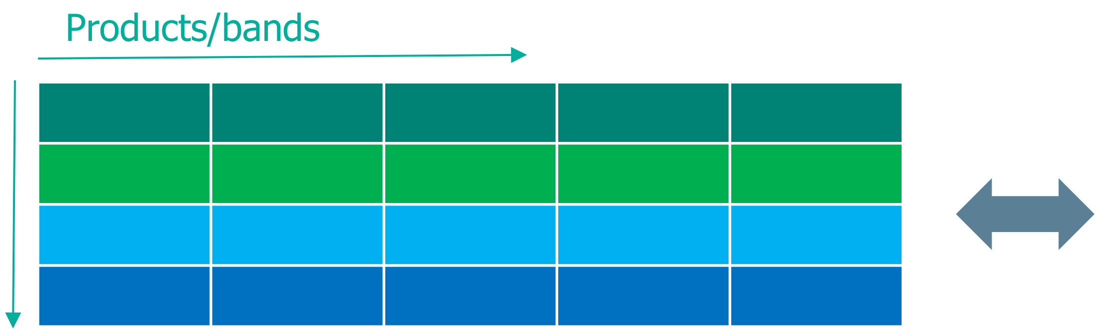


+ extraction statistics based on extraction protocol…

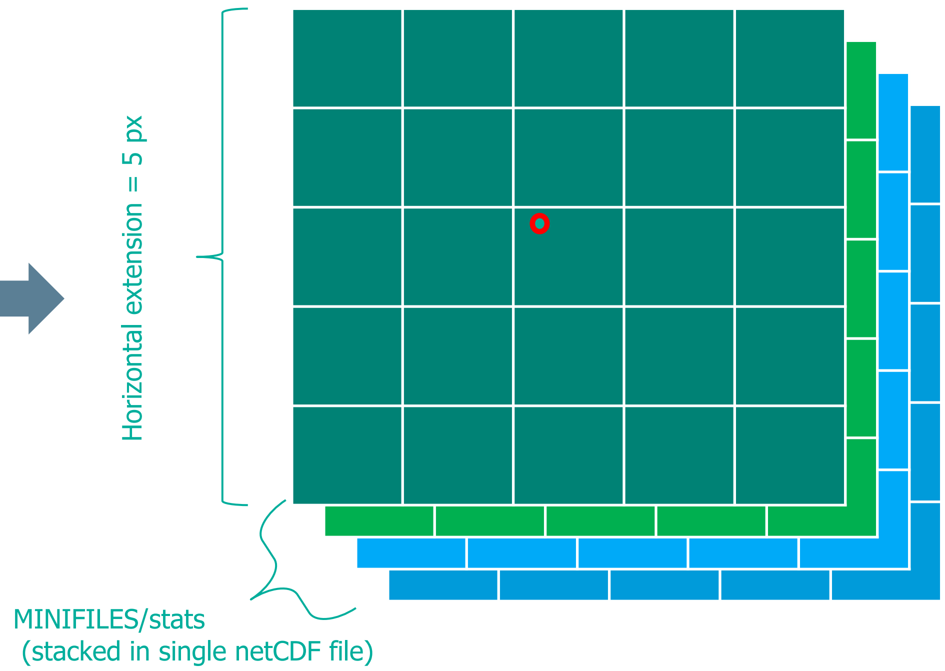
MDB file

1. Merging insitu and extractions according to matchup pairs
2. Statistical metrics calculated + scatter/spectral plots

In situ data base (IDB) file



Extraction data base (EDB) file



MDB: indexed by matchup pair ID
Time interpolation (nearest in time) applicable

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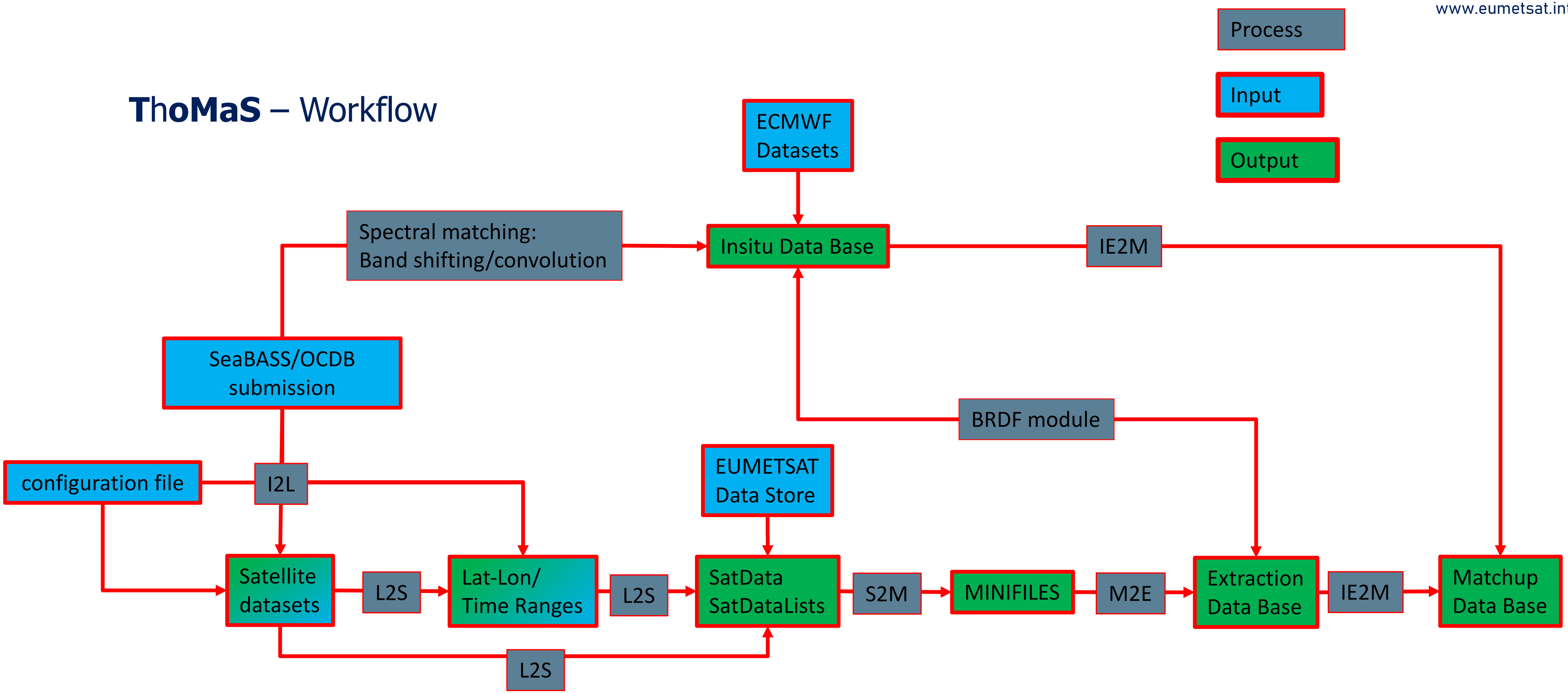
ThoMaS – Workflow



3. Usage: Summary on the terminology

- **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.

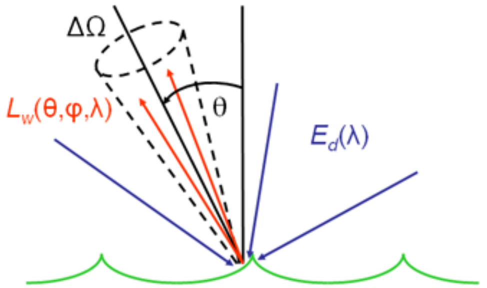
- **MDB** (Match-up Data Base): All the information from IDB and EDB combined and re-indexed according to matchup pairs + matchup statistics.

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

4. Some background: match-ups

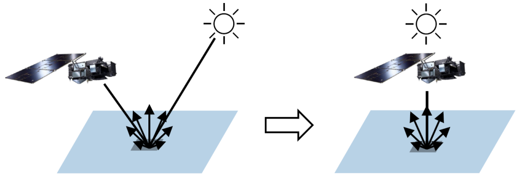
Definition of Rrs

$$R_{rs}(\theta, \phi, \lambda) \equiv \frac{L_w(\text{in air}, \theta, \phi, \lambda)}{E_d(\text{in air}, \lambda)} \quad (\text{sr}^{-1}) \,.$$

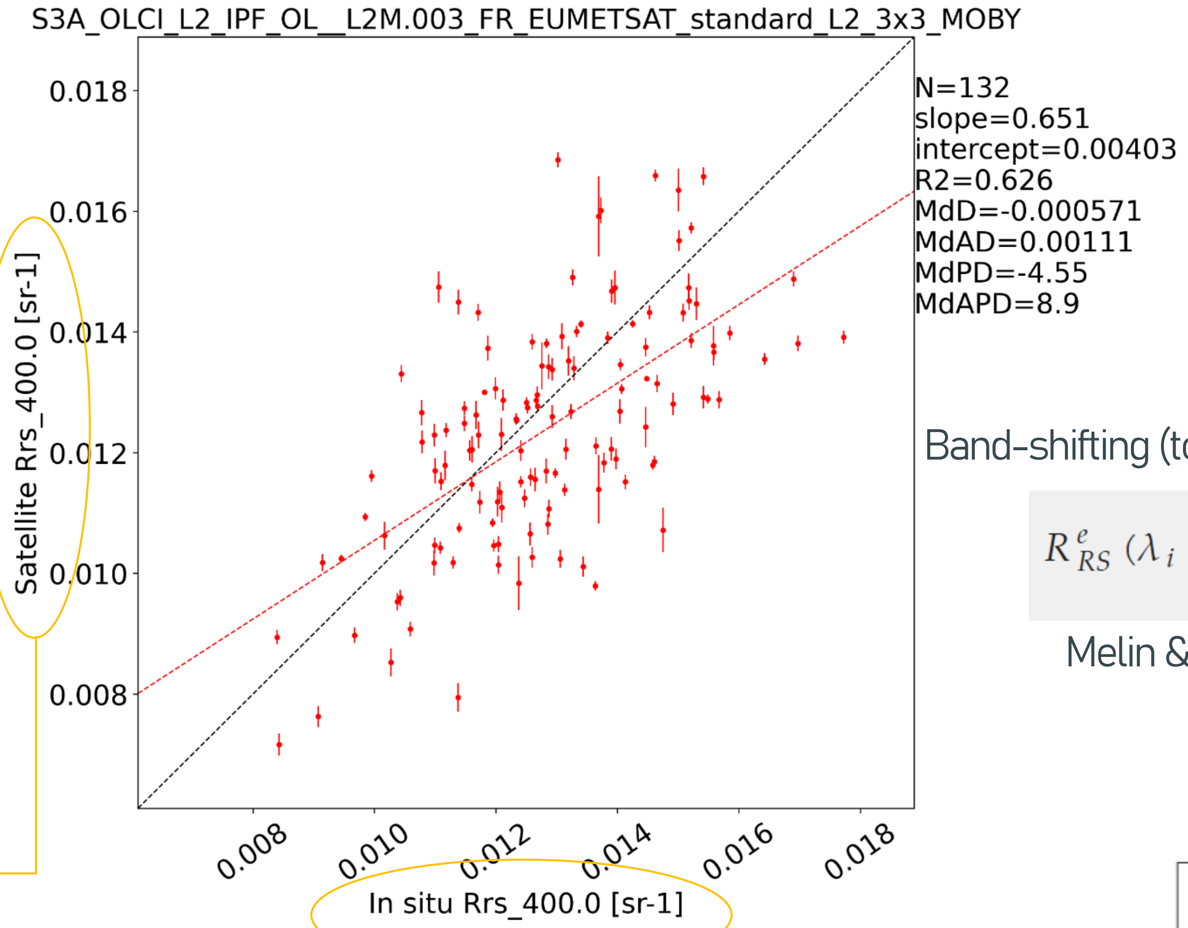


OO Web Book, Mobley, Boss & Roesler

BRDF correction:



D'Alimonte et al.
Morel et al. 2002 supported in ThoMaS

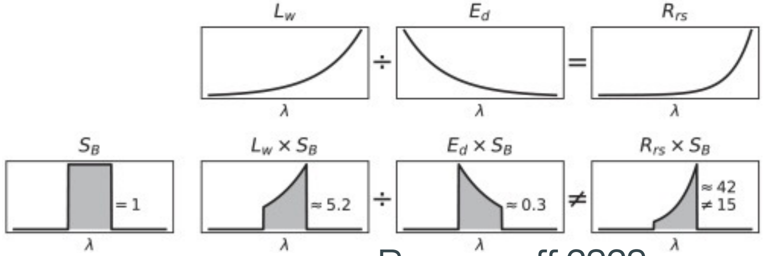


Band-shifting (to pair multispectral to multispectral)

$$R^{e}_{RS}(\lambda_i \rightarrow \lambda_t) = R^{f}_{RS}(\lambda_t)\frac{R_{RS}(\lambda_i)}{R^{f}_{RS}(\lambda_i)}$$

Melin & Sclep 2015 supported in ThoMaS

Spectral convolution



Burggraaff 2020

Are we comparing 🍎 with 🍎?

→ What is the definition of Rrs?

→ Are these two compatible "spectrally"? → convolution/band-shifting

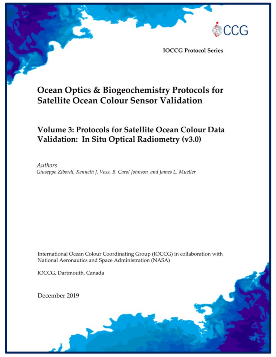
→ Are these two compatible "directionally"? → BRDF correction

4. Some background: match-ups

Quality of insitu

ThoMaS still **<u>does not</u>** consider any quality flag to process insitu data… but stay tuned ☺…

fiducial reference measurements for satellite ocean colour


IOCCG Protocol Series

Ocean Optics & Biogeochemistry Protocols for Satellite Ocean Colour Sensor Validation

Volume 3: Protocols for Satellite Ocean Colour Data Validation: In Situ Optical Radiometry (v3.0)

Authors
Giuseppe Zibordi, Kenneth J. Voss, B. Carol Johnson and James L. Mueller

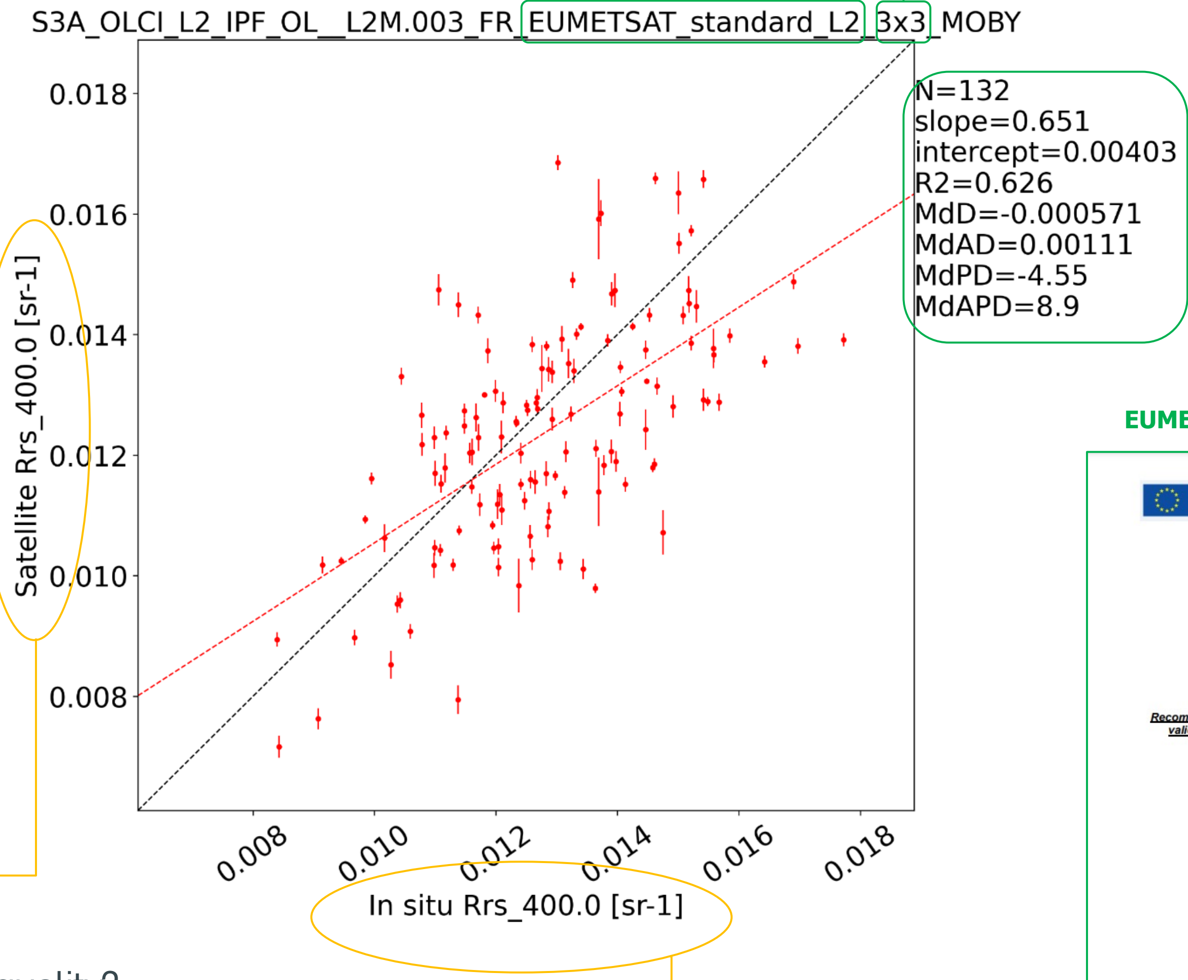
International Ocean Colour Coordinating Group (IOCCG) in collaboration with National Aeronautics and Space Administration (NASA)

IOCCG, Dartmouth, Canada

December 2019

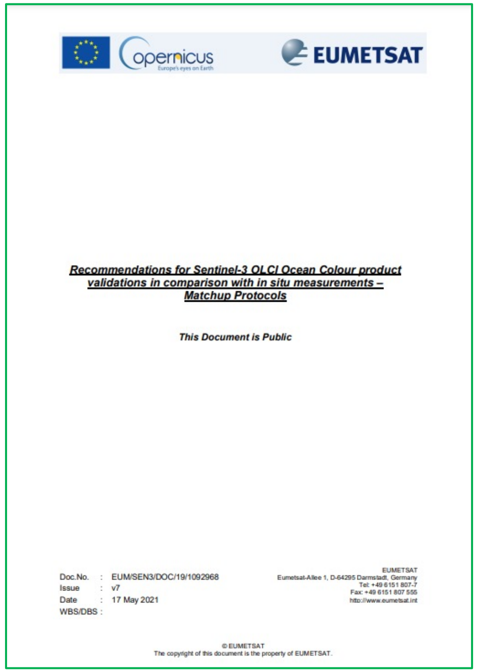
Define your extraction statistics!

Define your extraction window size!



Define the matchup statistics!

EUMETSAT's Matchup Protocols


<u>Recommendations for Sentinel-3 OLCI Ocean Colour product validations in comparison with in situ measurements – Matchup Protocols</u>

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<u>Are we comparing 🍎 with 🍎</u>?

→ Are the insitu measurements of sufficient quality?
→ Are insitu and satellite measurements temporally-spatially comparable?
→ What value (and uncertainty) shall I extract from the satellite data?

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

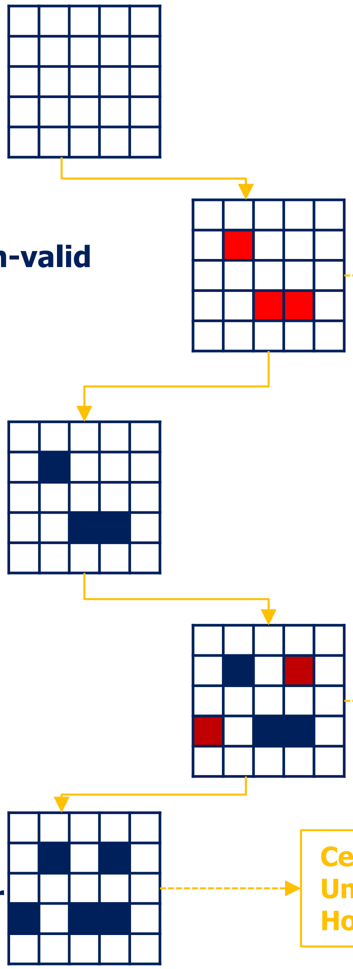
Window size recommended: 5x5 or 3x3
Tolerable insitu-satellite time difference: 1 hr or 3 hrs

Set BFOR: 5x5 window

Detection of non-valid pixels (flagged pixels)

Set BOR: without flagged pixels

Set final: without flagged & outlier



Pixels are masked/removed if flagged by any of the following:

CLOUD, CLOUD_AMBIGUOUS, CLOUD_MARGIN, INVALID, COSMETIC, SATURATED, SUSPECT, HISOLZEN, HIGHGLINT, SNOW_ICE, AC_FAIL, WHITECAPS, ADJAC, RWNEG_O2, RWNEG_O3, RWNEG_O4, RWNEG_O5, RWNEG_O6, RWNEG_O7, RWNEG_O8

Macropixel is discarded if:

$N_{BOR} < 50\% \; N_{BFOR}$

Pixel 'X' is considered <u>outlier</u> if:

$|value@X - \mu_{BOR}| < 1.5\sigma_{BOR}$

Central value: $median_{final}$
Uncertainty measure (Type B): σ_{final}
Homogeneity measure: CV_{final}

Macropixel is discarded if:

$CV_{final}(560)>20\%$

μ → Mean
σ → Standard deviation

ThoMaS can be run with many other extraction protocols, that you define

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

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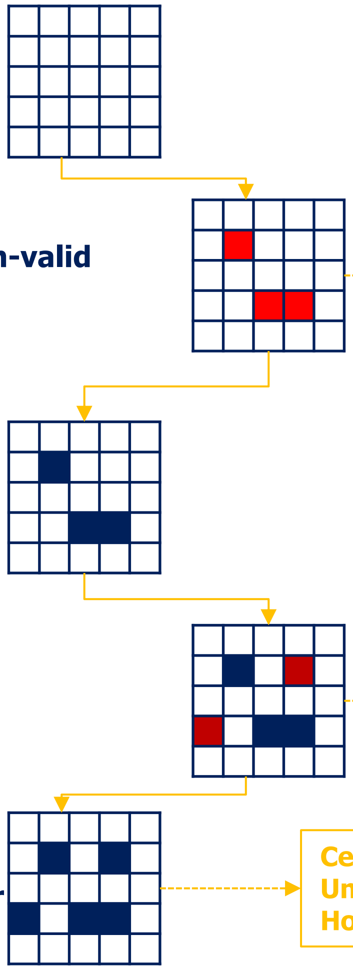


Pixels are masked/removed if flagged by any of the following:

ATMFAIL, LAND, HIGLINT, HILT, HISATZEN, STRAYLIGHT, CLDICE, COCCOLITH, HISOLZEN, LOWLW, CHLFAIL, NAVWARN, MAXAERITER, CHLWARN, ATMWARN, SEAICE, NAVFAIL, ABSAER, MODGLINT

Macropixel is discarded if:

$N_{BOR} < 50\% \ N_{BFOR}$

Pixel 'X' is considered outlier if:

$|\text{value@X} - \mu_{BOR}| < 1.5\sigma_{BOR}$

Macropixel is discarded if:

Median[CV(Rrs(410-551));CV(AOT(869))]>15%

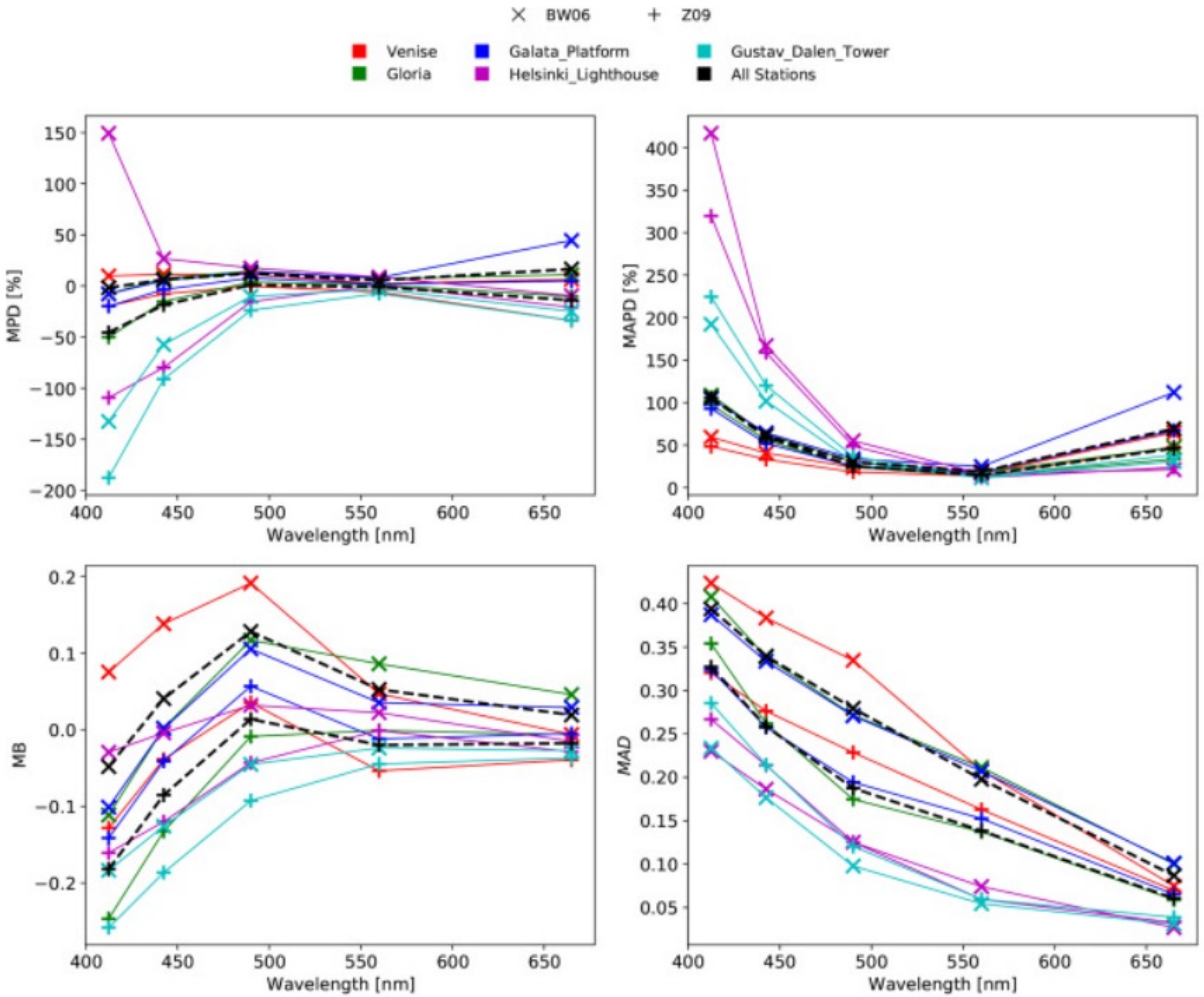
Central value: median_{final}
Uncertainty measure (Type B): σ_{final}
Homogeneity measure: CV_{final}

ThoMaS can be run with many other extraction protocols, that you define

μ → Mean
σ → Standard deviation

4. Some background: match-ups: what protocol to use?

Should we care about what matchup protocol we use?

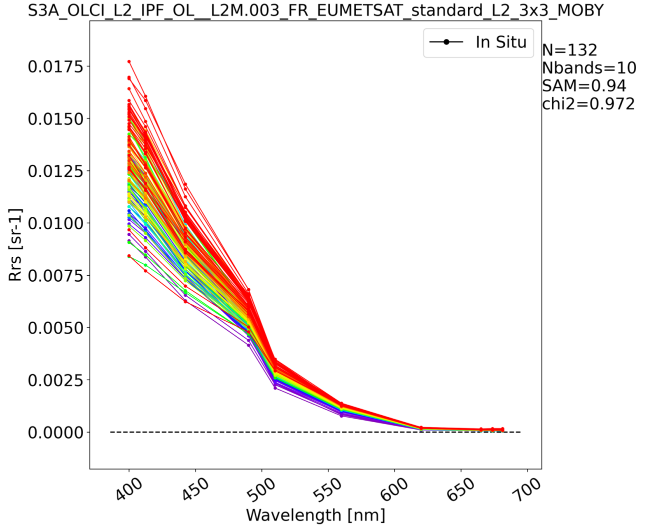


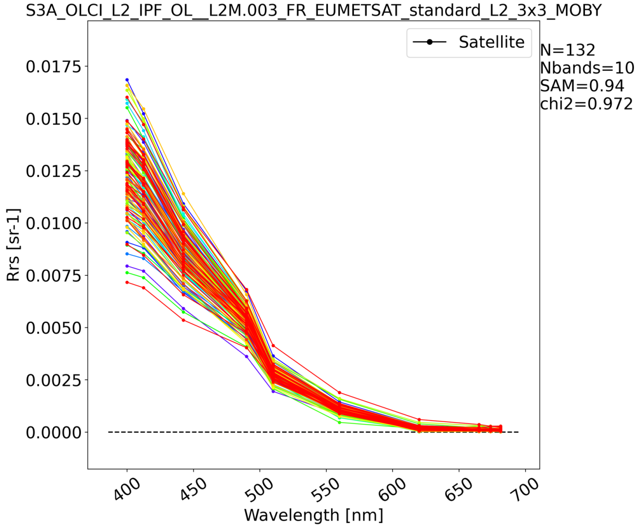
[Concha et al. 2021]

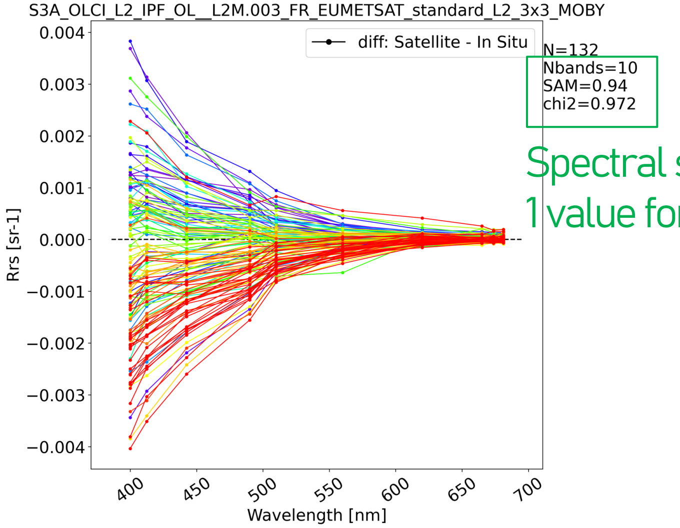
4. Some background: match-ups

www.eumetsat.int

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

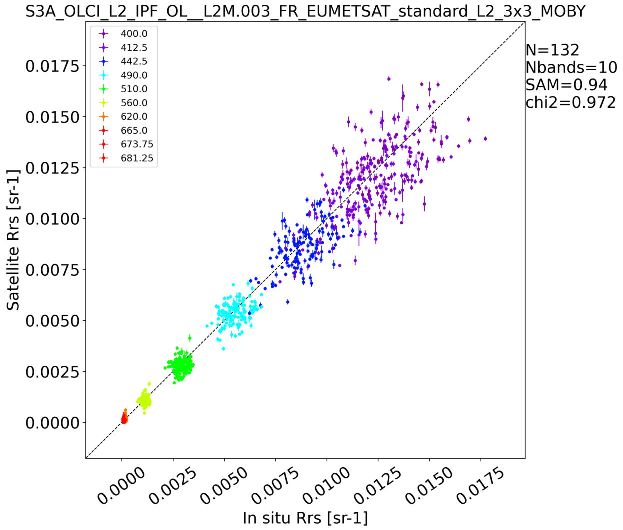


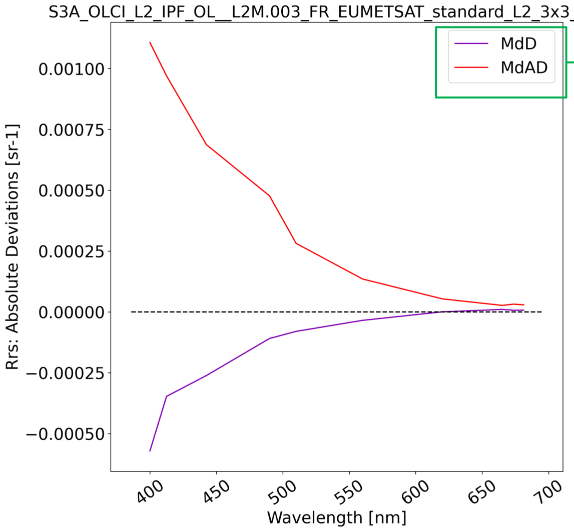


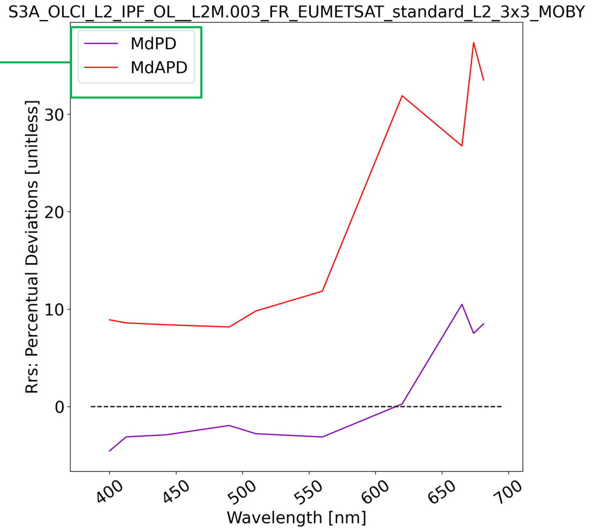


Spectral statistics
1 value for the whole set

statistics band-by-band, plotted spectrally

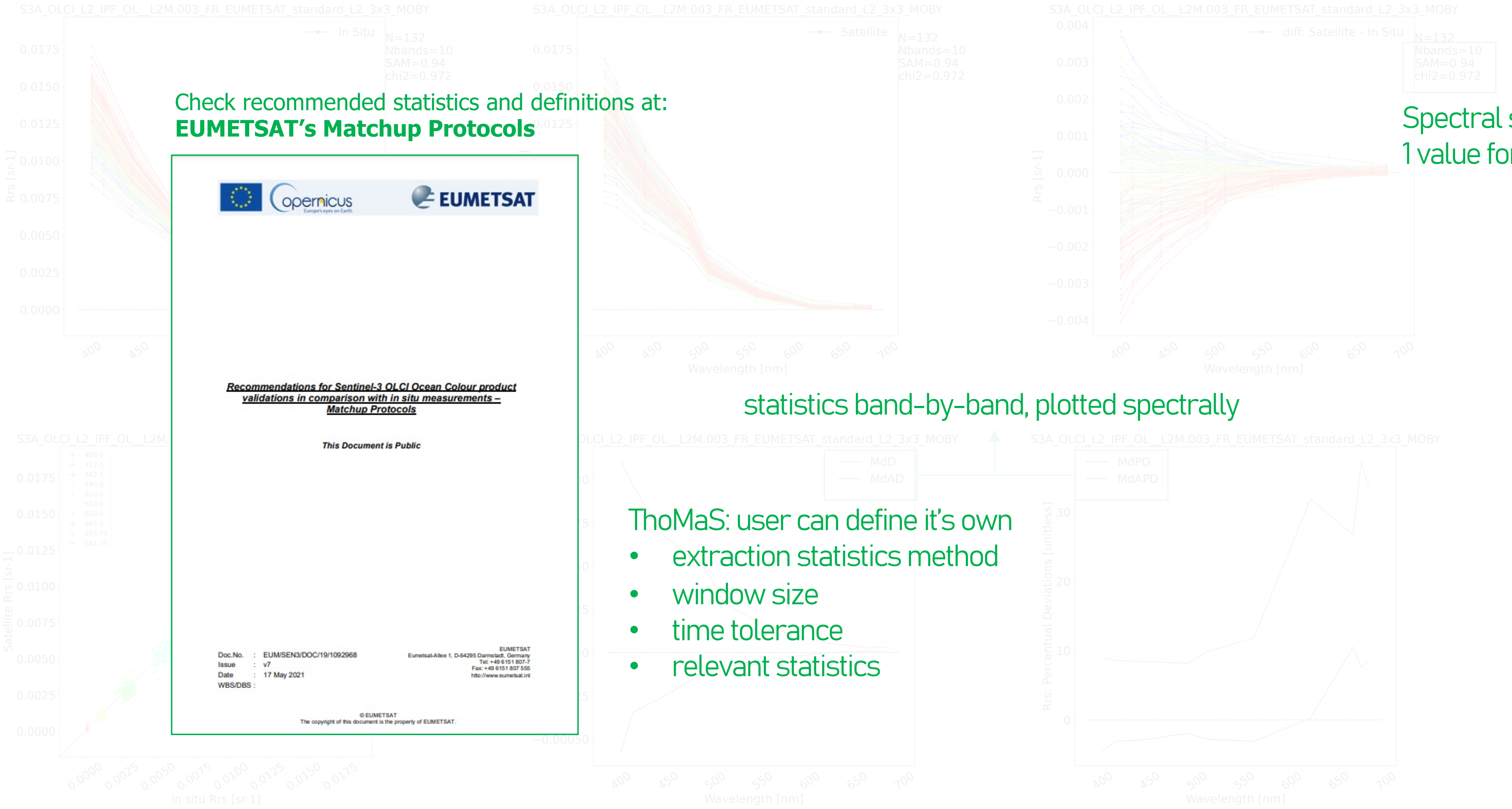






4. Some background: match-ups

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



Check recommended statistics and definitions at:
EUMETSAT's Matchup Protocols

Copernicus — Europe's eyes on Earth
EUMETSAT

Recommendations for Sentinel-3 OLCI Ocean Colour product validations in comparison with in situ measurements – Matchup Protocols

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Spectral statistics
1 value for the whole set

statistics band-by-band, plotted spectrally

ThoMaS: user can define it's own

- extraction statistics method
- window size
- time tolerance
- relevant statistics

5. 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.txt**
5. ECMWF: Register to ADS/CDS and get url and key.
6. ECMWF: store ADS/CDS url/keys under **~/.ecmwf_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
jupyter	1.0.0	Unspecified	https://anaconda.org/anaconda/jupyter

Conda will take care of this…

5. Getting the code

- Git way:

```
cd ~
mkdir ThoMaS
cd ThoMaS
git clone --depth 1 https://gitlab.eumetsat.int/eumetlab/oceans/ocean-science-studies/ThoMaS .
```

- Direct download:

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

Recent updates were done on the code

```
git fetch
git pull
```

6. Setting the environment

- Once conda and ThoMaS are installed, create the thomas env:

```
cd ~
cd ThoMaS
conda env create –f environment.yml
conda activate thomas
```

→ **libmamba** is the best choice for those of you who are stuck in the "**Solving environment step**"

7. Required inputs: SeaBASS/OCDB file

www.eumetsat.int

```
/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,…
/units=none,yyyymmdd,hh:mm:ss,degrees,degrees,m,%,degrees,unitless,mg/L,mg/m^3,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,…
/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,…
```

7. Required inputs: SeaBASS/OCDB file

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/processed=20190101
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/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,…
/units=none,yyyymmdd,hh:mm:ss,degrees,degrees,m,%,degrees,unitless,mg/L,mg/m^3,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,1/sr,…
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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,…
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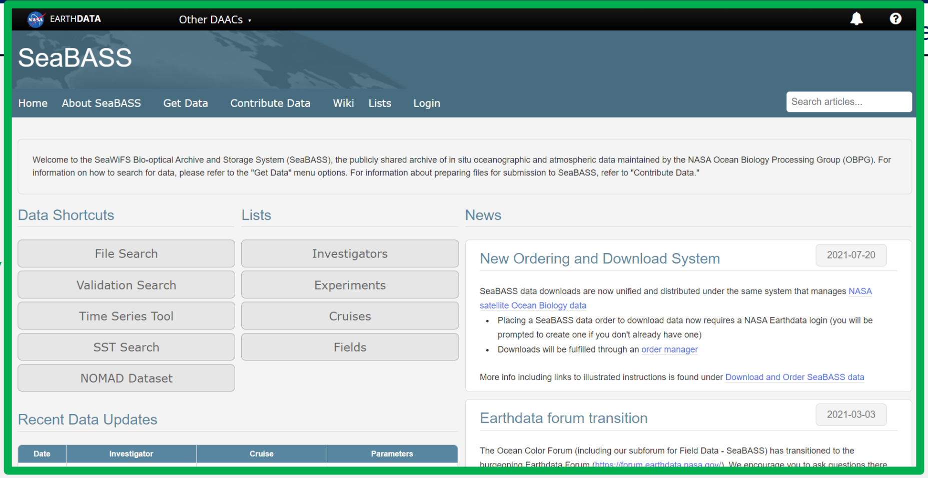
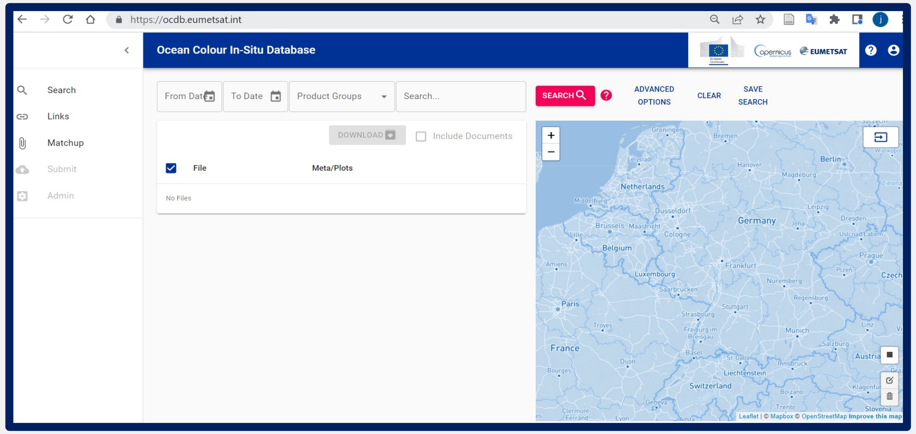
SeaBASS
seabass.gsfc.nasa.gov



Inter-operable

OCDB
ocdb.eumetsat.int



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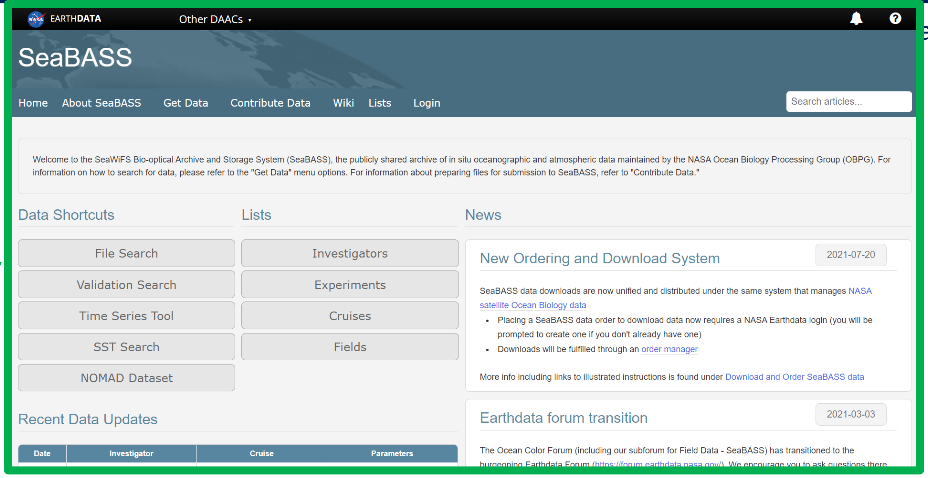

Inter-operable

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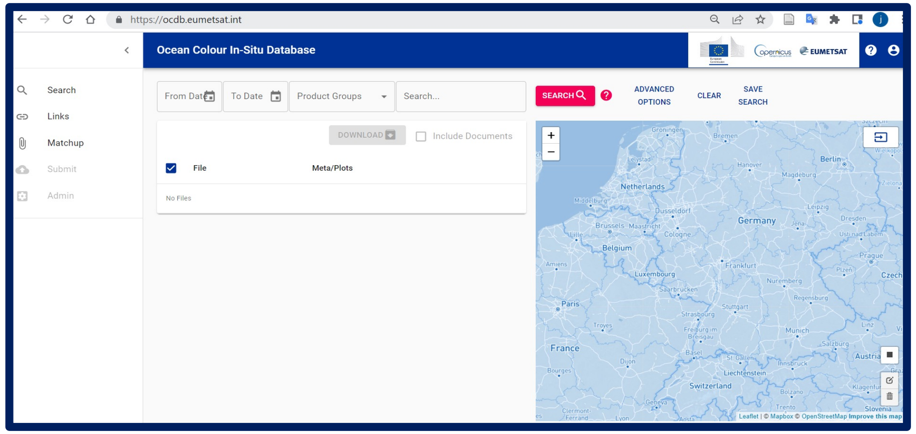


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/data_type=cast
/data_status=final
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/BRDF_option=None
/instrument_model=RAMSES
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/calibration_date=NA
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! COMMENTS
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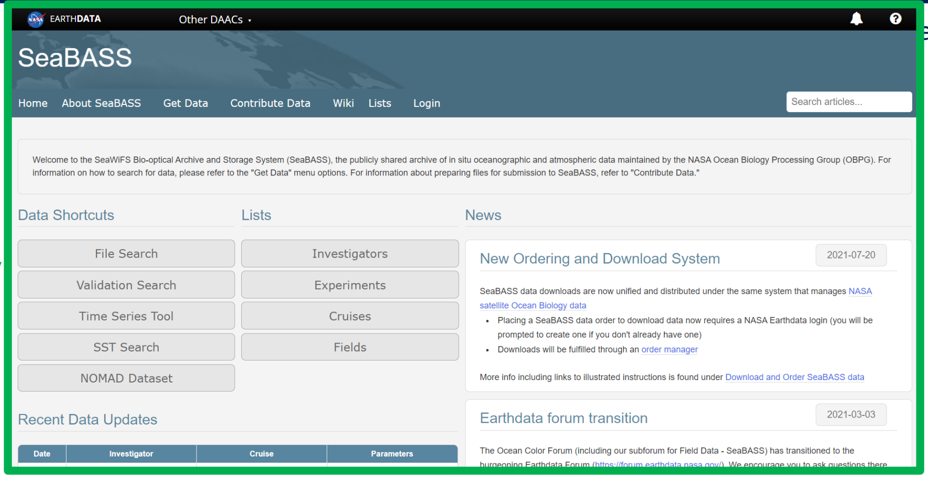
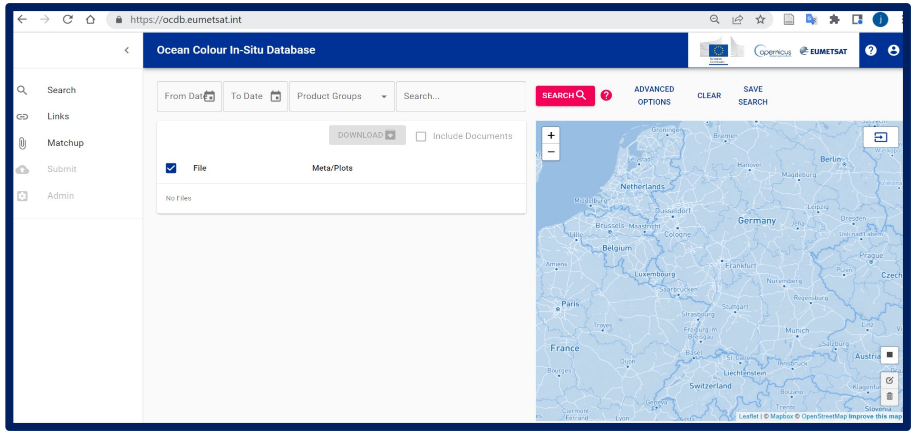
TestStation003,20201014,12:16:00,-32.0209,26.9584,0.01,0,134.7,0.2388,0.1,0.1,0.001918189,0.002097384,0.002191946,0.002353893,0.002567901,0.002792078,0.00307,…
TestStation004,20210910,09:40:00,3,-3,0.01,0,134.9,0.2388,0.1,0.1,0.001271305,0.001359205,0.00139314,0.001432681,0.001487187,0.00153414,0.00160502,0.00165816,…
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,…
```

SeaBASS
seabass.gsfc.nasa.gov

Inter-operable

OCDB
ocdb.eumetsat.int





at.int

ThoMaS demo

Thank you!

Questions are welcome.

Contacts and further information

For information on our training programme

training@eumetsat.int

For information on EUMETSAT services

ops@eumetsat.int

For our training calendar

https://trainingevents.eumetsat.int/trui/

More information:

Data Store

Access: https://data.eumetsat.int/

Help: https://eumetsatspace.atlassian.net/wiki/spaces/DSDS/overview

EUMDAC

Source : https://gitlab.eumetsat.int/eumetlab/data-services/eumdac/

Help: https://eumetsatspace.atlassian.net/wiki/spaces/EUMDAC/overview

Gitlab

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

https://gitlab.eumetsat.int/eumetlab/oceans/ocean-training

Training courses

https://trainingevents.eumetsat.int/trui/

Course materials

https://training.eumetsat.int/course/view.php?id=492