→ 4th ESA ADVANCED TRAINING
ON OCEAN REMOTE SENSING

Validation of Ocean Colour Data

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Part 1

WHAT IS VALIDATION?
WHY DO WE BOTHER DOING IT?

Water Framework Directive

- Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000 establishing a framework for Community action in the field of water policy

- The purpose of the Directive is to establish a framework for the protection of inland surface waters (rivers and lakes), transitional waters (estuaries), coastal waters and groundwater.

- It will **ensure** that all aquatic ecosystems and, with regard to their water needs, terrestrial ecosystems and wetlands meet '**good status**' by 2015.

Quantification

WFD Classes

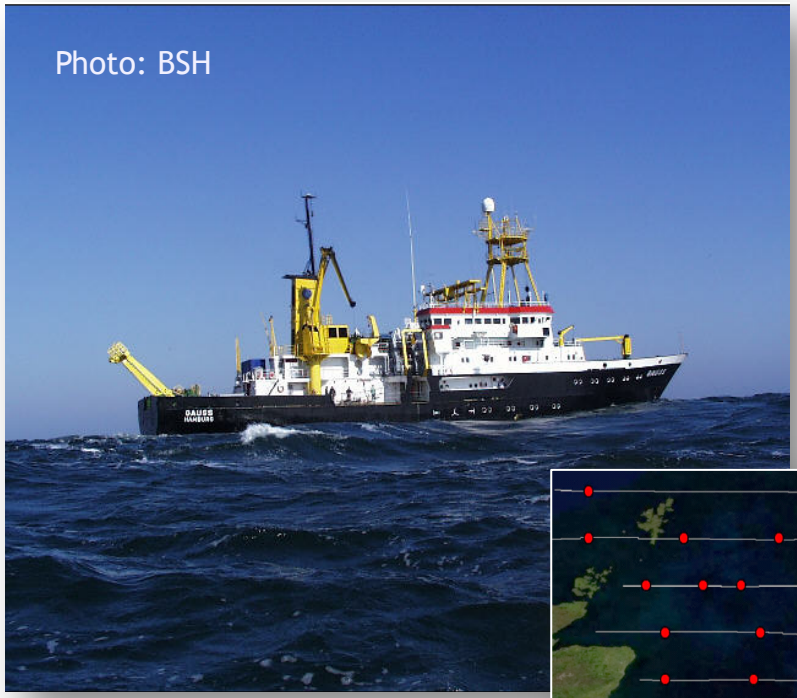
- high
- good
- moderate
- poor
- bad
- uncertain
- N/A

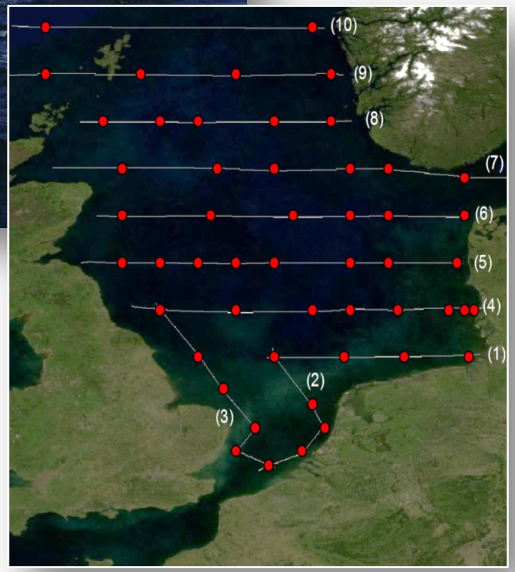
Get the assessment right!
Provide evidence!

✓ ↓

✘ → **measures**

Regular Monitoring Cruises





Fernerkundungsanwendungen
Küste * BAW * 01.12.2011

In-situ Data: BSH, 2006-2010

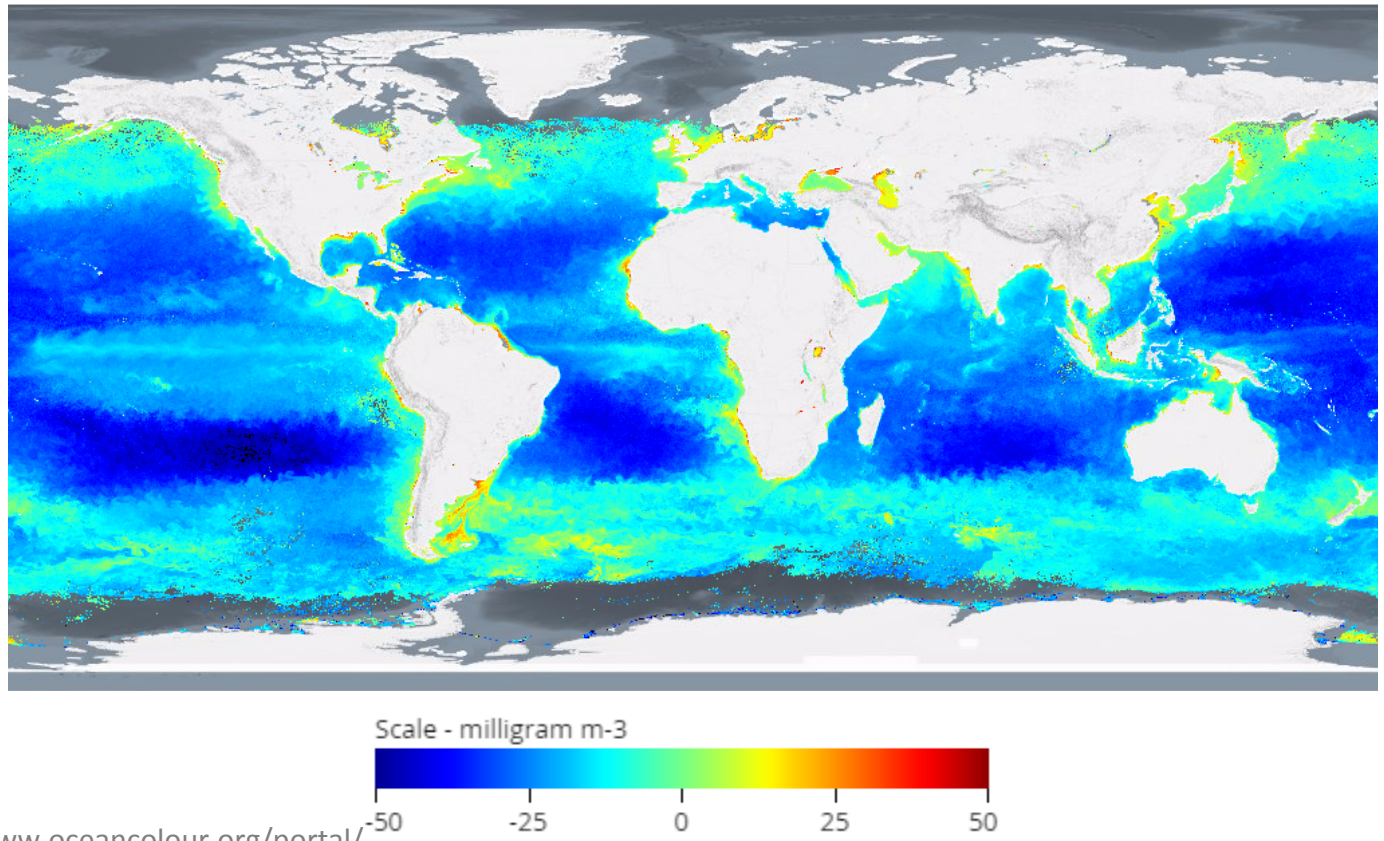
Climate Change

- GCOS – Global Climate Observing System
  - Serving the IPCC Reports
  - Intercovernmental Panel on Climate Change
- Essential Climate Variables: ECVs
  - Chlorophyll-a concentration
- Accuracy & Precision

	Accuracy			Precision		
	Goal	Breakthrough	Threshold	Goal	Breakthrough	Threshold
Chl-a	5% (max)	8.5% (max)	25% (max)	-	-	-

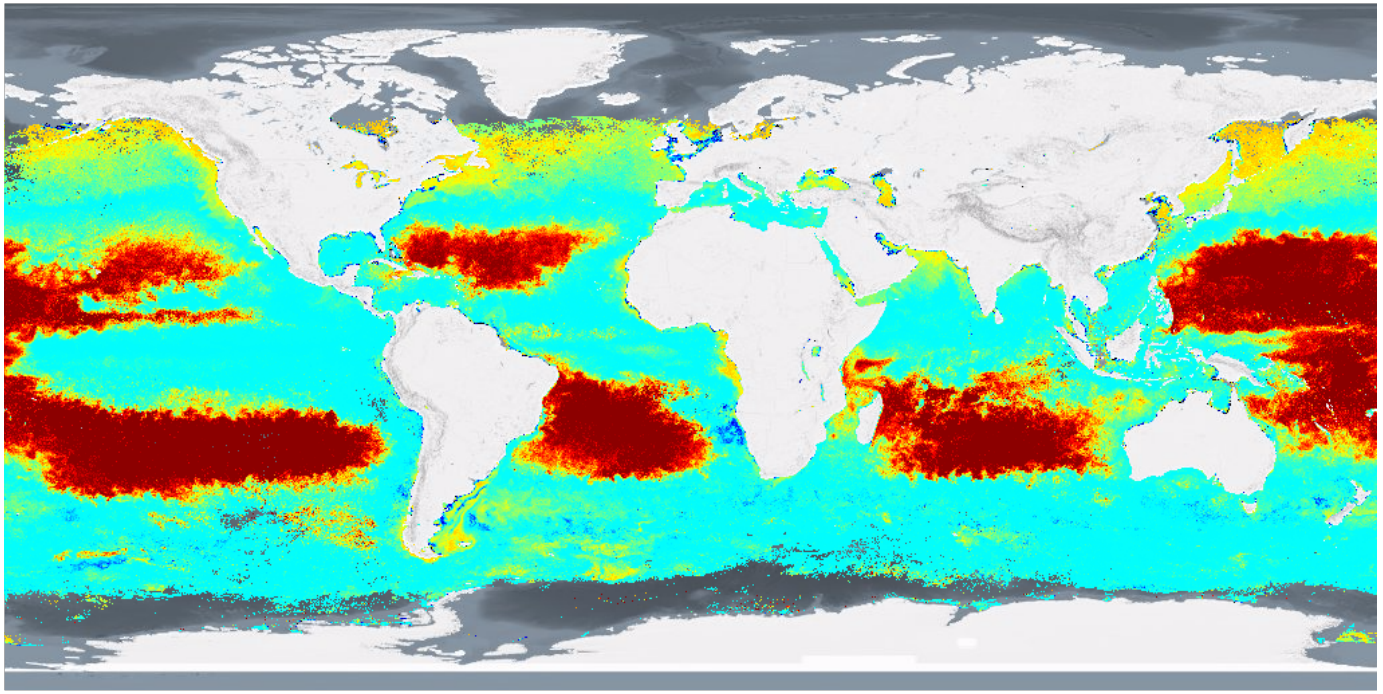
source: ESA Ocean Colour CCI, User Requirements document, http://www.esa-oceancolour-cci.org/

OC CCI Chl



source: http://www.oceancolour.org/portal/

OC CCI Chl Uncertainty



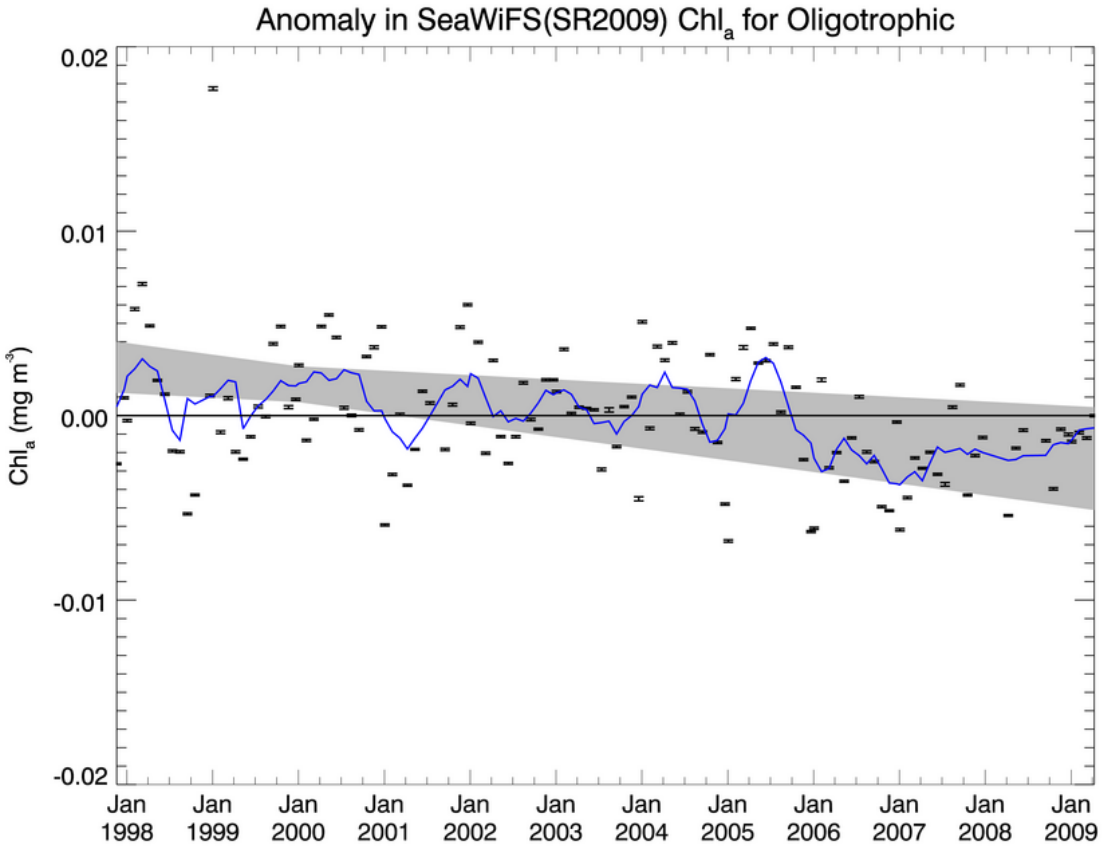
source: http://www.oceancolour.org/portal/

Climate Change - Stability

Ocean chlorophyll	**Stability (over 10 years)**		
Source of requirement	Goal	Breakthrough	Threshold
Requirement from GCOS	-	-	-
Requirement from CMUG			
Requirement from CCI - Modellers	1%	1%	10%
Requirement from CCI – EO scientists	1%	1-2 %	5%

source: ESA Ocean Colour CCI, User Requirements document, http://www.esa-oceancolour-cci.org/

Long Term Trends



source: Bryan Franz: Methods for Assessing the Quality and Consistency of Ocean Color Products, http://oceancolor.gsfc.nasa.gov/DOCS/methods/sensor_analysis_methods.html

Algorithms & Products

- **Algorithm**
  - procedure to transform variable A into variable B
  - based on
    - physical principles
    - empirical relationship
    - combination of both
  - subject to
    - assumptions
    - limitations
    - scope (e.g. min and max of concentrations)
  - algorithm Validation:
    - test if expected behaviour is confirmed
    - using simulated data (radiative transfer simulations)
    - using in-situ measurements (no satellite overpass required)

Advantages:
- full control on input data (simulations)
- Large number of measurements available (historic in-situ measurements)
- assumptions and limitations respected
- systematic studies
- assessing the error behaviour

Disadvantages:
- idealised world, lower limit of real error

Algorithms & Products

- **Product** Validation
  - Generating output variables B with satellite measurements A as input
  - Applying one or more methods to compare B with
    - reference data (in-situ, other remote sensing data)
    - expectation (plausibility checks)

Advantages:
- real world being studied
- estimate of overall uncertainty

Disadvantages:
- assumptions and limitations may not be completely true
- unknown input error
- output variables B and reference measurements differ
- no complete test coverage
- often not enough reference data to systematically study dependencies

SWOT

What are strengths, weaknesses, opportunities and threats when comparining …

	satellite observation vs in-situ observation	sattelite observations vs numerical model
Strength		
Weakness		
Opportunity		
Threat		

Part 2

RIGHT AND WRONG

Please answer!

How would you characterise a good validation?

Definitions

- Accuracy
- Precision
- Stability
- Error
- Uncertainty

Comparing Fruits

- What measures the satellite
  - the radiance emitted from the ocean surface of a certain spatial extent (typically 1km^2)
  - a snapshot in time
  - subject to uncertainties in instrument characterisation and instrument calibration

Comparing Fruits

- What measures the satellite: TOA radiances
- From this derive with an algorithm
  - water leaving reflectance
    - subject to uncertainties in characterisation of the atmosphere (atmosphere mode)
  - optical properties of the water column (absorption, scattering, attenuation)
    - vertically integrated over the depth of the euphotic zone
    - subject to uncertainties in characterisation of the water coloum (water model)
  - concentrations of water constituents (Chl-a, TSM)
    - vertically averaged over the euphotic zone
    - subject to uncertainties in the conversion factors from optical properties to concentrations
  - all for an area of typicall 1km^2 and for short snapshot in time!

Comparing Fruits

- What measures the satellite: TOA radiances
  - ~ 1km², short snapshot in time
- From this derive with an algorithm: Rrs, IOPs, concentrations
  - 1km², short snapshot in time, vertically integrated
- In-situ we measure
  - aerosol optical properties → verification of characterisation of the atmosphere
    - The aerosol properties are a by-product of the AC.
  - above / below water radiance field → validation of Rrs
  - optical properties of the water → validation of IOPs
  - concentrations → validaton of concentrations
    - different techniques (e.g HPLC, spectro-radiometric, fluorometric for Chl-a)
  - from ships, buoys, towers, gliders
    - no spatial extent of the measurement
    - sequence of point measurements in time (time series, transect)

How to compare apples with apples

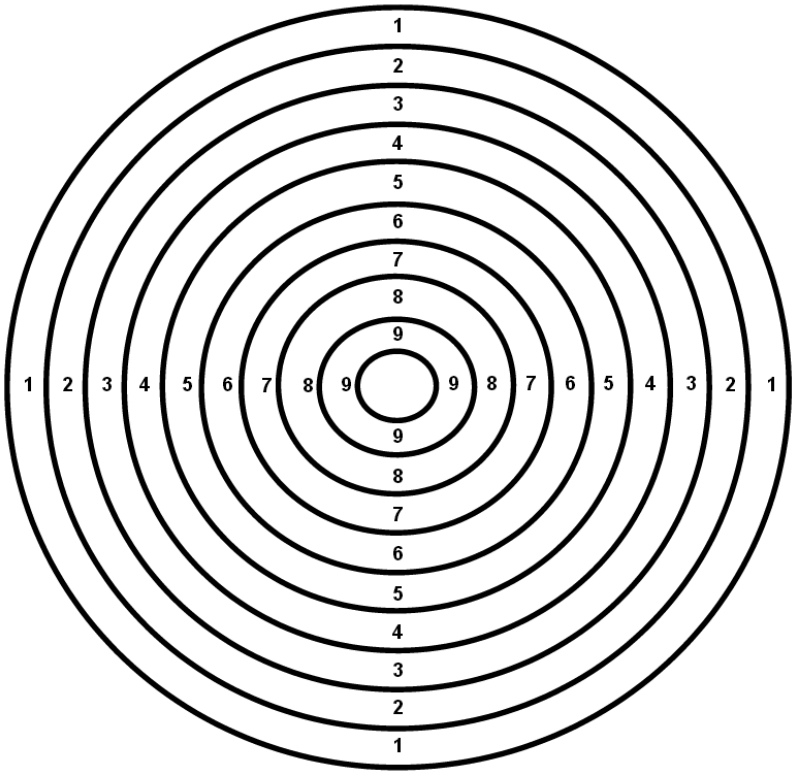
- Understand your satellite data
  - the ATBD explains the methods, e.g. calibration with HPLC in-situ measurements
  - do the assumption made for the algorithm agree with the properties of the water I am studying (concentration ranges, species composition = SIOPs, …)

- Understand your reference data
  - read the protocol. If no protocol is available, be very careful!

- Consider the spatial, vertical and temporal representativeness
  - what are typical current vecolicites → which time interval is acceptable between satellite and reference measurements
  - how is the spatial homogeneity in the area of investigation → can I average several pixel? How many pixel?
  - how is the vertical distribution in the area at that time of the year? How does this compare with the assmptions of the satellite algorithm?

Target Diagram

Explain **accuracy** and **precision** with the target circle



Part 3

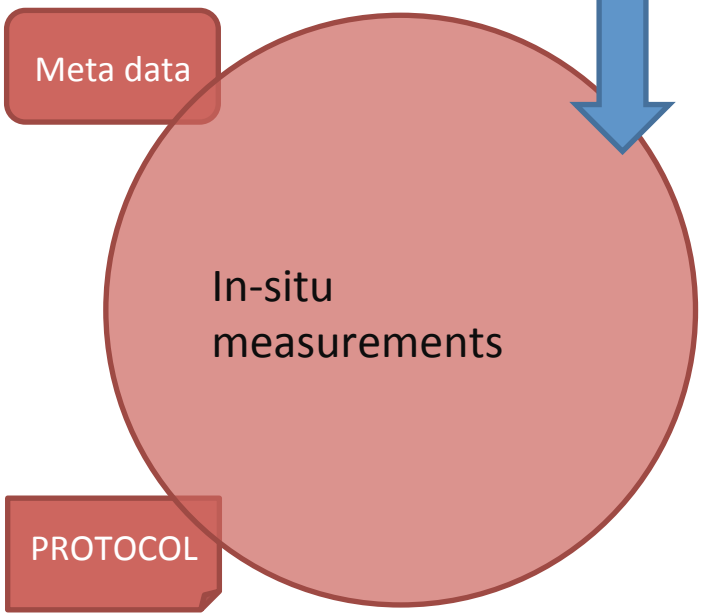
PROTOCOLS AND IN-SITU DATA SOURCES

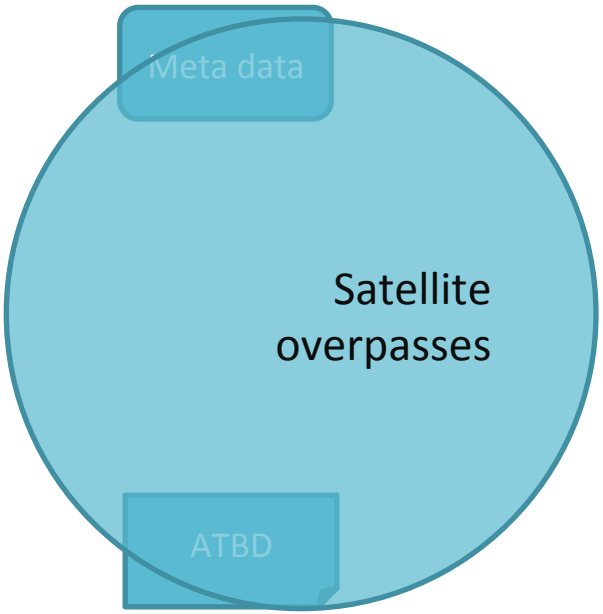
In-situ data and match-ups

match-ups

PROTOCOL

Location: tolerance (±distance; pixel averaging)
Time: tolerance (±time shift; cycles)
Parameter: „fruits“ (Chl HPLC vs Fluor. or not; radiance normalisation)
Filtering: quality criteria (cloudiness, homogeneity, measurement error)
Statistics: RMS, bias, …
…



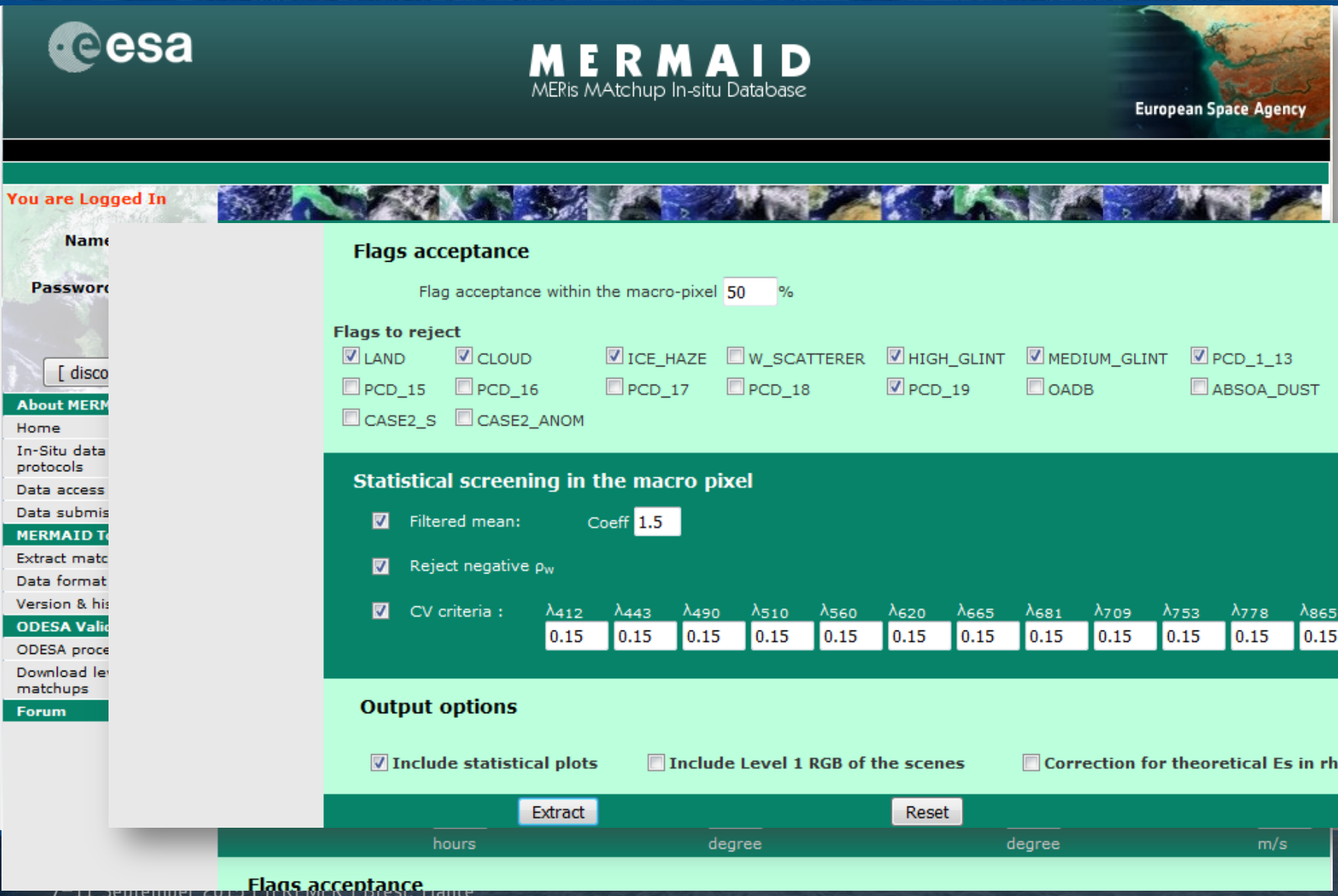


Algorithm Theoretical Basis Document

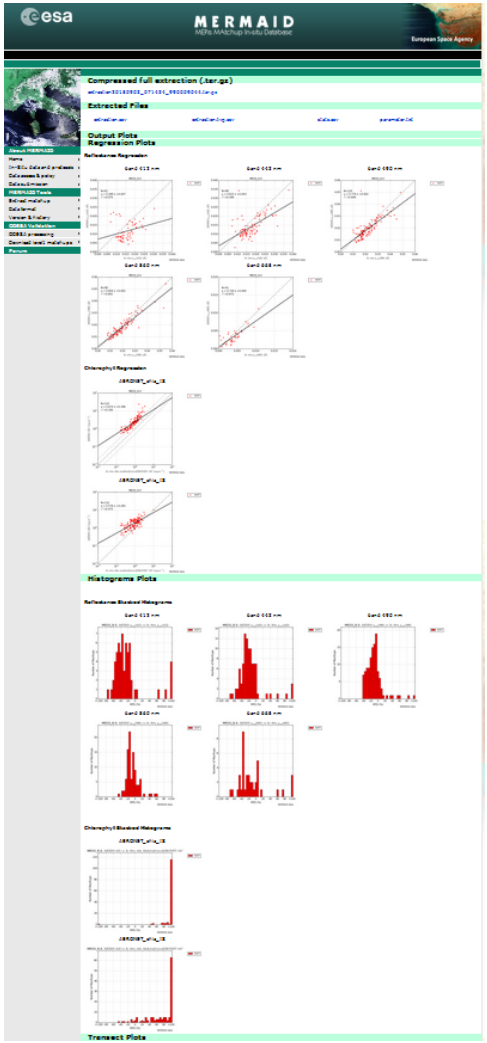
In-situ data sources

- Europe/ESA: MERMAID
  - Rrs, concentrations
  - tailored to validation of MERIS and S3-OLCI
  - http://mermaid.acri.fr/home/home.php
- US/NASA: SeaBAS & NOMAD
  - Rrs, concentrations
  - validation of ocean colour sensors, but concentrating on SeaWiFS spectral bands
  - http://seabass.gsfc.nasa.gov/seabasscgi/news.cgi
  - http://seabass.gsfc.nasa.gov/wiki/article.cgi?article=NOMAD
- Aeronet-OC
  - Rrs & aerosol optical properties
  - http://aeronet.gsfc.nasa.gov/cgi-bin/type_one_station_seaprism_new?site=Lucinda&nachal=2&level=1&place_code=10
- National programmes
  - e.g. UK CEFAS Smart Buoys
  - http://cefasmapping.defra.gov.uk/Smartbuoy/Map

Example: MERMAID **Product** Validaton



Example: MERMAID **Product** Validaton



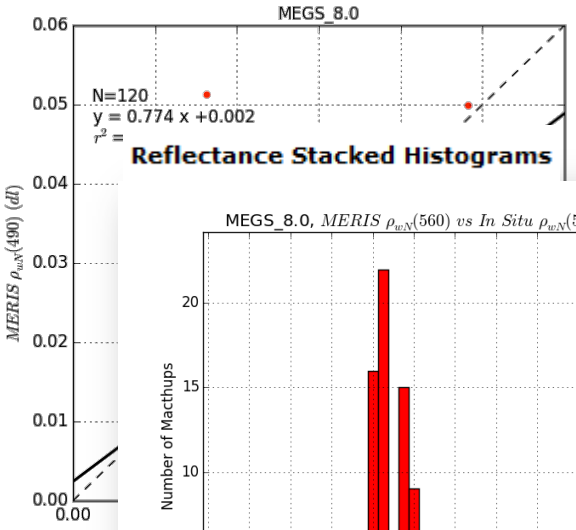
Compressed full extraction (.tar.gz)

extraction20150903_071434_990009044.tar.gz

Extracted Files

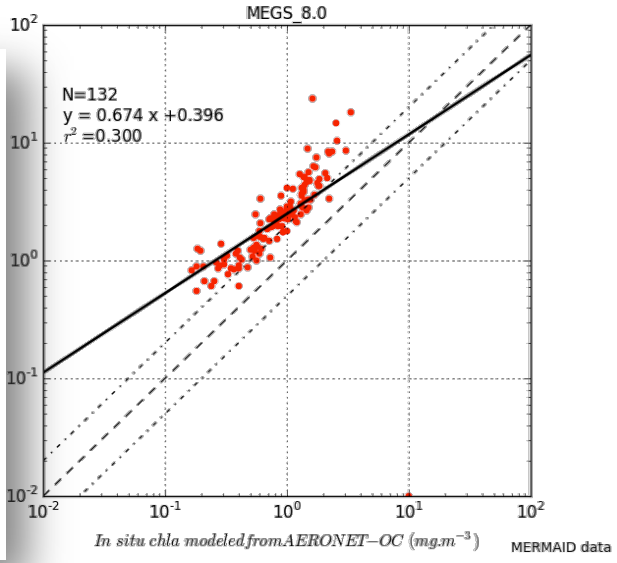
extraction.csv extractionAvg.csv stats.csv parameter.txt

Reflectance Regression

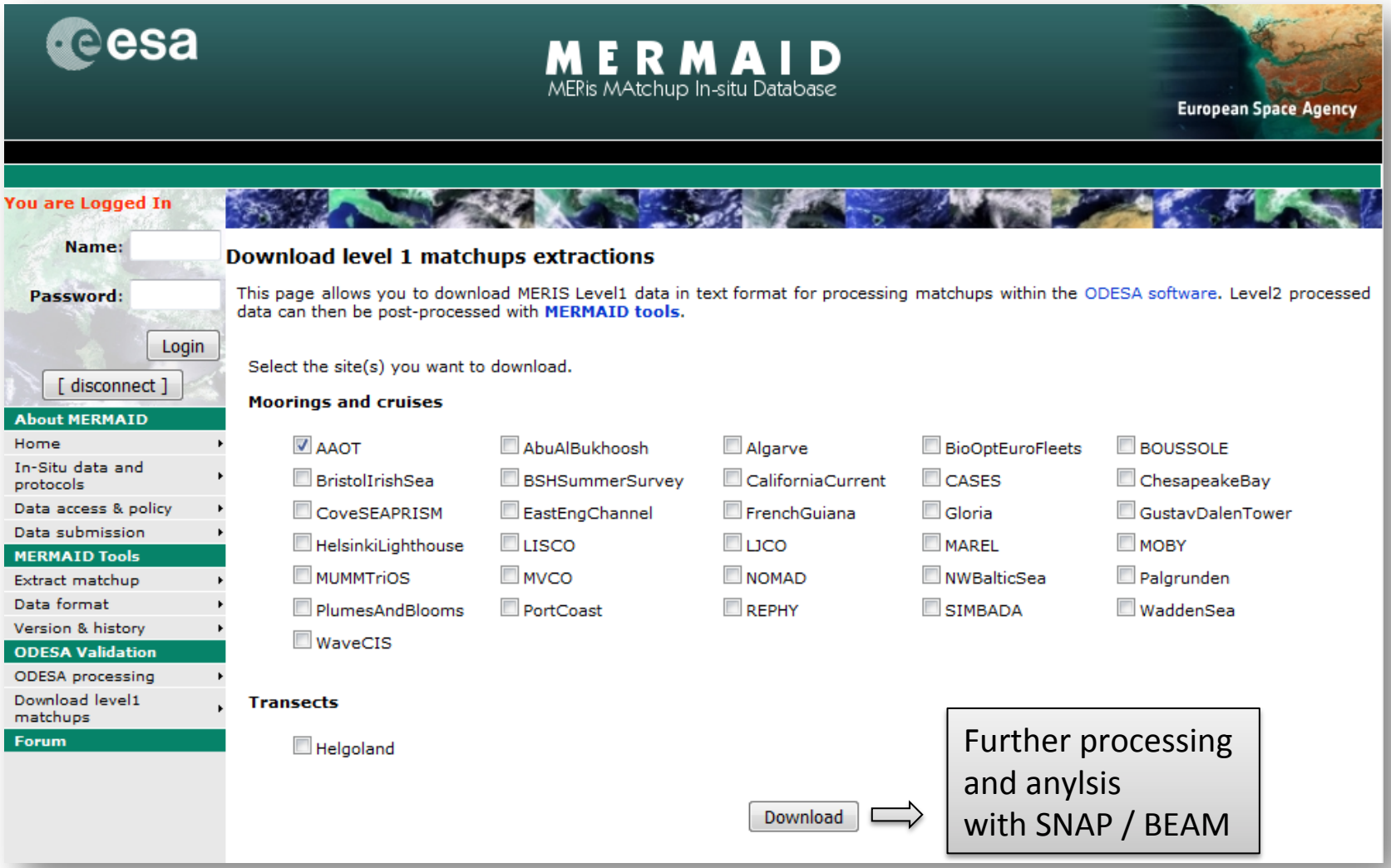


Reflectance Stacked Histograms

Chlorophyll Regression



Example: MERMAID **Algorithm** Validaton

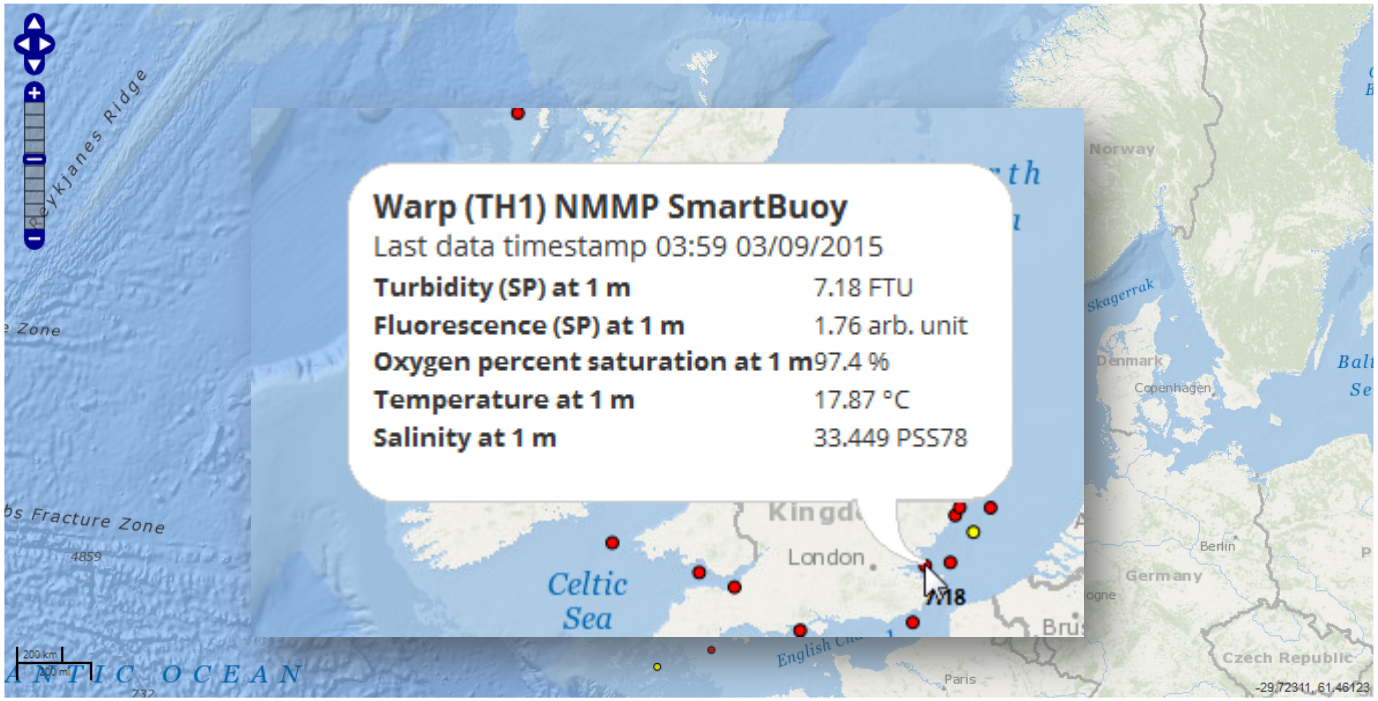


Example: Cefas SMART Buoy Time Series

Marine monitoring interactive map

Basic mode: Hover over point for basic information, click point for further information. click+drag pans map.

Advanced mode: Select multiple points by clicking and dragging a selection rectangle to view and download data from multiple platforms.



View selected

- Historic deployments
- Future deployments
- Current deployments

Labelling

Turbidity (SP) (FTU) at 1 m

Visibility:

- Barrow Waverider
- Blackstones WaveNet Site
- CandyFloss NERC SSB SmartBuoy
- Dowsing SmartBuoy
- EAOW DWR Site C Waverider
- Firth of Forth WaveNet Site
- Hastings WaveNet Site
- Hinkley Point Waverider
- Liverpool Bay Coastal Observatory
- Moray Firth WaveNet Site
- Poole Bay WaveNet Site
- Scarweather WaveNet Site
- Sizewell Waverider
- South Knock WaveNet Site

Select all | Select none

Save view* | Load view | Clear save/Reset

Map Esri, DeLorme, GEBCO, NOAA NGDC, and other contributors.
Data last loaded: 07:41:57 GMT+0200 Thu Sep 03 2015

Example: Cefas SMART Buoy Time Series

Details

Latest data values from 'Warp (TH1) NMMP SmartBuoy' (WMO ID: 6201072) provided by 'Cefas', located at 51°31'.53N, 001°01'.70E

Locate on map

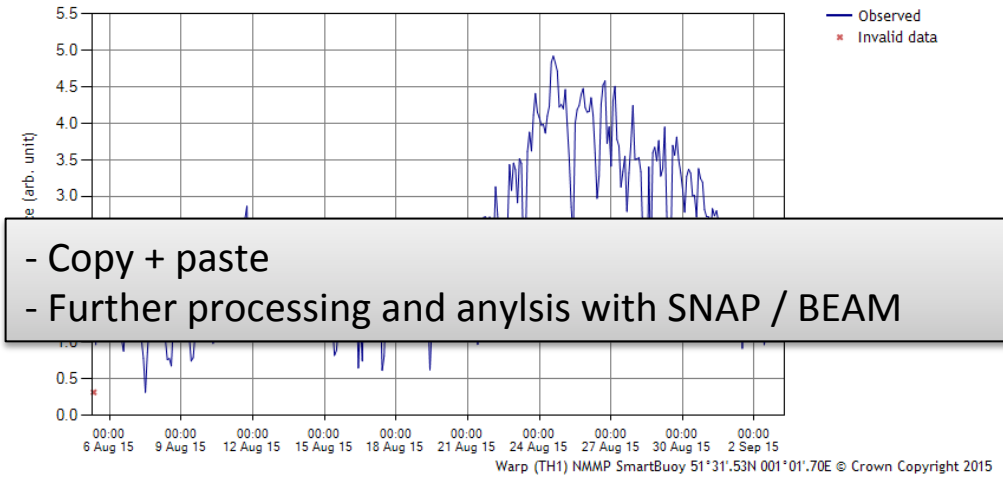
Cefas

Time (GMT)	Salinity (PSS78)	Sea temperature (°C)	Turbidity (OBS) (FTU)	Fluorescence (arb. unit)	PAR irradiance (µE m-2 s-1)	O2 saturation (%)
03-Sep-15 03:59	33.449	17.87	7.18	1.76		97.4
03-Sep-15 01:59	33.341	17.91	10.38	1.66		97.7
02-Sep-15 23:59	33.221	17.98	32.82	1.55		97.1

Tabular data | Graphs | Additional Information

Printable view

Fluorescence



- Copy + paste
- Further processing and anylsis with SNAP / BEAM

Time	O2 saturation (%)
03-Se	97.4
03-Se	97.7
02-Se	97.1
02-Se	97.8
02-Se	98.2
02-Se	98.1
02-Se	101.2
02-Se	101.1
02-Se	98.1
02-Se	98.3
02-Se	96.9
02-Se	97.8
02-Se	98.1
01-Se	97.9
01-Se	98.6
01-Sep-15 19:59	98.3

Example: NOMAD

SeaBASS

NOMAD: NASA bio-Optical Marine Algorithm Dataset

Home | Data Users | Data Contributors | Data Search | NOMAD | Data Archive | Wiki | Lists | Contact Us

NOMAD: NASA bio-Optical Marine Algorithm Dataset

NOMAD is a publicly available, global, high quality in situ bio-optical data set for use in ocean color algorithm development and satellite data product validation activities. Data products include coincident observations of wate… s the date, time, and coordinates of data collection and binary processing … cients) and aerosol optical thicknesses have been or will be included in th… Downloads. Additional background details, such as the motivation for creati… Verdell and Bailey reference listed below.

NOMAD is available for research uses only. It was compiled by … generous data contributions from the ocean color research comm… interpolation (OI) sea surface temperature (SST) data were acqui… National Geophysical Data Center. NOMAD Data access and … identified outliers to the SeaBASS Administrator.

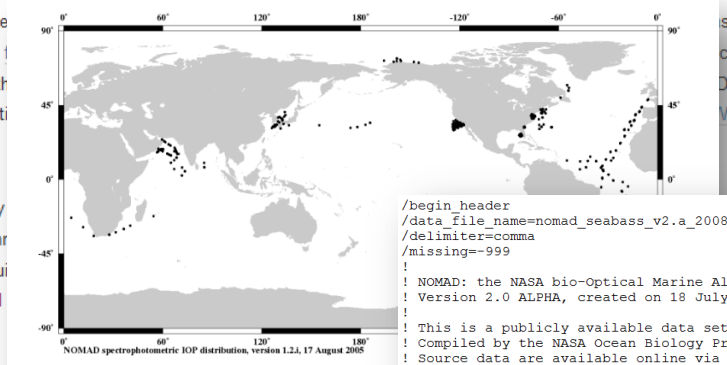


Figure 1. Global map of spectrophotometric ab…

IOP data processing documentation

Evaluation, processing, and distribution of Inherent Optical Properties
Spectrophotometric absorption processing evaluation data set (map)
Backscattering processing evaluation data set (map)

Downloads

Download Version (right click and choose "save as")	Map	Date Last Updated
Current NOMAD data set (version 2.a)	Map v2.a	18 July, 2008
Original NOMAD data set (version 1.3)	Map v1.3	19 Sept, 2005

```
/begin_header
/data_file_name=nomad_seabass_v2.a_2008200.txt
/delimiter=comma
/missing=-999
!
! NOMAD: the NASA bio-Optical Marine Algorithm Data set
! Version 2.0 ALPHA, created on 18 July 2008
!
! This is a publicly available data set for research use only.
! Compiled by the NASA Ocean Biology Processing Group, Goddard Space Flight
! Source data are available online via the SeaBASS Web site (http://seabass.
! Please contact the SeaBASS Administrator with questions (seabass@seabass.g
!
! ~~~~ ALL USERS ARE ASKED TO ACKNOWLEDGE BOTH THE INDIVIDUAL DATA CONTRIBUT
!
! Data were contributed by participants in the NASA SIMBIOS Program (NRA-96-
! and NRA-99-OES-09) and by voluntary contributors.  A cruise name accompani
! data record.  Cruise details, including contributors' names, are available
! using the "General Search" and "Cruise Search" utilities on the SeaBASS We
! (http://seabass.gsfc.nasa.gov/search.html).
!
! CITATION: Werdell, P.J. and S.W. Bailey, 2005: An improved in situ
! bio-optical data set for ocean color algorithm development and satellite
! data product validation.  Remote Sensing of Environment, 98(1), 122-140.
!
! IOP-RELATED DOCUMENTATION:
! http://seabass.gsfc.nasa.gov/data/werdell_nomad_iop_qc.pdf
!
! alphabetical description of data products
! -----------------------------------------
! a          ~ total absorption coefficient (m-1)
! ad      ~ detrital (non-algal) absorption coefficient (m-1)
```

Further processing and anylsis with SNAP / BEAM

Protocols – In-situ

- Protocols include requirements and procedures for
  - Radiometry: instruments, deployment, data processing
  - Water samples: procedures, chemical treatment …
  - Processing: radiance normalisation, corrections, conversion, …
  - Documentation, meta data

- Radiometry (Aeronet-OC):
  Zibordi et al (2009): AERONET-OC: A Network for the Validation of Ocean Color Primary Products. AMS Volume 26, Issue 8 (August 2009).
  http://journals.ametsoc.org/doi/abs/10.1175/2009JTECHO654.1

- In-situ measurements:
  Tilstone and Martinez-Vicente (2012): ISECA Protocols for the Validation of Ocean Colour Satellite data in Case 2 European Waters. INTERREG IVA 2 Mers Seas Zeeen Cross-border Cooperation Programme 2007 – 2013.
  https://www.google.de/url?sa=t&rct=j&q=&esrc=s&source=web&cd=3&ved=0CDEQFjACahUKEwiArLjvxNLHAhWEltsKHQh6ACE&url=http%3A%2F%2Fwww.vliz.be%2Fimisdocs%2Fpublications%2F254220.pdf&ei=St_jVYDfPISt7gaI9IGIAg&usg=AFQjCNGFUaKxNm7WfNrNdtaocmJWGSutMQ&cad=rja

- MERMAID:
  Barker et al (2013):
  - Part A: In-situ Measurement Protocols. Apparent optical properties.
    http://mermaid.acri.fr/dataproto/CO-SCI-ARG-TN-0008_In-situ_Measurement_Protocols-AOPs_Issue2_Mar2013.pdf
  - Part B: Inherent Optical Properties and in-water constituents.
    http://mermaid.acri.fr/dataproto/CO-SCI-ARG-TN-0008_In-situ_Measurement_Protocols-IOPs-Constituents_Issue1_Mar2013.pdf

Example

Pigment extraction and sample preparation

For pigment extraction 2 ml of 90 % acetone is added to the filter which is ultrasonicated using an ultrasonic probe for 20 secs as described in Llewellyn et al. (2005). The extracting solvent also has an internal standard (typically Apo-8'-Carotenal (trans)). The concentration of internal standard must be chosen in such a way that pigments and standard peak areas are comparable.

After extraction, the sample is micro centrifuged for 2 minutes The extract is then injected through a 100 µl loop into the HPLC system.

Protocols - Processing

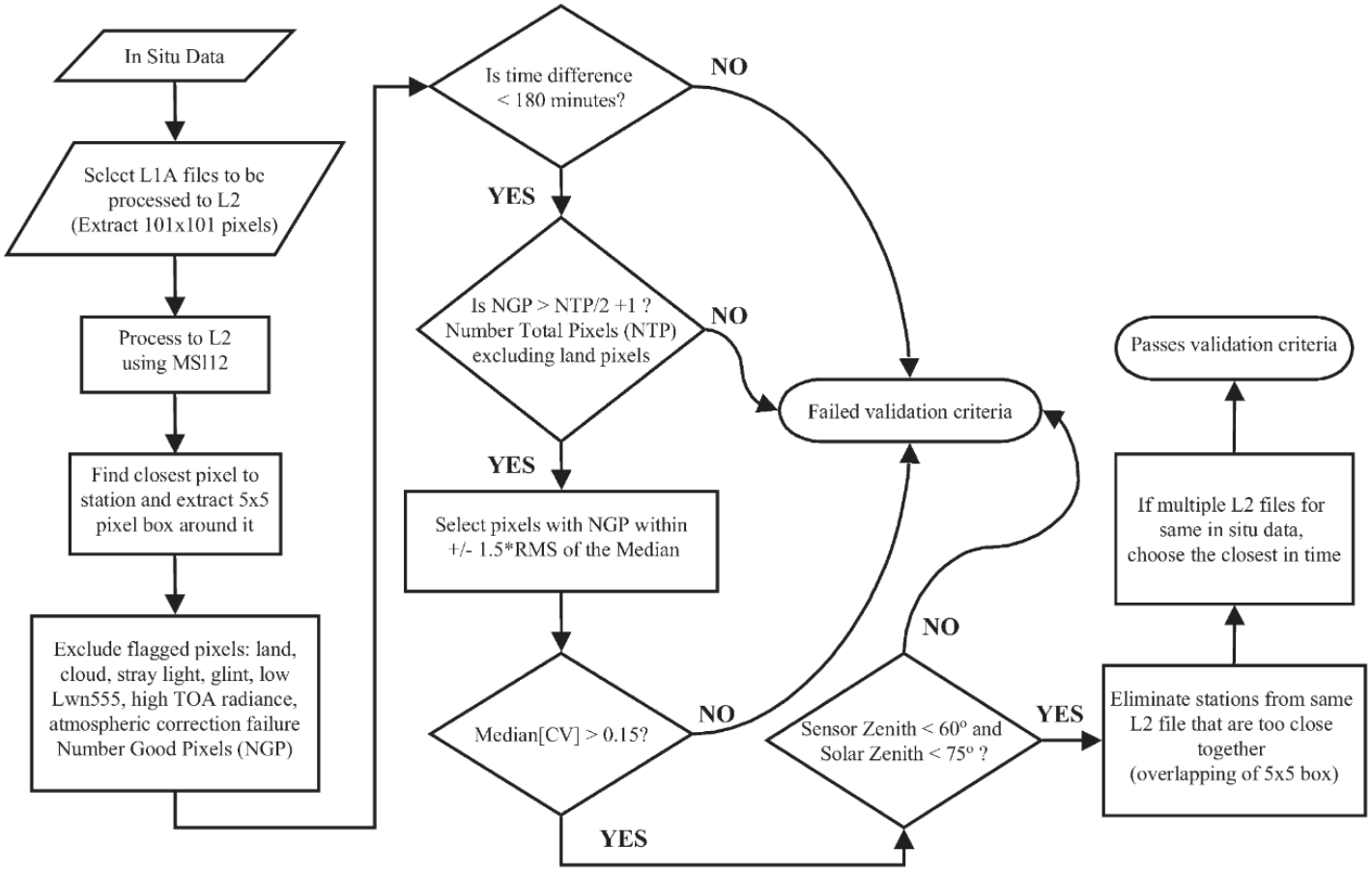


Fig. 1. Flowchart of the validation process highlighting the applied exclusion criteria.

Source: Bailey & Werdell, 2006: A multi-sensor approach for the on-orbit validation of ocean color satellite data products. RSE 102 (2006)

Please answer!

- Case 1 waters: only one variable determines the water colour. This is typically the Chlorophyll-a concentration. All other optically active substances covary with the chl-a concentrations.

- Case 2 waters are all other waters. There the colour is depending on several uncorrelated substances (typically 3-5 different components)

- Why is validation in Case 1 waters different from validation in Case 2 waters? Name a few issues!

Part 4

VALIDATION TECHNIQUES

Please answer!

What validation methods do you know,
or could imagine?

Overview

- First impression: looking at images!
- Decorrelation analysis (“invalidation”)
- Match-up analysis
- Frequency distributions
- Time series
- Transects

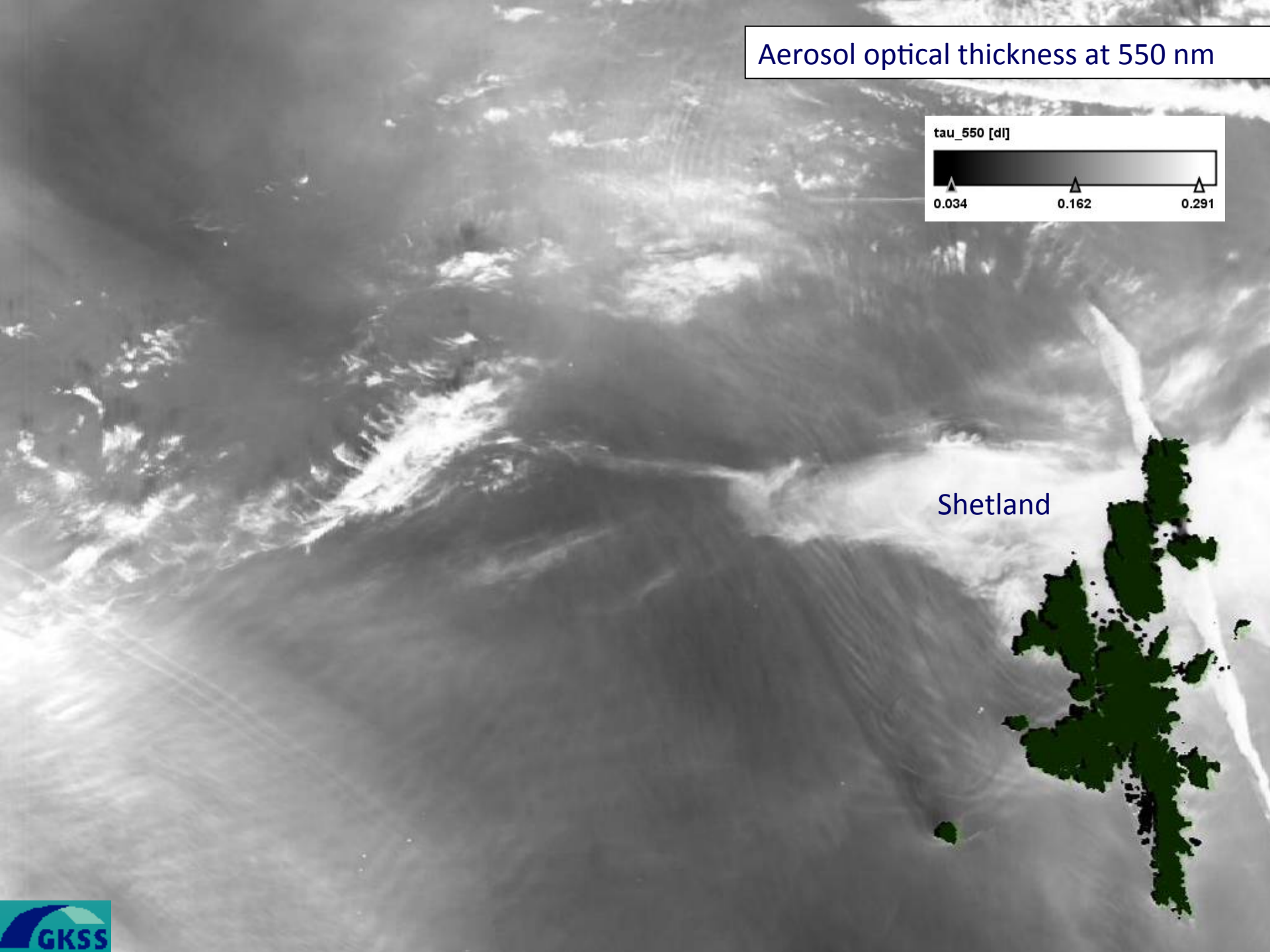
Visual Analysis

- The following example has been prepared by Roland Doerffer

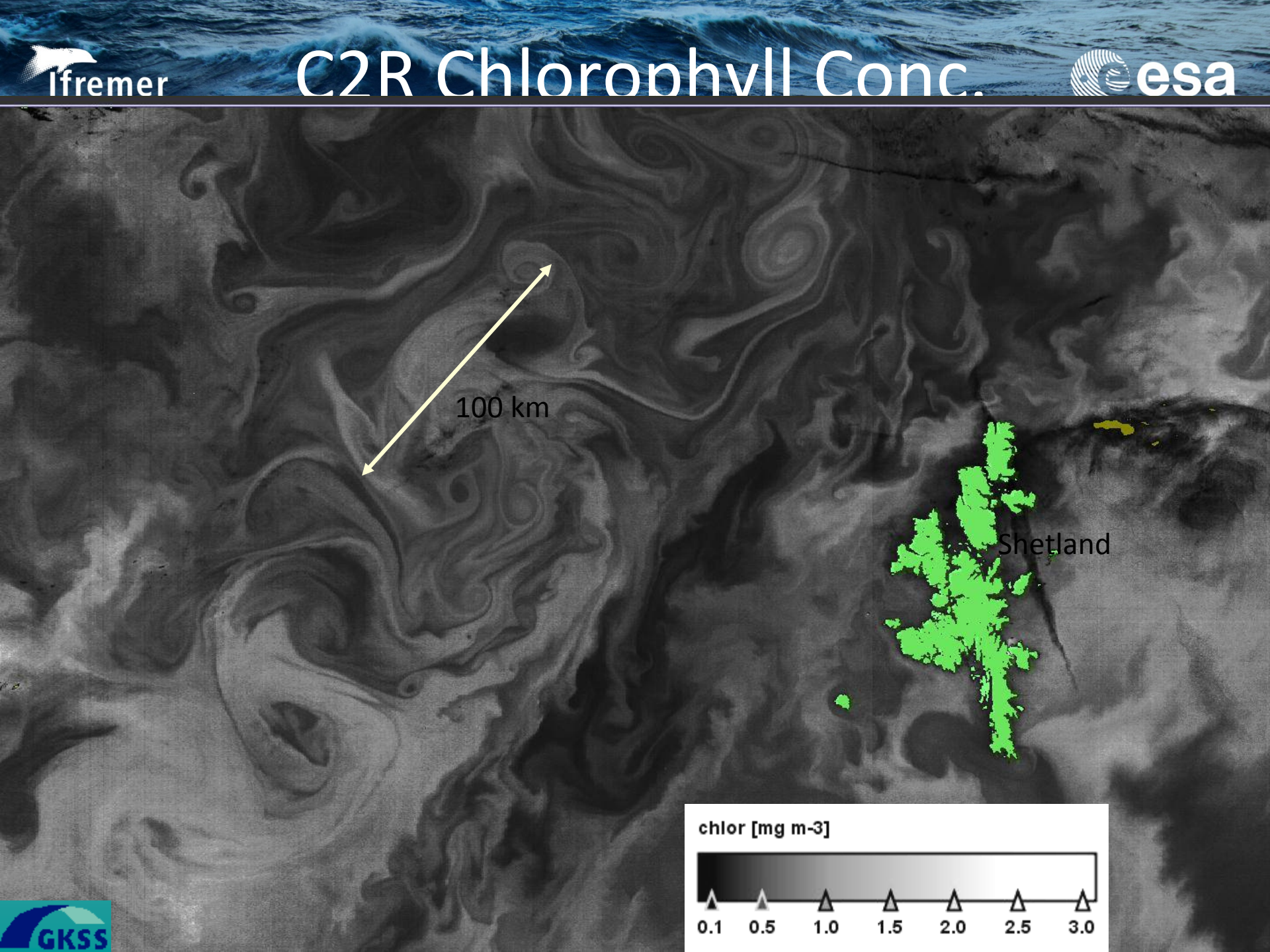
- It shows top-of-atmosphere radiance, aerosol optical thickness and chlorophyll concentration
  - TOA image gives an impression on the integrated signal
  - Aerosol optical thickness and chlorophyll concentration should be decorrelated
  - Features visible in aerosol optical thickness should look like atmospheric structures
  - Features in the chlorophyll concetration should look likes water

  (this requires experience from working onboard ships and with satellite images)


TOA
Radiance reflectance
RLw RGB
Shetland


Aerosol optical thickness at 550 nm
tau_550 [dl]
0.034
0.162
0.291
Shetland

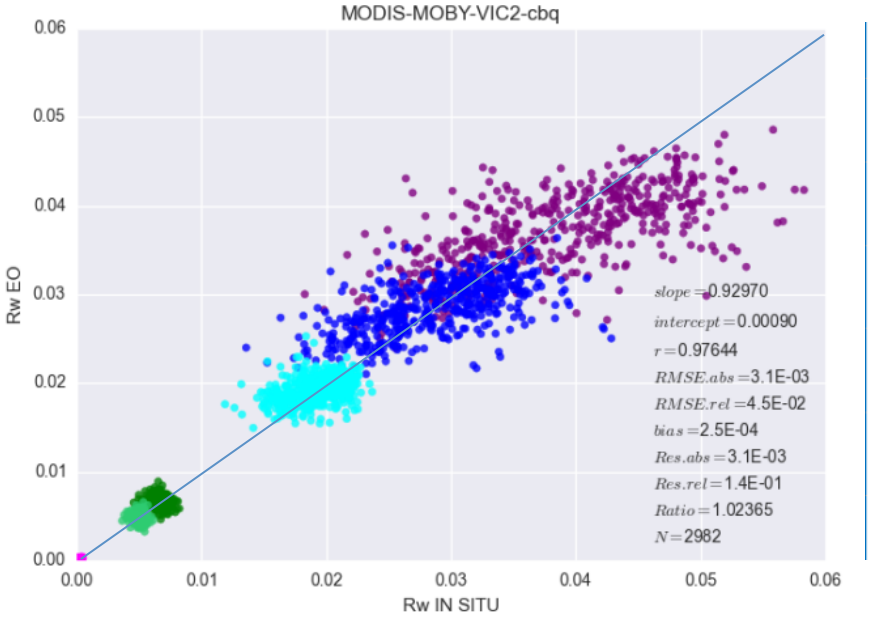
C2R Chlorophyll Conc.



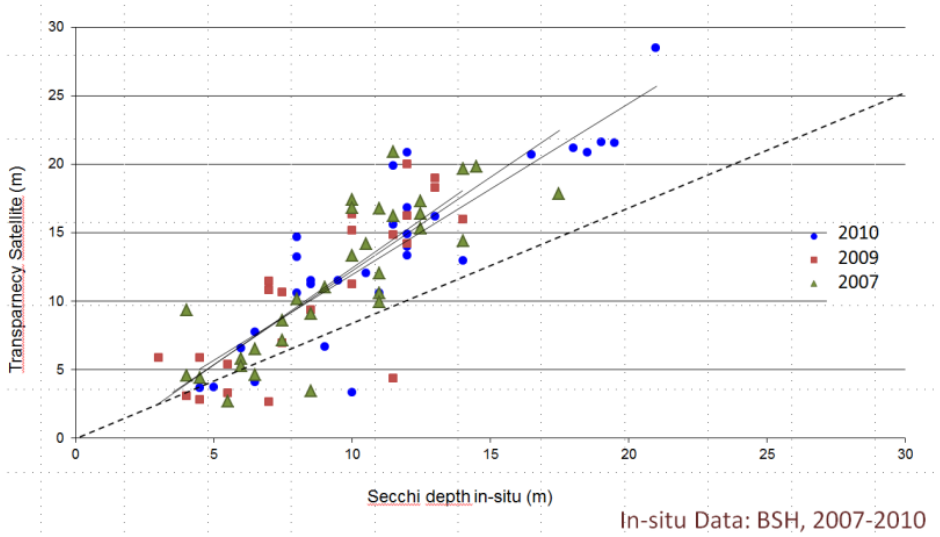
Match-up Analysis

Tools: scatter plots & statistics

Example 1: Radiometry, MOBY site



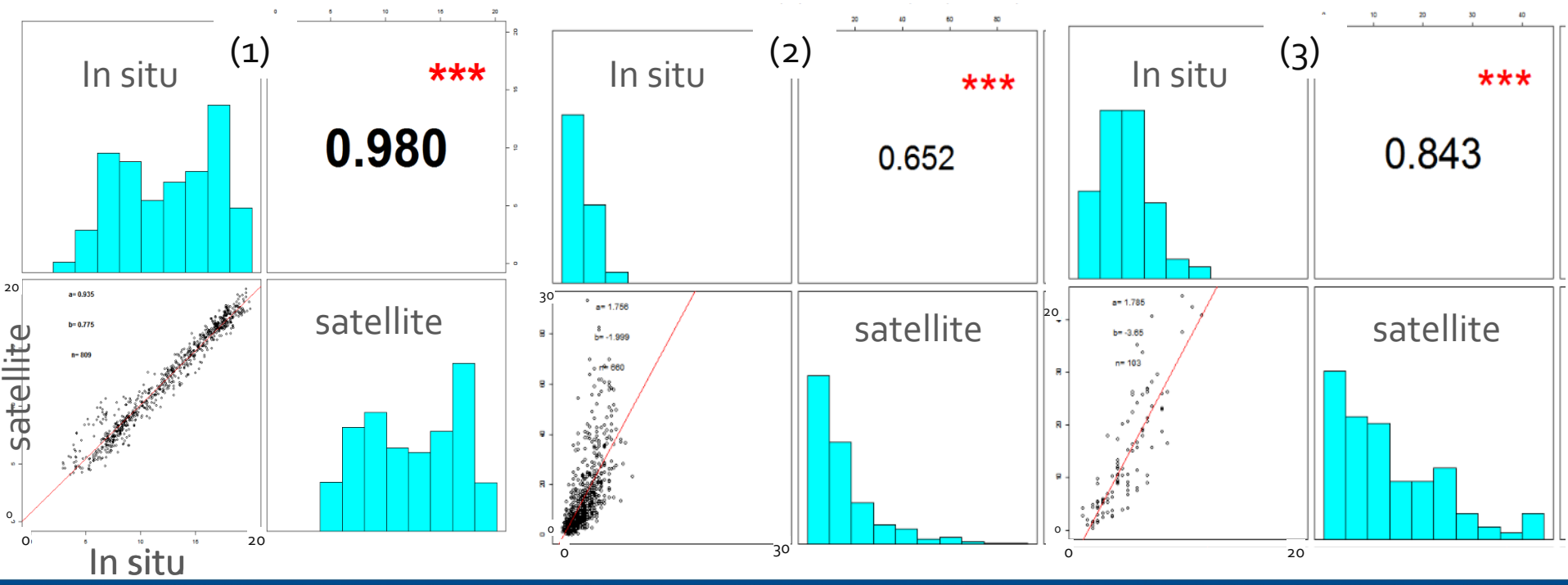
Example2 : Secchi Depth, comparison of 3 years



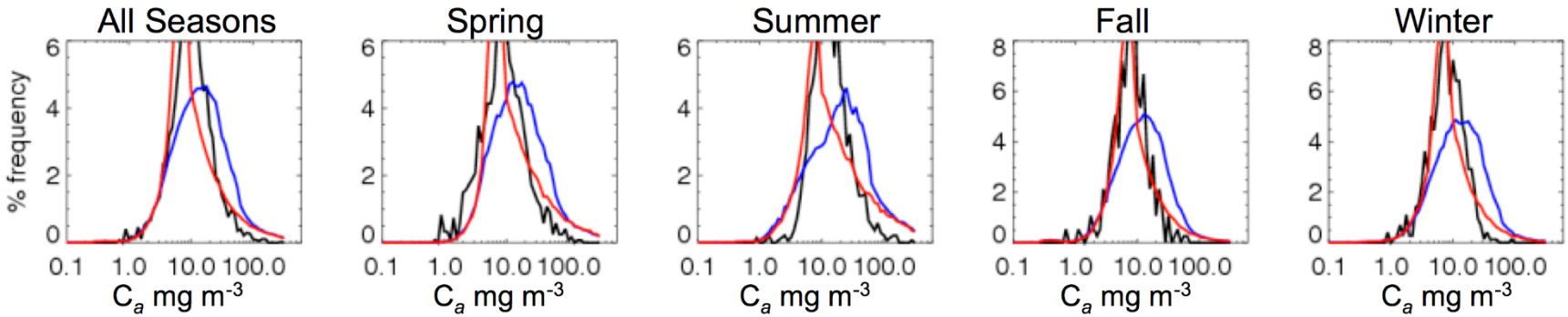
Match-ups & Distribution

Comparison of different algorithms and in-situ

- (1) SST, North Sea
- (2) Transparency (Algo 1), Med. Sea
- (3) Transparency (Algo 2), Med. Sea



Distributions

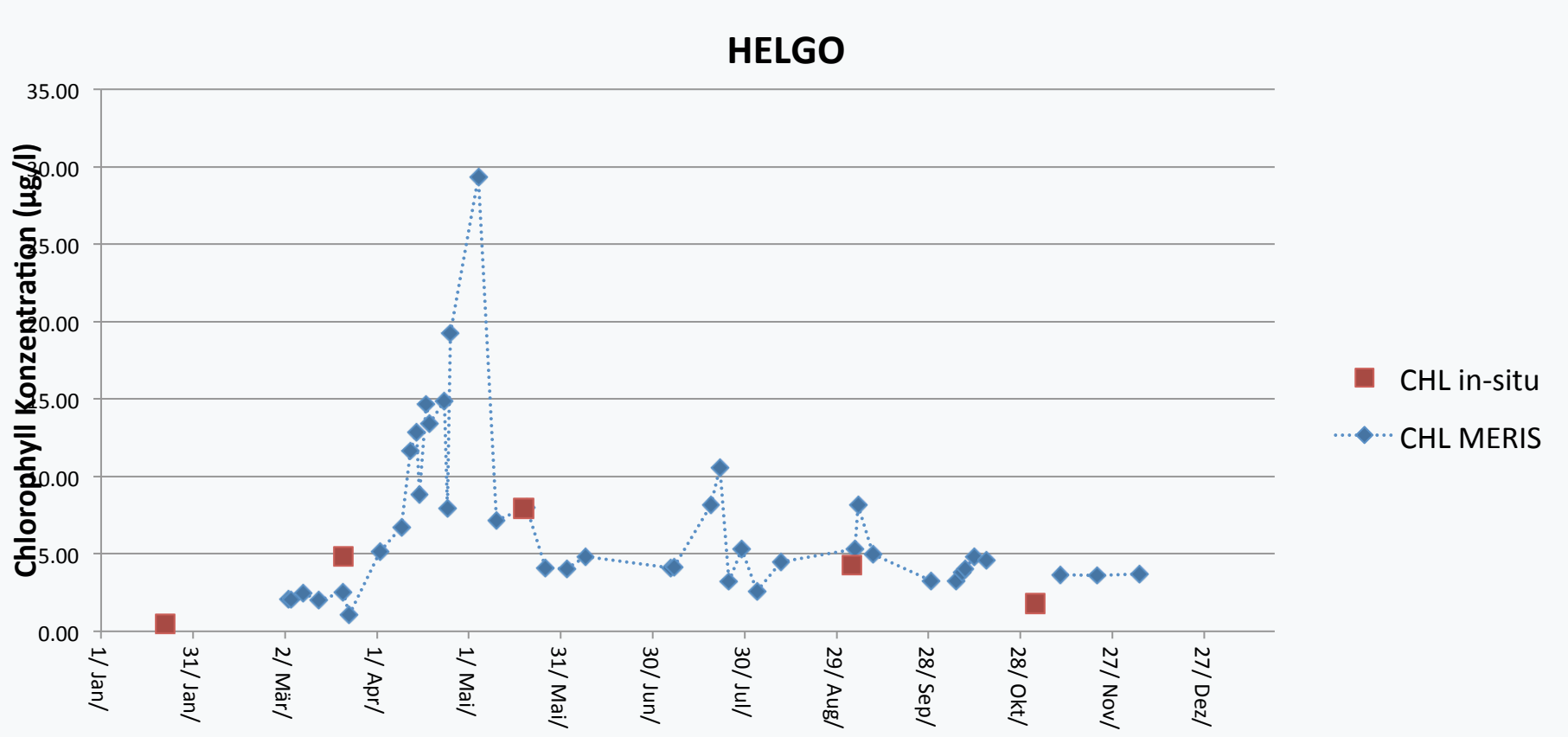


Color Code: in situ, SeaWiFS before, SeaWiFS after

Example of a regional analysis against bulk in situ statistics. The plots show seasonal distributions of SeaWiFS chlorophyll-a retrievals, before (blue) and after (red) a particular algorithm change, with the regional distribution of in situ measurements (black).

Source: B. Franz: ethods for Assessing the Quality and Consistency of Ocean Color Products. http://oceancolor.gsfc.nasa.gov/DOCS/methods/sensor_analysis_methods.html

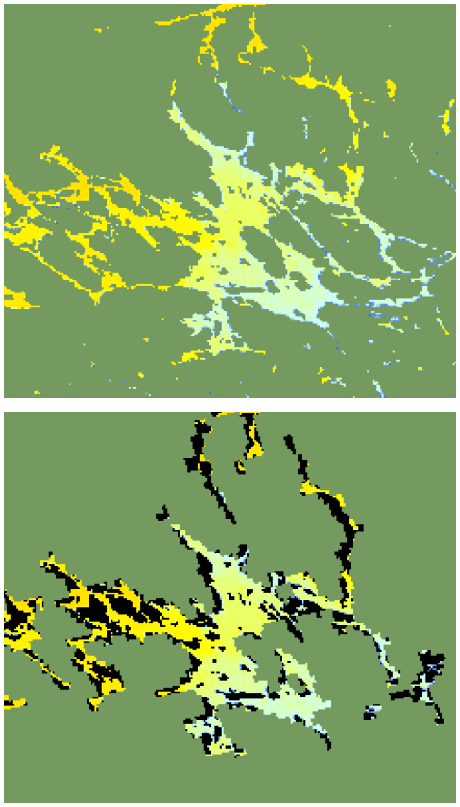
Time Series

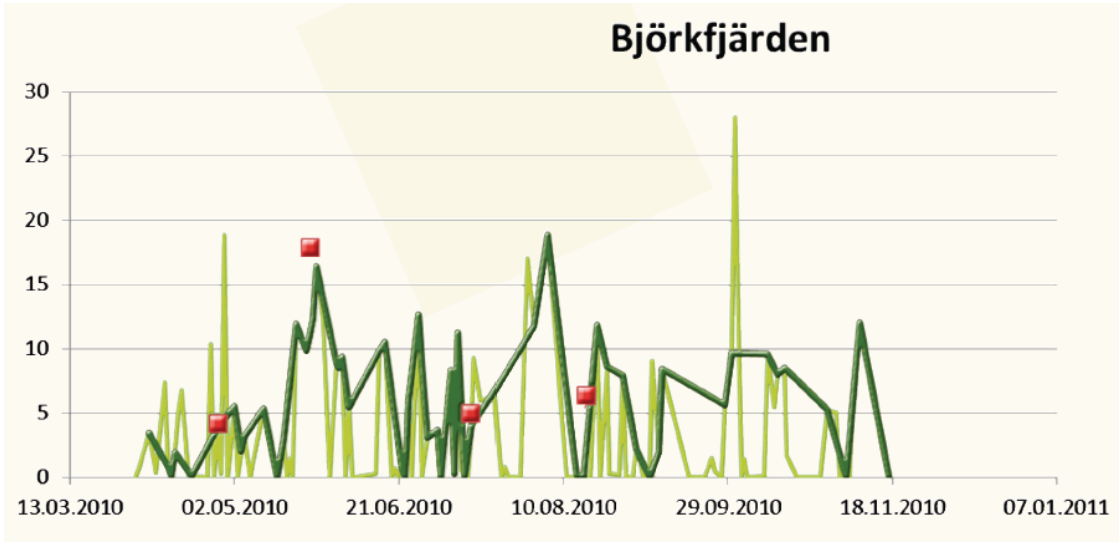


Satellite data: WAQSS Service, Brockmann Consult

In situ data: BSH/IOW 2010

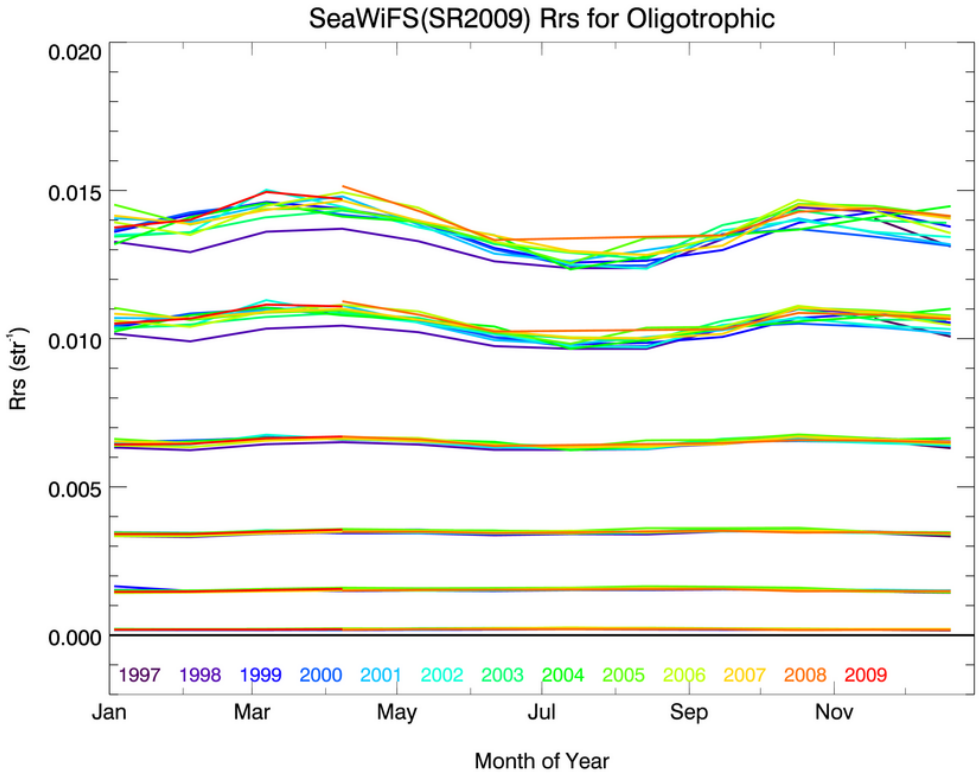
Filtering and the effect on time series





Light green line: no filtering on the satellite data
→ a lot of scatter; hard to detect anything
Dark blue line: after filtering
→ reducing outliers, trend becomes clear
→ but: reducing the number of points

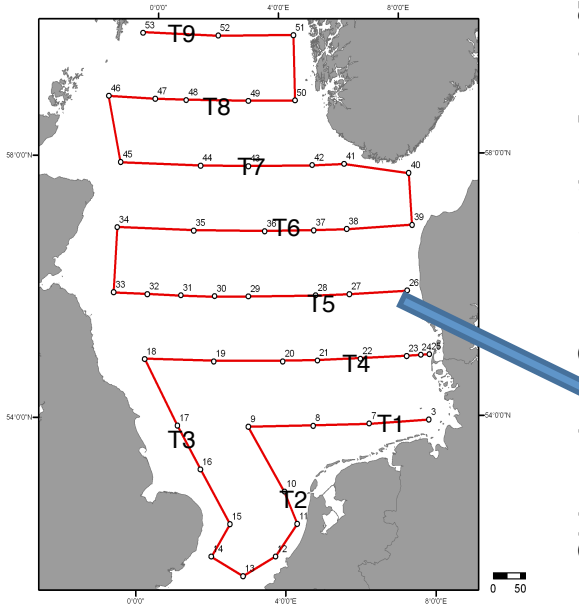
Time Series Plausibility

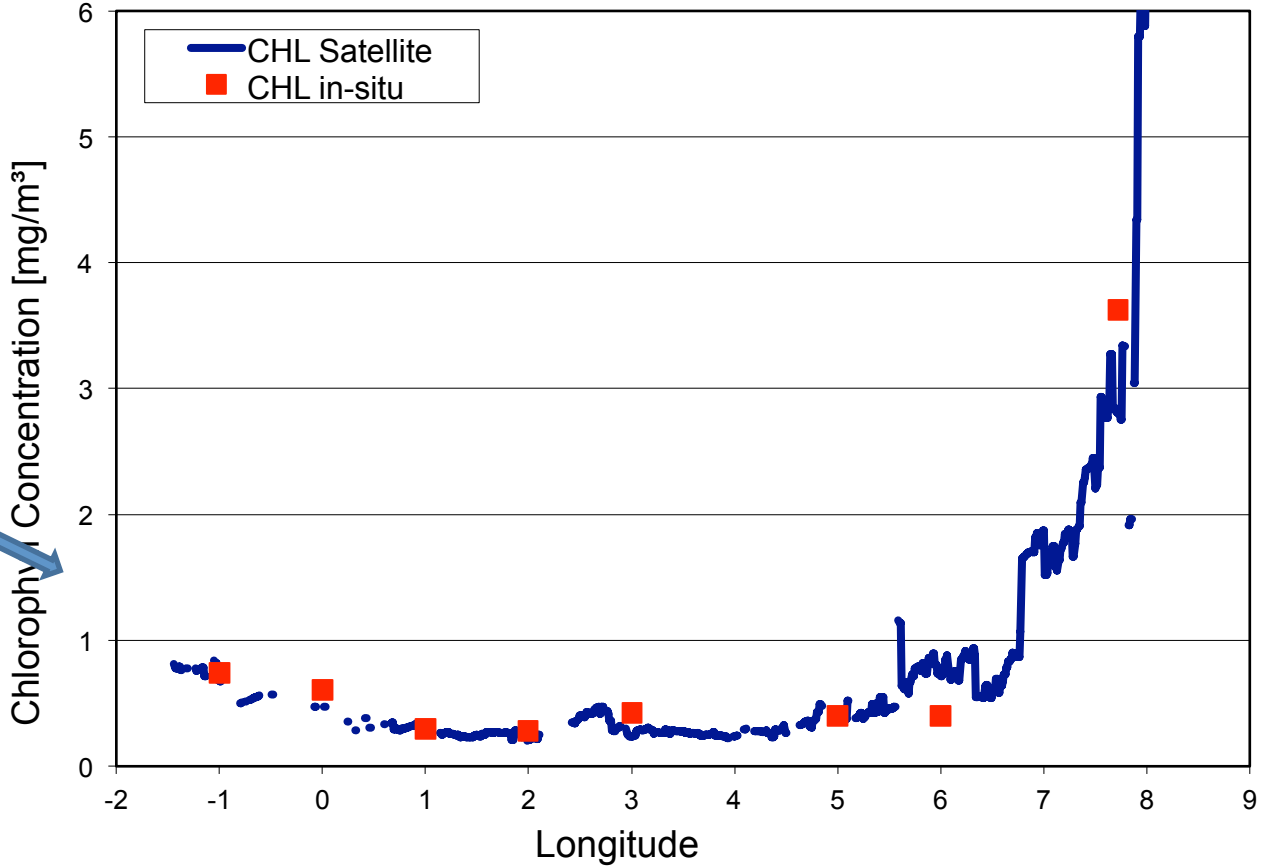


An example of a trend analysis is the SeaWiFS annual cycle for Rrs. In the absence of any major geophysical events, we expect the trend in global deep-water or global oligotrophic-water Rrs to repeat from year to year. Low-level differences may be due to geographic sampling biases or real geophysical changes, but on the large-scale these plots tell us that SeaWiFS products are, to first order, self-consistent over time

Source: B. Franz: ethods for Assessing the Quality and Consistency of Ocean Color Products. http://oceancolor.gsfc.nasa.gov/DOCS/methods/sensor_analysis_methods.html

Transects





Satellite data: WAQSS Service, Brockmann Consult

In-situ Data: BSH, 2006

Summarize!

Method	Strength	Weakness
Visual inspection		
Match-up sat vs in-situ		
Match-up sat vs sat		
Distributions		
Time series		
Transects		

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