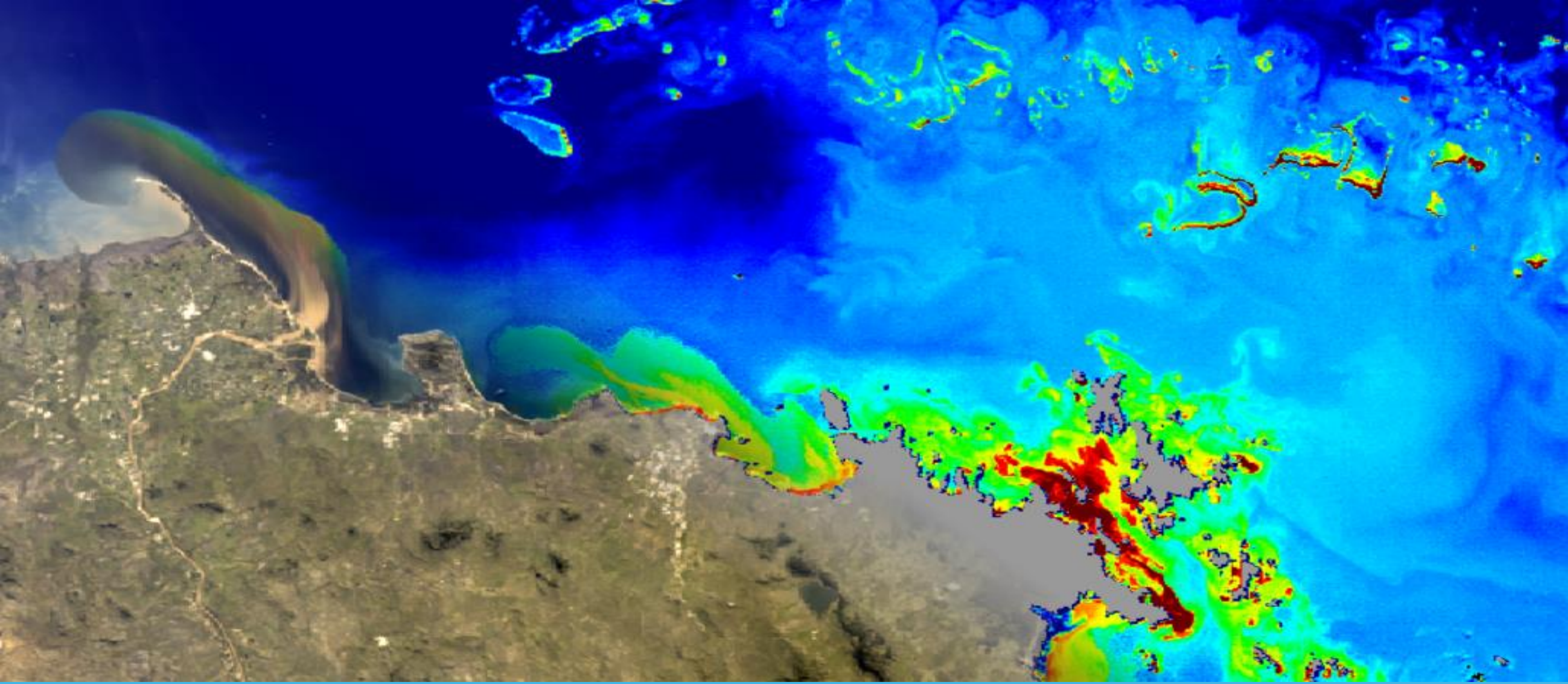

Migration of the MERIS FUB Coastal Water Processor to Sentinel-3 OLCI

Schroeder T. , Schaale M., Lovell J. Blondeau-Patissier D., Boadle D., and Baker B.

7-9 May 2019 S3VT meeting, ESA-ESRIN, Frascati (Rome), Italy

CSIRO OCEANS & ATMOSPHERE
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IMOS

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This presentation

- Brief recap of FUB algorithm approach – from MERIS to S3
- S3 validation
- New plug-in features – eVT filter, pixel-based uncertainties
- TBDs
- Updates from the Lucinda Jetty Coastal Observatory
- Summary & Outlook

Very brief FUB algorithm recap

Approach:
Inverse modeling of coupled ocean-atmosphere radiative transfer simulations using artificial neural networks (ANNs).

International Journal of Remote Sensing
Vol. 28, No. 24, 20 December 2007, 5627–5632

Taylor & Francis
Taylor & Francis Group

Retrieval of atmospheric and oceanic properties from MERIS measurements: A new Case-2 water processor for BEAM

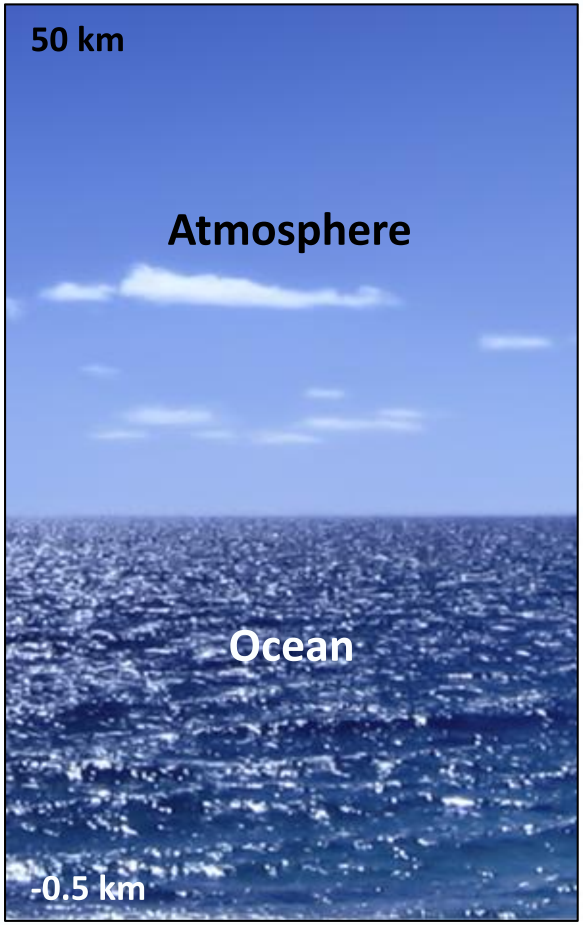
TH. SCHROEDER*†‡, M. SCHAALE† and J. FISCHER†
†Free University Berlin, Institute for Space Sciences, Berlin, Germany
‡CSIRO Land & Water, Environmental Remote Sensing Group, Canberra, Australia

Atmospheric correction algorithm for MERIS above case-2 waters

TH. SCHROEDER*†, I. BEHNERT‡§, M. SCHAALE†, J. FISCHER† and R. DOERFFER‡
†Free University Berlin, Institute for Space Sciences, Berlin, Germany
‡GKSS Research Centre, Institute for Coastal Research, Geesthacht, Germany
§CIMEL Electronique, Paris, France

Forward model

Coupled ocean-atmosphere radiative transfer model, matrix-operator method (FUB). Simulates the upward radiance field (TOA & BOA) for a variety of different Sun and observing geometries depending on the concentration of different types of atmospheric and oceanic constituents.



- Vertical profile (US-Standard)
- Ozone (344 DU)
- Rayleigh (980hPa, 1040hPa)
- Aerosols (8-Types)
- Optical depths (5)
- Single scattering albedos
- Phase functions

- Vertical homogenous mixing of CHL, TSM, YEL
- No bottom-up effects (optically deep water)
- Phase functions
- $a=a_w+a_{p1}(CHL)+a_{p2}(TSM)+a_y(YEL)$
- $b=b_w+b_{p1+p2}(TSM)$

Inverse model

- **MERIS 4 ANNs** (1 ATMCOR + 3 WQ retrieval) – **Sentinel-3** now **20 ANNs** (4 x 5)
- Used MERIS LUT for S3 but **extended** the **viewing geometry**
- Task of the ANNs is to perform **non-linear function approximation**
- Networks free parameters (weights) are adapted during a **supervised learning procedure**
- ANN advantage: **Universal function approximator**, fast, can be robust against input errors (noise)
- ANN disadvantage: **No analytical method to derive optimum network architecture**, under-fitting, over-fitting ...
- **Train various networks** by varying the number of hidden layer neurons & account for different transformations (PCA), input noise levels
- Optimum architecture is assessed through **validation against "real-world" (in-situ) data**

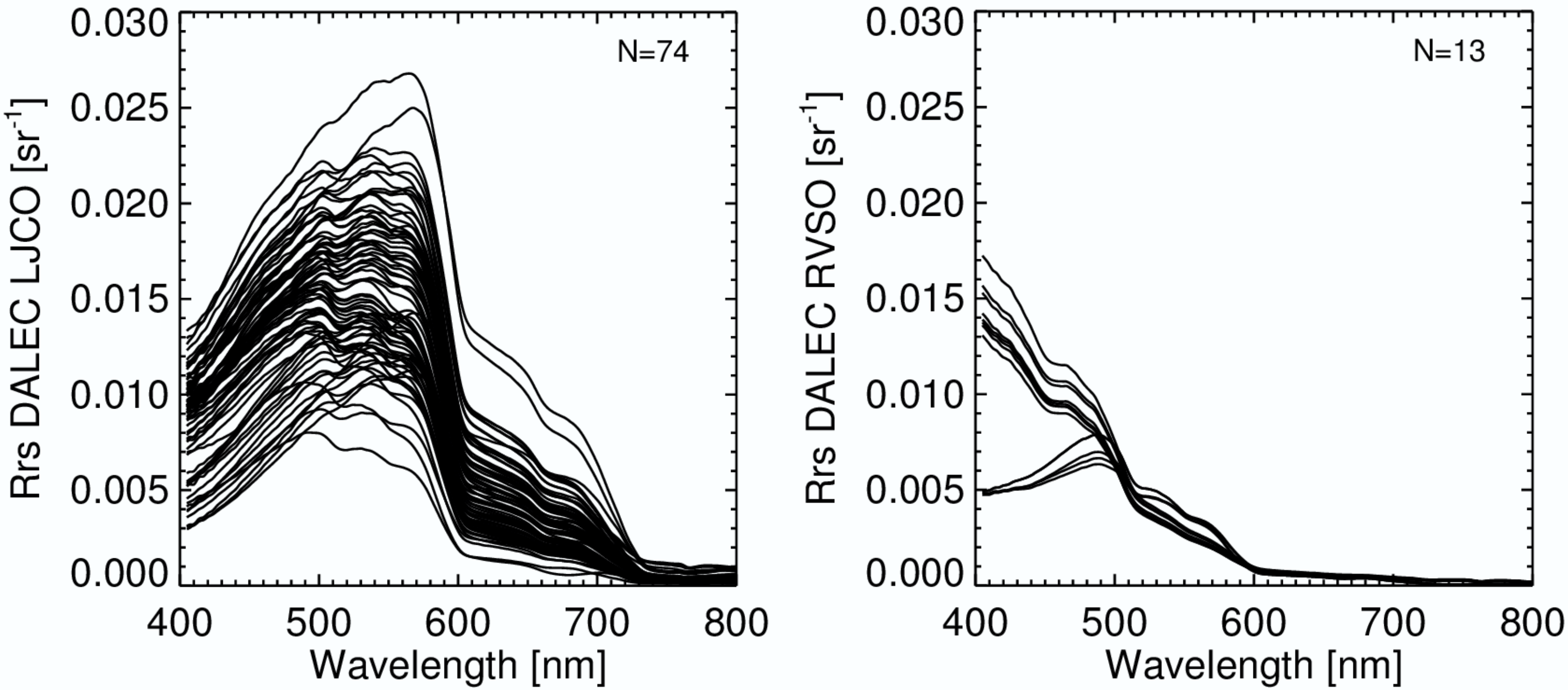
S3 radiometric validation – hyper-spectral DALEC

Fixed platform deployments (LJCO) and transects (AIMS RV Solander)

3 Zeiss MMS1 UV-VIS NIR spectrometer (Lu, Lsky, Ed) 400-1050 nm, 256 bands, 16 bit ADC
Motorized azimuth control, integrated GPS, roll pitch and heading


DALEC spectra matching S3A at ΔT±30 min, N=87

Fixed platform deployments (LJCO) and transects (AIMS RV Solander)



Mix of coastal and open ocean waters

Match-ups extractions and additional QC
Radiometry

IPF: OL_1 ≥6.07, OL_2 ≥6.11
Processing Baseline: ≥2.23

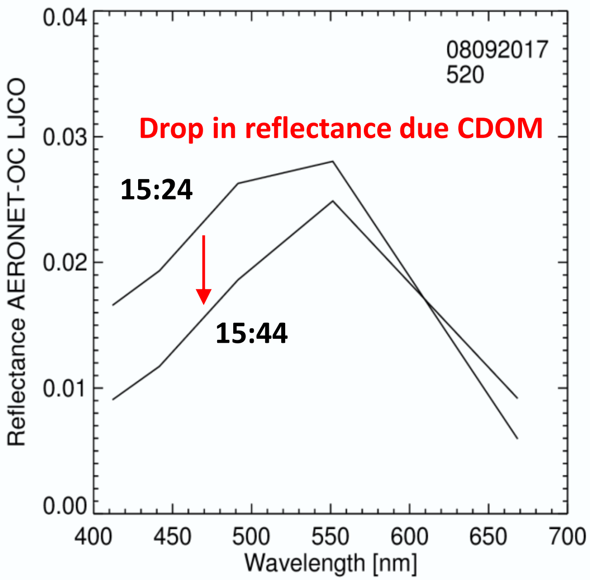
L1 flags: land, coastline, bright, straylight_risk, invalid, sun_glint_risk
L2 flags: AC_fail
NN_flags: min/max I/O ranges (convexity test)

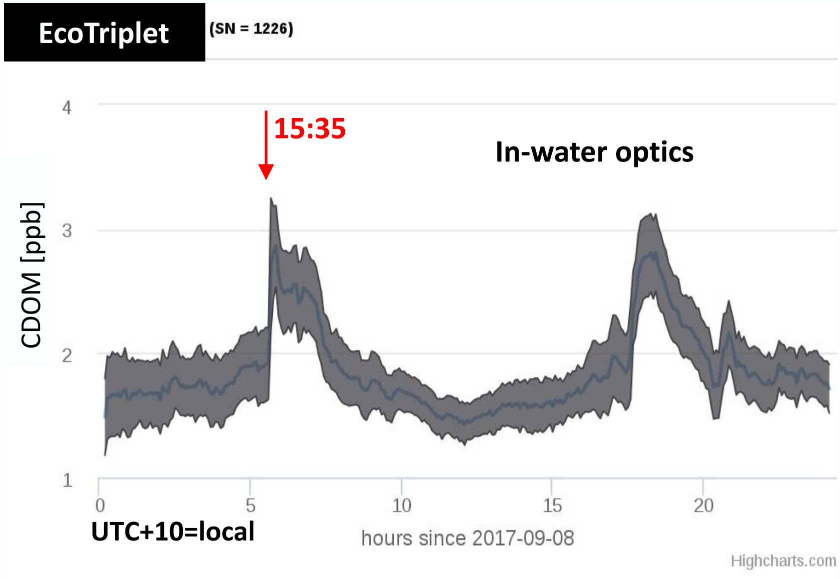
Match area: 3x3 no flags raised
Time difference: ΔT =±30 min – strong tidal gradients at LJCO
Standard deviation within match-up area lower 40% of median
Visual inspection of RGB macro region – filtering scattered clouds and haze

Finally N=50 high quality match-ups within ±30 min to S3A

Tidal fronts at LJCO

Large spectral changes within 2 subsequent SeaPRISM observations possible



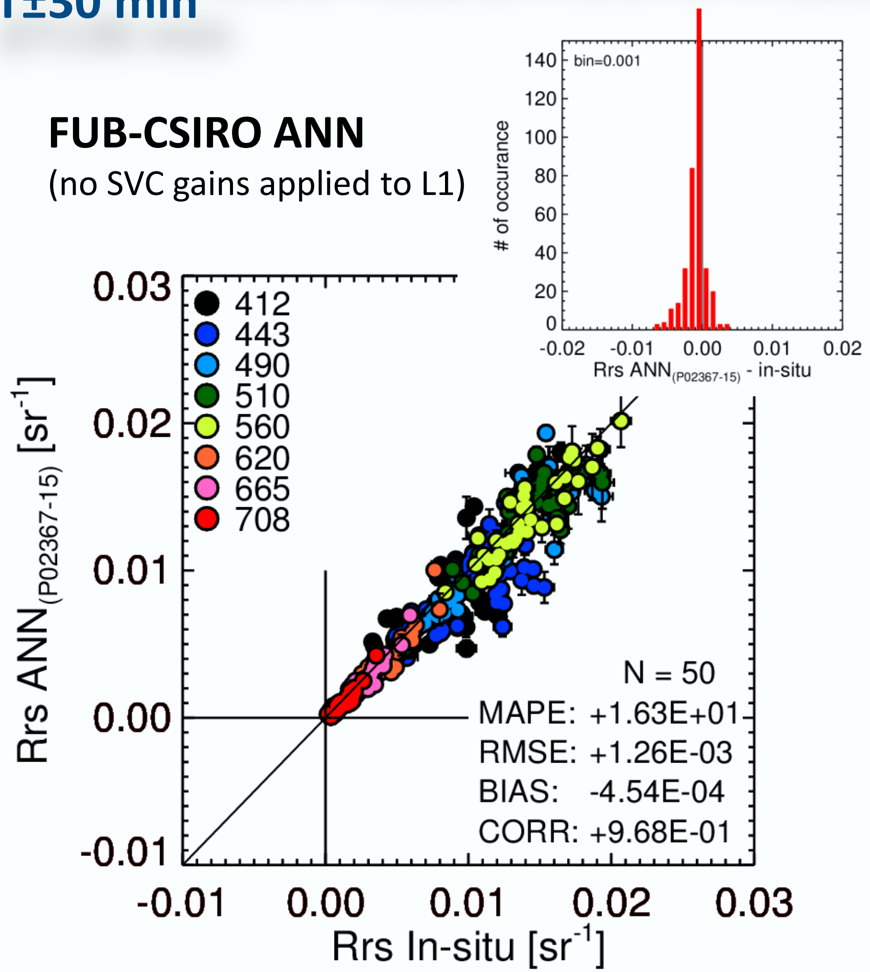


S3A-DALEC radiometric match-ups

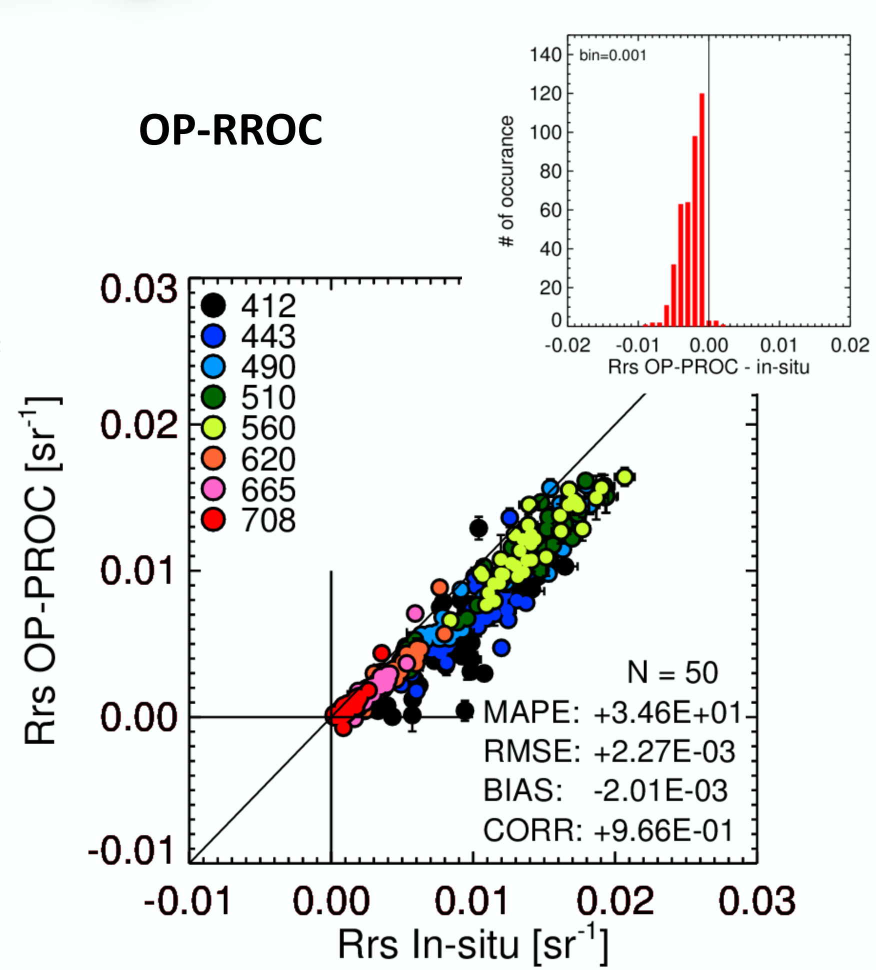
ΔT±30 min

FUB-CSIRO ANN

(no SVC gains applied to L1)

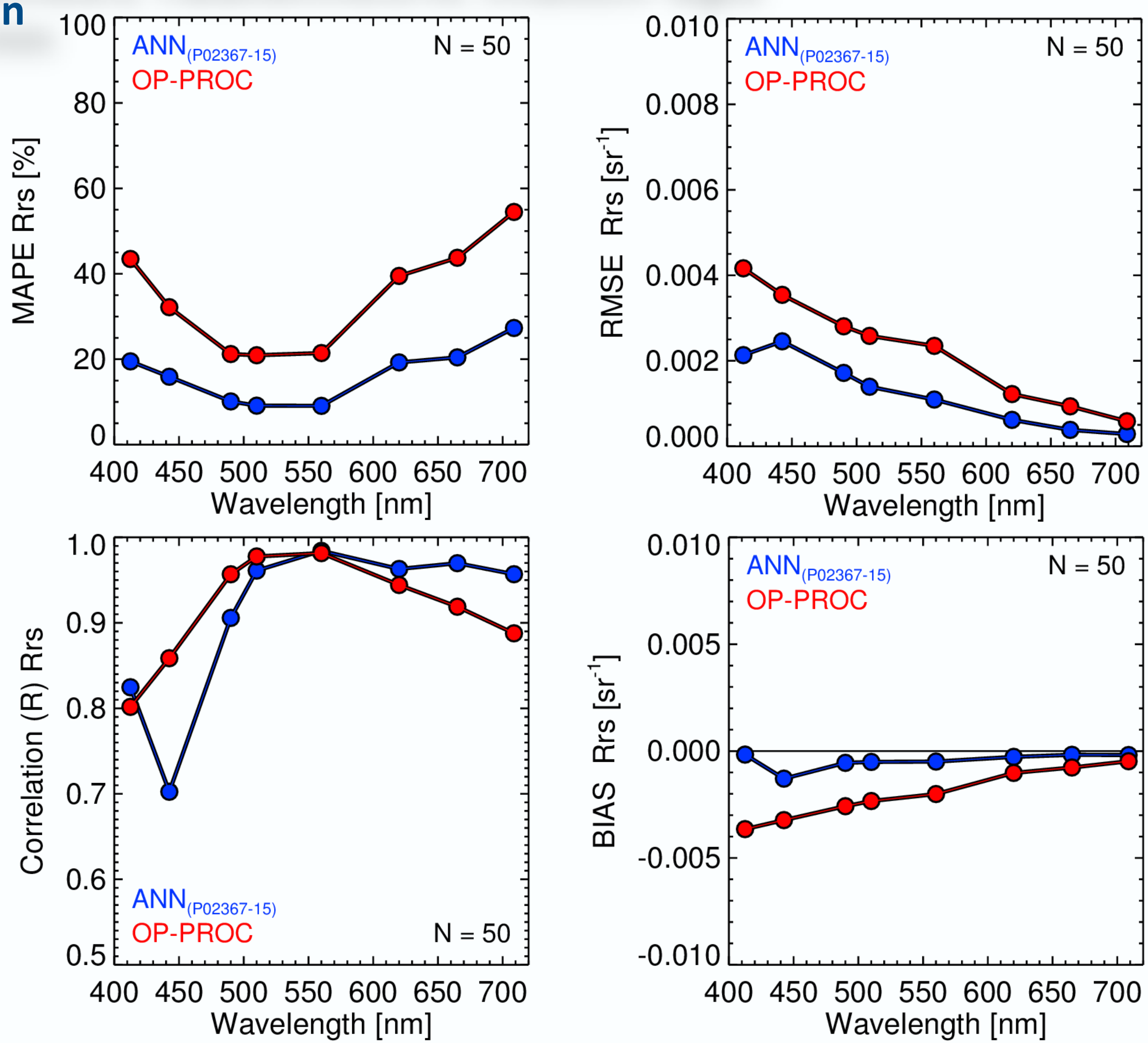


OP-RROC



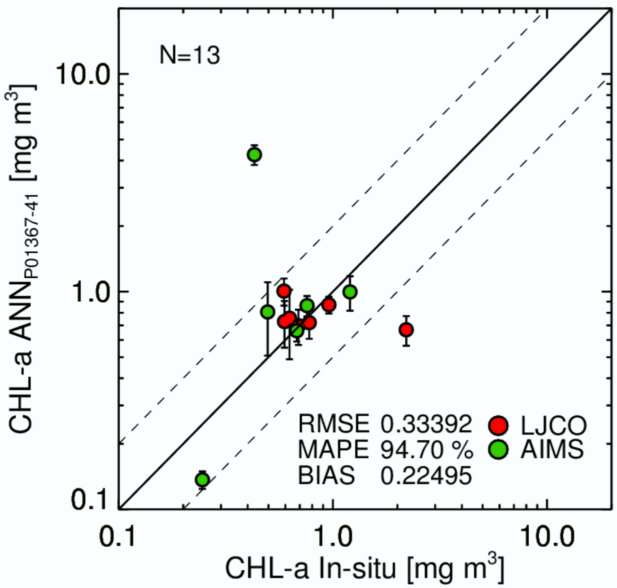
S3A-DALEC radiometric match-ups

ΔT±30 min

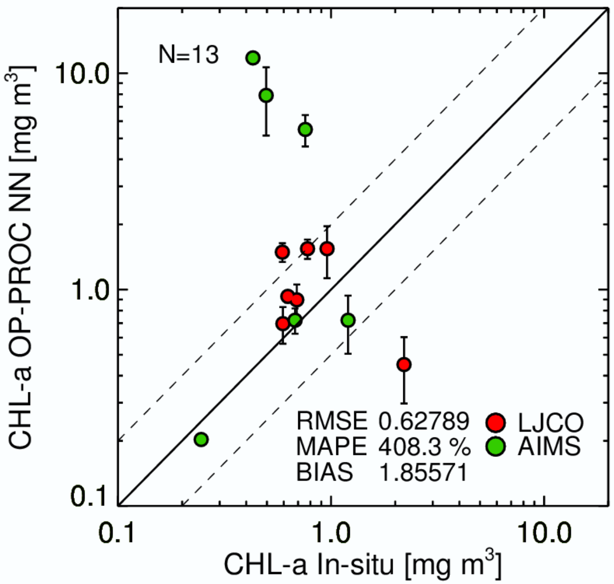


S3A water quality match-ups – Chl-a
ΔT±30 min

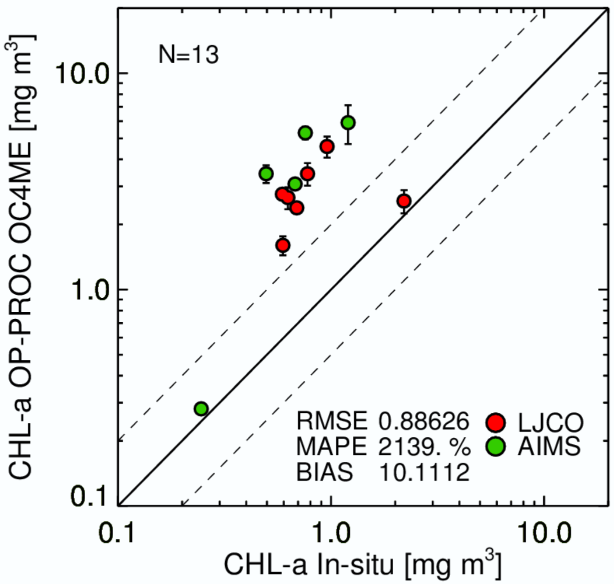
FUB-CSIRO ANN



OP-PROC NN



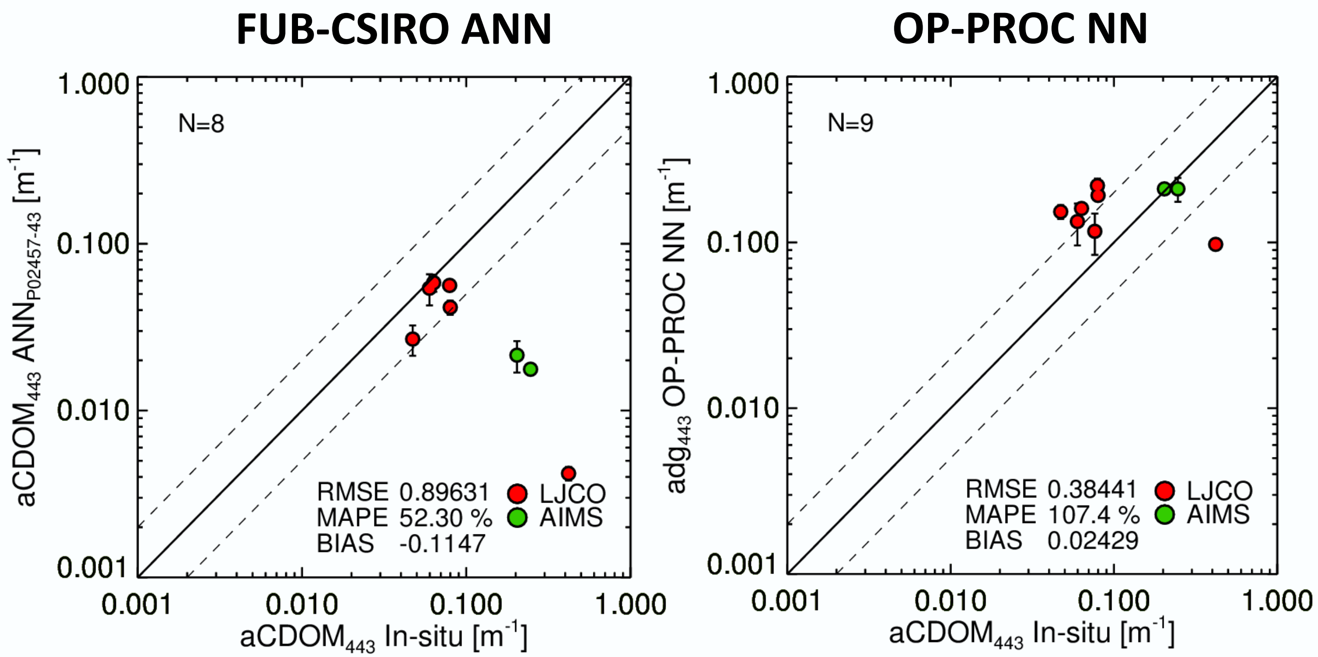
OP-PROC OC4ME



Same QC as for radiometry plus L2 flags: AC_fail, OC4ME_fail, OCNN_fail

Very preliminary – more data required

S3A water quality match-ups – aCDOM $_{443}$ agd $_{443}$
ΔT±30 min

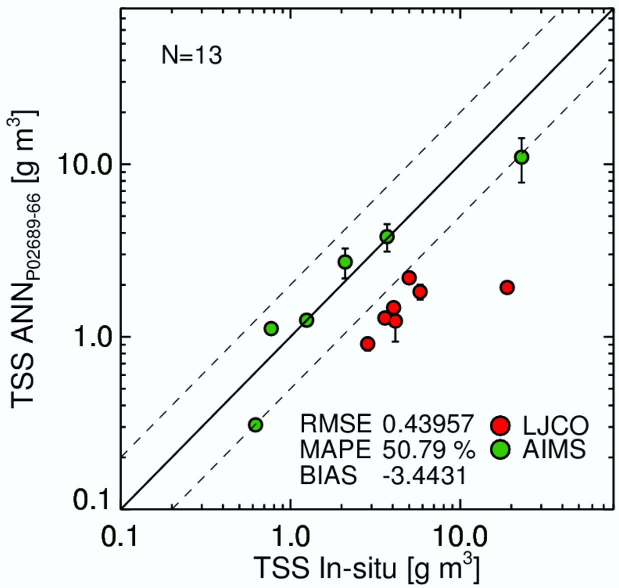


Very preliminary – more data required

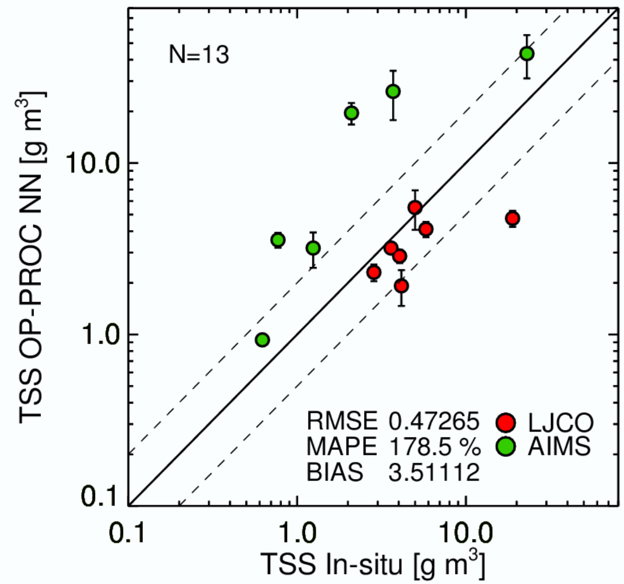
S3A water quality match-ups – TSS

ΔT±30 min

FUB-CSIRO ANN



OP-PROC NN

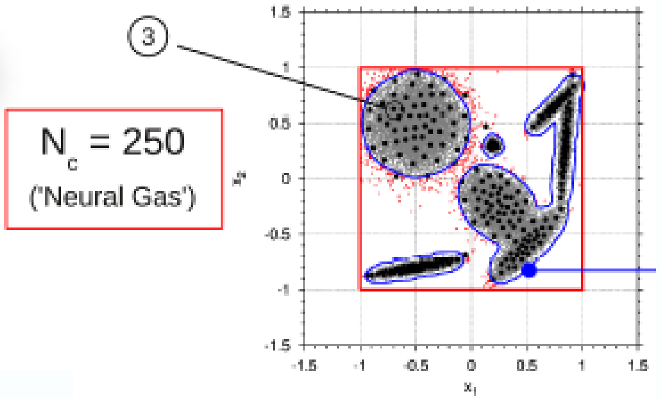


Very preliminary – more data required

New plug-in features

Data (density) validation test (VT)

Improved out-of-scope detection

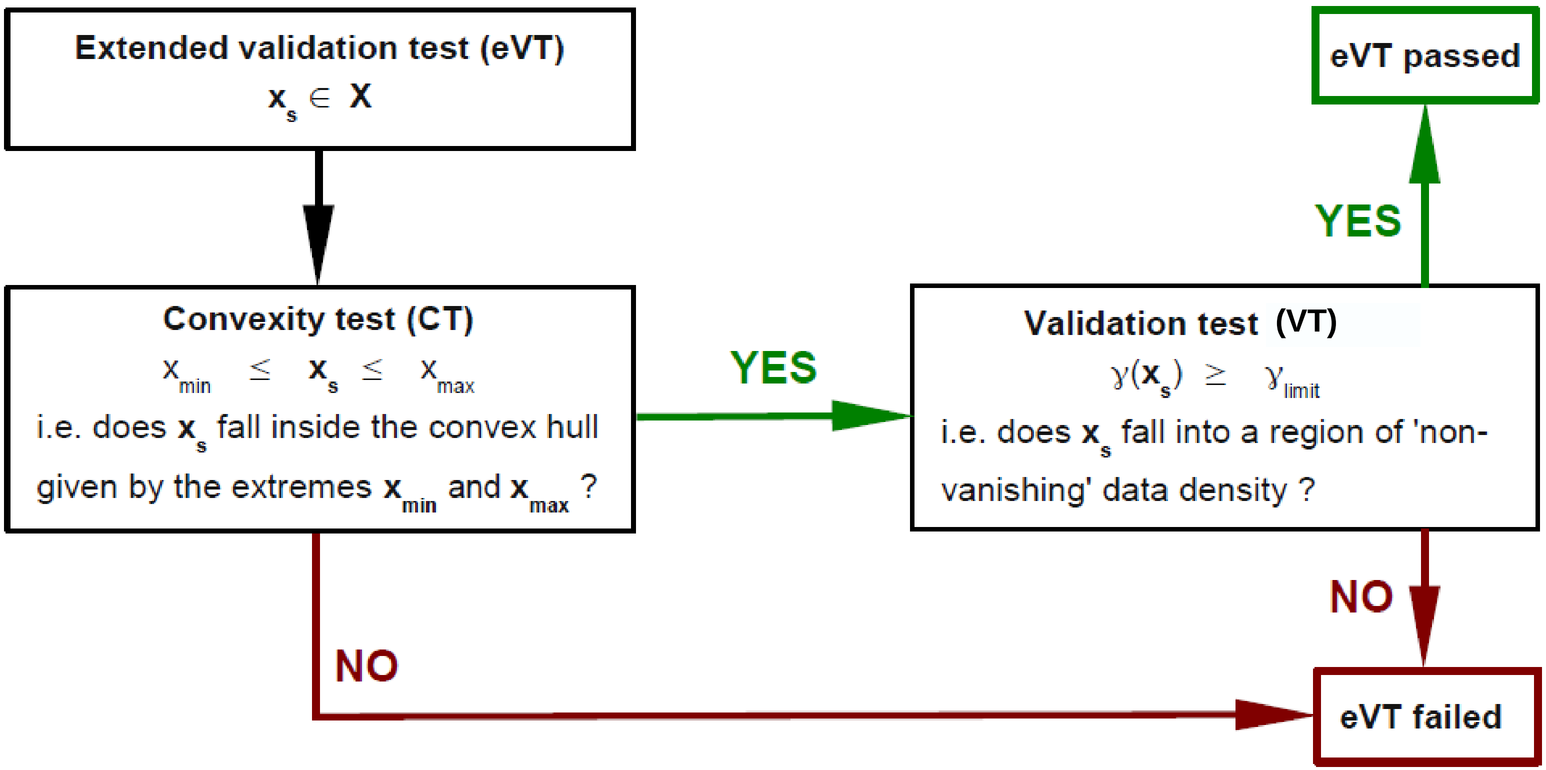


- Simulated data space not filled completely
- Approximation of data density by a kernel density estimator (1D normalized Gaussian kernels)
- Kernel centers are estimated from a vector quantization algorithm
- Spread of centers estimated by nearest neighbor heuristics
- Cut off density estimated from 2% quantile of the integrated training data's density histogram

Schaale M., Schroeder T., (2013),
"An extended validation test for data input into parameterized retrieval algorithms"
AIP Conf. Proc., 1531, 951, DOI:10.1063/1.4804929

Extended validation test (eVT) = CT + VT

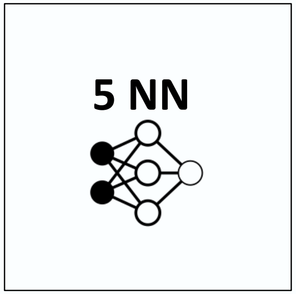
Improved out-of-scope detection



Error bar estimates on a pixel-by-pixel basis

3 sources of uncertainty accounted for and estimated

1. Inverse model variance



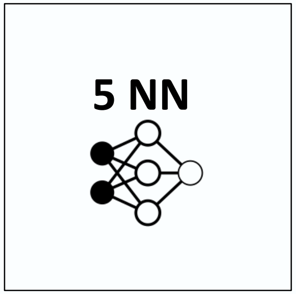
Estimation of the inherent model uncertainty requires computation of the Hessian matrix (2nd derivative of the ANN with respect to the weights) – computationally very demanding job.

More pragmatic approach averaging multiple ANNs of same architecture but trained with a different random seed initializing the network weights. Different starting conditions = different local minima.

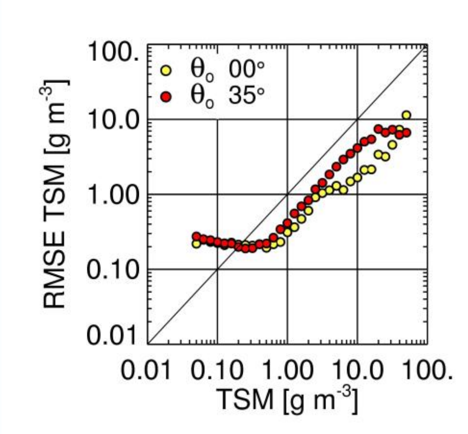
Error bar estimates on a pixel-by-pixel basis

3 sources of uncertainty accounted for and estimated

1. Inverse model variance



2. Prediction variance



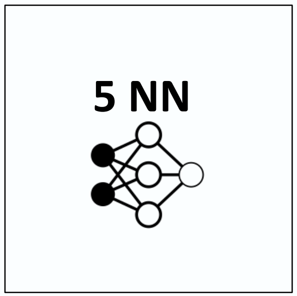
Estimated from a recall with unlearnt LUT data (100.000 samples) for each ANN ensemble.

Conservative estimate as the retrieval error for a given concentration or reflectance interval (bin) corresponds to a very wide range of atmospheric and oceanic conditions.

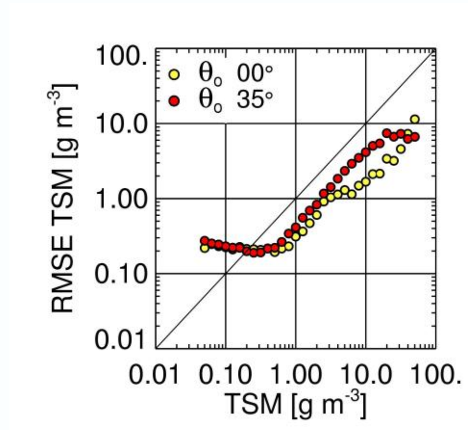
Error bar estimates on a pixel-by-pixel basis

3 sources of uncertainty accounted for and estimated

1. Inverse model variance

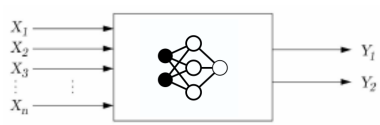


2. Prediction variance



3. Instrument noise variance (Averaged SNRs: EUM/OPS-SEN3/MAN/17/907205)

$$C_X = \begin{bmatrix} \sigma^2_{X_1} & \sigma_{X_1X_2} & \cdots & \sigma_{X_1X_n} \\ \sigma_{X_2X_1} & \sigma^2_{X_2} & \cdots & \sigma_{X_2X_n} \\ \vdots & \vdots & & \vdots \\ \sigma_{X_nX_1} & \sigma_{X_nX_2} & \cdots & \sigma^2_{X_n} \end{bmatrix}$$

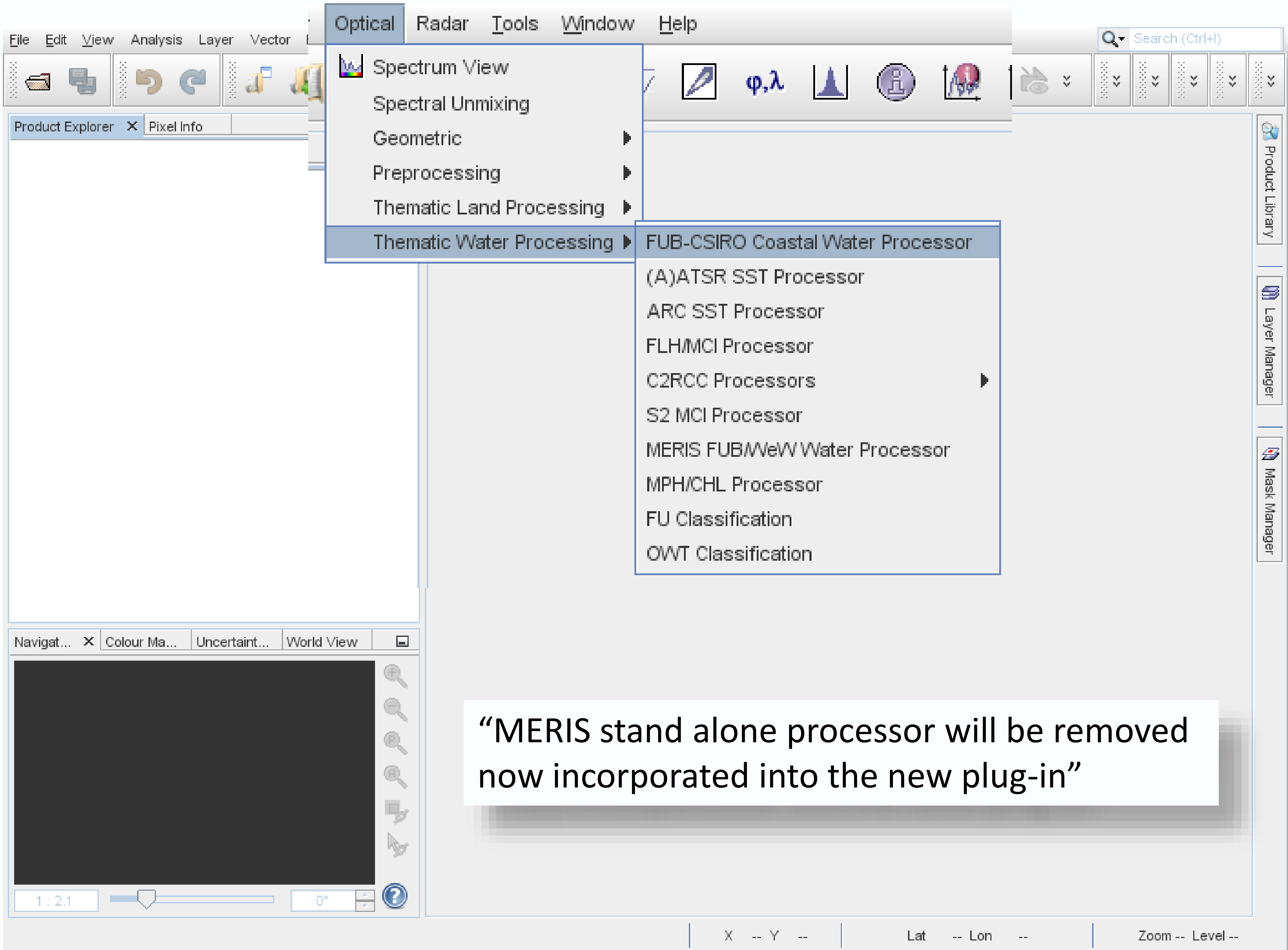


$$C_Y = \begin{bmatrix} \sigma^2_{Y_1} & \sigma_{Y_1Y_2} \\ \sigma_{Y_2Y_1} & \sigma^2_{Y_2} \end{bmatrix}$$ or $$C_Y = F_X C_X F_X^T$$

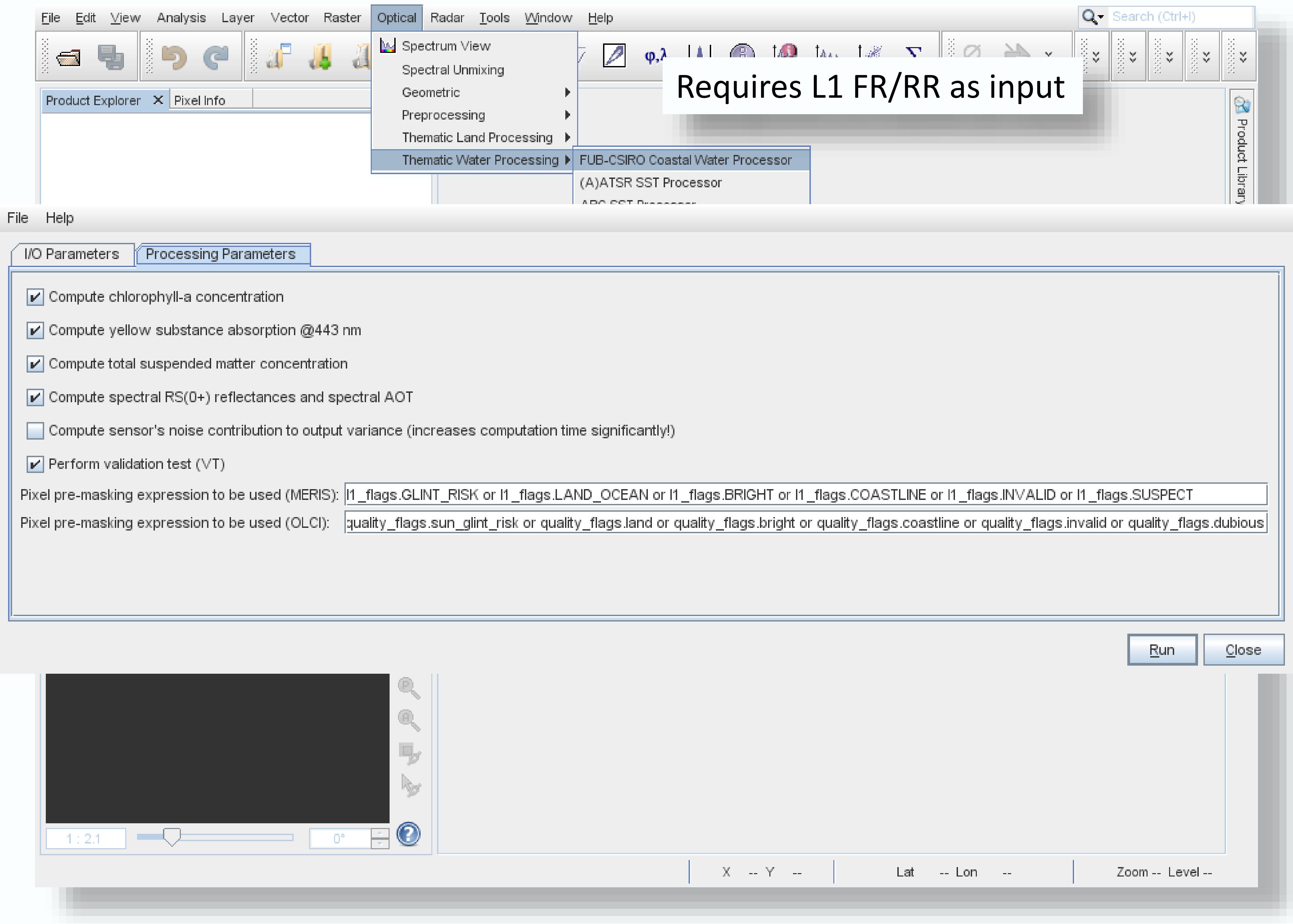
(Modified from Arras 1998)

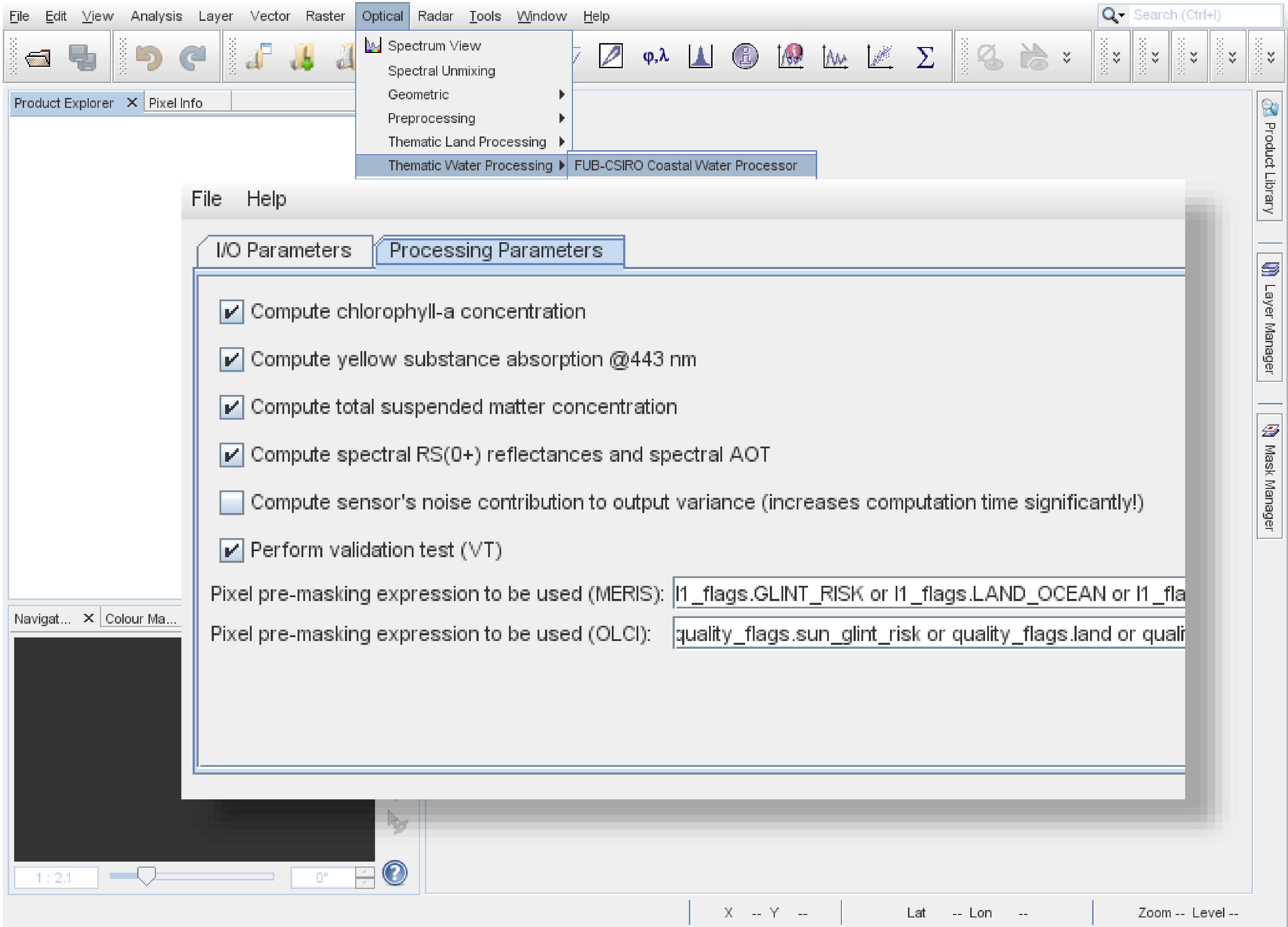
First order error propagation. Calculate the contribution of an input error e.g. covariance matrix (Cx) describing instrument noise (SNR) to the output variance by utilizing the network Jacobian matrix (Fx).

Integration into SNAP (as a Python module)



"MERIS stand alone processor will be removed now incorporated into the new plug-in"


Requires L1 FR/RR as input
File Edit View Analysis Layer Vector Raster Optical Radar Tools Window Help
Search (Ctrl+I)
Product Explorer
Pixel Info
Spectrum View
Spectral Unmixing
Geometric
Preprocessing
Thematic Land Processing
Thematic Water Processing
FUB-CSIRO Coastal Water Processor
(A)ATSR SST Processor
Product Library
File Help
I/O Parameters
Processing Parameters
Compute chlorophyll-a concentration
Compute yellow substance absorption @443 nm
Compute total suspended matter concentration
Compute spectral RS(0+) reflectances and spectral AOT
Compute sensor's noise contribution to output variance (increases computation time significantly!)
Perform validation test (VT)
Pixel pre-masking expression to be used (MERIS):
l1_flags.GLINT_RISK or l1_flags.LAND_OCEAN or l1_flags.BRIGHT or l1_flags.COASTLINE or l1_flags.INVALID or l1_flags.SUSPECT
Pixel pre-masking expression to be used (OLCI):
quality_flags.sun_glint_risk or quality_flags.land or quality_flags.bright or quality_flags.coastline or quality_flags.invalid or quality_flags.dubious
Run
Close
1 : 2.1
0°
X -- Y --
Lat -- Lon --
Zoom -- Level --



File Edit View Analysis Layer Vector Raster Optical Radar Tools Window Help
Search (Ctrl+I)
Spectrum View
Spectral Unmixing
Geometric
Preprocessing
Thematic Land Processing
Thematic Water Processing
FUB-CSIRO Coastal Water Processor
Product Explorer
Pixel Info
Product Library
Layer Manager
Mask Manager
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File Help
I/O Parameters
Processing Parameters
Compute chlorophyll-a concentration
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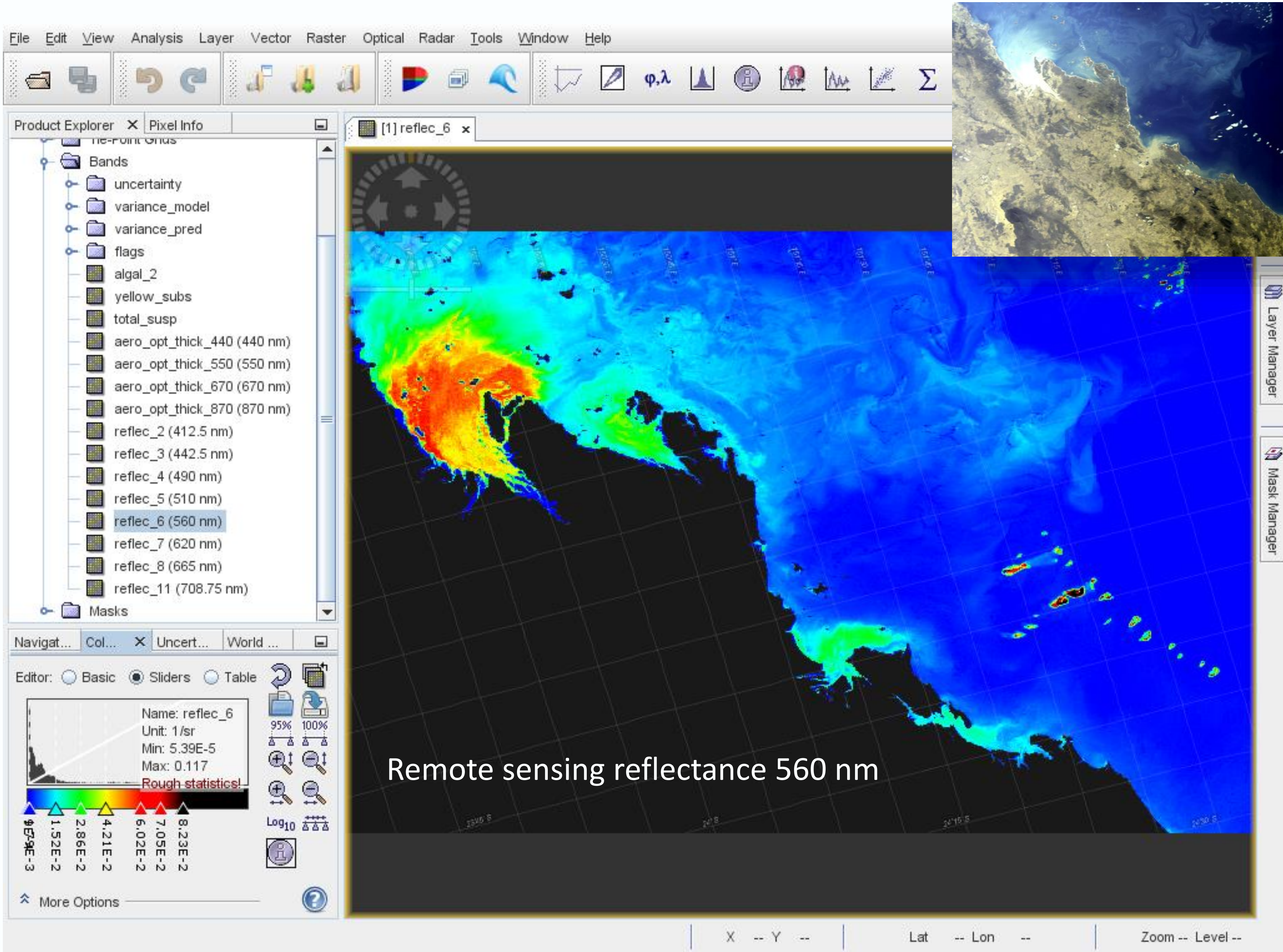
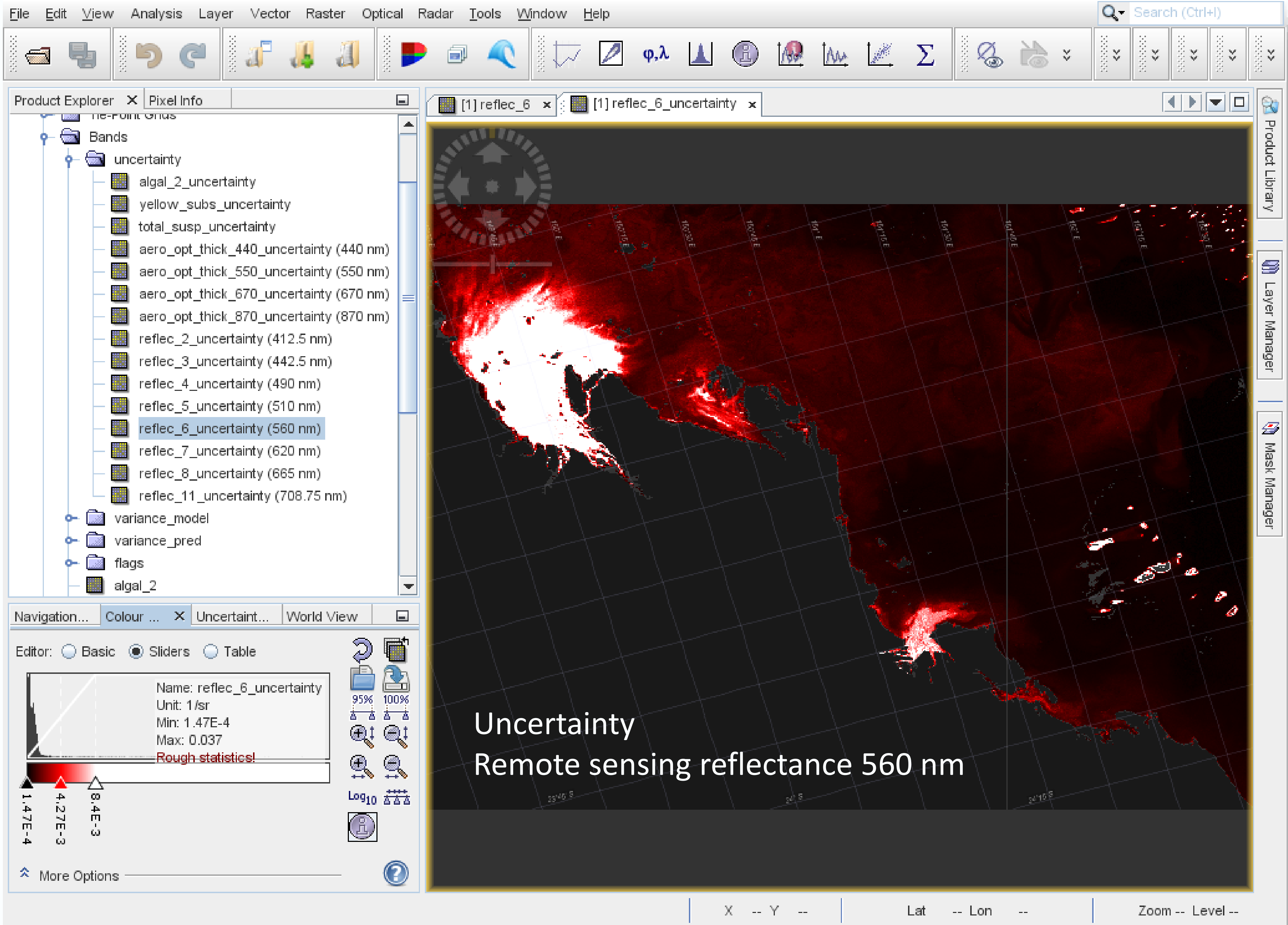
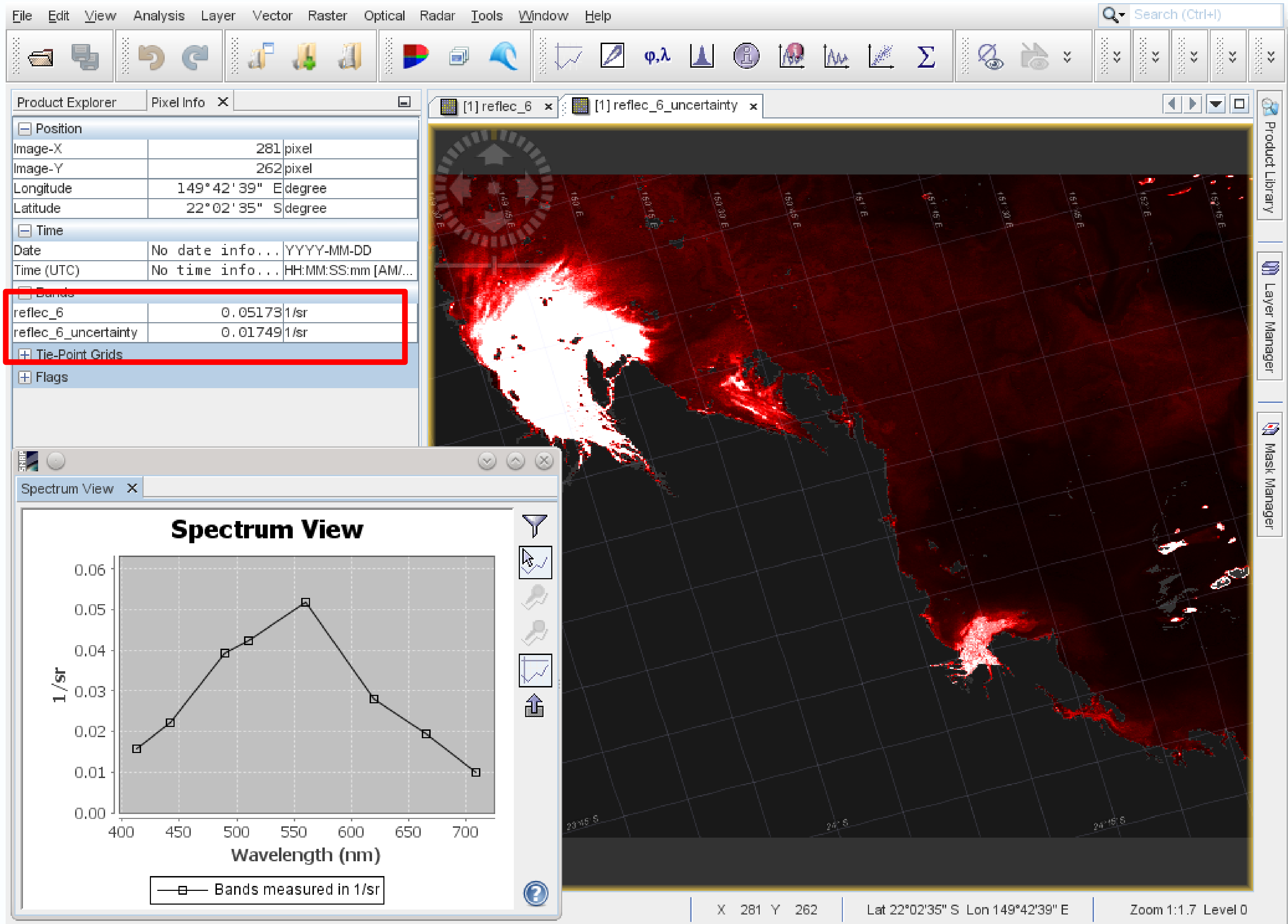
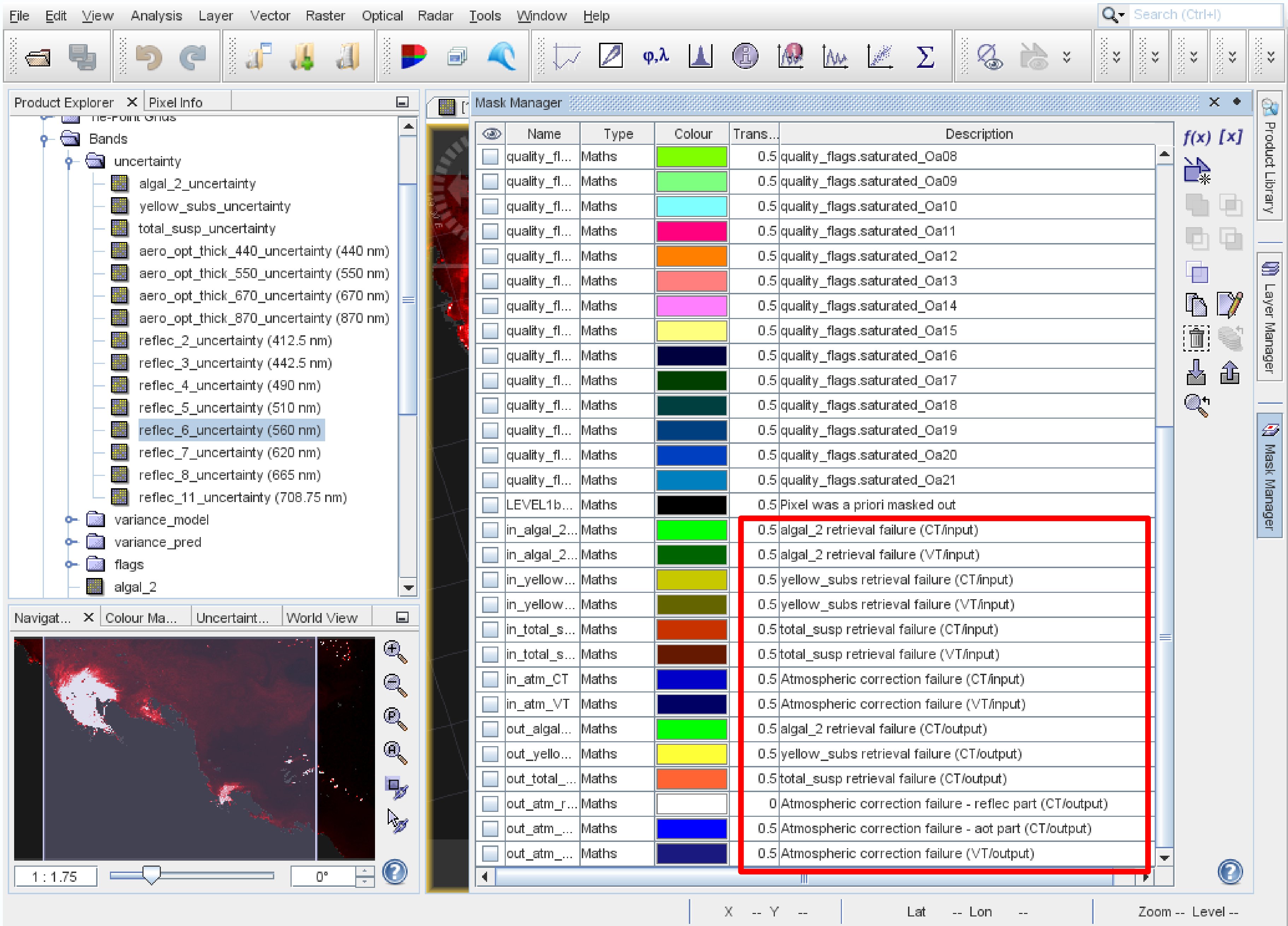
Compute total suspended matter concentration
Compute spectral RS(0+) reflectances and spectral AOT
Compute sensor's noise contribution to output variance (increases computation time significantly!)
Perform validation test (VT)
Pixel pre-masking expression to be used (MERIS):
l1_flags.GLINT_RISK or l1_flags.LAND_OCEAN or l1_fla
Pixel pre-masking expression to be used (OLCI):
quality_flags.sun_glint_risk or quality_flags.land or quali
X -- Y --
Lat -- Lon --
Zoom -- Level --

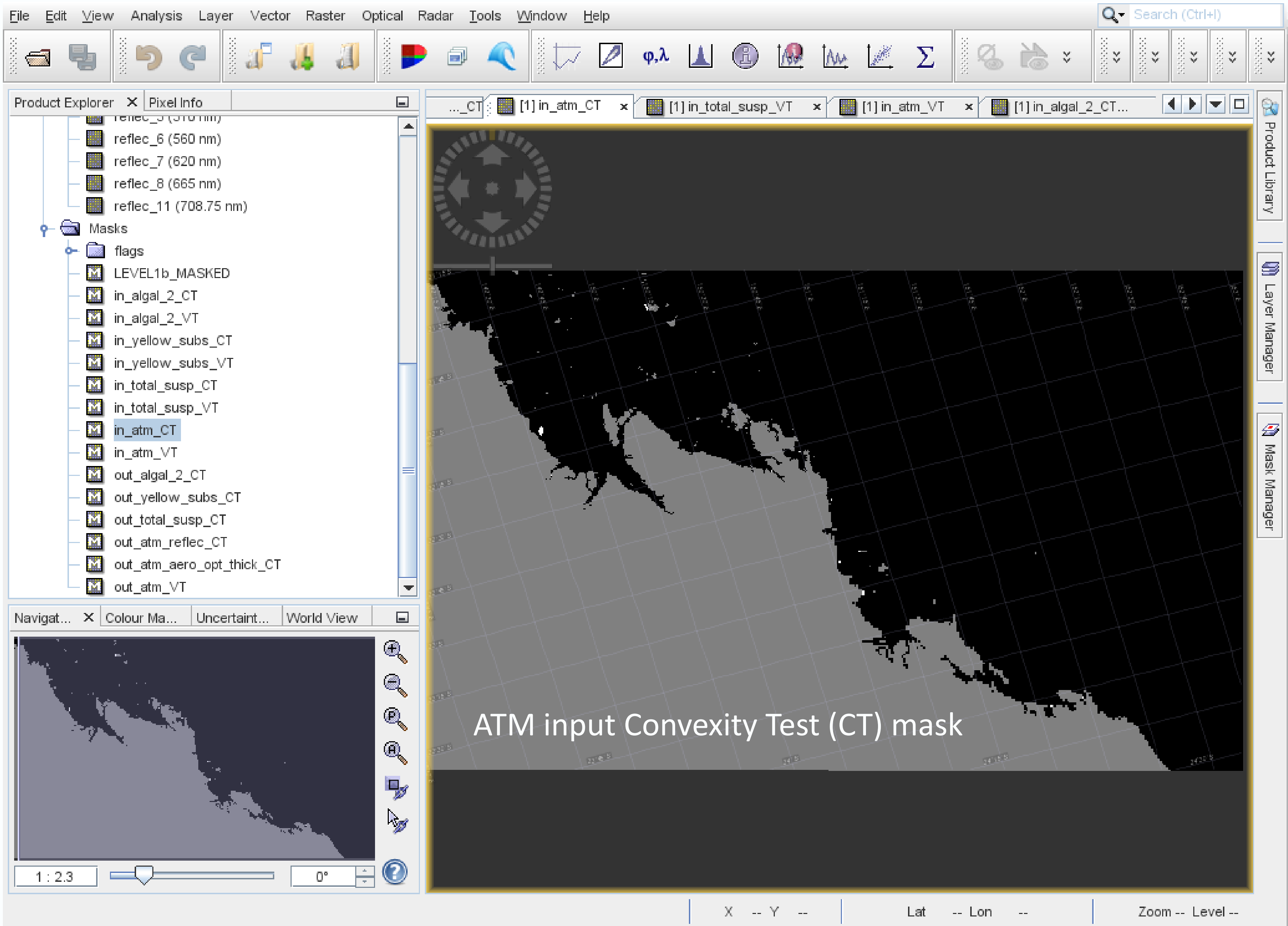

File Edit View Analysis Layer Vector Raster Optical Radar Tools Window Help
Product Explorer
Pixel Info
[1] reflec_6
Bands
uncertainty
variance_model
variance_pred
flags
algal_2
yellow_subs
total_susp
aero_opt_thick_440 (440 nm)
aero_opt_thick_550 (550 nm)
aero_opt_thick_670 (670 nm)
aero_opt_thick_870 (870 nm)
reflec_2 (412.5 nm)
reflec_3 (442.5 nm)
reflec_4 (490 nm)
reflec_5 (510 nm)
reflec_6 (560 nm)
reflec_7 (620 nm)
reflec_8 (665 nm)
reflec_11 (708.75 nm)
Masks
Navigat...
Col...
Uncert...
World ...
Editor: Basic Sliders Table
Name: reflec_6
Unit: 1/sr
Min: 5.39E-5
Max: 0.117
Rough statistics!
1.52E-2
2.86E-2
4.21E-2
6.02E-2
7.05E-2
8.23E-2
95%
100%
Log10
More Options
Layer Manager
Mask Manager
Remote sensing reflectance 560 nm
X -- Y --
Lat -- Lon --
Zoom -- Level --


File Edit View Analysis Layer Vector Raster Optical Radar Tools Window Help
Search (Ctrl+I)
Product Explorer
Pixel Info
Bands
uncertainty
algal_2_uncertainty
yellow_subs_uncertainty
total_susp_uncertainty
aero_opt_thick_440_uncertainty (440 nm)
aero_opt_thick_550_uncertainty (550 nm)
aero_opt_thick_670_uncertainty (670 nm)
aero_opt_thick_870_uncertainty (870 nm)
reflec_2_uncertainty (412.5 nm)
reflec_3_uncertainty (442.5 nm)
reflec_4_uncertainty (490 nm)
reflec_5_uncertainty (510 nm)
reflec_6_uncertainty (560 nm)
reflec_7_uncertainty (620 nm)
reflec_8_uncertainty (665 nm)
reflec_11_uncertainty (708.75 nm)
variance_model
variance_pred
flags
algal_2
Navigation...
Colour ...
Uncertaint...
World View
Editor: Basic Sliders Table
Name: reflec_6_uncertainty
Unit: 1/sr
Min: 1.47E-4
Max: 0.037
Rough statistics!
1.47E-4
4.27E-3
8.4E-3
95%
100%
Log10
More Options
[1] reflec_6
[1] reflec_6_uncertainty
Uncertainty
Remote sensing reflectance 560 nm
Product Library
Layer Manager
Mask Manager
X -- Y --
Lat -- Lon --
Zoom -- Level --

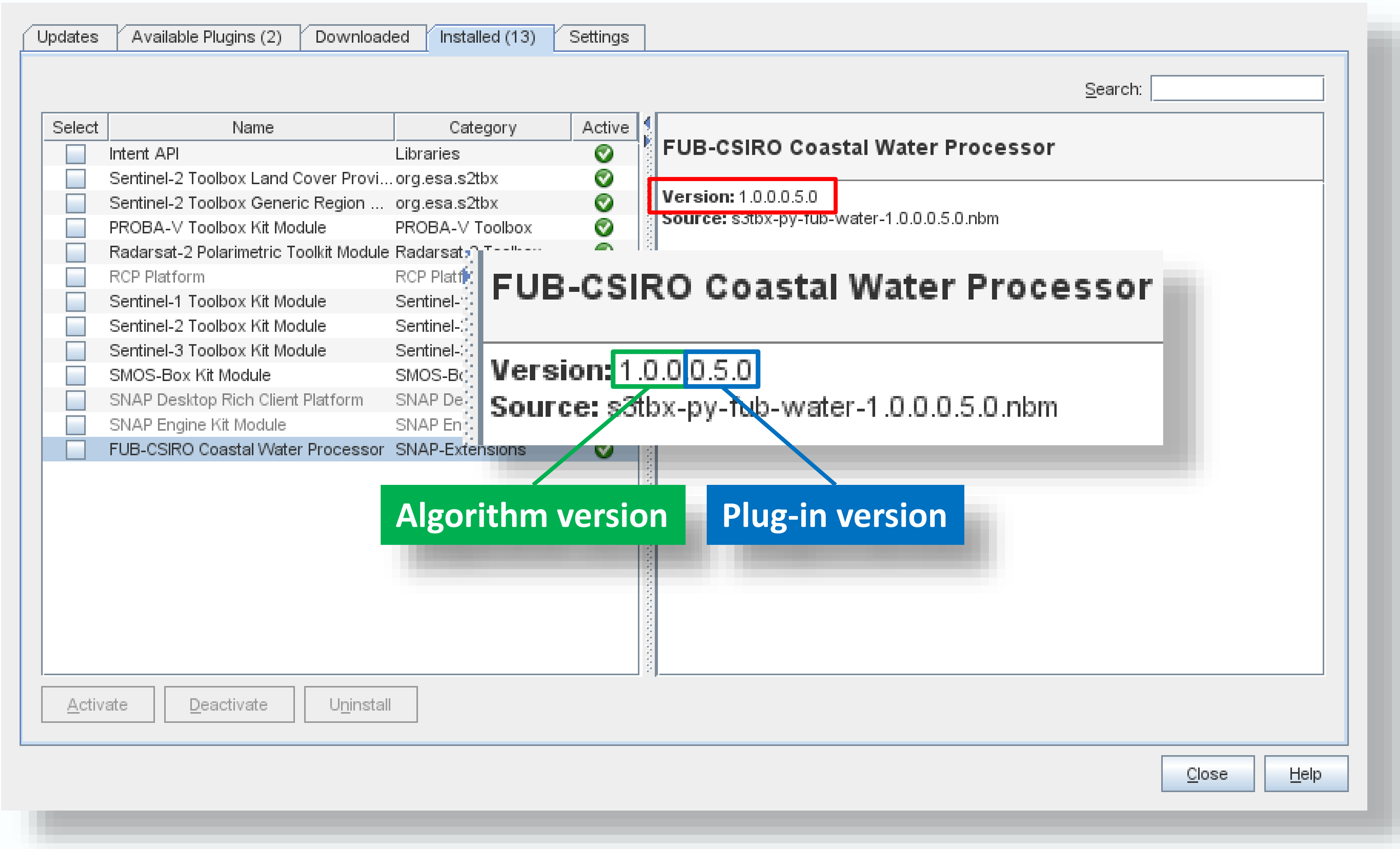

File Edit View Analysis Layer Vector Raster Optical Radar Tools Window Help
Search (Ctrl+I)
Product Explorer
Pixel Info
Position
Image-X 281 pixel
Image-Y 262 pixel
Longitude 149°42'39" E degree
Latitude 22°02'35" S degree
Time
Date No date info... YYYY-MM-DD
Time (UTC) No time info... HH:MM:SS:mm [AM/...
Bands
reflec_6 0.05173 1/sr
reflec_6_uncertainty 0.01749 1/sr
Tie-Point Grids
Flags
[1] reflec_6
[1] reflec_6_uncertainty
Product Library
Layer Manager
Mask Manager
Spectrum View
Spectrum View
0.06
0.05
0.04
0.03
0.02
0.01
0.00
1/sr
400 450 500 550 600 650 700
Wavelength (nm)
Bands measured in 1/sr
X 281 Y 262
Lat 22°02'35" S Lon 149°42'39" E
Zoom 1:1.7 Level 0



File Edit View Analysis Layer Vector Raster Optical Radar Tools Window Help
Search (Ctrl+I)
Product Explorer
Pixel Info
Bands
uncertainty
algal_2_uncertainty
yellow_subs_uncertainty
total_susp_uncertainty
aero_opt_thick_440_uncertainty (440 nm)
aero_opt_thick_550_uncertainty (550 nm)
aero_opt_thick_670_uncertainty (670 nm)
aero_opt_thick_870_uncertainty (870 nm)
reflec_2_uncertainty (412.5 nm)
reflec_3_uncertainty (442.5 nm)
reflec_4_uncertainty (490 nm)
reflec_5_uncertainty (510 nm)
reflec_6_uncertainty (560 nm)
reflec_7_uncertainty (620 nm)
reflec_8_uncertainty (665 nm)
reflec_11_uncertainty (708.75 nm)
variance_model
variance_pred
flags
algal_2
Navigat...
Colour Ma...
Uncertaint...
World View
1 : 1.75
0°
Mask Manager
Name Type Colour Trans... Description
quality_fl... Maths 0.5 quality_flags.saturated_Oa08
quality_fl... Maths 0.5 quality_flags.saturated_Oa09
quality_fl... Maths 0.5 quality_flags.saturated_Oa10
quality_fl... Maths 0.5 quality_flags.saturated_Oa11
quality_fl... Maths 0.5 quality_flags.saturated_Oa12
quality_fl... Maths 0.5 quality_flags.saturated_Oa13
quality_fl... Maths 0.5 quality_flags.saturated_Oa14
quality_fl... Maths 0.5 quality_flags.saturated_Oa15
quality_fl... Maths 0.5 quality_flags.saturated_Oa16
quality_fl... Maths 0.5 quality_flags.saturated_Oa17
quality_fl... Maths 0.5 quality_flags.saturated_Oa18
quality_fl... Maths 0.5 quality_flags.saturated_Oa19
quality_fl... Maths 0.5 quality_flags.saturated_Oa20
quality_fl... Maths 0.5 quality_flags.saturated_Oa21
LEVEL1b... Maths 0.5 Pixel was a priori masked out
in_algal_2... Maths 0.5 algal_2 retrieval failure (CT/input)
in_algal_2... Maths 0.5 algal_2 retrieval failure (VT/input)
in_yellow... Maths 0.5 yellow_subs retrieval failure (CT/input)
in_yellow... Maths 0.5 yellow_subs retrieval failure (VT/input)
in_total_s... Maths 0.5 total_susp retrieval failure (CT/input)
in_total_s... Maths 0.5 total_susp retrieval failure (VT/input)
in_atm_CT Maths 0.5 Atmospheric correction failure (CT/input)
in_atm_VT Maths 0.5 Atmospheric correction failure (VT/input)
out_algal... Maths 0.5 algal_2 retrieval failure (CT/output)
out_yello... Maths 0.5 yellow_subs retrieval failure (CT/output)
out_total_... Maths 0.5 total_susp retrieval failure (CT/output)
out_atm_r... Maths 0 Atmospheric correction failure - reflec part (CT/output)
out_atm_... Maths 0.5 Atmospheric correction failure - aot part (CT/output)
out_atm_... Maths 0.5 Atmospheric correction failure (VT/output)
f(x) [x]
Product Library
Layer Manager
Mask Manager
X -- Y --
Lat -- Lon --
Zoom -- Level --



ATM input Convexity Test (CT) mask



Updates
Available Plugins (2)
Downloaded
Installed (13)
Settings
Search:
Select
Name
Category
Active
Intent API
Libraries
Sentinel-2 Toolbox Land Cover Provi...
org.esa.s2tbx
Sentinel-2 Toolbox Generic Region ...
org.esa.s2tbx
PROBA-V Toolbox Kit Module
PROBA-V Toolbox
Radarsat-2 Polarimetric Toolkit Module
RCP Platform
Sentinel-1 Toolbox Kit Module
Sentinel-2 Toolbox Kit Module
Sentinel-3 Toolbox Kit Module
SMOS-Box Kit Module
SNAP Desktop Rich Client Platform
SNAP Engine Kit Module
FUB-CSIRO Coastal Water Processor
SNAP-Extensions
FUB-CSIRO Coastal Water Processor
Version: 1.0.0.0.5.0
FUB-CSIRO Coastal Water Processor
Version: 1.0.0 0.5.0
Source: s3tbx-py-fub-water-1.0.0.0.5.0.nbm
Algorithm version
Plug-in version
Activate
Deactivate
Uninstall
Close
Help

TBDs before public release

SNAP installation does not provide working Python bridge

Separate uncertainty outputs for Rrs and AOT*) to enable combined spectrum view plotting of product and corresponding error

Provide WQ outputs on linear scale to enable easier interpretation of error bars

*) **AOT product not validated** – recommended not to be used for algorithm version 1.0.0 – will be replaced by a separate ANN

Lucinda Jetty Coastal Observatory

New instrumentation – Satlantic hyper-spectral system

Installation June 2019

Summary & outlook

- FUB processor successfully ported to S3 SNAP
- Robust validation of radiometry – good performance compared to OP-PROC
- Further validation in pipeline using Aeronet-OC (collab. ACRI)
- Number of WQ match-ups insufficient – preliminary results
- Pixel-by-pixel uncertainties and improved out-of-scope detection will lead to increased data confidence
- In-situ data sharing important to improve algorithms
- All our data available to S3VT and the public (portal.aodn.org.au)

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