IOCCG Training Course on Ocean Colour Remote Sensing

Uncertainties in ocean colour remote sensing
Lecure 2: algorithms, validation

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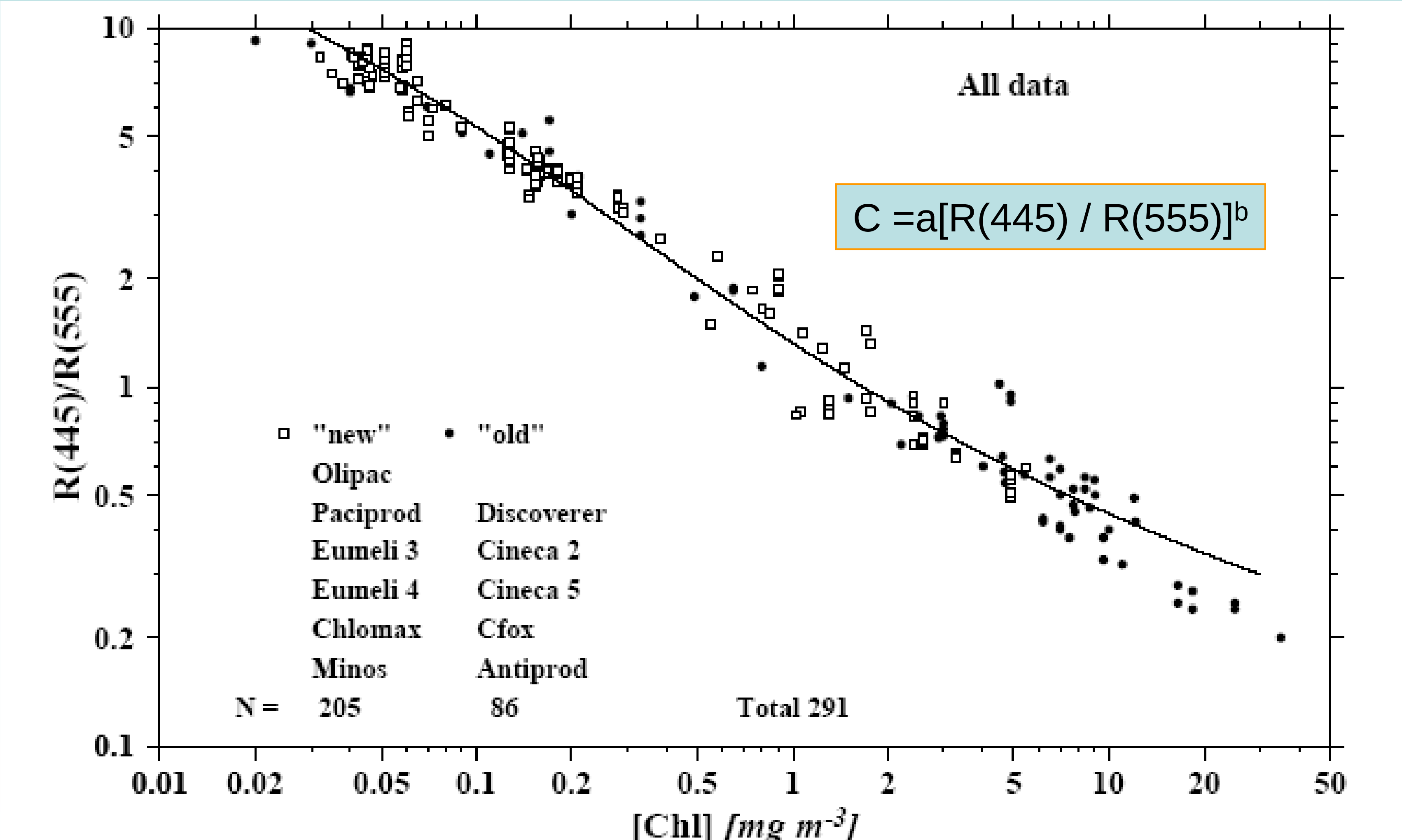
IOCCG
International Ocean Colour research Coordination Group

Algorithms and uncertainties

- Inversion schemes
- Saturation and masking effects
- Out of scope conditions
- Verification
- Validation
- Strategies for validation
- Summary and conclusions

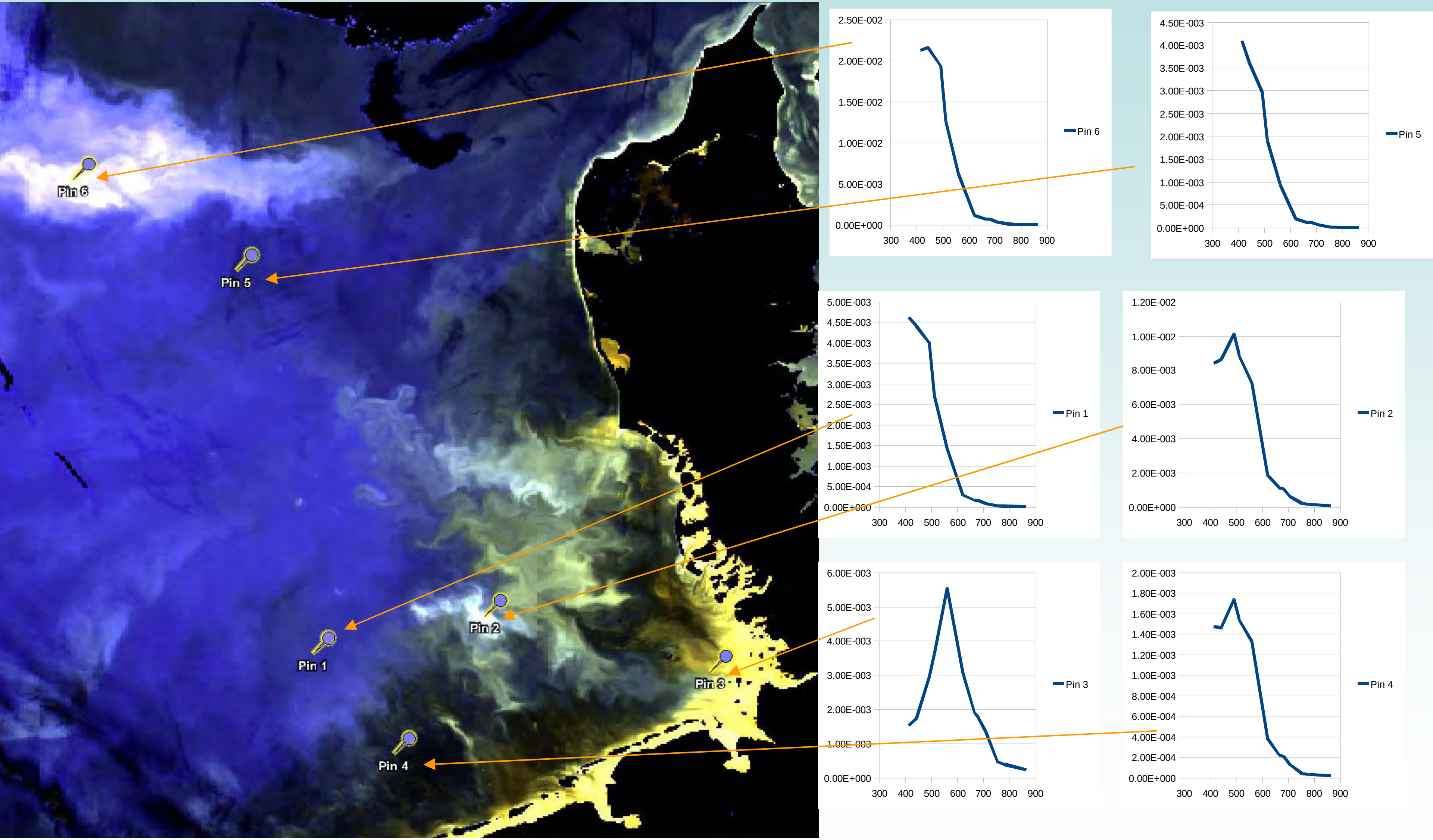
Case 1 water algorithm based on reflectance ratio model R445 / R555



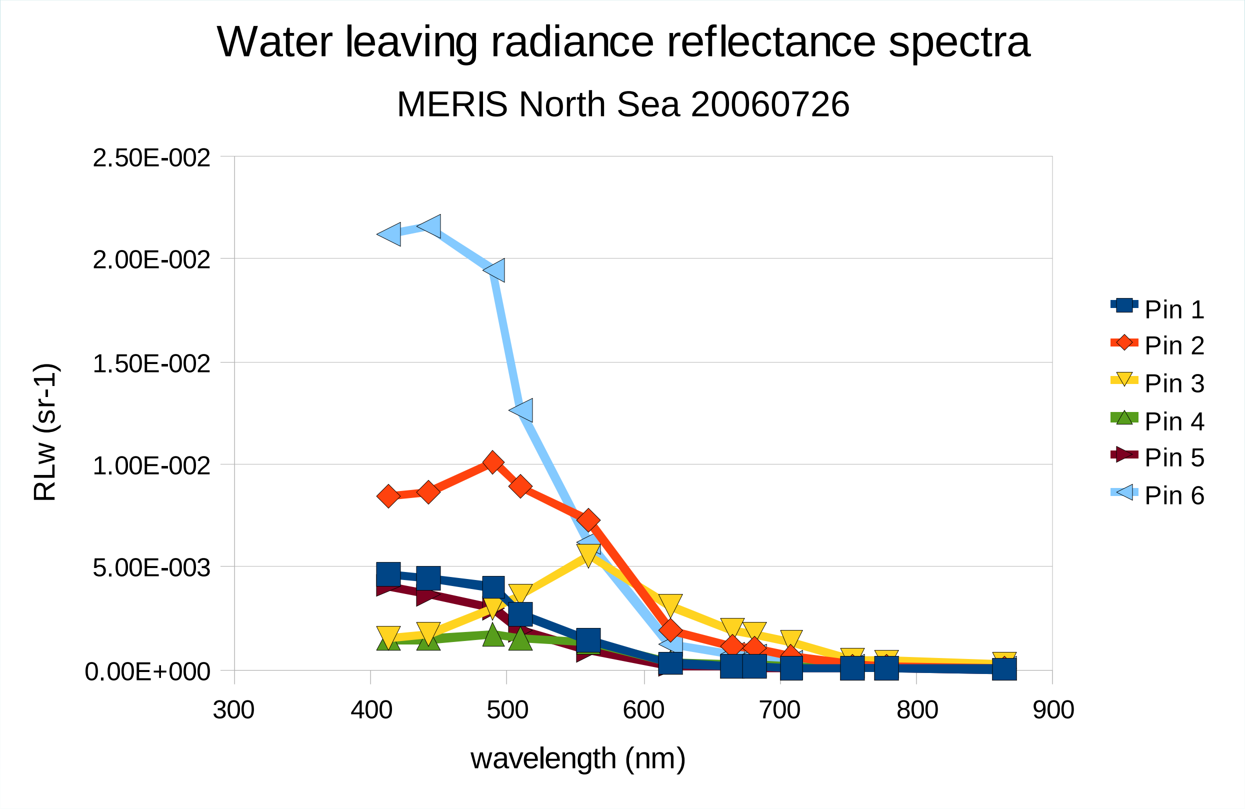
Case 1 water:

Morel / Antoine MERIS Case 1 water ATBD

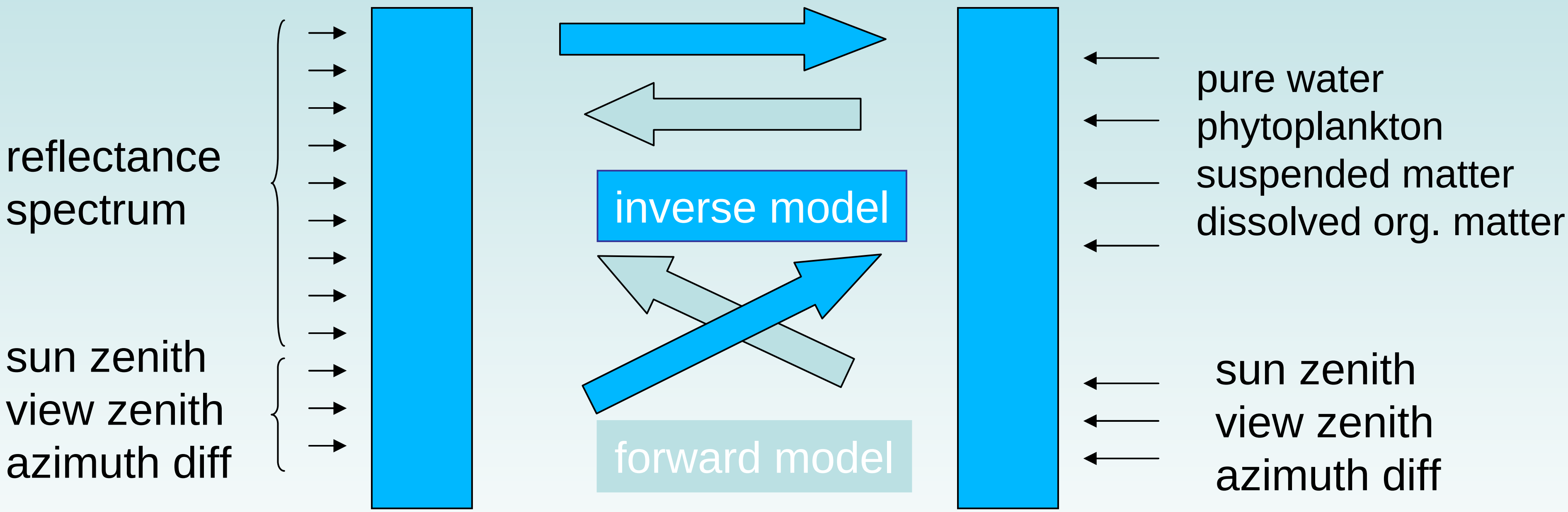
Water leaving radiance reflectance spectra in coastal water



Variability of water leaving reflectance spectra



The inverse problem

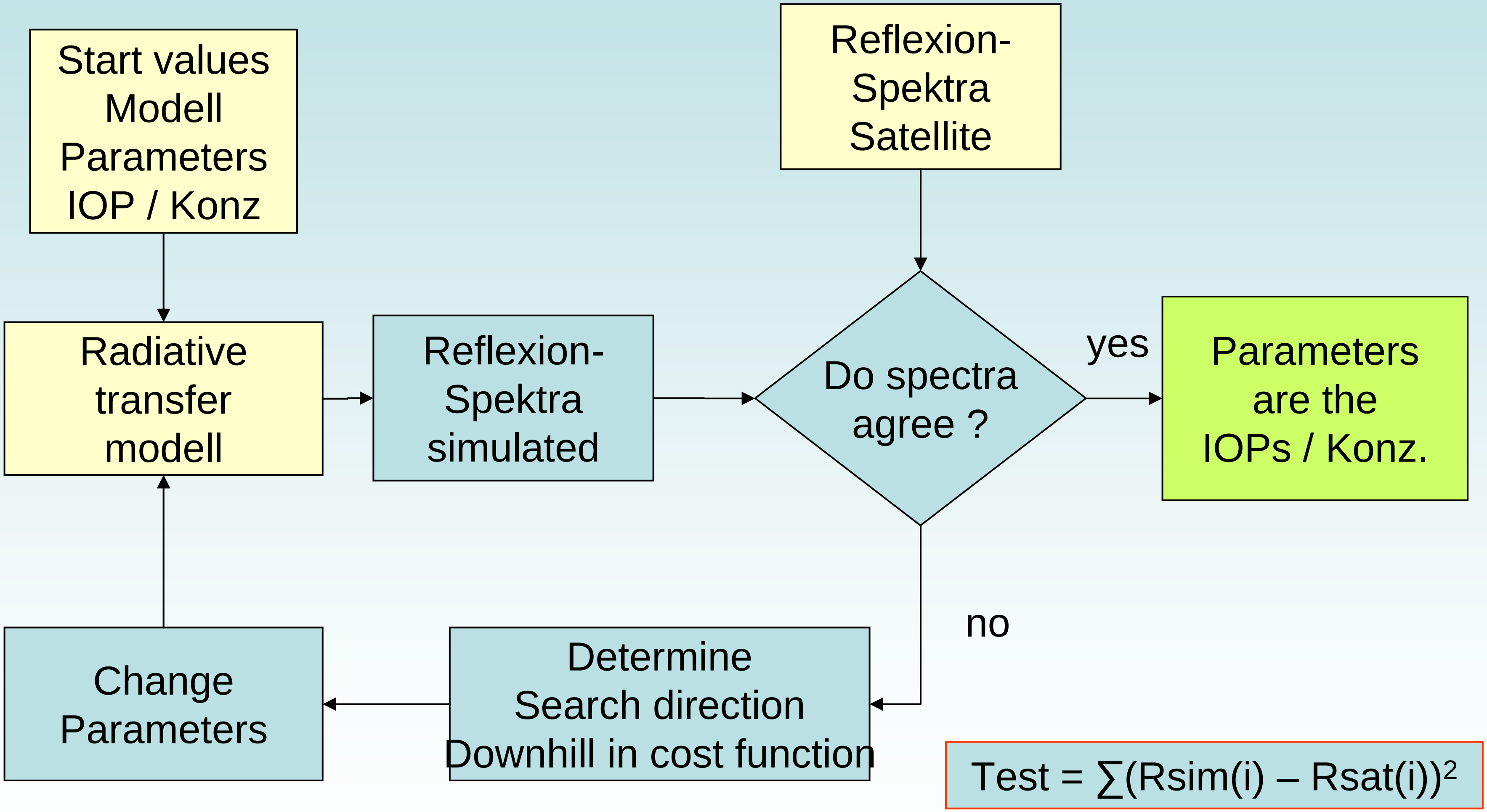


- Matrix inversion
- Inversion by optimization
- Inversion by neural network

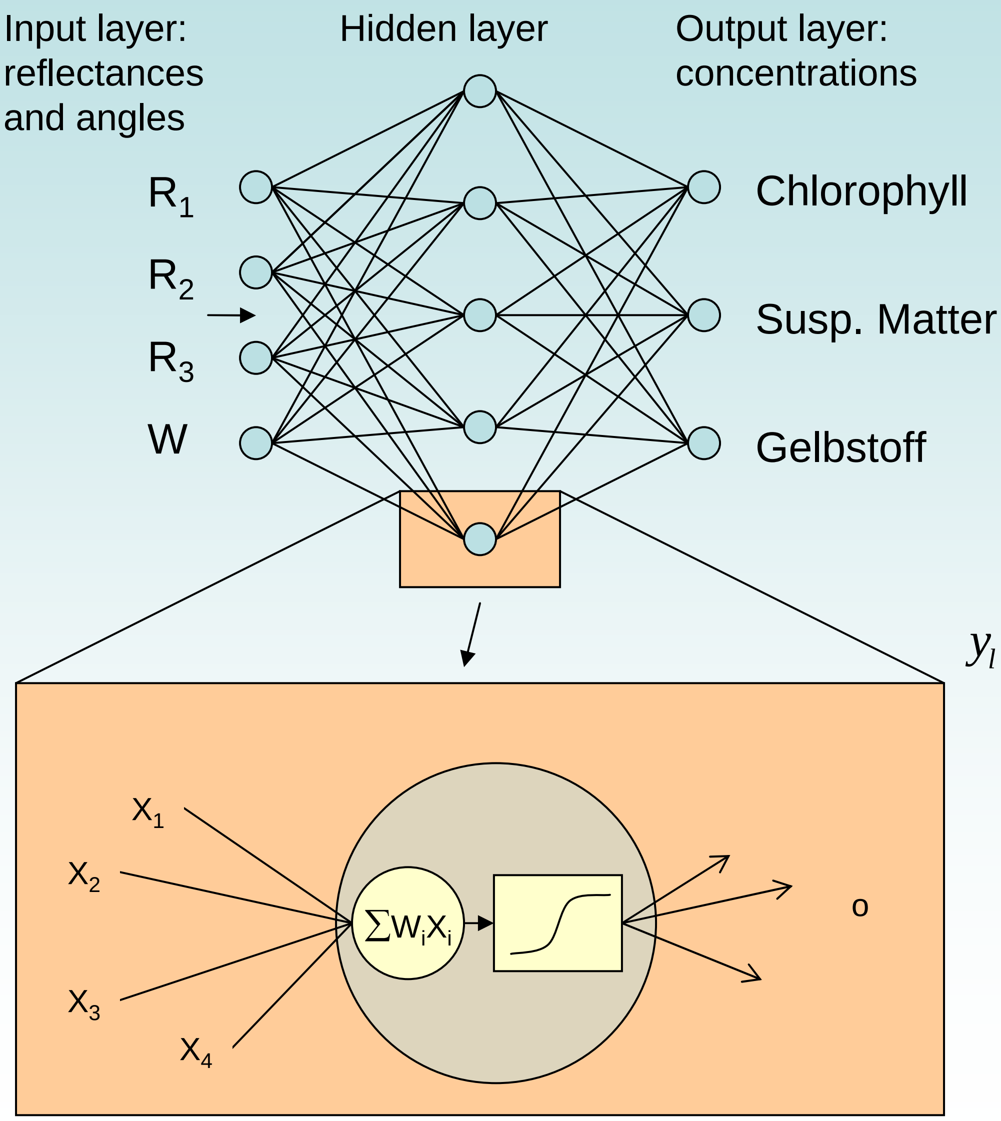
Success depends on:

- Bio-optical model
- ambiguities

Inverse Modellierung using Optimization Procedures



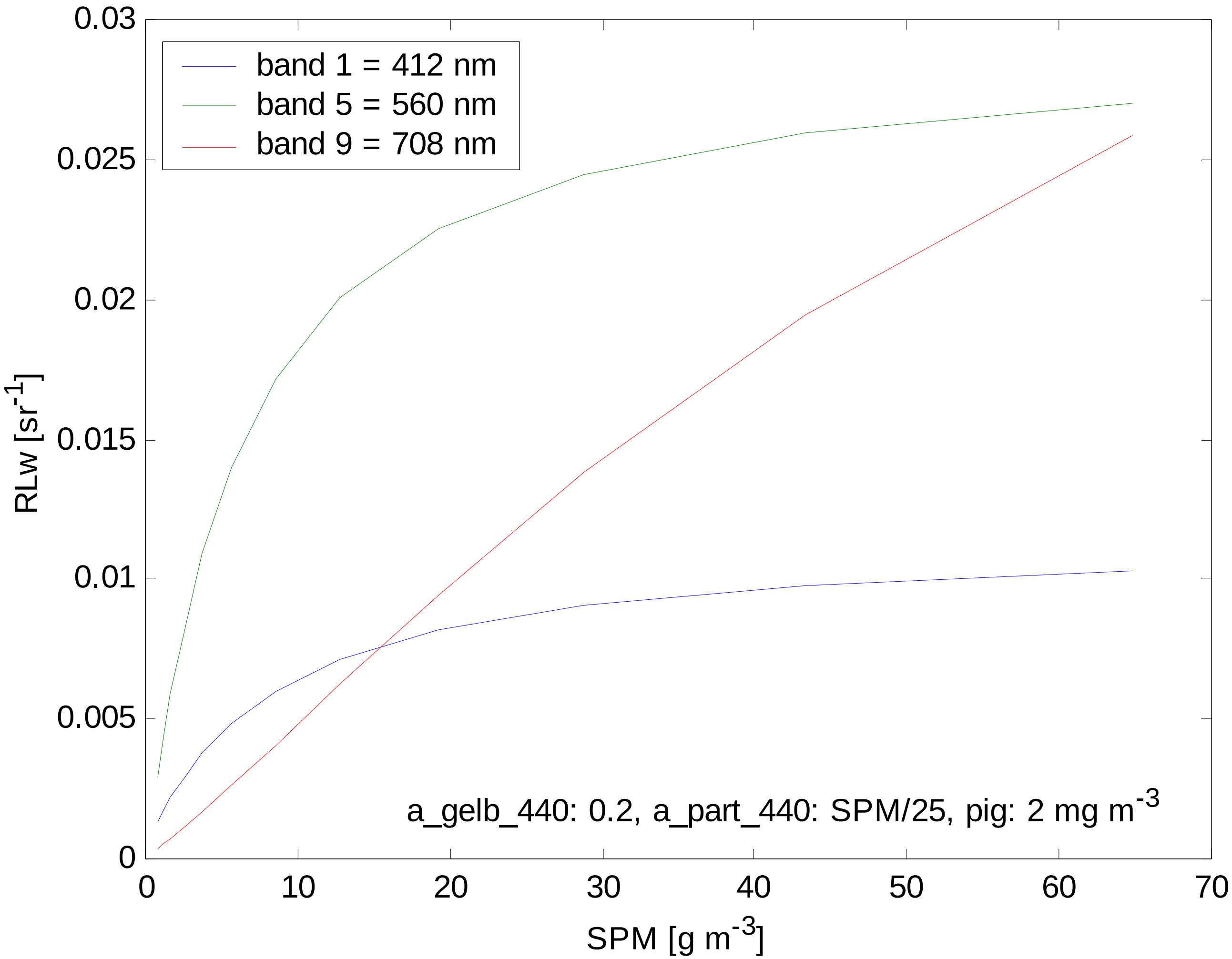
Simplified scheme of NN Algorithm



$$y_l = s(-d_l + \sum_{k=1}^{3} w_{kl} \cdot s(-c_k + \sum_{j=1}^{5} v_{jk} \cdot s(-b_j + \sum_{i=1}^{4} u_{ij} x_i)))$$

Sensitivity at different concentration ranges and spectral bands

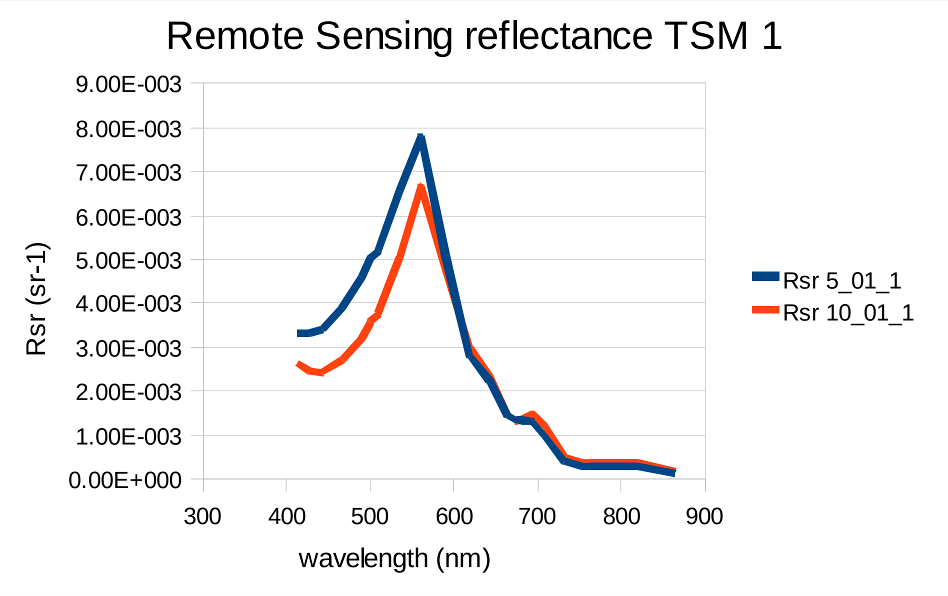
RLw for MERIS bands 1 (412 nm), 6 (560 nm), 10 (708 nm)

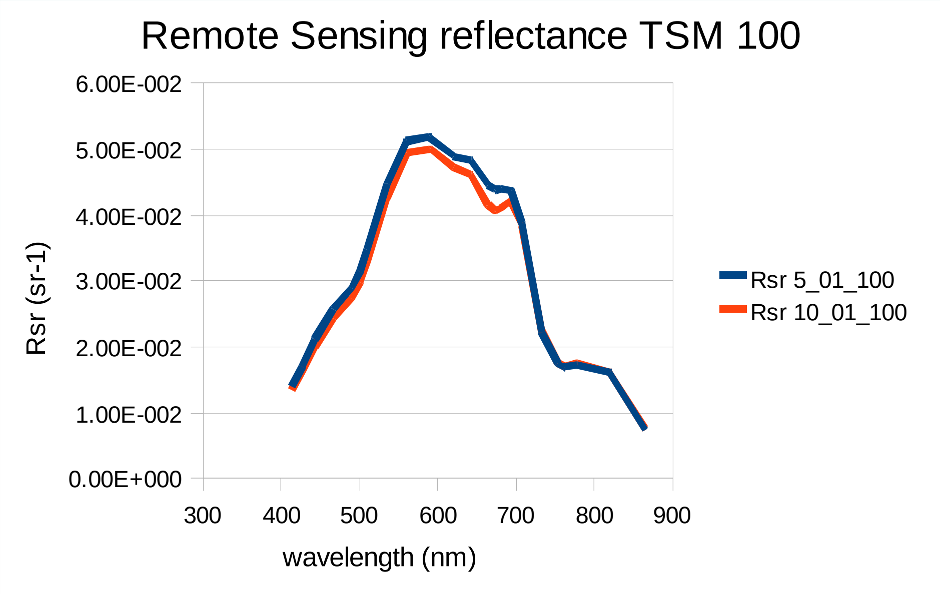


Sensitivity of the reflectance at a spectral band depends on the concentration

To cover a large concentration range many bands from the blue to NIR range are necessary

Sensitivity at different concentration ranges and spectral bands



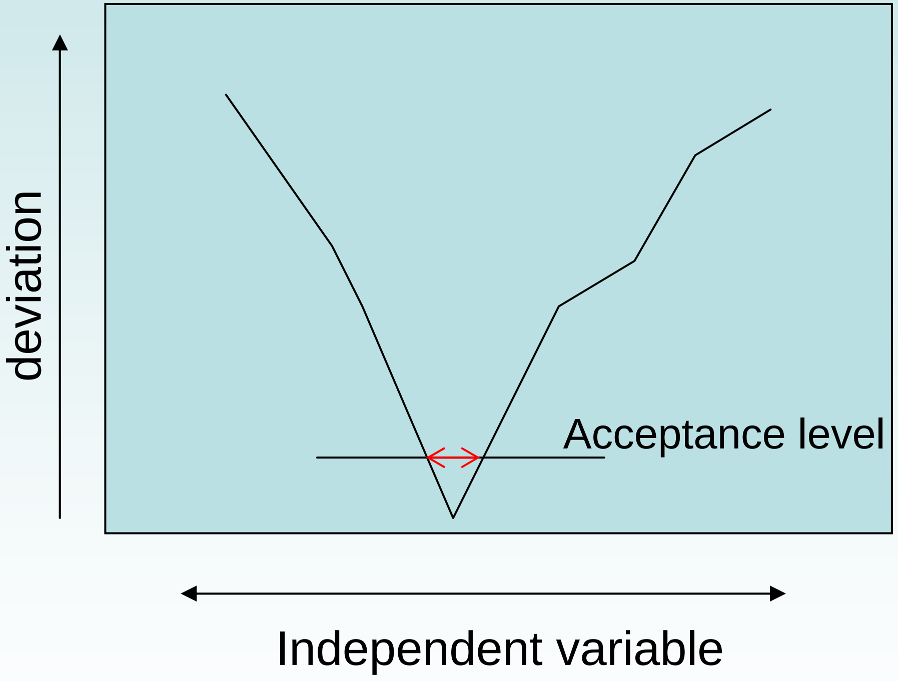


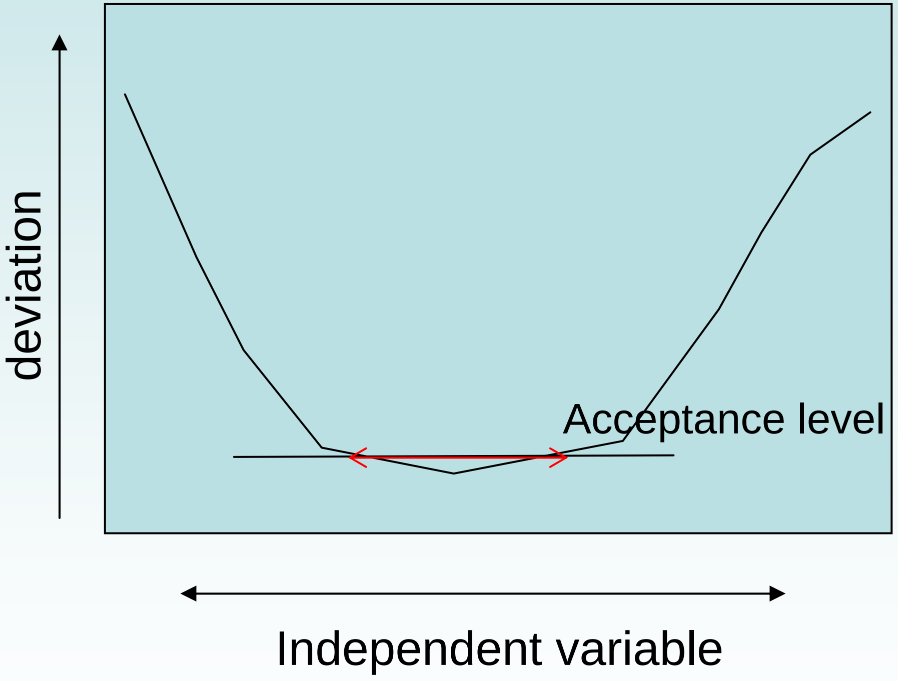
Chl. 5/10 mg m-3
TSM 1 g m-3
aYS(443) 0.1 m-1

Chl. 5/10 mg m-3
TSM 100 g m-3
aYS(443) 0.1 m-1

Searching for minimum: principle, 1D case

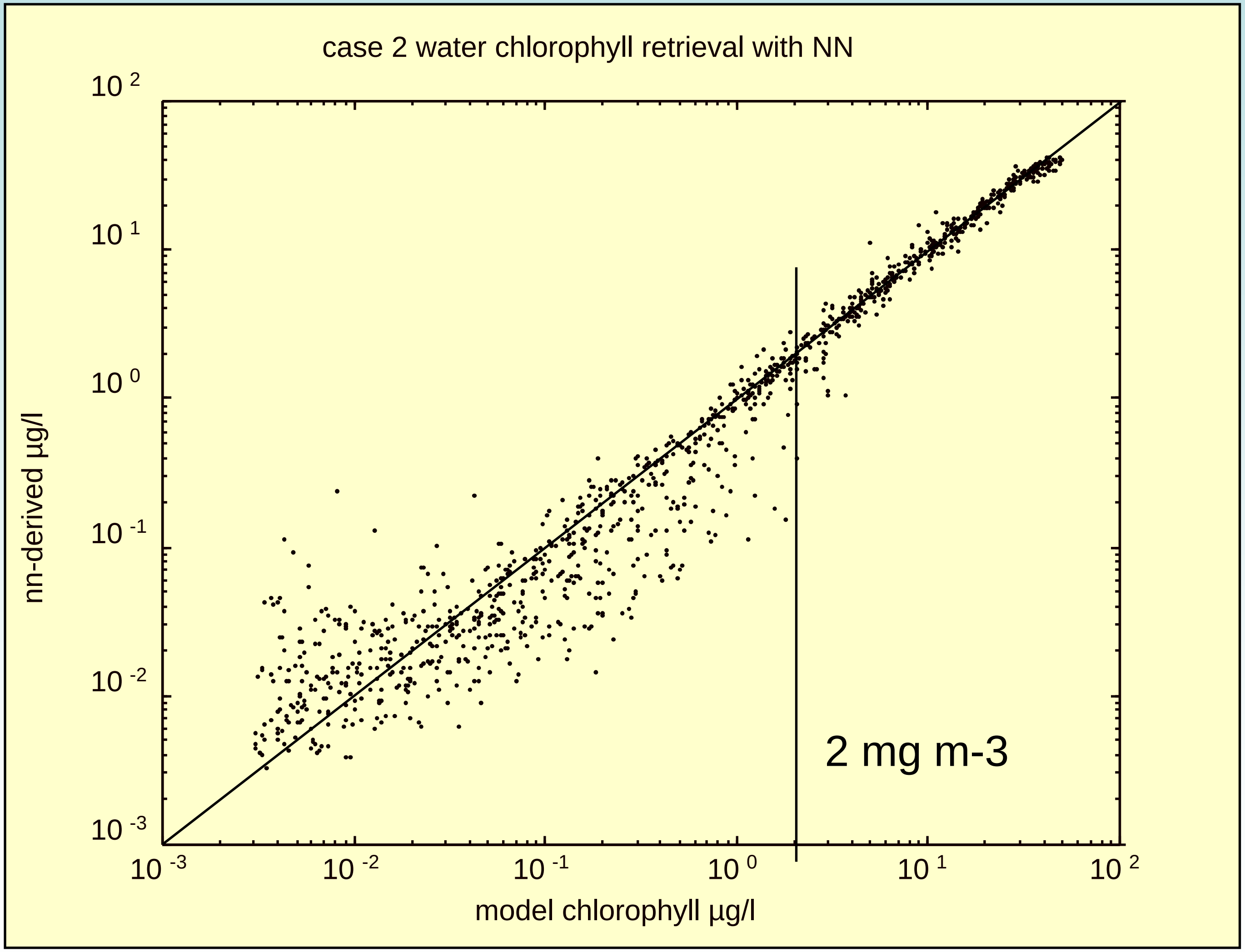
Search for minimum: Deviation between measured and simulated spectrum





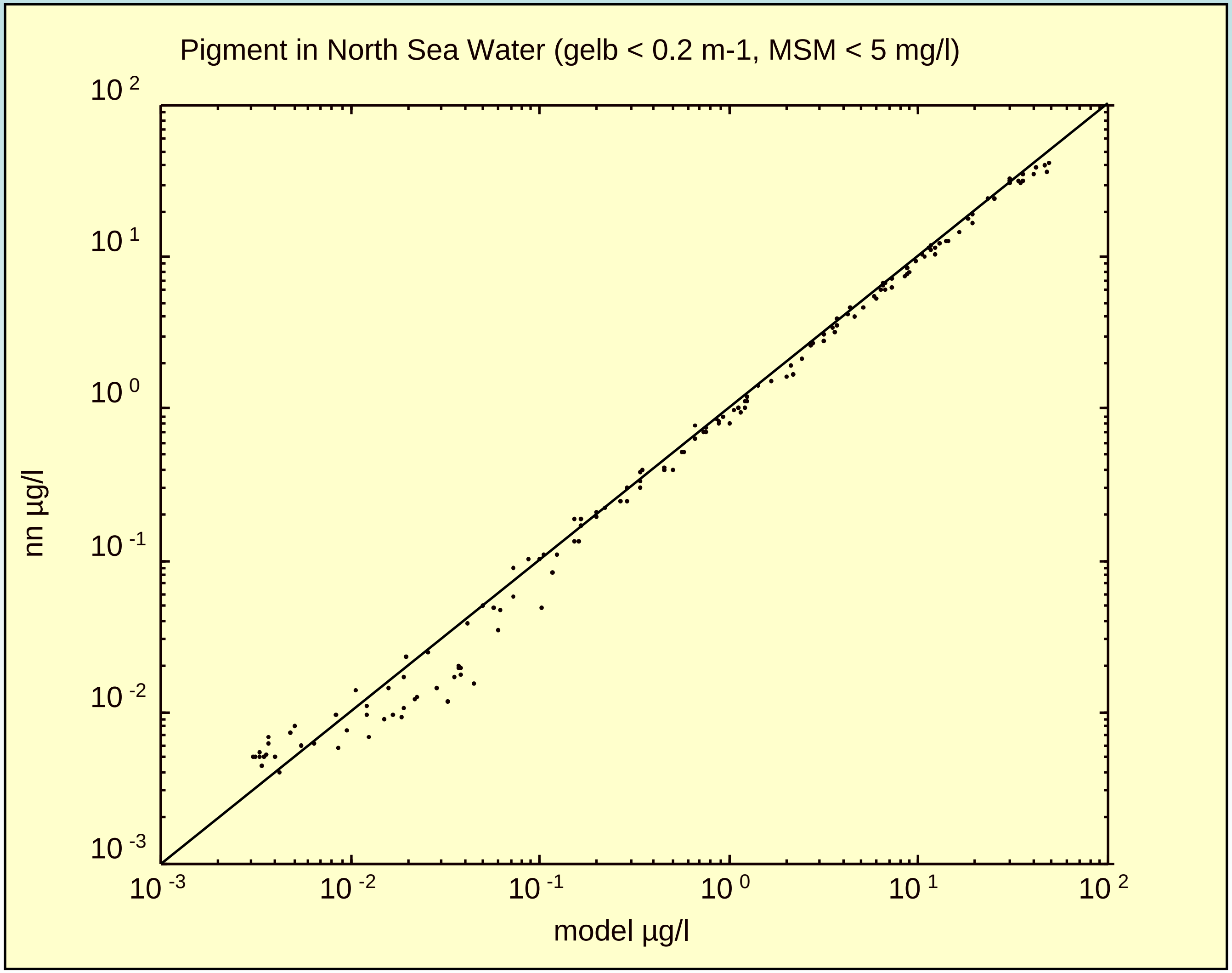
Width can be estimated from the 2nd order derivative (Hessean matrix)

Uncertainties due to ambiguities for different concentration mixtures



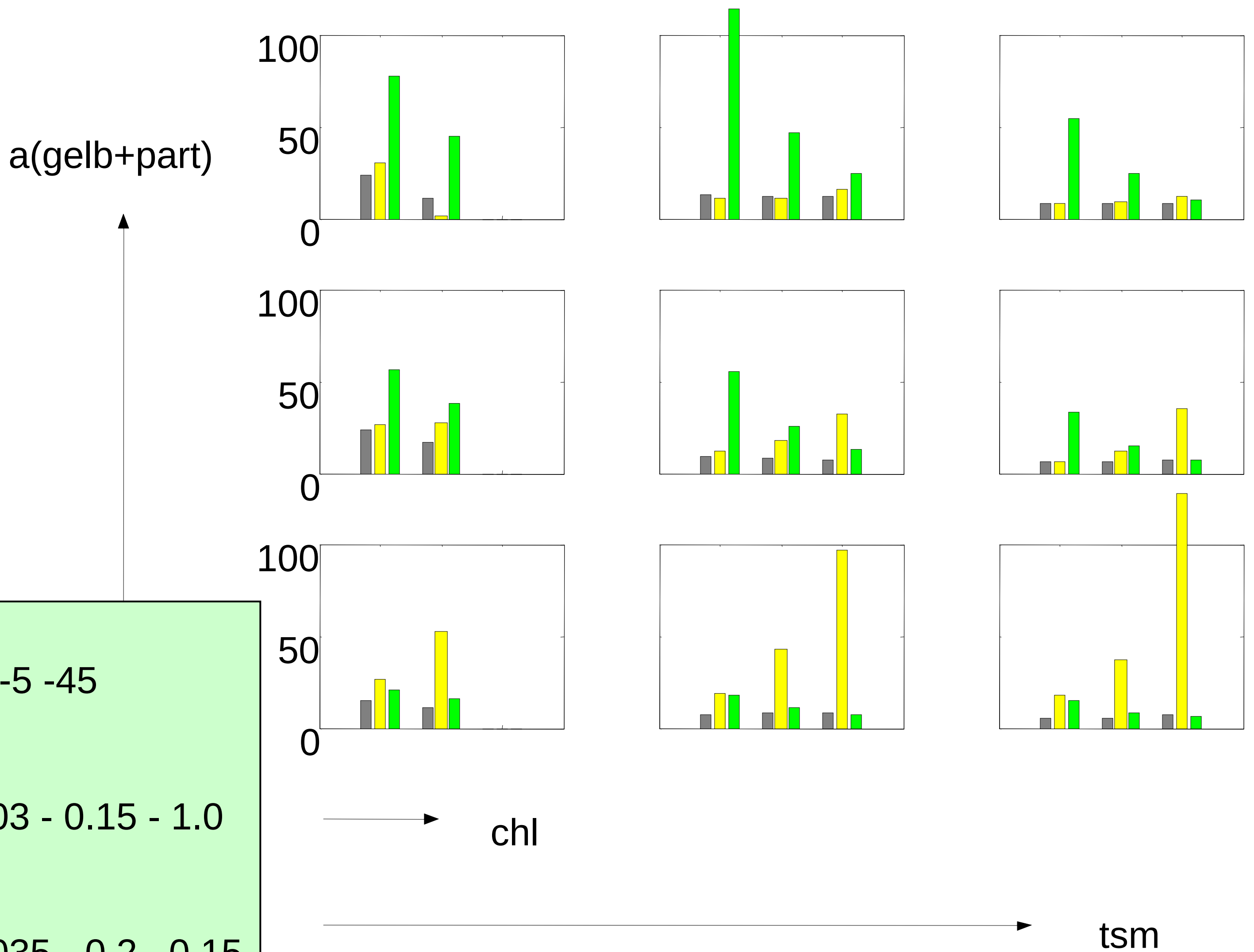
All cases of turbid water

Ambiguities 2



Typical North Sea coastal water: ay_443: < 0.2 m-1, TSM < 5 mg /l

Determine uncertainties on a pixel by pixel basis II



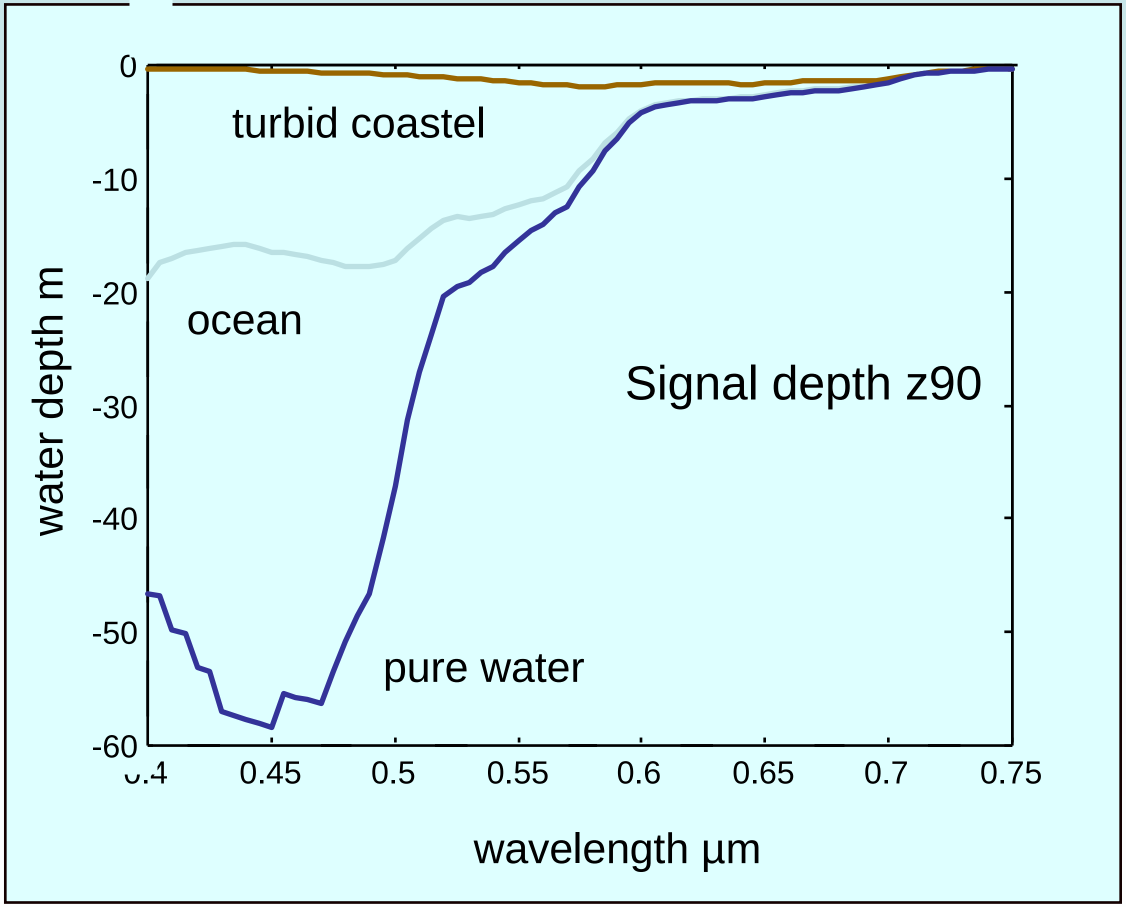
conc_bp
0.05 - 0.5 -5 -45

conc_pig
0.005 - 0.03 - 0.15 - 1.0

conc_gelb
0.005 - 0.035 - 0.2 –0.15

Signal depth at different spectral bands

Multiband algorithms: the information for each band may come from a different water layer



$z_{90}=1/k$

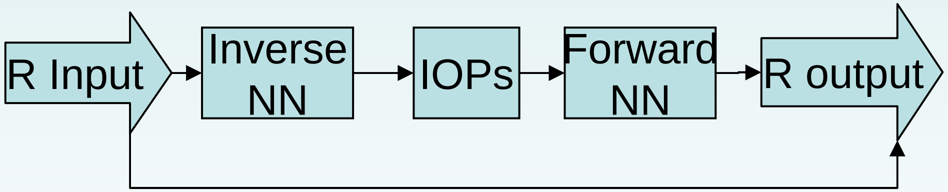
coastal:
TSM=5 mg/l
Chlor.=5µg/l
Gelb=a_{380}=1m^{-1}

open ocean:
Chlor.=1µg/l

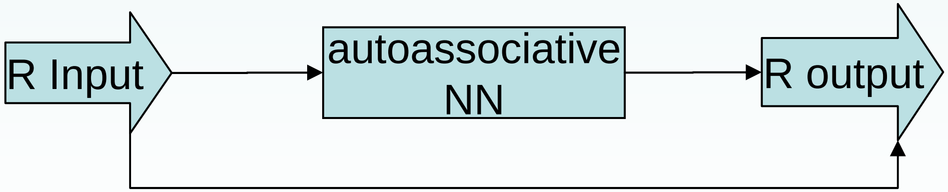
Detection of out of scope conditions

- 2 Procedures have been developed
  - **Combination of an inverse and forward Neural Network**
  - **Use of an autoassociative Neural Network**
- Both produce a reflection spectrum, which is compared with the input spectrum
- Deviation between input and output spectrum can be computed as a chi2
- A threshold can be used to trigger an out of scope warning flag

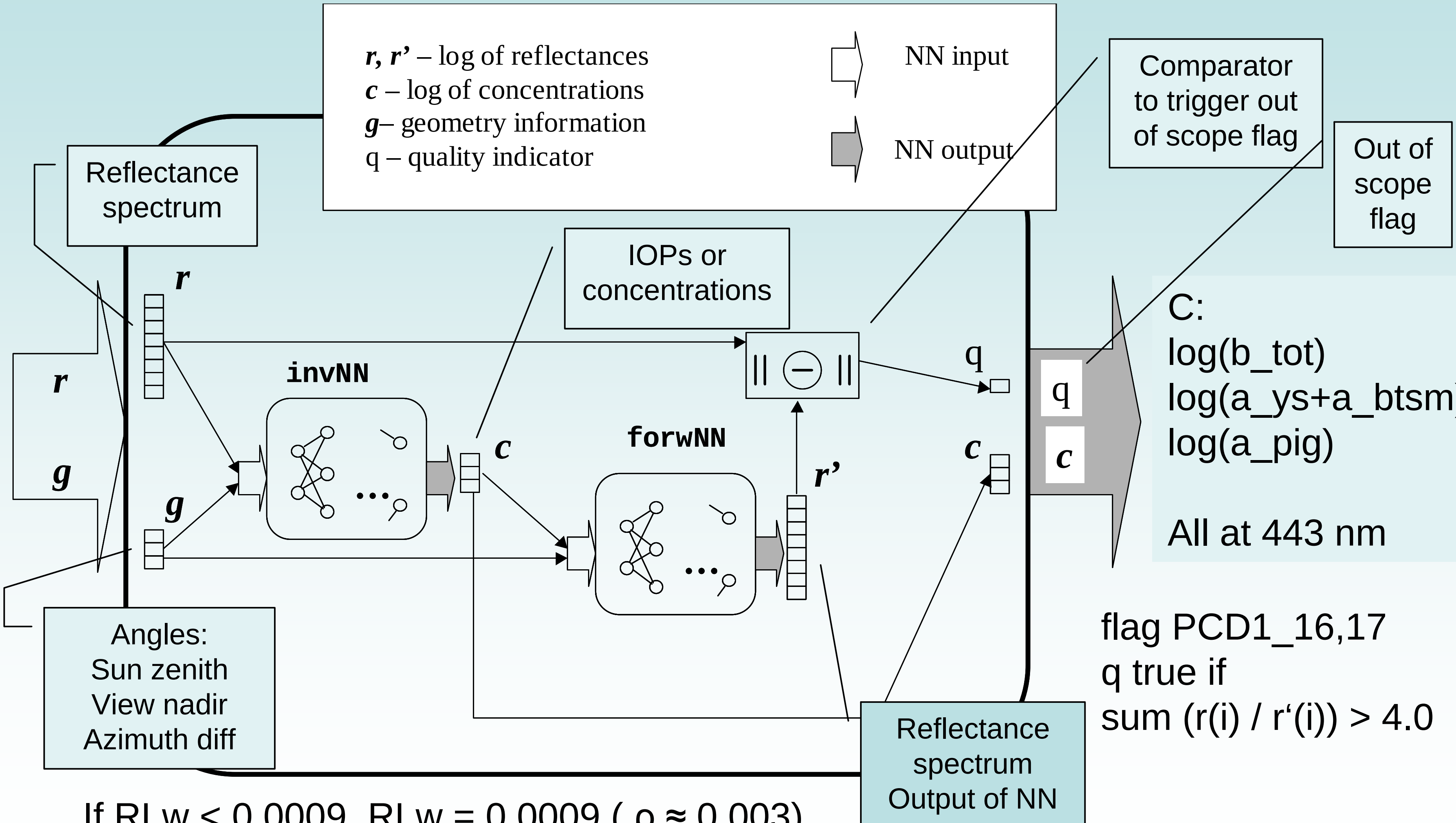
- Combination of inverse and forward NN



- Auto-associative NN



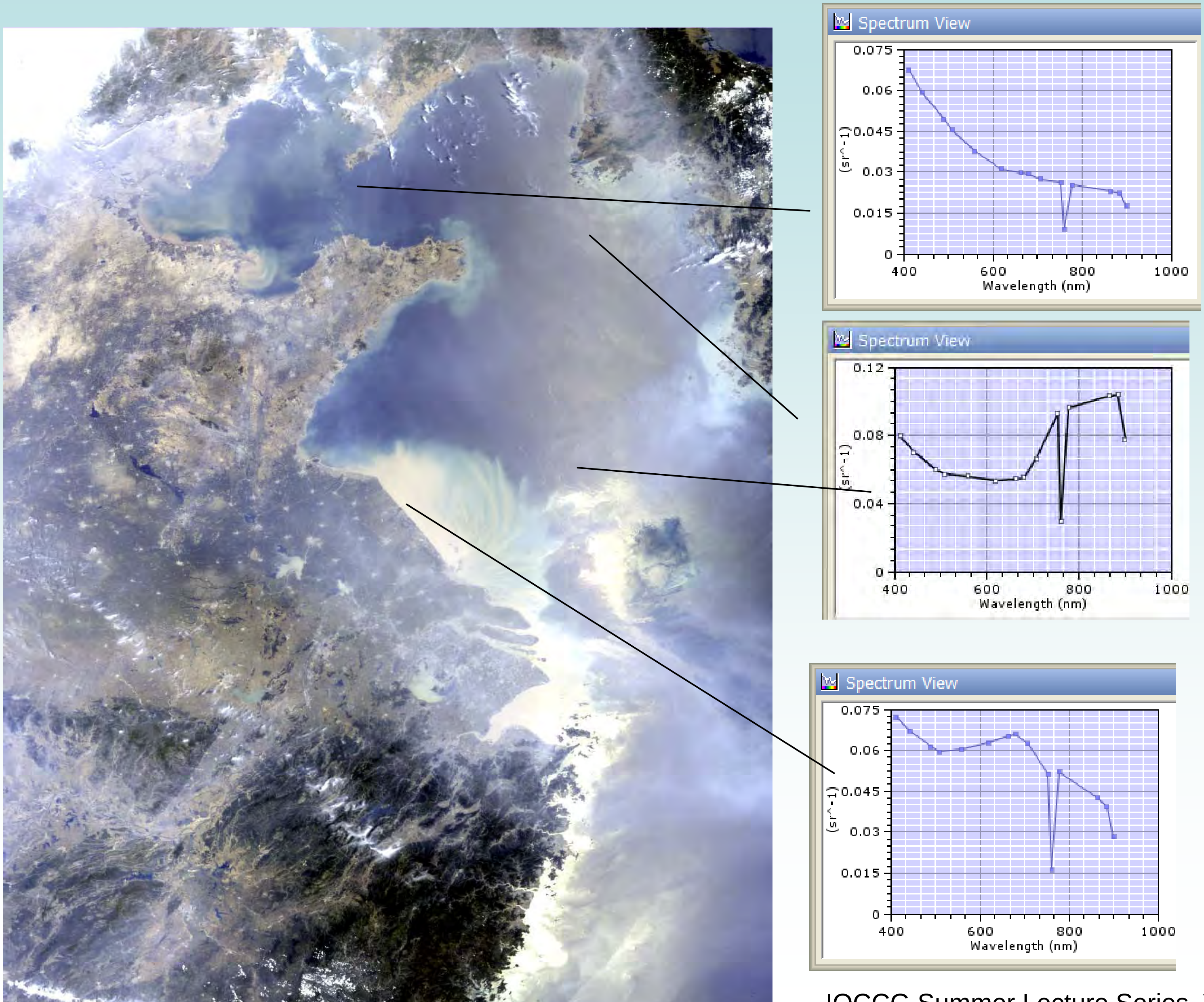
Detection of out of scope conditions (MERIS processor)



flag PCD1_16,17
q true if
sum (r(i) / r'(i)) > 4.0

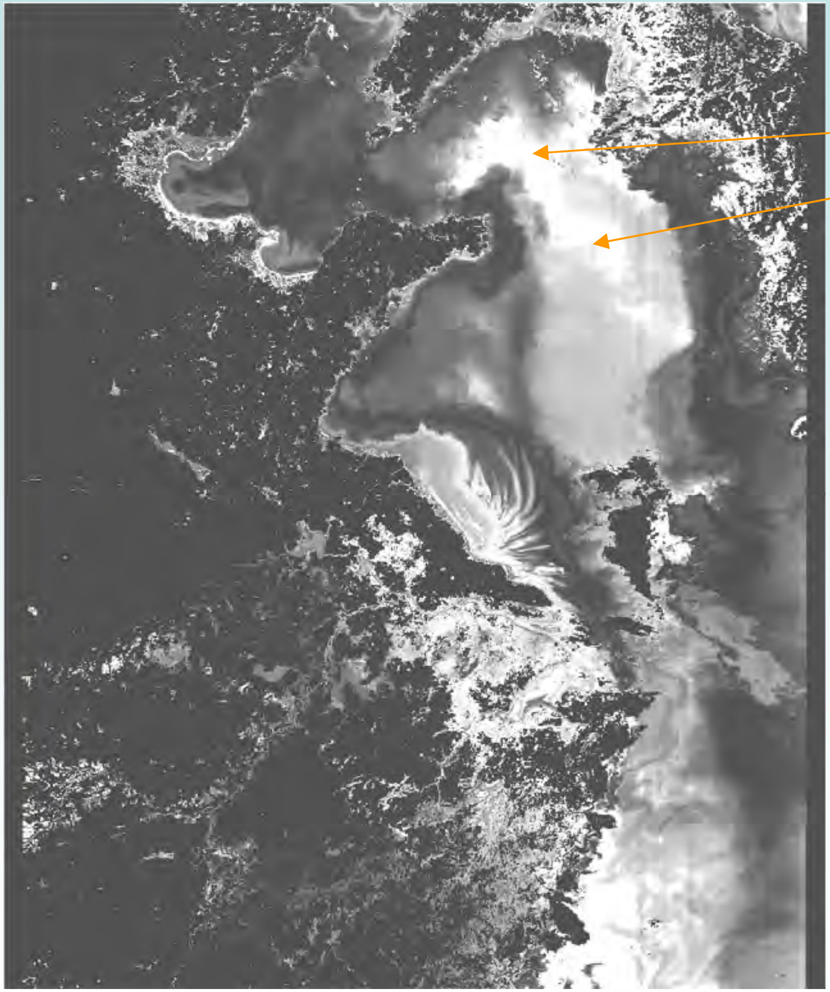
If RLw < 0.0009, RLw = 0.0009 (ρ ≈ 0.003)

Detection of out of scope conditions (MERIS processor)



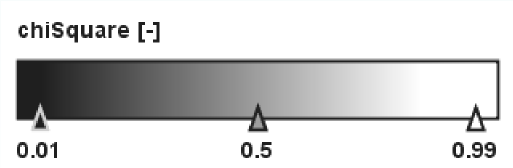
Top of atmosphere radiance spectra at normal and critical locations

Detection of out of scope conditions (MERIS processor)



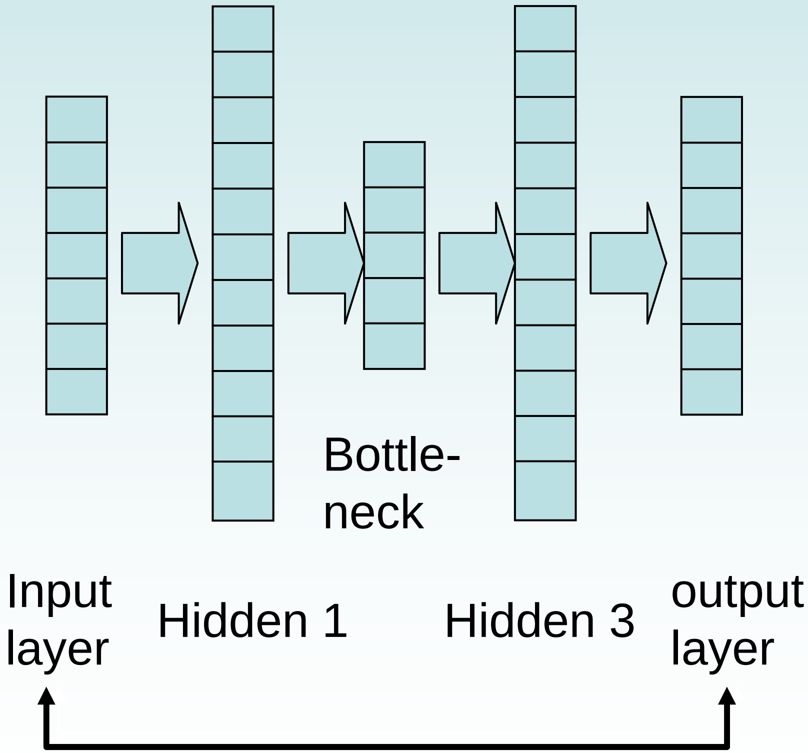
Exeptional bloom,
Indicated by high Chi_square value

Chi_square is computed by comparing
The input reflectance spectrum with the output of the forward NN



Detection of out of scope conditions using an aaNN

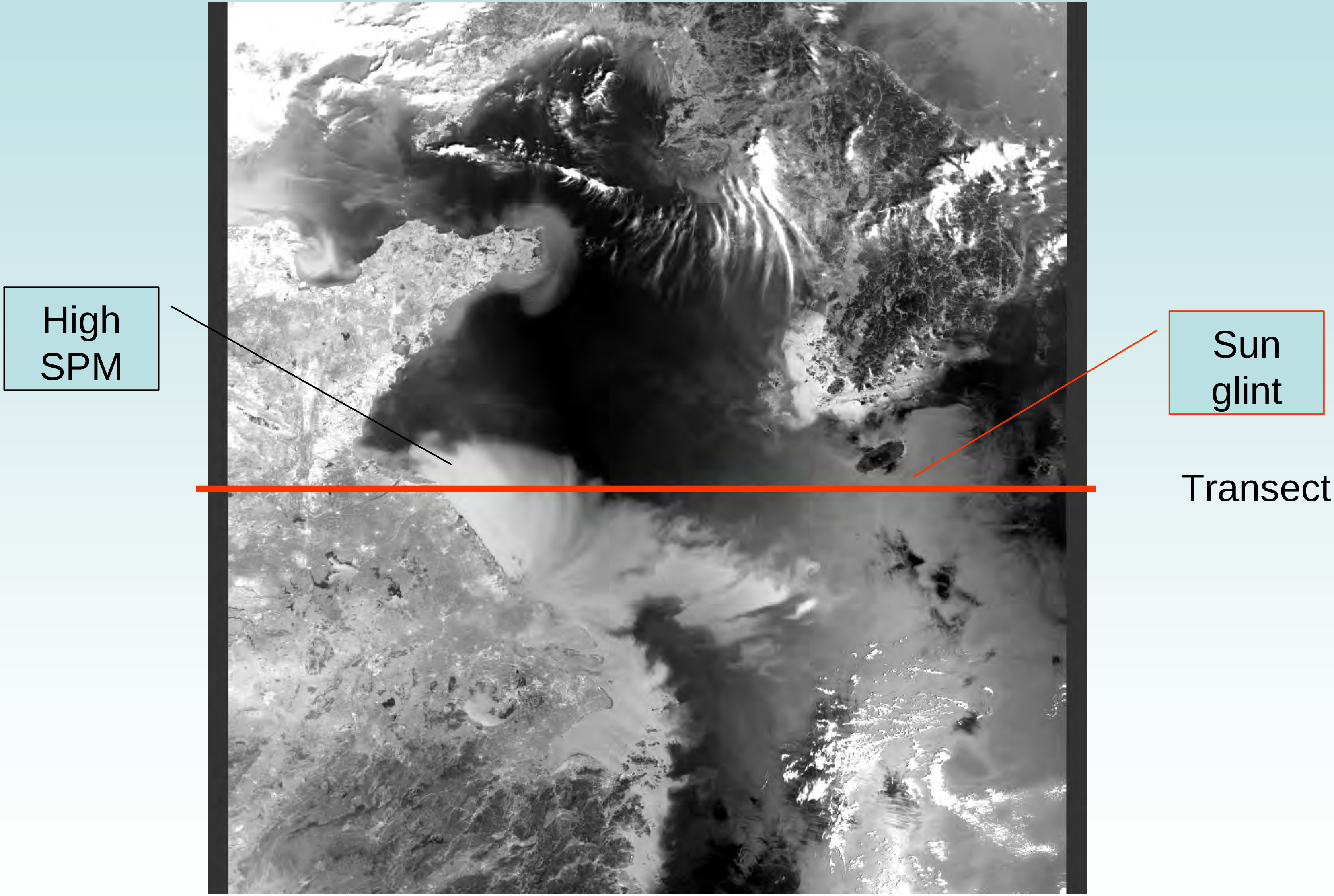
- Important to detect toa radiance specta which are not in the simulated training data set
- These are out of scope of the atmospheric correction algorithm
- Autoassociative neural network with a bottle neck layer



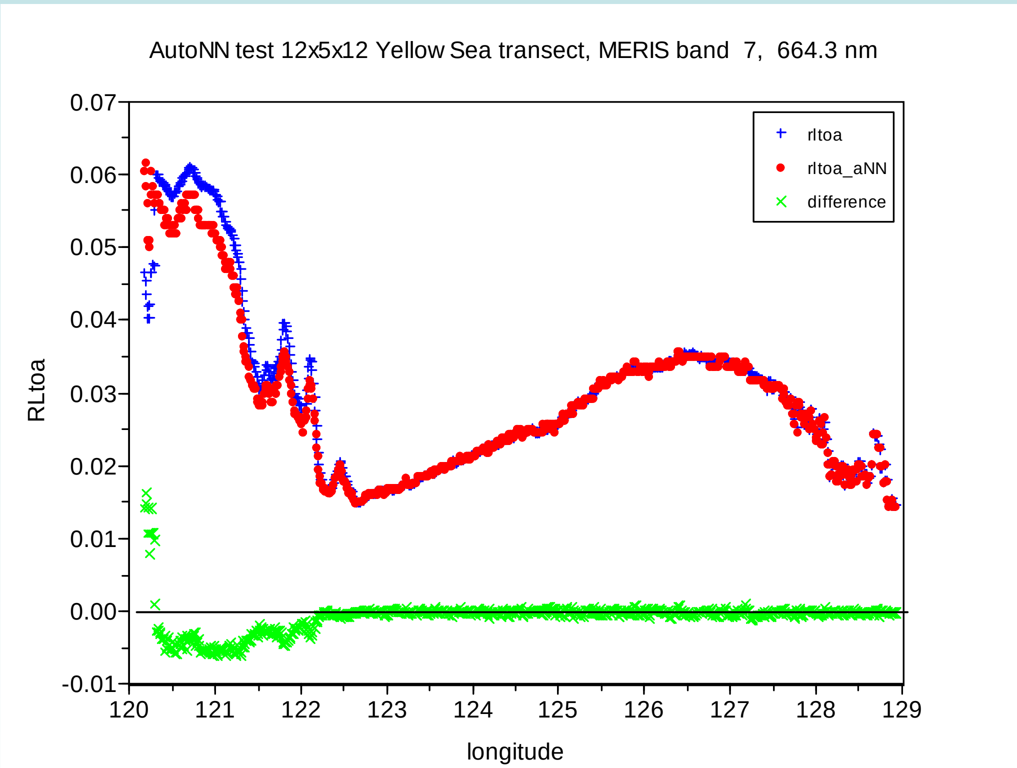
Functions also
as nonlinear PCA
i.e. bottle neck number of
neurons
Provide estimate of
Independent components

For the GAC training data
Set of ~ 1Mio. Cases
Bottleneck minimum was 4-5

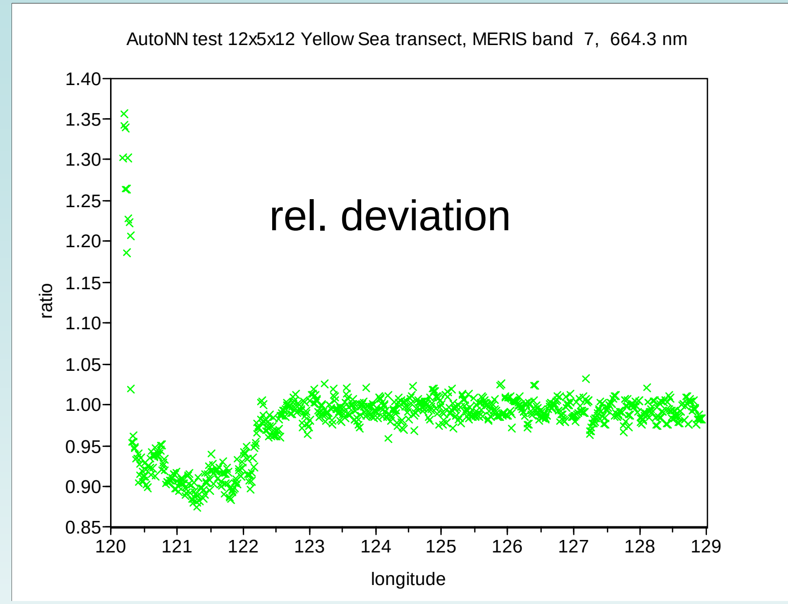
Detection of out of scope conditions aaNN: example for L1 (TOA) data

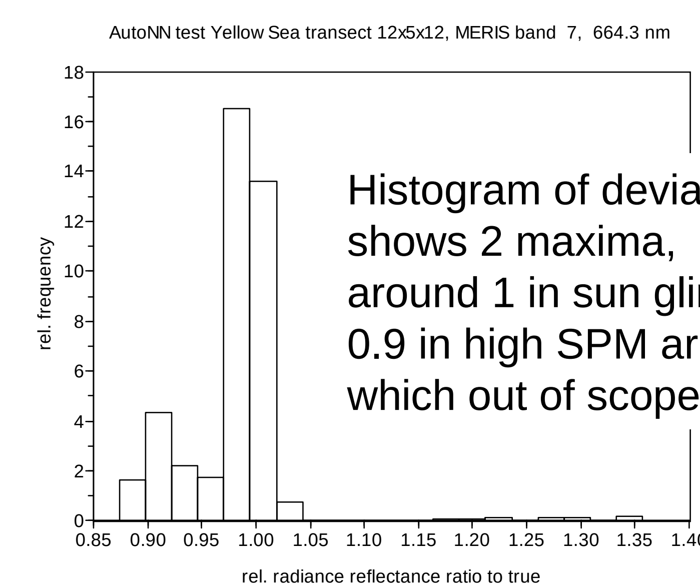


Detection of out of scope conditions aaNN: example



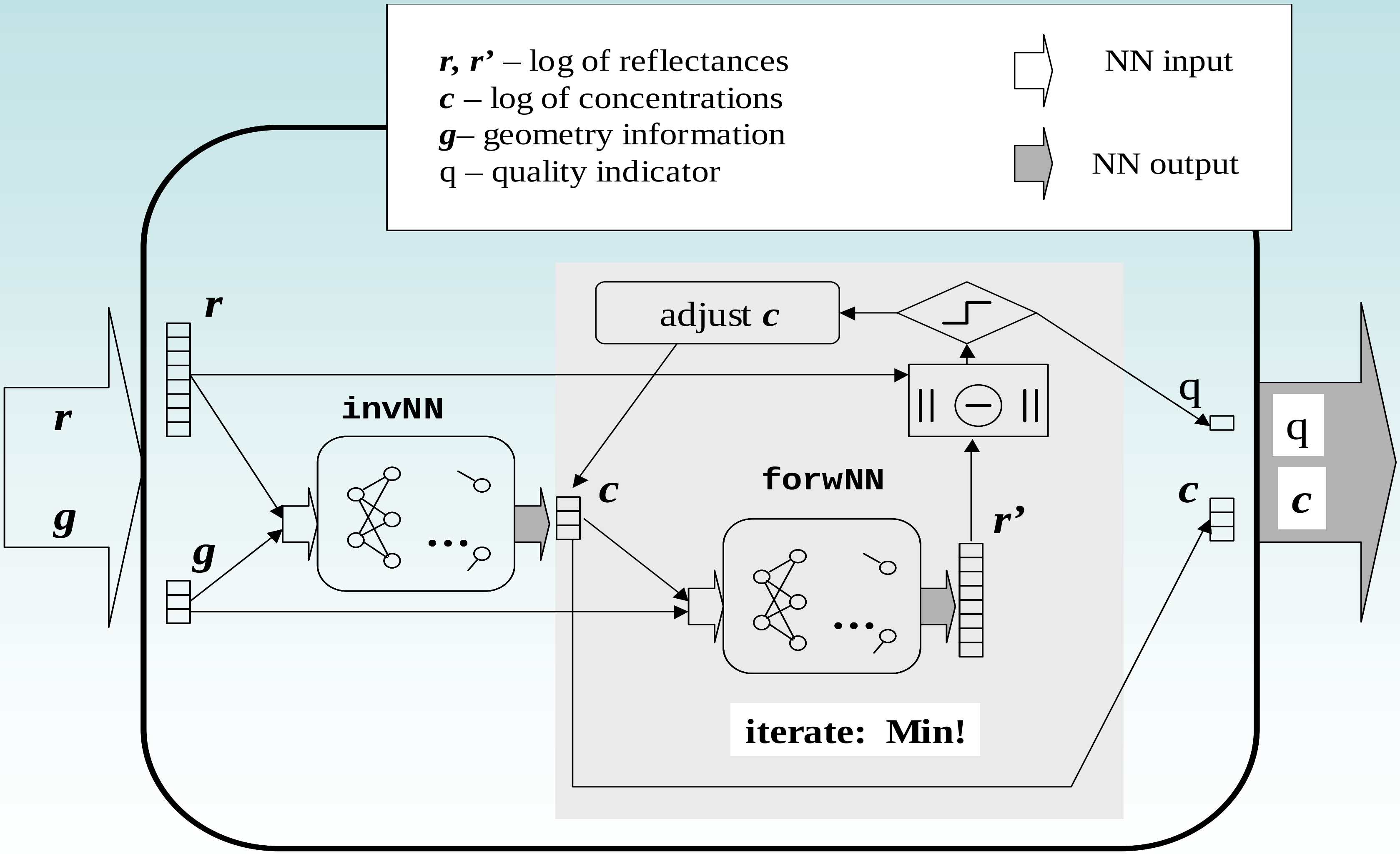
significant deviation in area with high SPM concentrations, but not in sun glint area



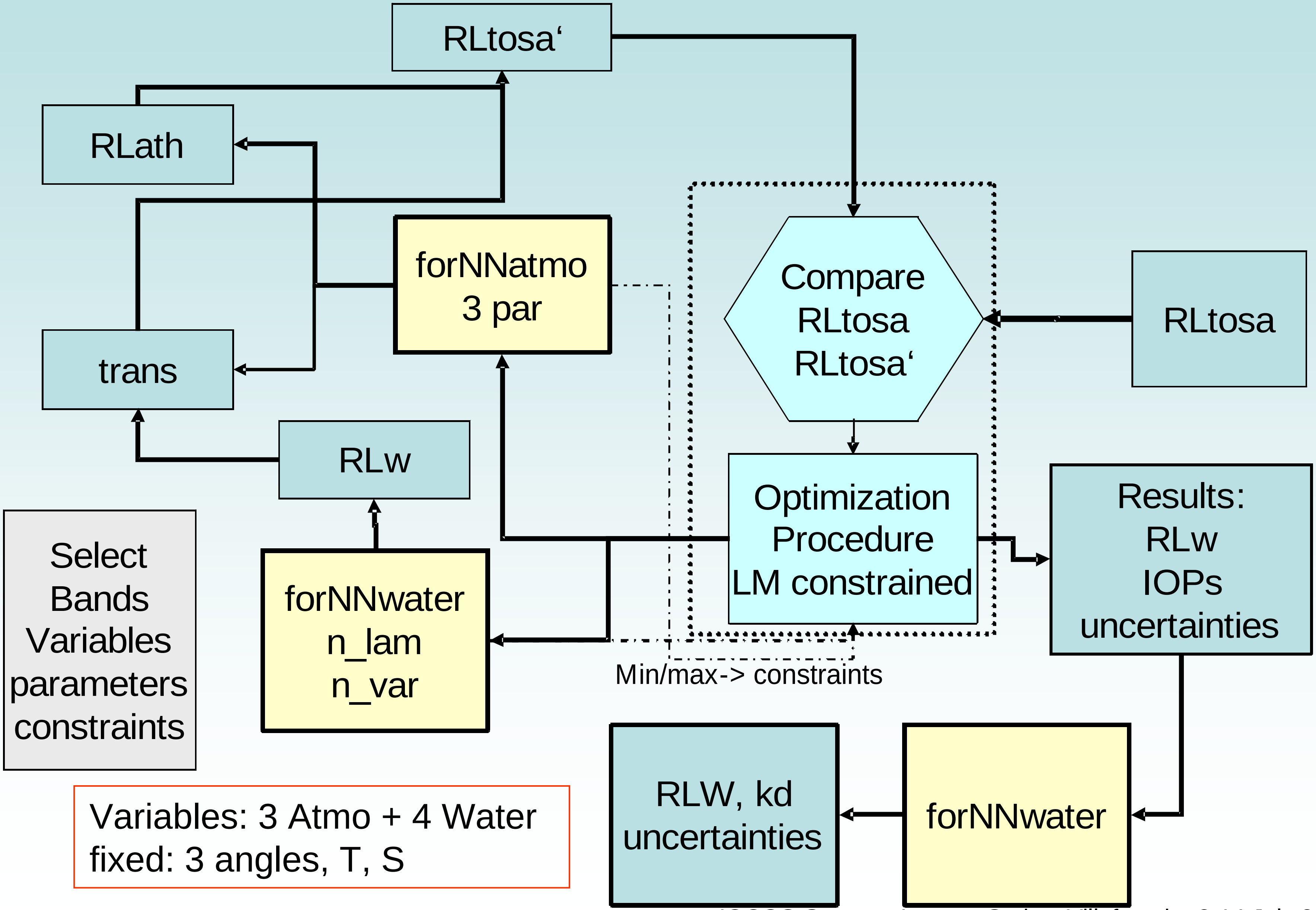


Histogram of deviations shows 2 maxima, around 1 in sun glint 0.9 in high SPM area, which out of scope

Determine uncertainties on a pixel by pixel basis combinations of inverse and forward model and optimization procedure



Computation of uncertainties on pixel-by-pixel basis

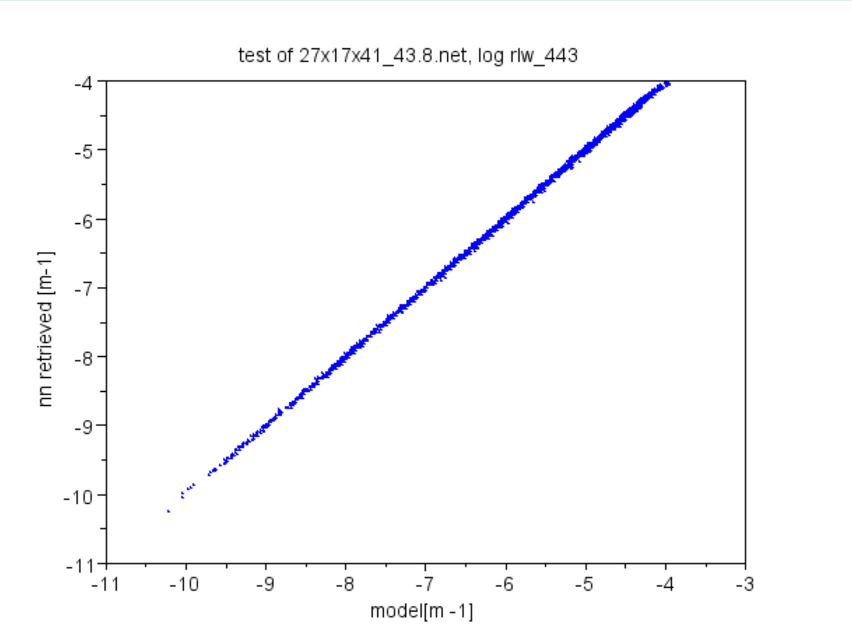


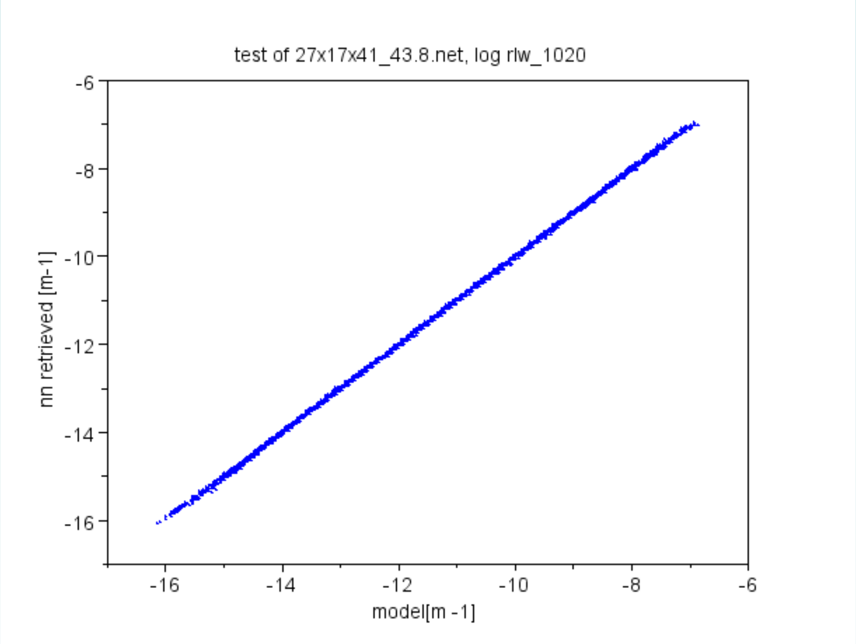
Variables: 3 Atmo + 4 Water
fixed: 3 angles, T, S

Verification

- Using simulated test data
- You can detect ambiguities
- Non linear behaviour
- Concentration ranges with failures
- It might be necessary to change bio-optical model
- Or range and frequency distribution of the training data set

Test of NN I 1

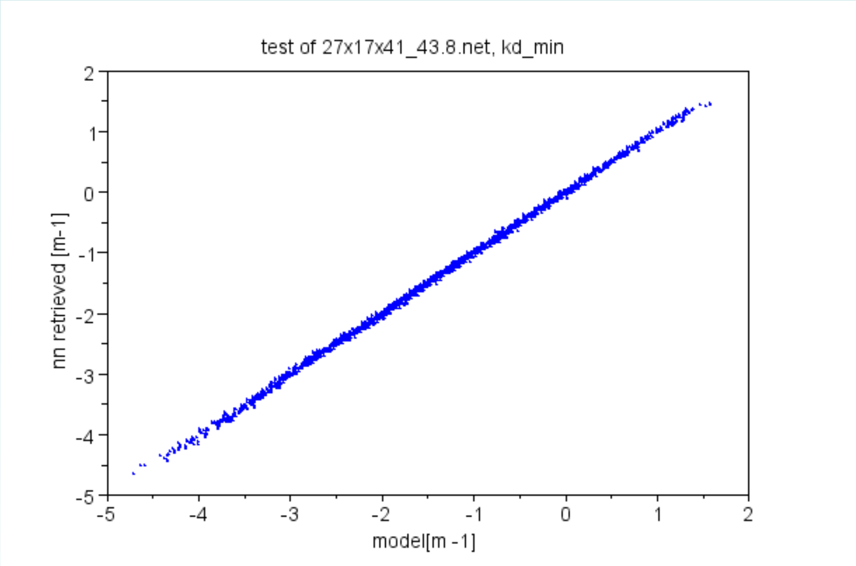


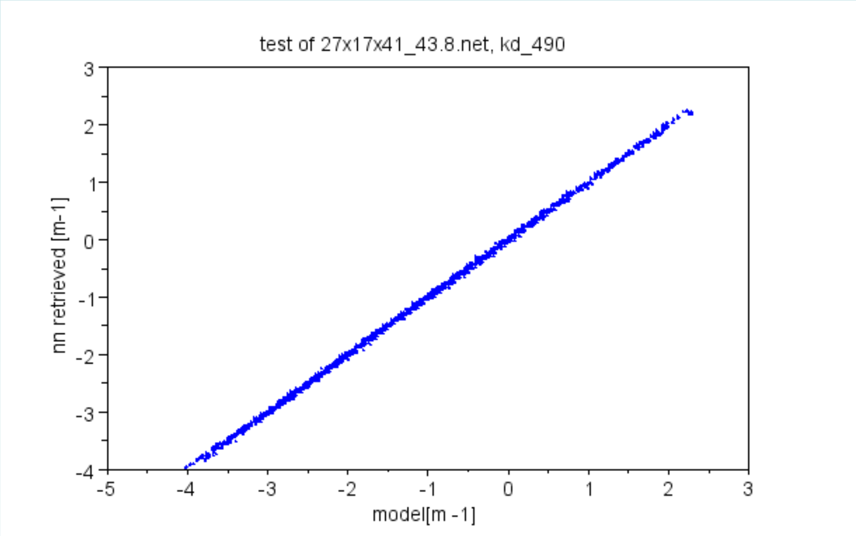


443 nm

1020 nm

Test of NN I 3

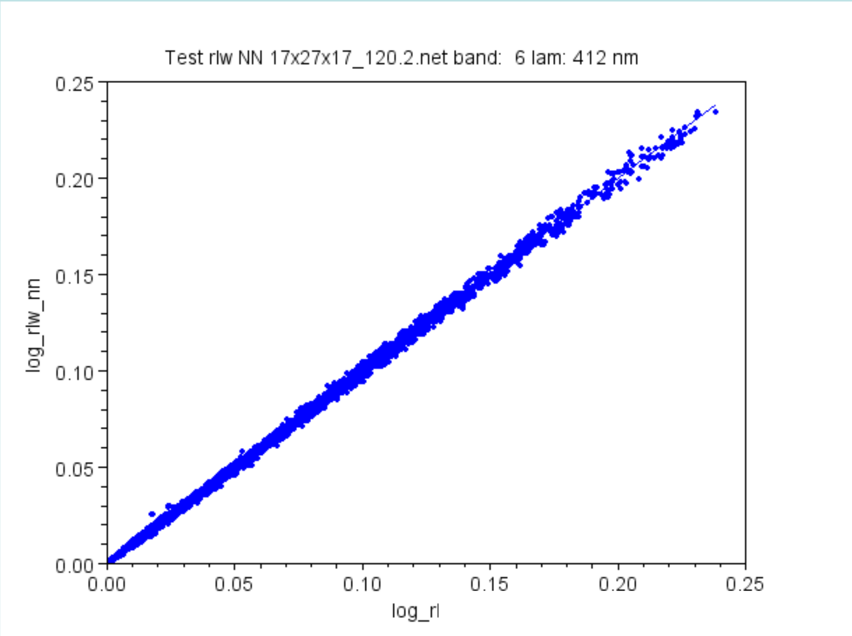


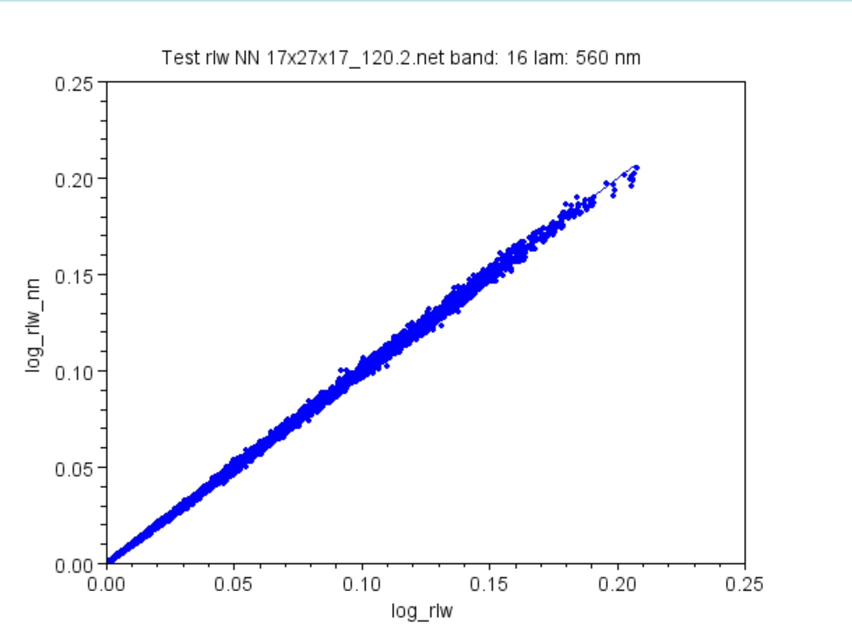


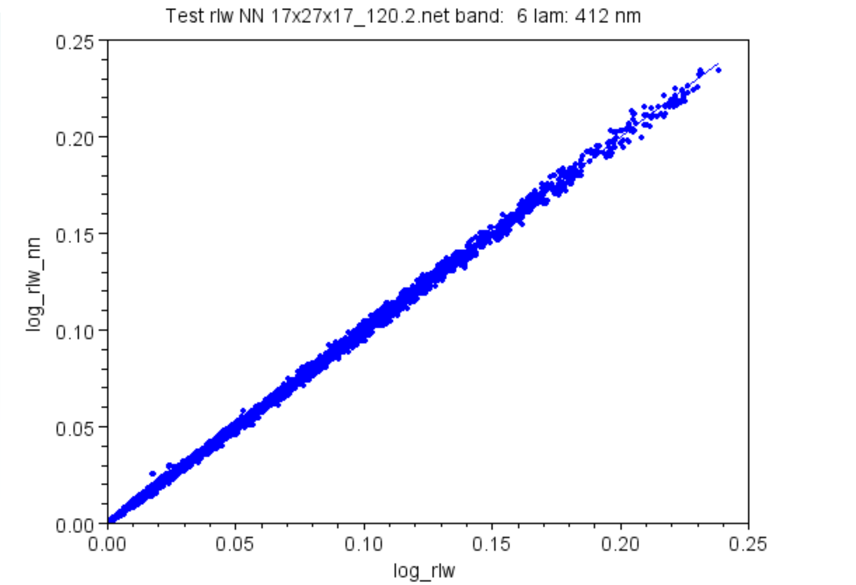
Kd_min

Kd_490

Test of NN 17x27x17, training with 5% random noise on RLw

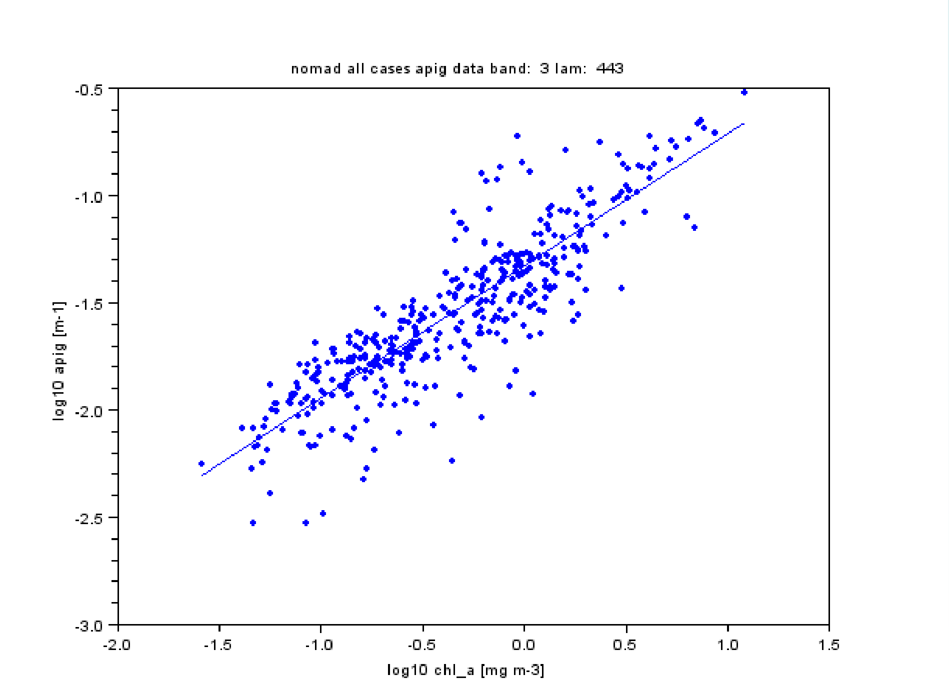






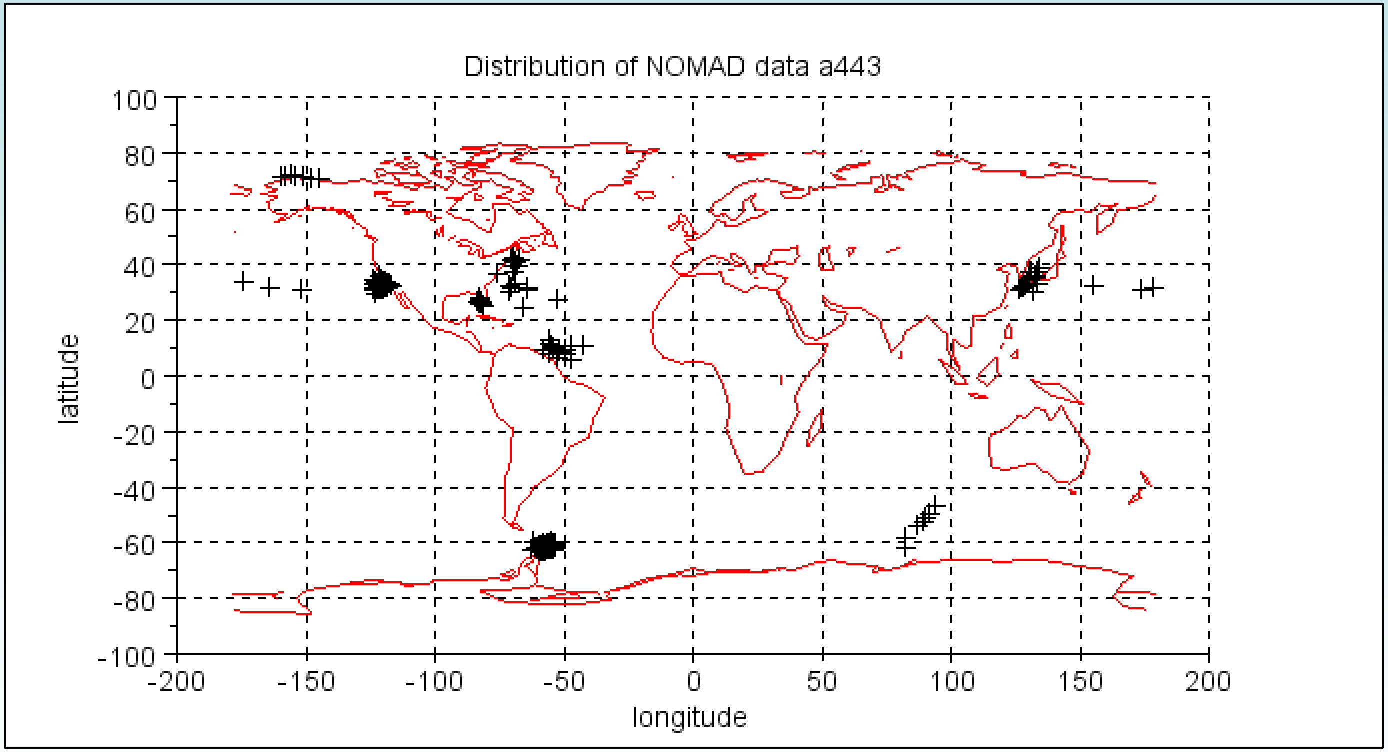
Validation

- NOMAD data set
  - Compiled, quality checked and maintained by OC group of NASA
  - In situ observations from different cruises, different teams, instruments, procedures, sky and wave conditions
  - Includes RLw at 6 MERIS bands (412,443,490, 510, 560,665)
  - a_total, b_total / bb_total at443
- Note: in situ data have their own variabilities and uncertainties!

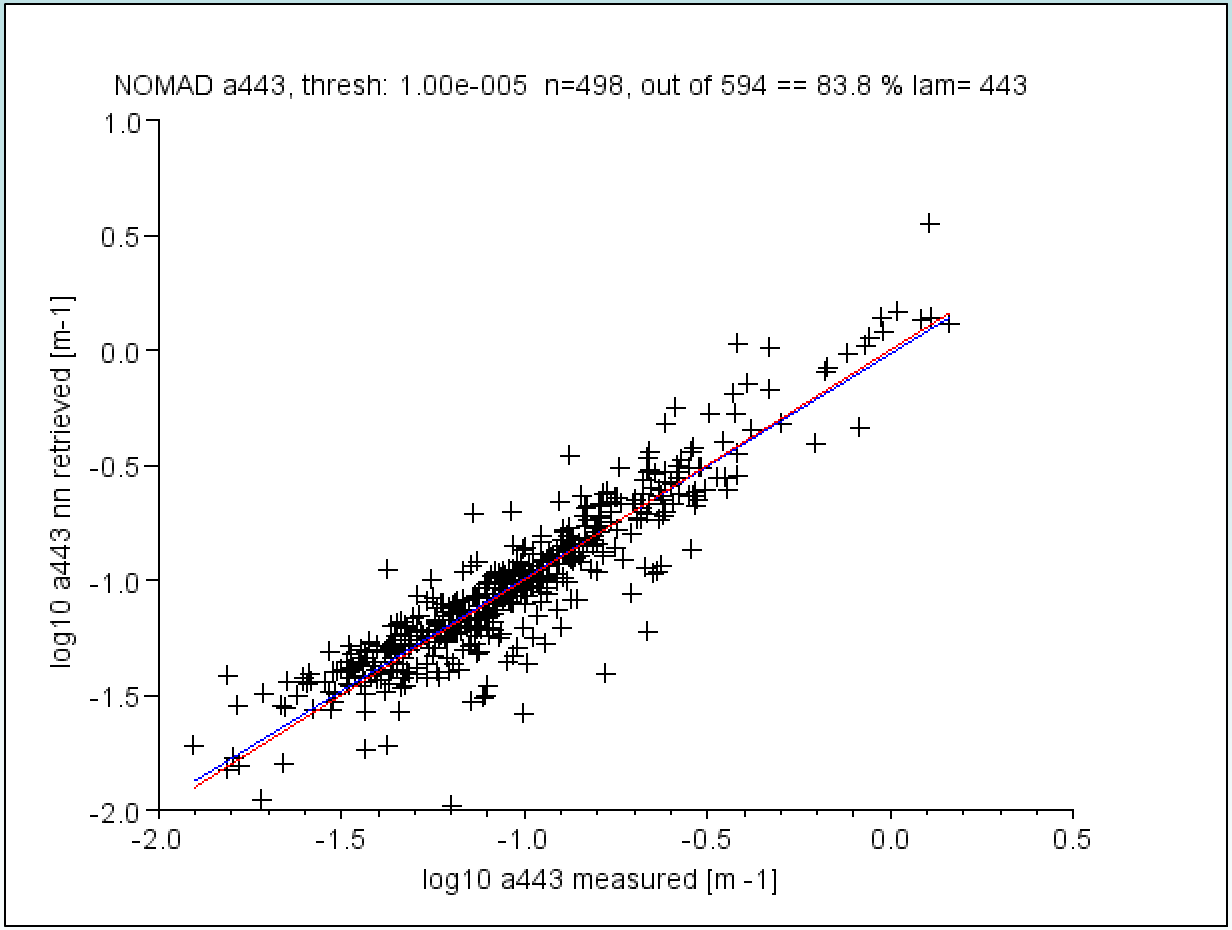


Relationship between chlorophyll a concentration and the absorption coefficient of phytoplankton pigments

Total absorption at 443 nm (water + constituents)

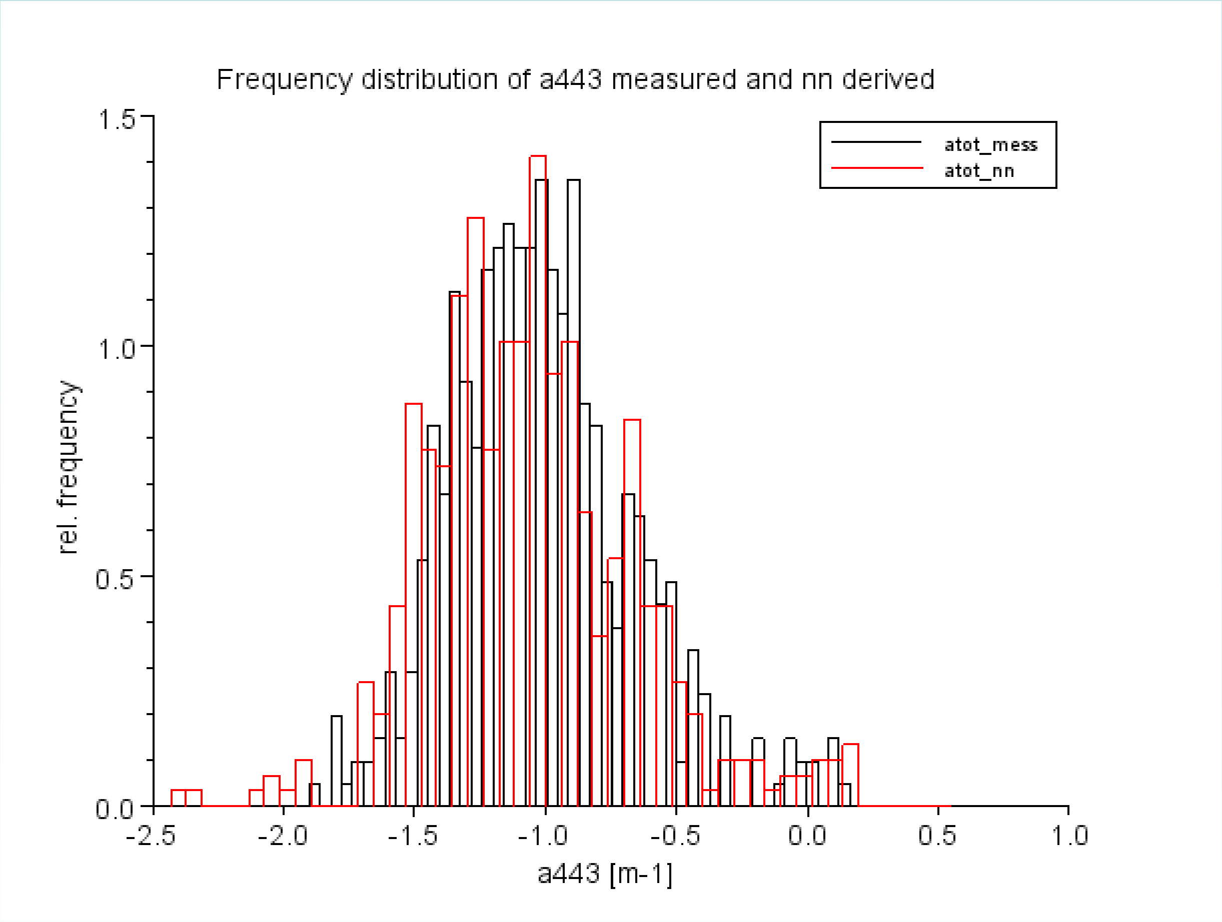


a443



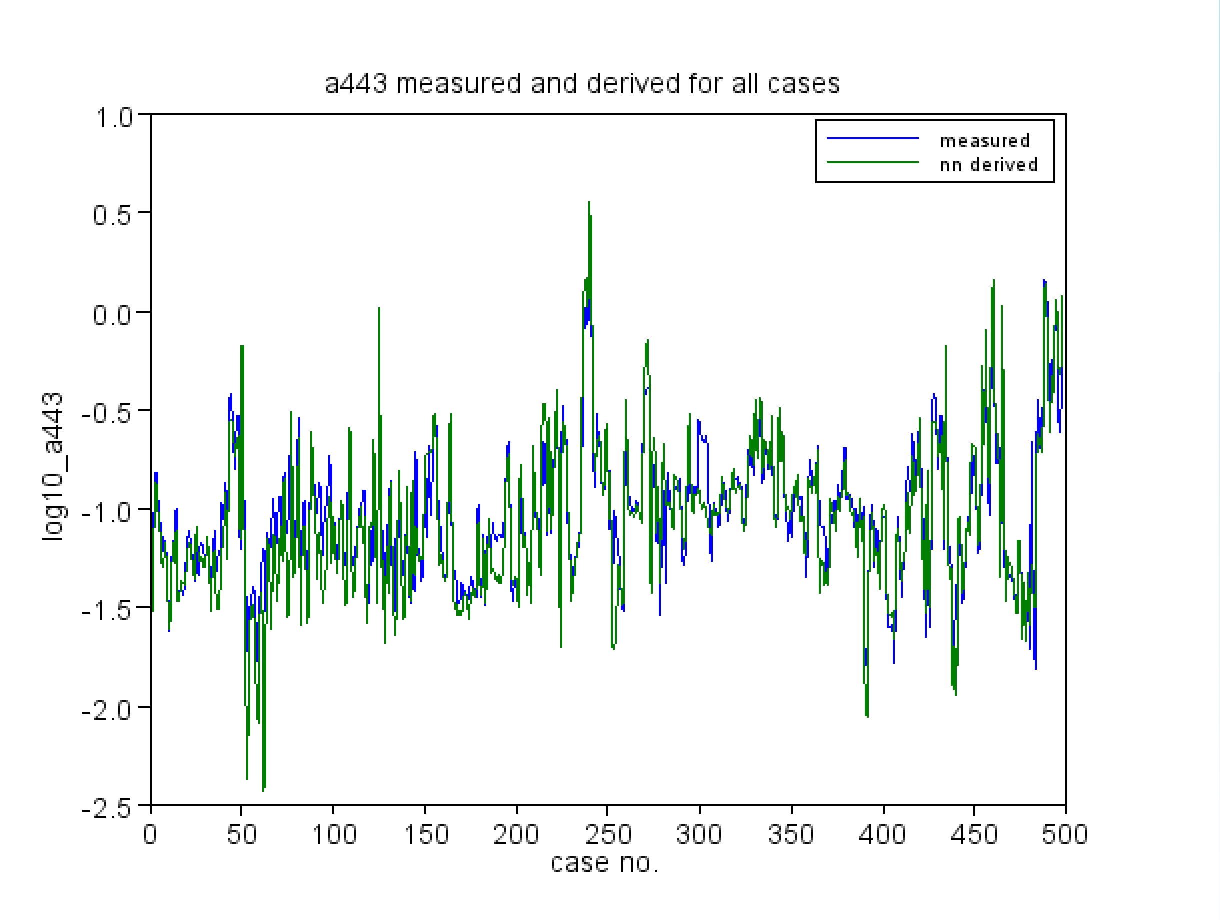
log10_a443_nn = log10_a443_measured * 0.977 - 0.0167, stdev = 0.141

Frequency distribution

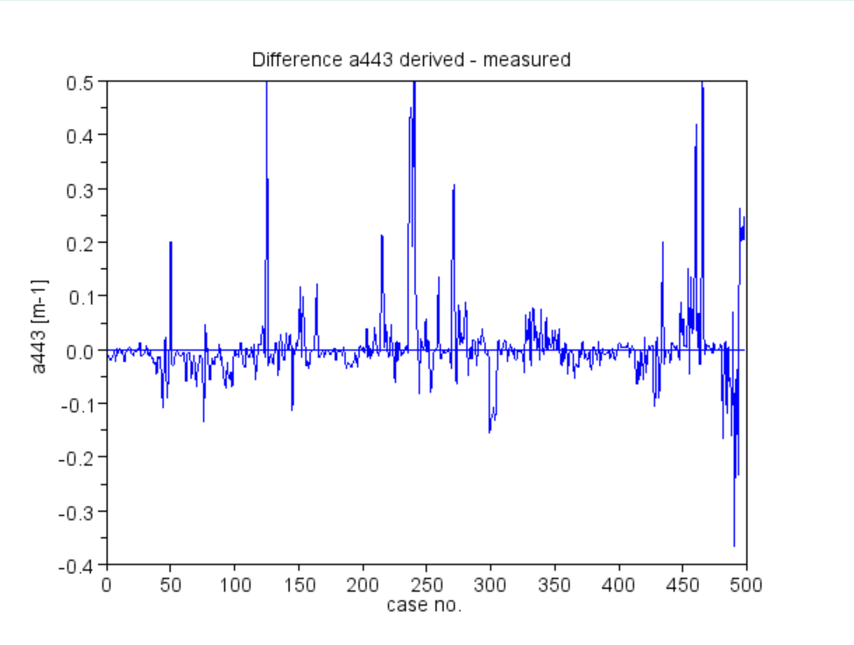


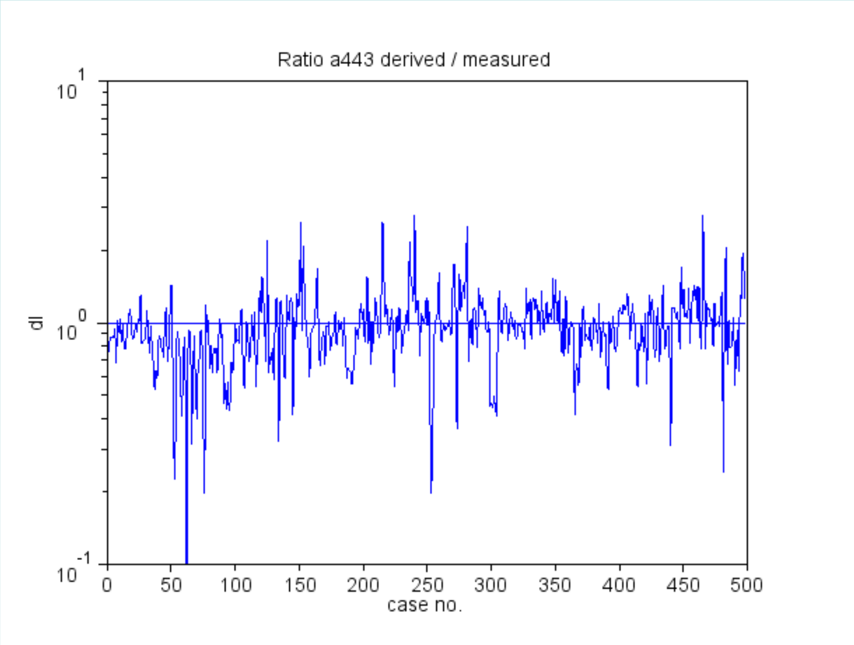
Frequency distributions of measured and derived a443 after removing outliers with sum_sq > 1.0 e-5

Measured and nn-derived a443 for all cases with sq <1.0e-5



Differences and rel.deviation



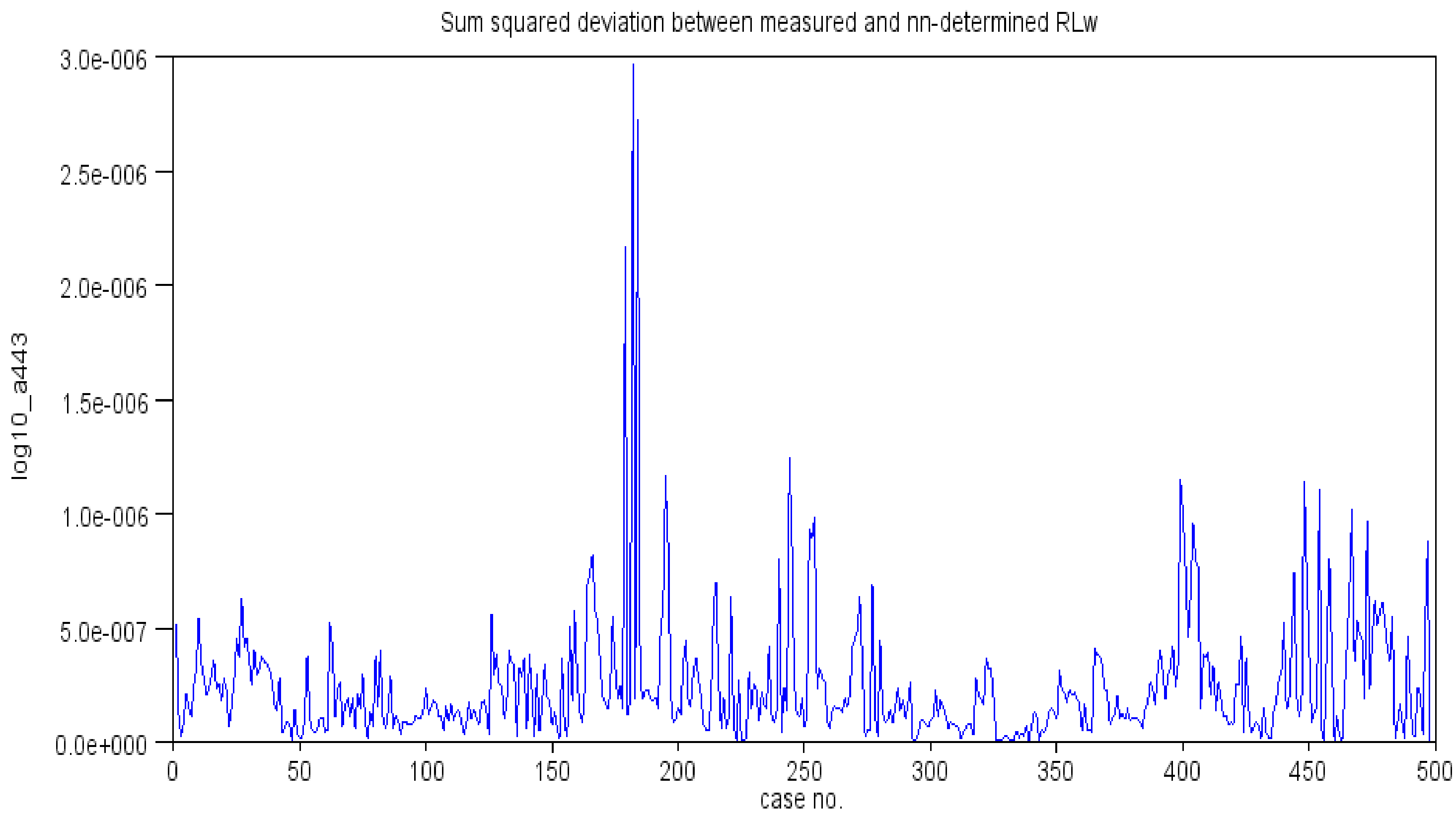


Log10 difference

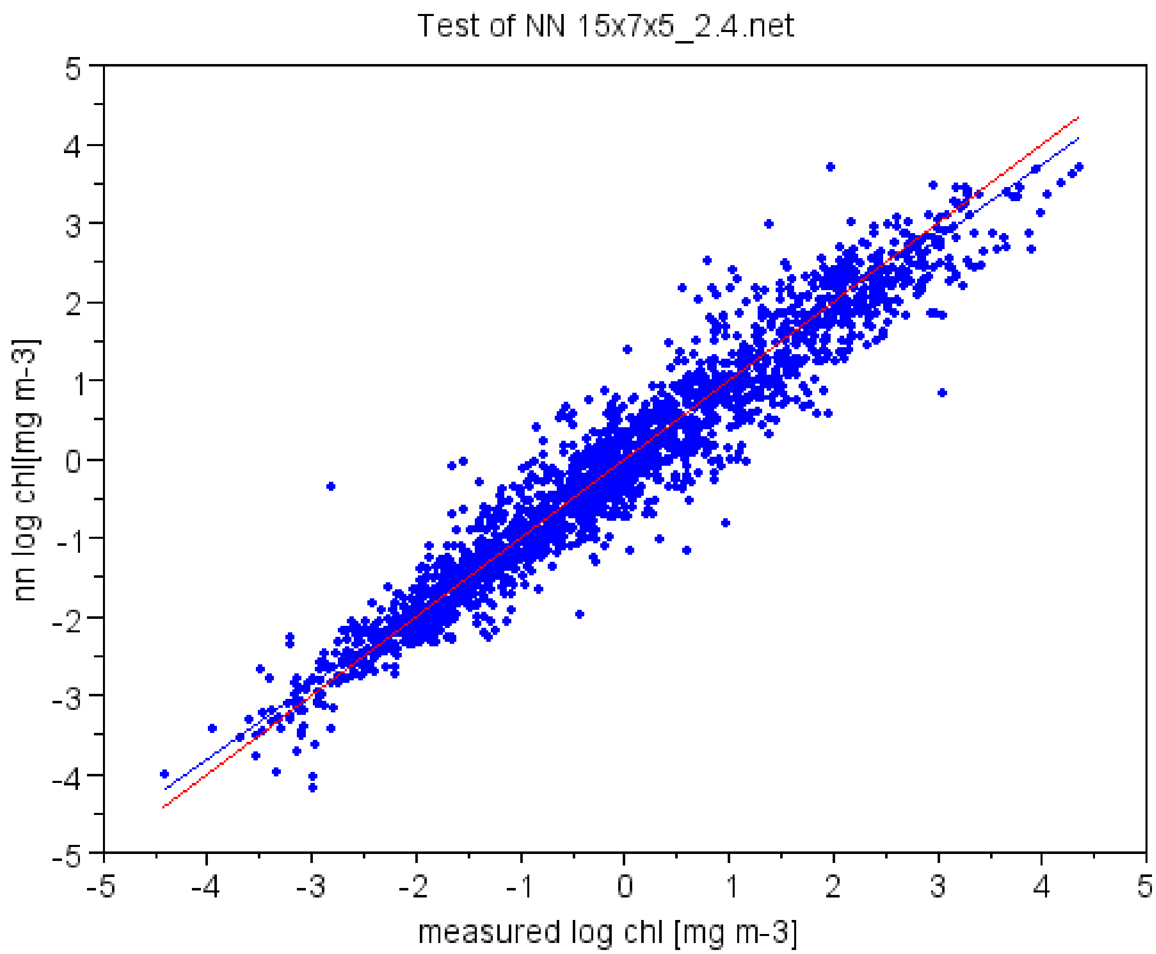
Log10 ratio

Mean difference: 0.0086102 m-1, stdev: 0.129
Mean ratio: 0.9717098, stdev: 0.334

Sum_sq of measured and nn derived reflectances

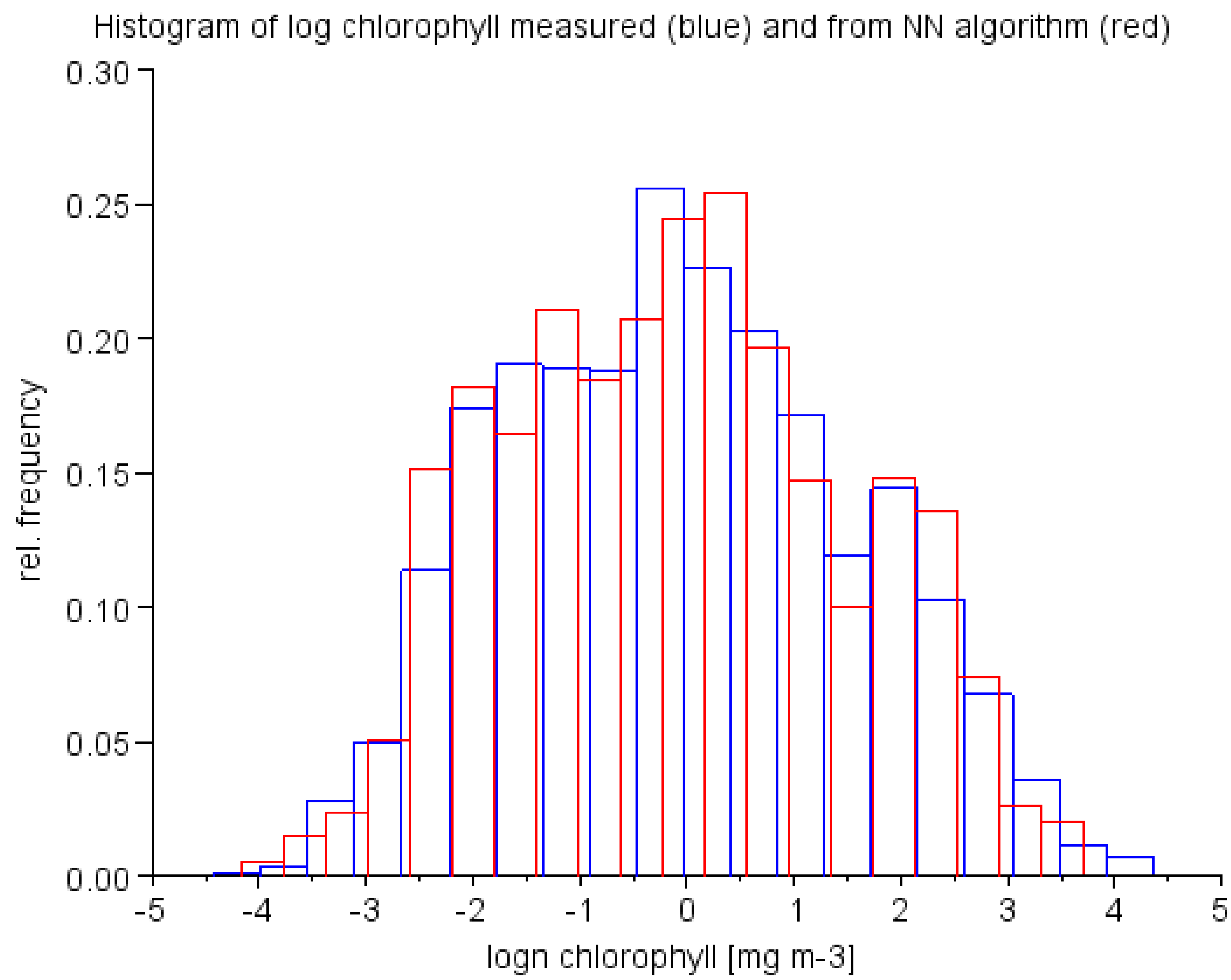


Test of NN based on measurements for chlorophyll

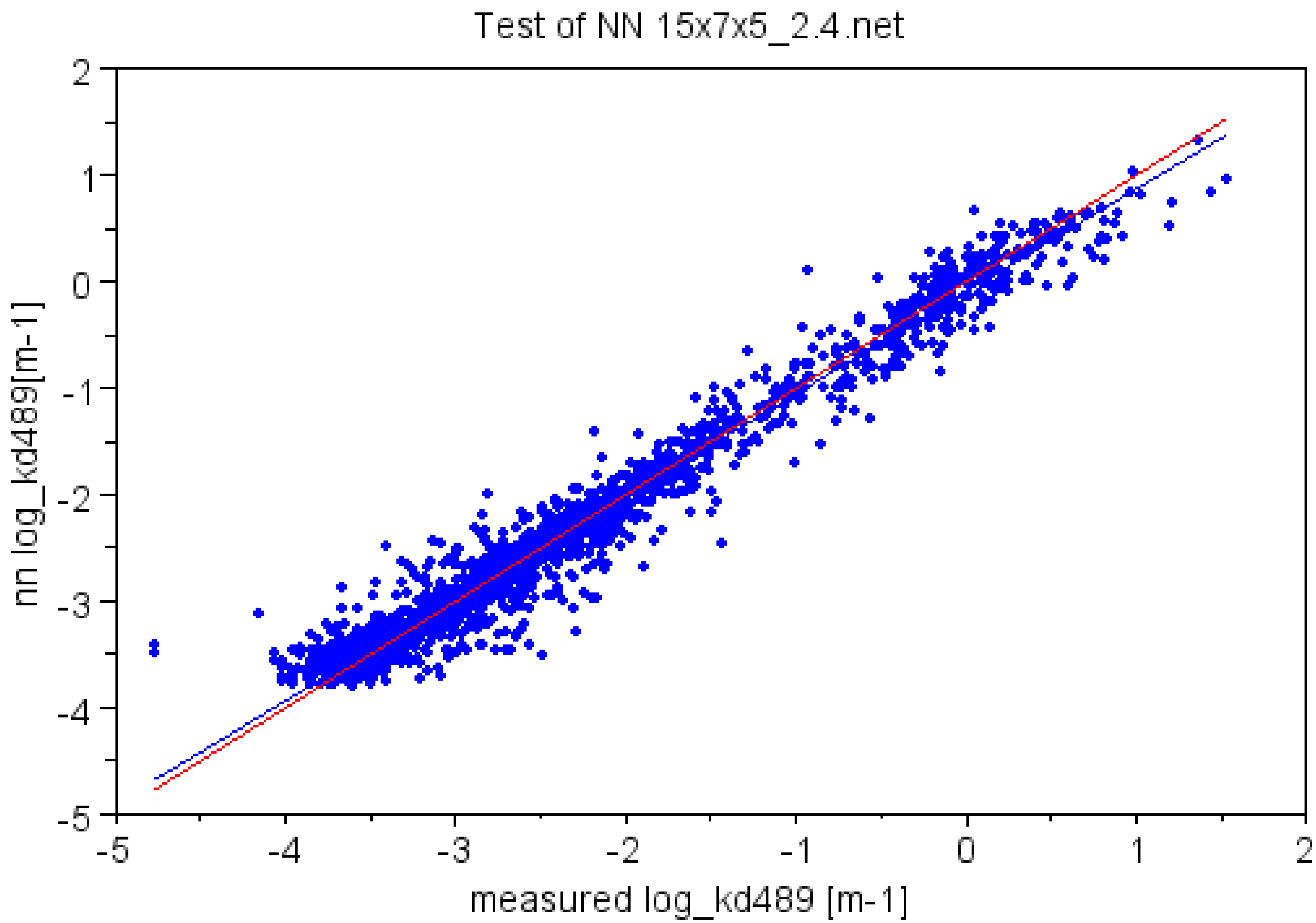


Log10 scale, red: 1 by 1 line

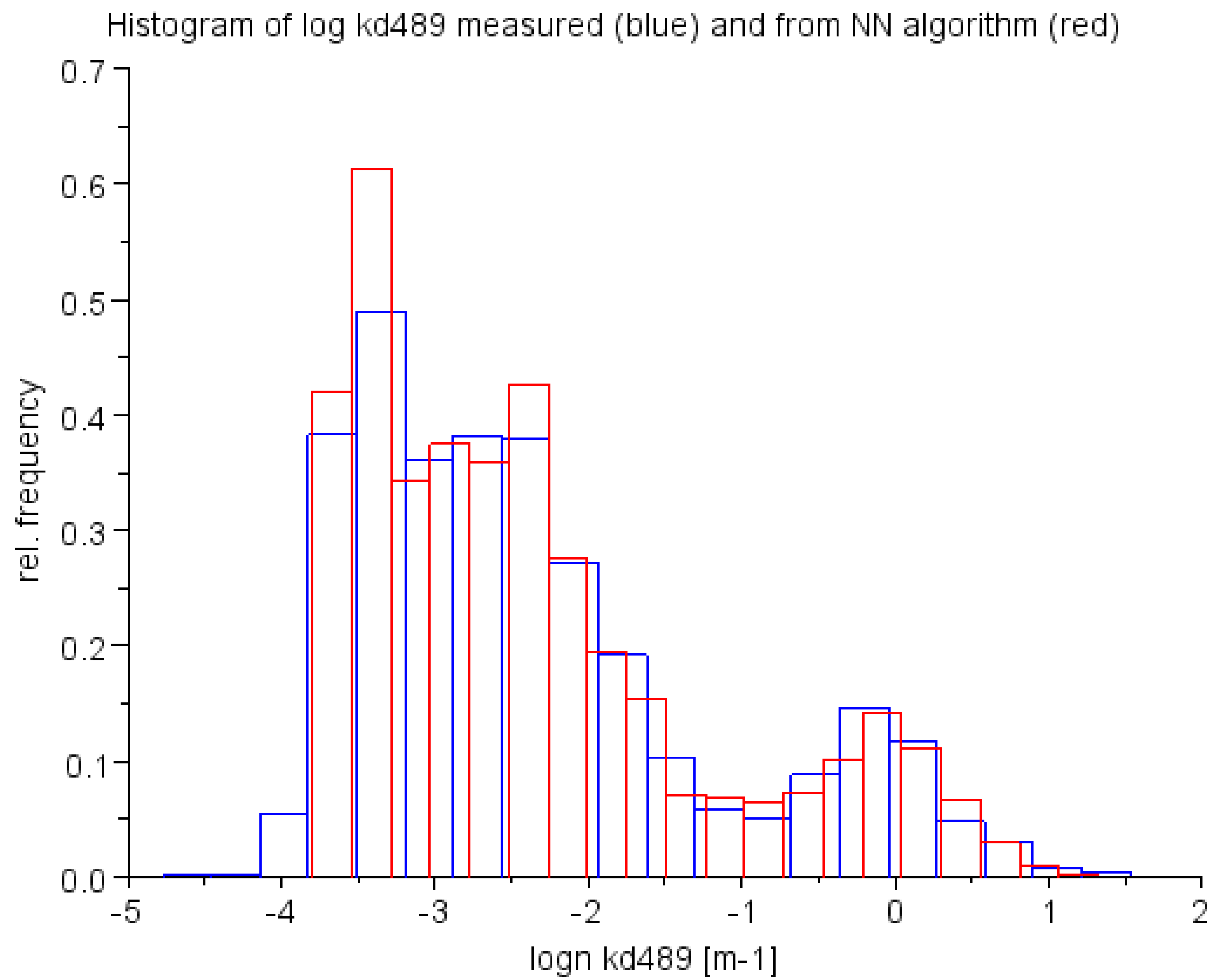
Comparison of histograms: measured, NN computed



NN for kd489


Test of NN 15x7x5_2.4.net
2
1
0
-1
-2
-3
-4
-5
nn log_kd489[m-1]
-5
-4
-3
-2
-1
0
1
2
measured log_kd489 [m-1]

Histogram kd489 measured and NN derived



Sensitivity analysis when algorithms are changed

- Chl.
  Algorithms

$$C_a = 10^{0.366-3.067R+1.930R^2+0.649R^3-1.532R^4}, \text{ where } R = log_{10}\left(\frac{R_{rs}443 > R_{rs}490 > R_{rs}510}{R_{rs}555}\right)$$

OC4v4 (SeaWiFS):

$$C_a = 10^{0.283-2.753R+1.457R^2+0.659R^3-1.403R^4}, \text{ where } R = log_{10}\left(\frac{R_{rs}443 > R_{rs}488}{R_{rs}551}\right)$$

OC3M (MODIS):

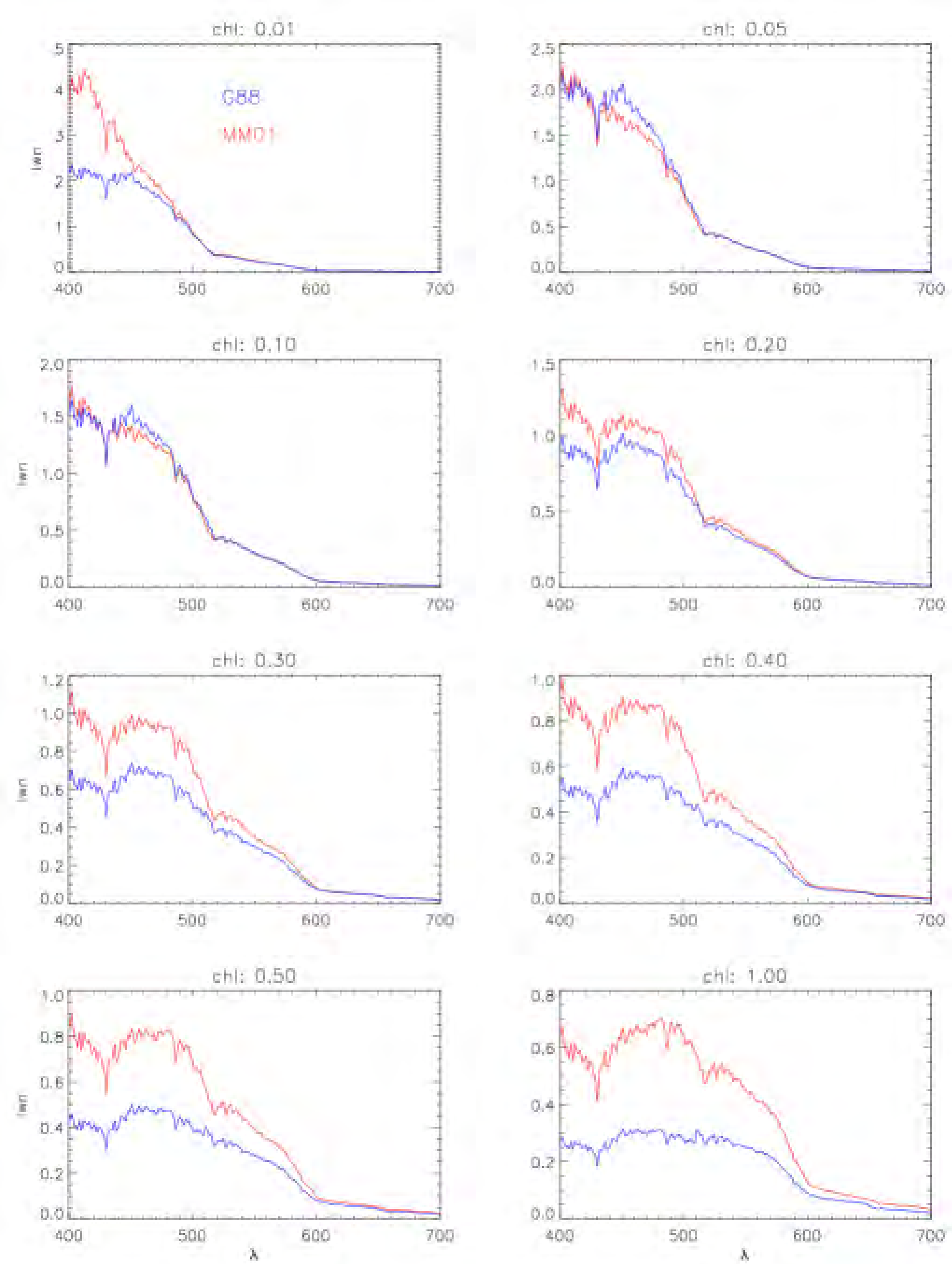
NASA GSFC Ocean colour group

Uncertainty Chl. Per 5% errror in input Rrs

	potential [chl] difference for 5% error in input Rrs											
input chl	10	5	3	2	1	0.5	0.4	0.3	0.2	0.1	0.05	0.01
OC4v4 percent difference	21	19	18	16	13	10	9	8	7	8	10	26
OC3M percent difference	18	17	16	15	13	10	10	8	8	8	11	24

Varying clear water radiance models

Compare Lwn spectra from two clear water radiance models:
Gordon et al. 1988 and
Morel and Maritorena 2001

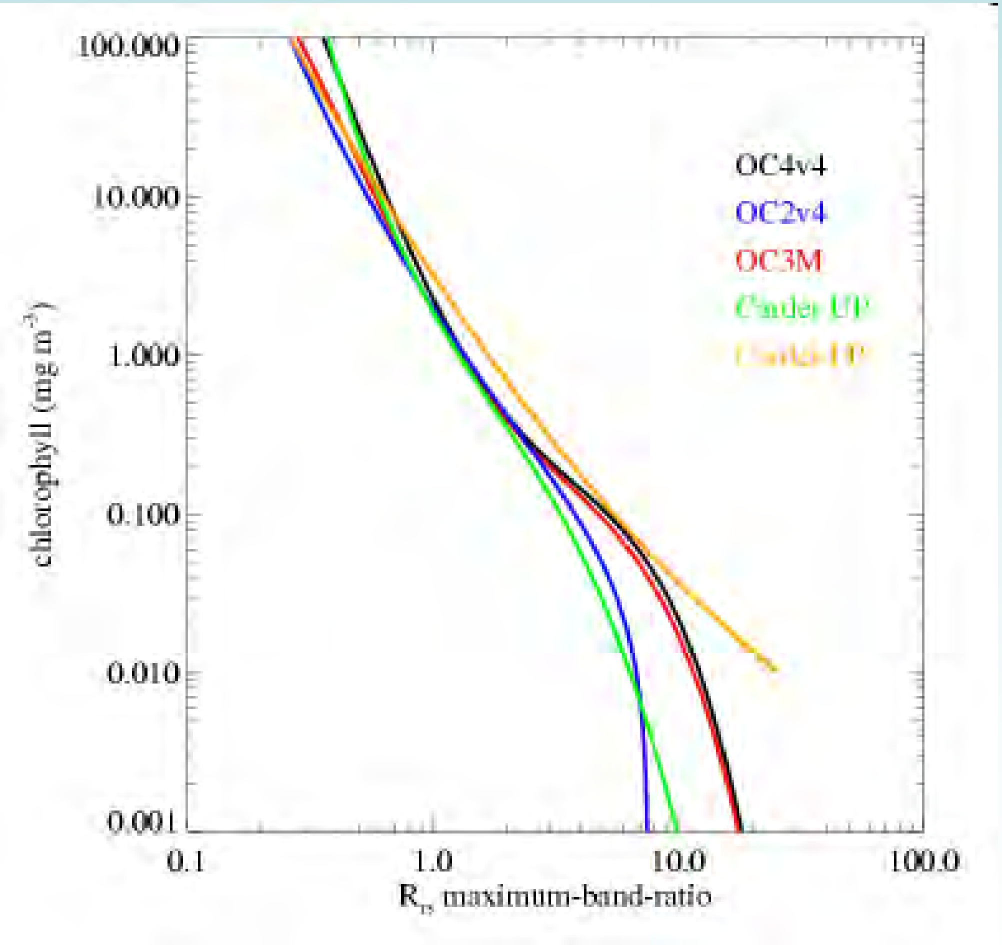


http://seabass.gsfc.nasa.gov/seabasscgi/oc.cgi

OC4 version 4 and other empirical chlorophyll algorithms

Display the functional form of various band-ratio algorithms

° Carder UP and FP indicate unpackaged and fully-packaged, respectively



http://seabass.gsfc.nasa.gov/seabasscgi/oc.cgi

http://seabass.gsfc.nasa.gov/seabasscgi/validation_search.cgi

Query results

Satellite: aqua
Products: adg,bbp,chlor_a
Dates: Jan 1, 2002 to Dec 31, 2012
North: 54.84375, South: 14.765625, West: -80.859375, East: -27.421875
Depth: greater than 0.0

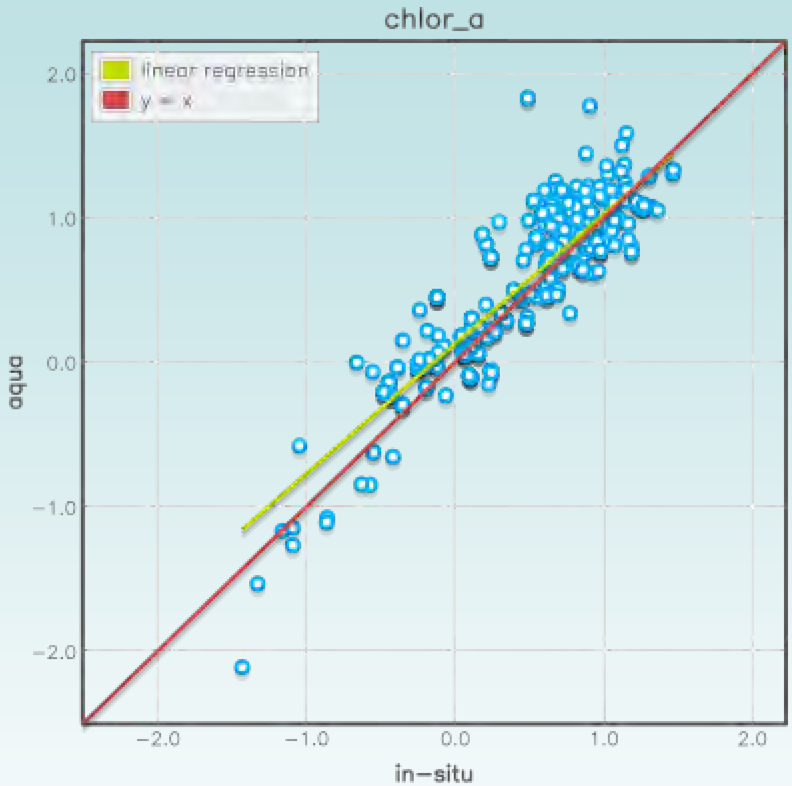
Total number of matchups: 434

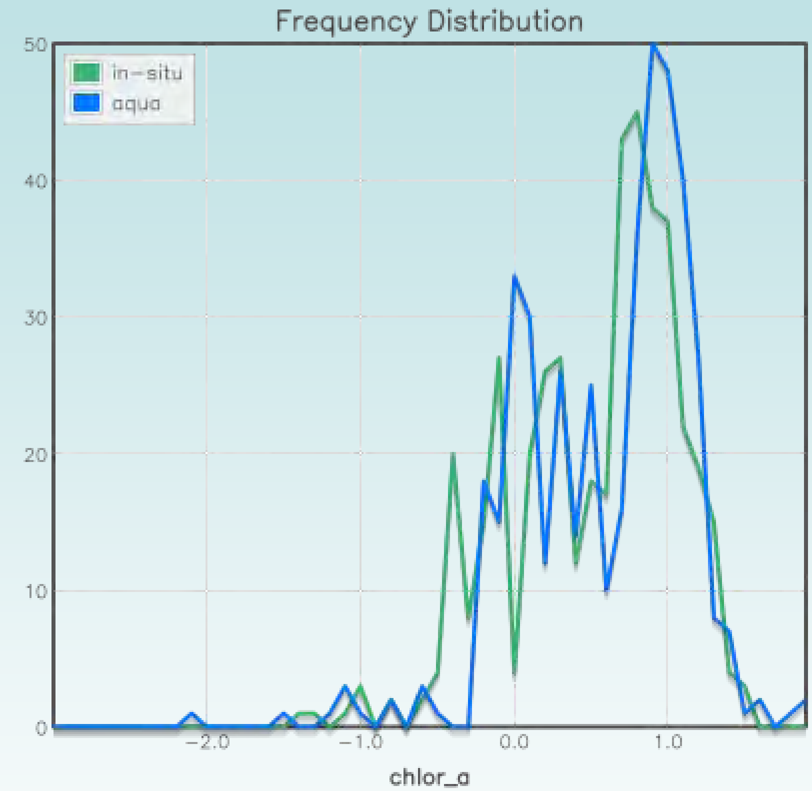
Date format is YYYY-MM-DD, time format is HH:MM:SS, and times are GMT.
Only products with matchups will be displayed. All log

Product Name	in-situ Range	aqua Range	N	Slope	Intercept
chlor_a	(-1.43180, 1.46790)	(-2.11162, 1.83166	434	0.897178	0.127466

R Squared	Median Ratio	Abs % Difference	RMSE
0.79997893	1.1060374	34.37675	0.243367

Result of query





Methods for Assessing the Quality and Consistency of Ocean Color Products

- Introduction http://oceancolor.gsfc.nasa.gov/DOCS/methods/sensor_analysis_methods.html

- This document provides details on several of the standard methods used by the Ocean Biology Discipline Processing Group (OBPG) at NASA/GSFC to evaluate the oceanic optical properties derived from spaceborne ocean color sensors. Many of these analyses are performed routinely for standard products, but they are also used to evaluate changes in processing algorithms or calibration. The analyses serve to verify the implementation of proposed changes and to provide quantitative feedback as to the impact of those changes on field-data comparisons, sensor-to-sensor agreement, temporal and spatial stability in derived product retrievals, and long-term sensor stability.

- Although not discussed here, any evaluation of instrument calibration or processing algorithm changes is normally preceded by a re-evaluation of the vicarious calibration (Franz et al., 2007). This effectively removes any bias on the mission-mean normalized water-leaving radiance retrievals at the vicarious calibration site. When comparing products from different sensors, any algorithm changes that are applicable to both sensors are applied equally, and both sensors are vicariously recalibrated to a common source (e.g., the Marine Optical Buoy, MOBY).

- The plots and images shown in this document come from various processing and testing events. They are provided as examples only, and thus they do not reflect the current state of product quality. This document is intended to describe the analysis methods. The analysis results are posted elsewhere.
- II. Comparison with in situ Observations

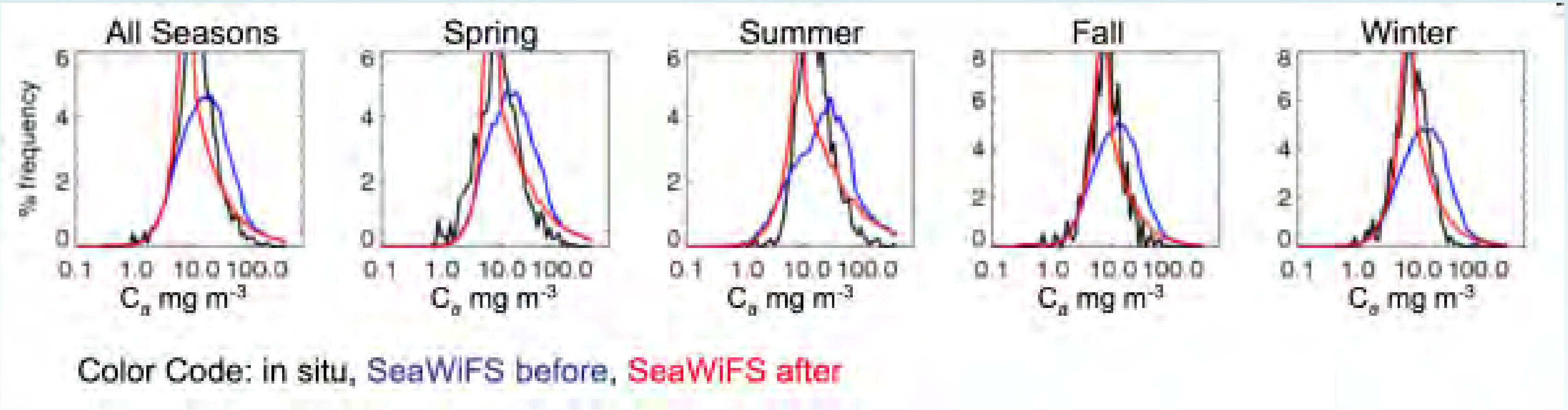
- The primary mechanism for assessing the quality of retrieved ocean color properties is through comparison with ground-truth measurements. A detailed description of the in situ match-up process is provided in Bailey and Werdell (2006), and current operational results are posted on the OBPG Validation Website. It should be recognized, however, that the temporal and geographic distribution of the in situ dataset is limited. These match-ups are generally not sufficient for assessing the quality of satellite remote sensed ocean color data over the full range of geometries through which the spaceborne sensor views the earth, or over the full temporal and geographic distribution of the Level-3 products, nor do they account for the effects of temporal and spatial averaging or systematic errors associated with Level-3 masking decisions.

Bryan Franz
NASA Goddard Space Flight Center
Ocean Biology Processing Group
18 January 2005

September 2009 (Update in Progress)

Level-2 Regional Analysis

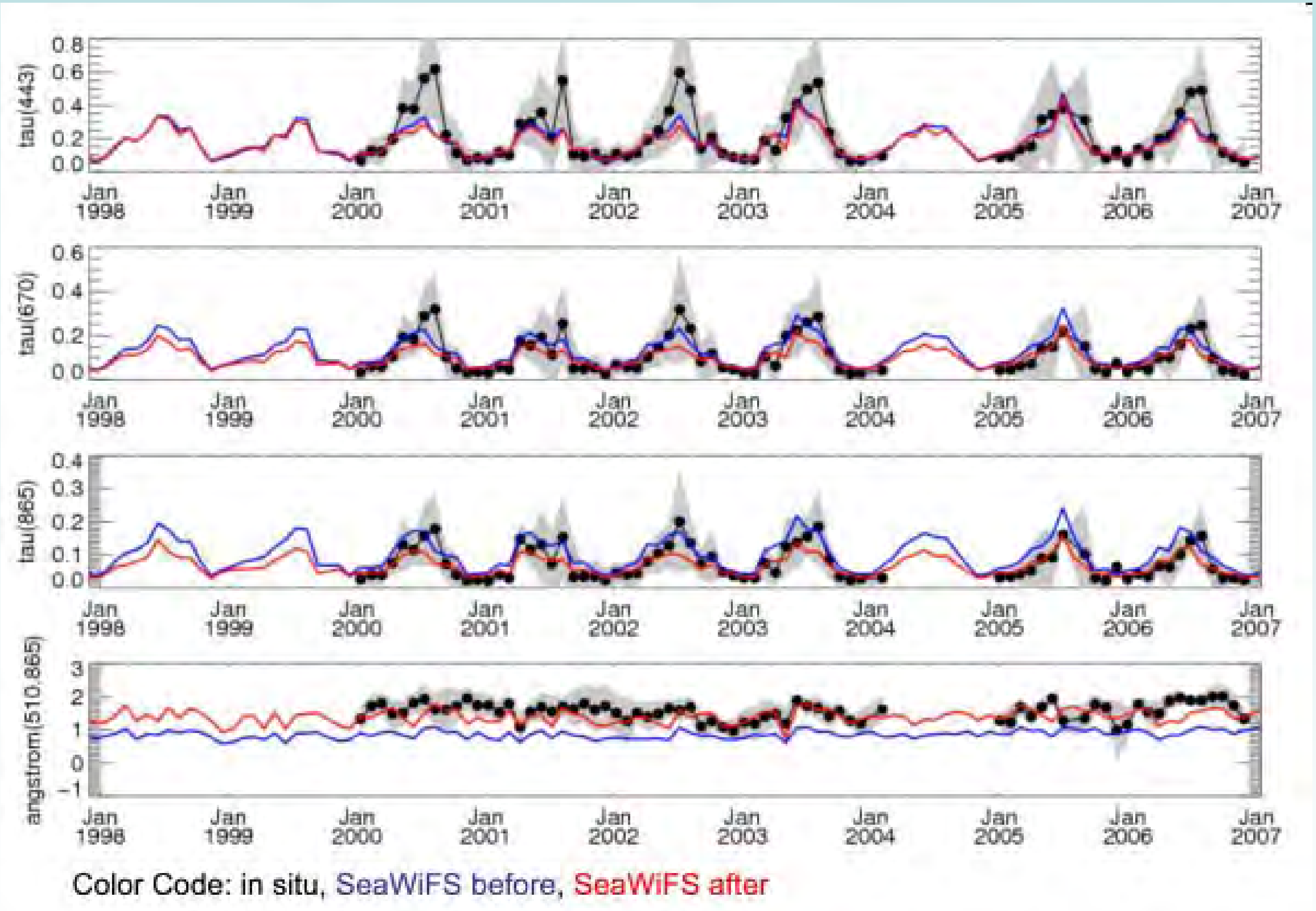
In situ data can be used to characterize the region, and the bulk statistics (e.g., seasonal histogram distributions, monthly-mean trends) can then be compared against equivalent statistics from the Level-2 satellite sensor retrievals. A one-for-one match-up between satellite retrievals and field observations is not required, so the "match-up" return is much higher.



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).

http://oceancolor.gsfc.nasa.gov/DOCS/methods/sensor_analysis_methods.html

Time series validation

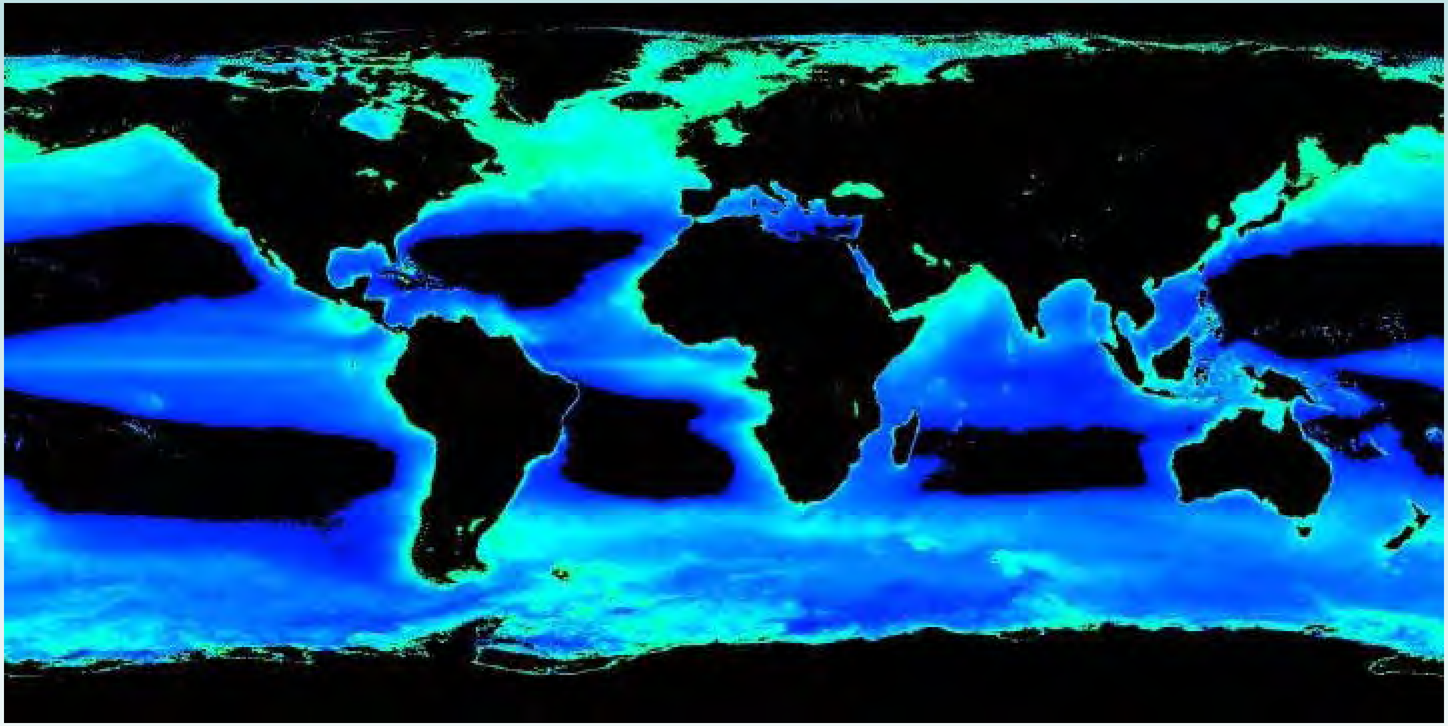


Example of a regional time-series analysis. The plots show SeaWiFS time-series aerosol property retrievals, before (blue) and after (red) a particular algorithm change, with the regional distribution of in situ measurements (black).

Level-3 Temporal Trending

- Level-3 trend analysis looks at long-term trends on global and regional spatial scales. It provides a standard mechanism for evaluating derived product consistency and sensor stability, and it quantifies the relative impact of calibration and algorithm changes on life-of-mission time scales.
- The Level-3 products are global binned, multi-day averages at 4.6 or 9-km resolution, with bins distributed in an equal-area, integerized sinusoidal projection
- From these multi-day global composites, a subset of the filled bins is selected and the binned products are averaged and trended with time.
- five global subsets are defined, corresponding to 1) all bins, 2) all deep water bins, and those bins from locations that are typically associated with 3) oligotrophic, 4) mesotrophic, 5) eutrophic conditions.
- The oligotrophic subset is all bins where 0.0 < chl < 0.1 mg/m^3. Similarly, mesotrophic and eutrophic subsets correspond to mean chl ranges between 0.1 to 1 and 1 to 10 mg/m^3, respectively.

Trend analysis

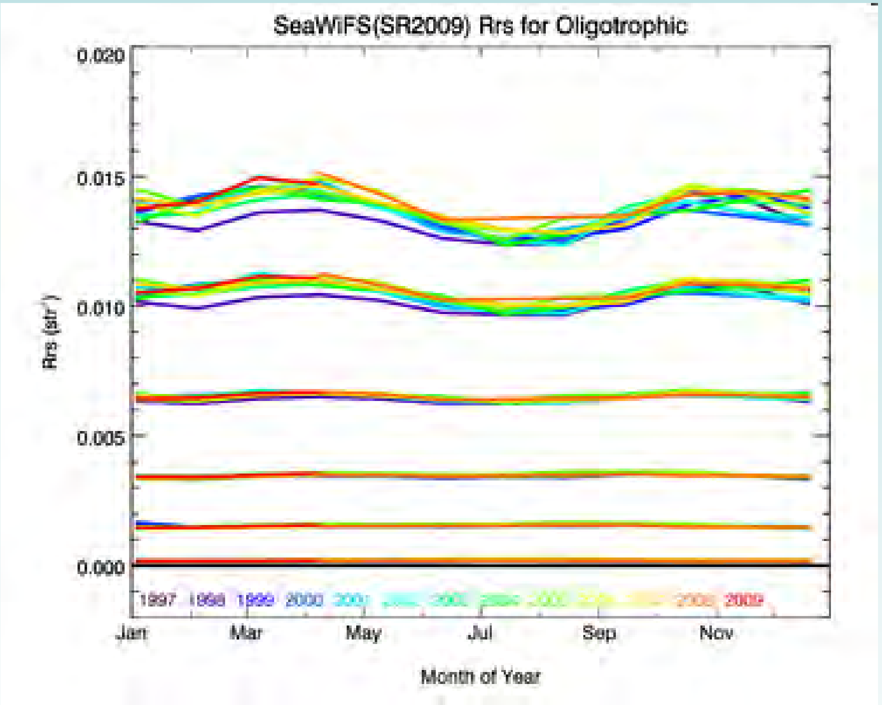


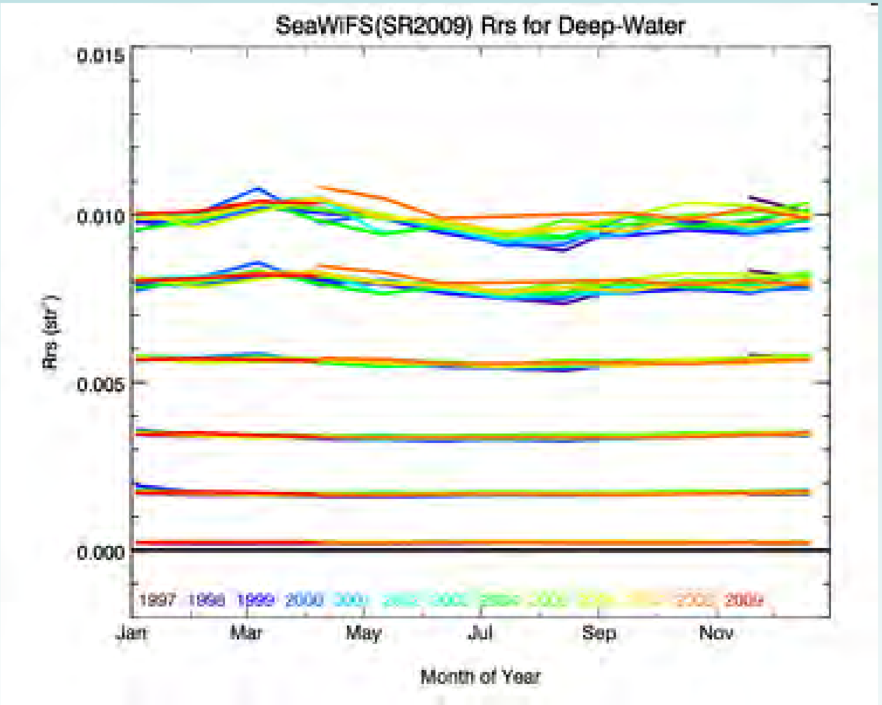
SeaWiFS mission mean chlorophyll showing the distribution of mesotrophic bins

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.

http://oceancolor.gsfc.nasa.gov/DOCS/methods/sensor_analysis_methods.html

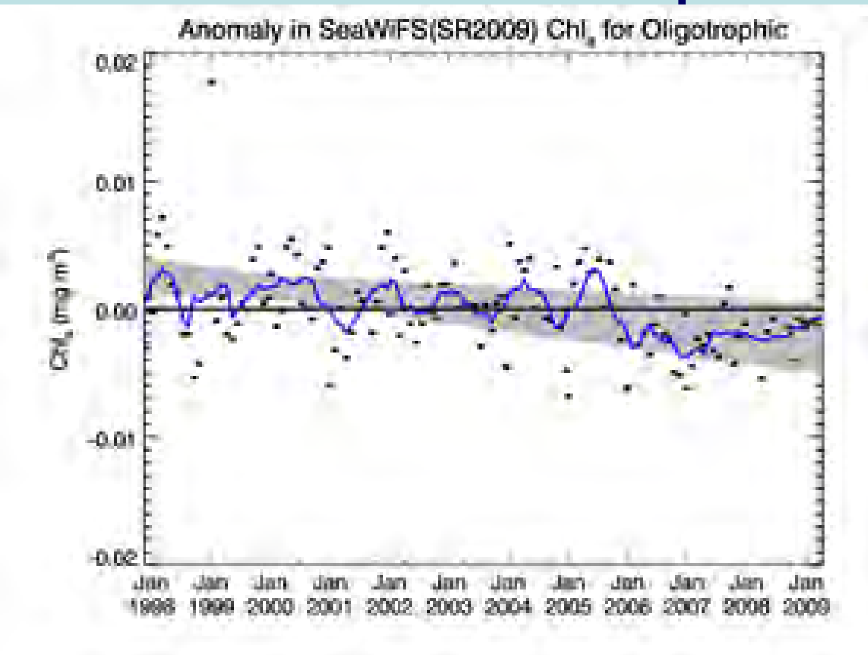
Trend Analysis II

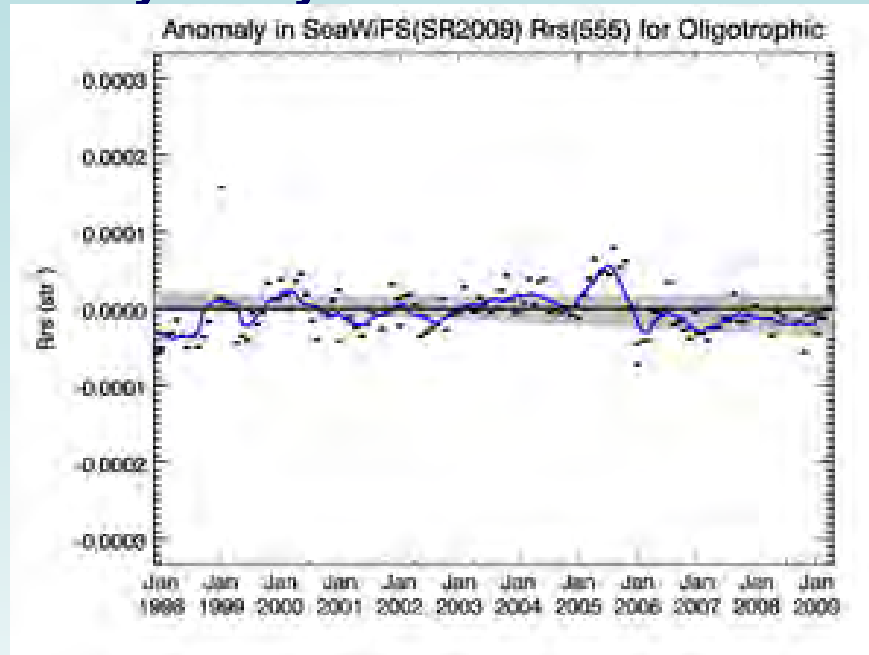




SeaWiFS annual cycle analysis for oligotrophic and deep-water subsets.
Plots show trends in remote sensing reflectance for the six visible channels

Temporal Anomaly Analysis



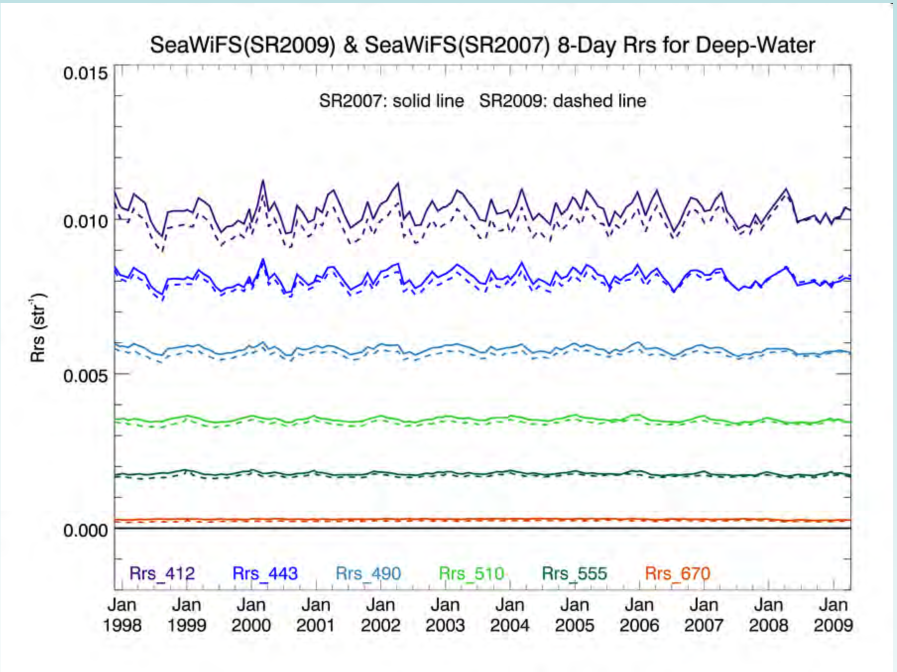


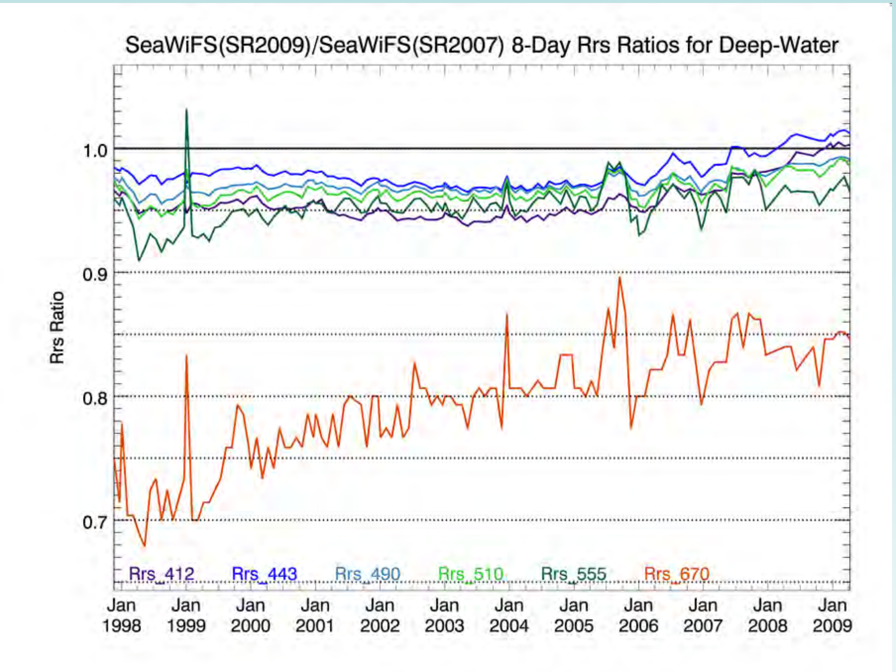
SeaWiFS anomaly trend relative to the mean annual cycle, for chlorophyll-a and nLw(555) in oligotrophic waters. Black symbols are the instantaneous subset mean minus the multi-year mean, with error bars indicating standard uncertainty on the mean. The Blue line is an 11-pt box-car average through the data points. The grey region is the range of linear fits that can be drawn through the data points (least squares fit, plus and minus twice the uncertainties on the fit coefficients).

Trend Comparisons and Common Bins

- Another useful tool for separating geophysical changes from sensor calibration and algorithm artifacts is to compare Level-3 trends between missions. Similarly, comparison of trends derived with different processing algorithms or sensor calibrations can help to verify proper implementation and to assess the impact of such changes on the global science products. This analysis looks at average values in coincident Level-3 retrievals on global and regional spatial scales, and presents the results as a comparative time-series over the common mission lifespan. We begin with Level-3 products composited over a common time period (usually 4 or 8 days). All OBPG Level-3 ocean color products use the same, equal area binning approach (Campbell et. al, 1995), but standard MODIS products are distributed at 4.6-km resolution while SeaWiFS is distributed at 9-km resolution. To allow for a direct, bin-for-bin comparison, the MODIS products are rebinned to the SeaWiFS 9-km resolution using standard binning algorithms. With Level-3 composited data products in an equivalent form, the datasets are further reduced to a set of common bins. This means that only those bins for which a retrieval exists for both sensors or both test processing configurations are included in subsequent averaging and trending. This is critical to the statistics, as some sensors show systematic data gaps even after 8-days of compositing, and this can result in geographic sampling bias if both sensors are not equivalently masked. Figure 6 shows an example of a trend comparison for remote sensing reflectance retrievals from two different SeaWiFS processing configurations (Reprocessing 2007 vs Reprocessing 2009).

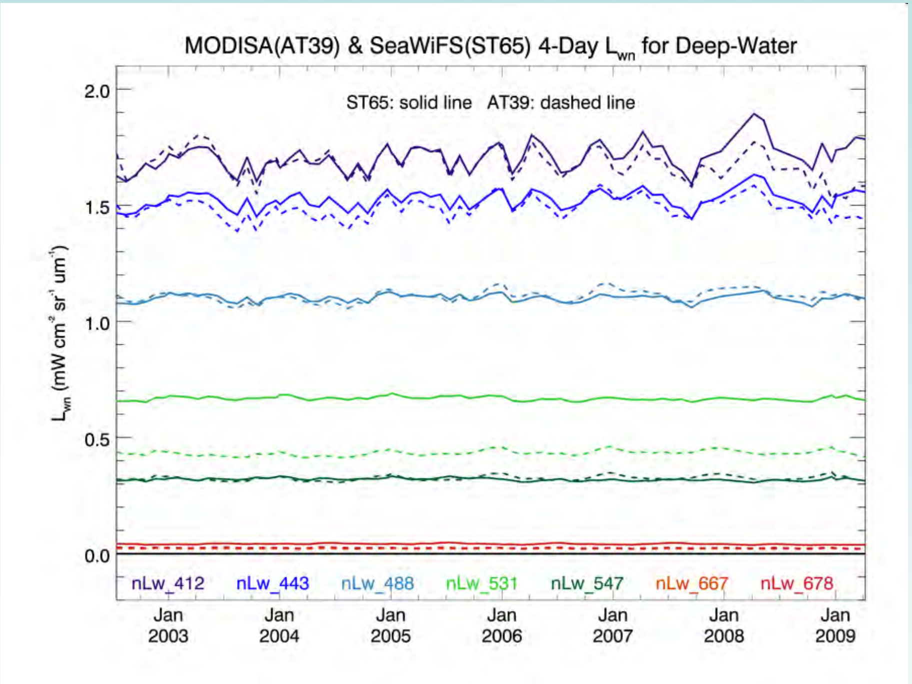
Trend Comparisons and Common Bins II

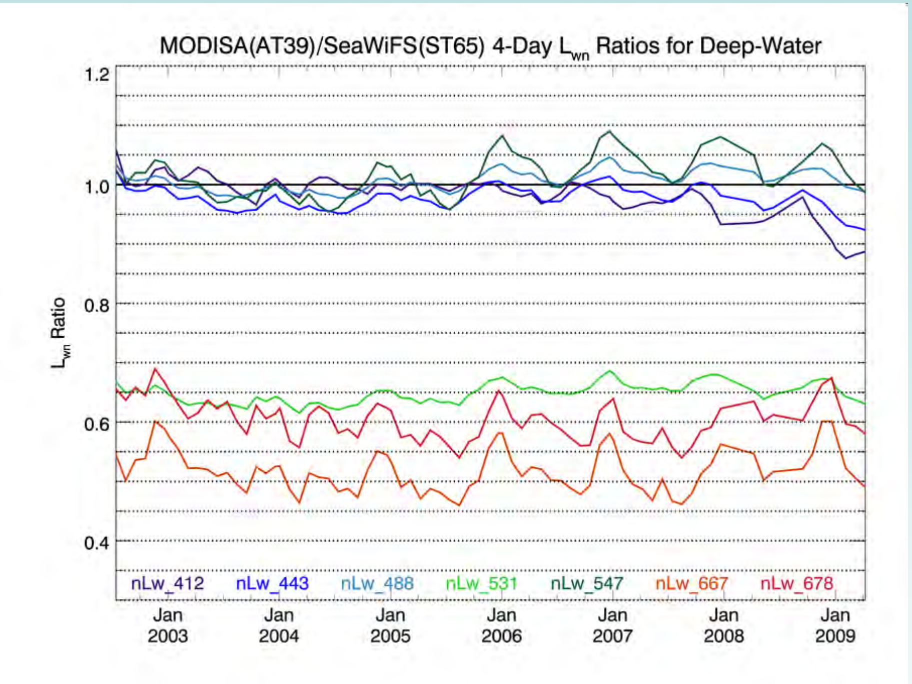




Example of a comparison for SeaWiFS remote sensing reflectance trends in the six visible wavelengths. The plot on the left is a direct comparison, while the plot on the right is a ratio of the two cases.

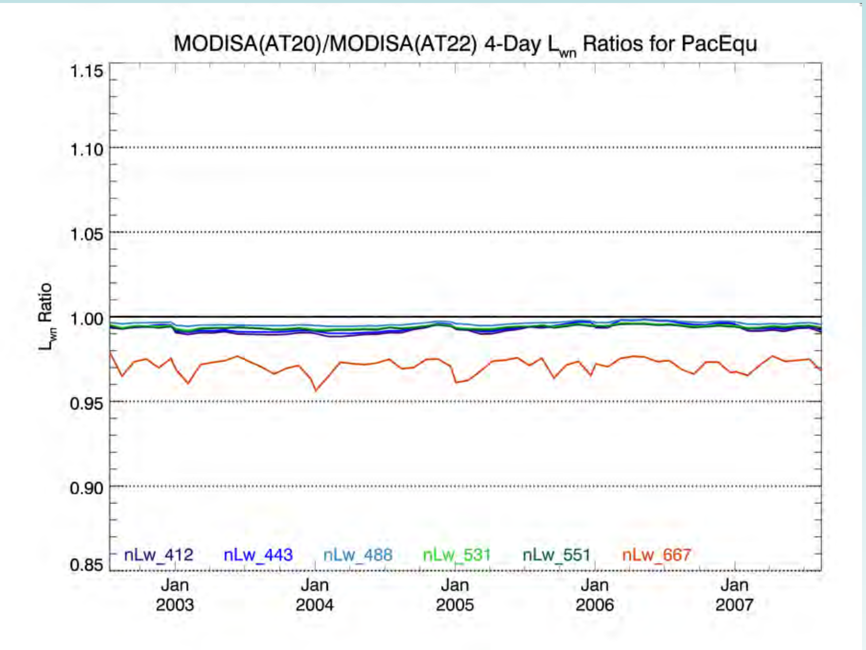
Trend Comparisons and Common Bins III

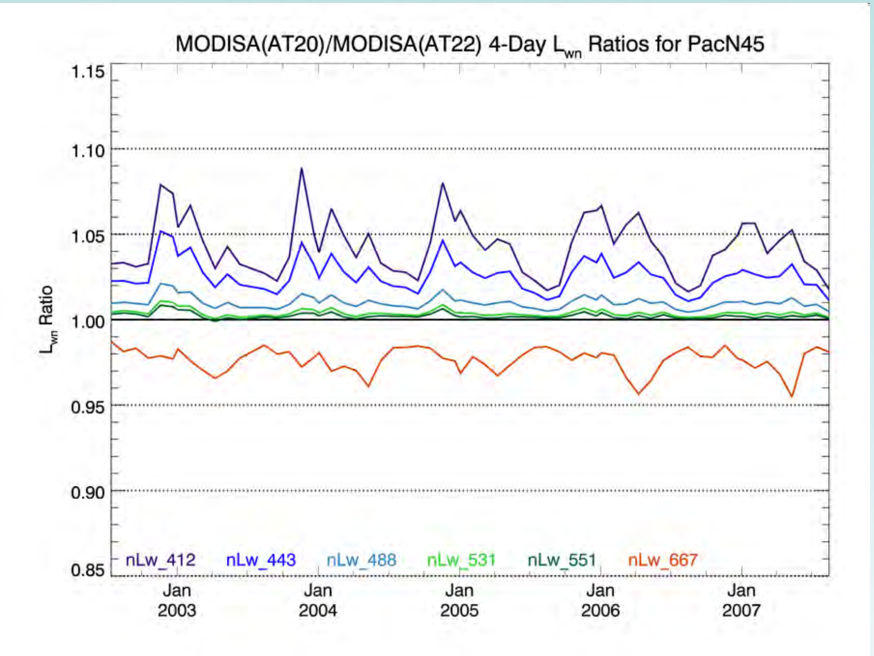




Example of a comparison between MODIS/Aqua and SeaWiFS normalized water-leaving radiance trends for seven visible wavelengths of MODIS. The plot on the left is a direct comparison, while the plot on the right is a ratio of the two sensors. The nearest wavelength bands of SeaWiFS are selected for the comparison, so MODIS 531-nm band is being compared to SeaWiFS 51--nm band, and both MODIS 667 and 678-nm bands are compared to SeaWIFS 670-nm band.

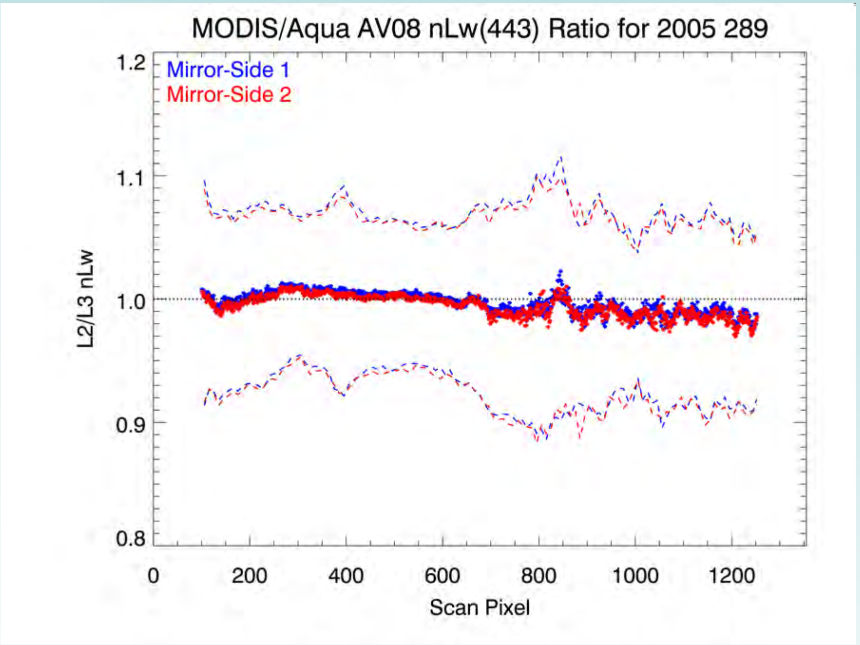
Effect of algorithm change: NO2

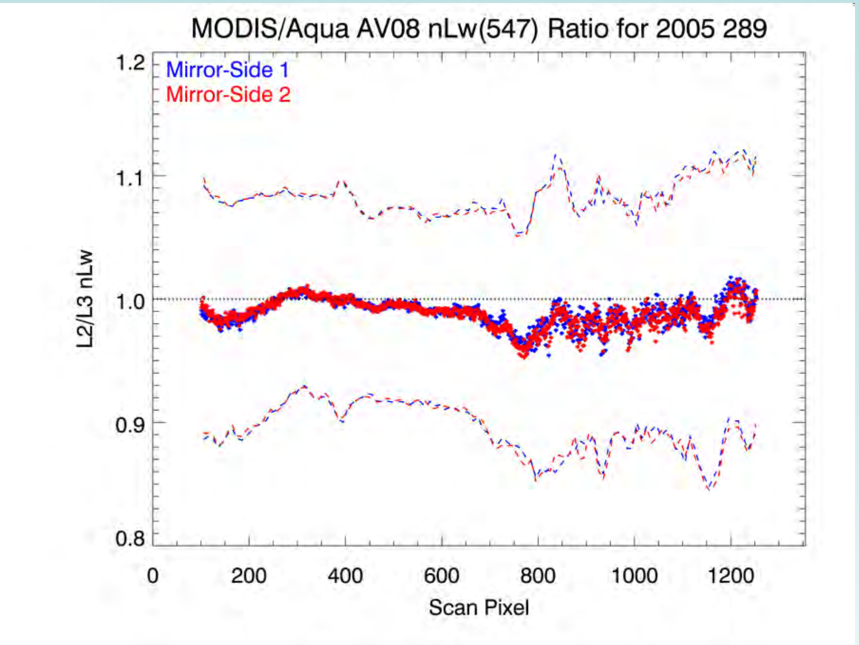




MODIS/Aqua water-leaving radiance ratios, before and after NO2 corrections. The left panel shows the effect at the equator while the right panel shows the effect at high latitude.

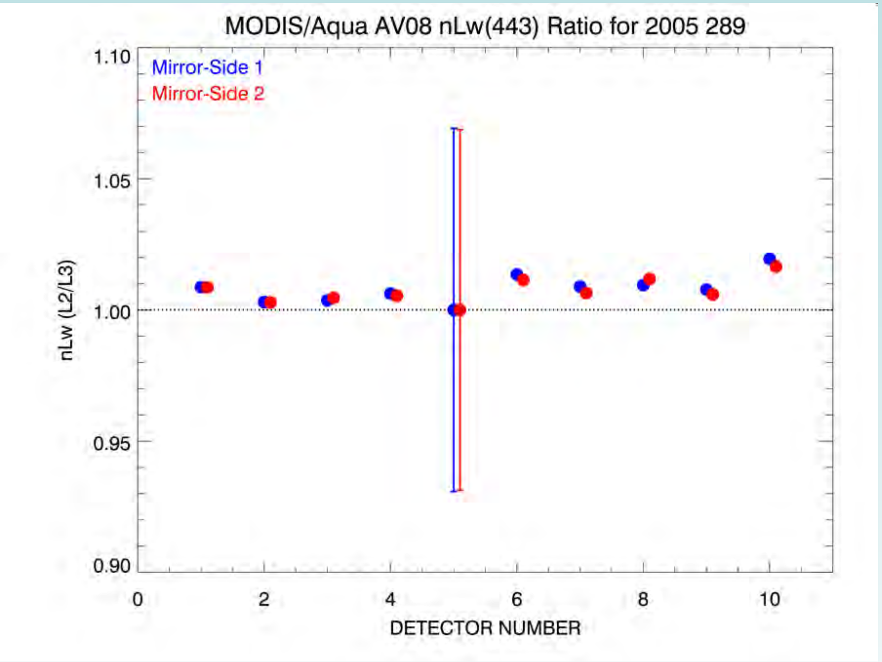
Level-2 to Level-3 Comparison

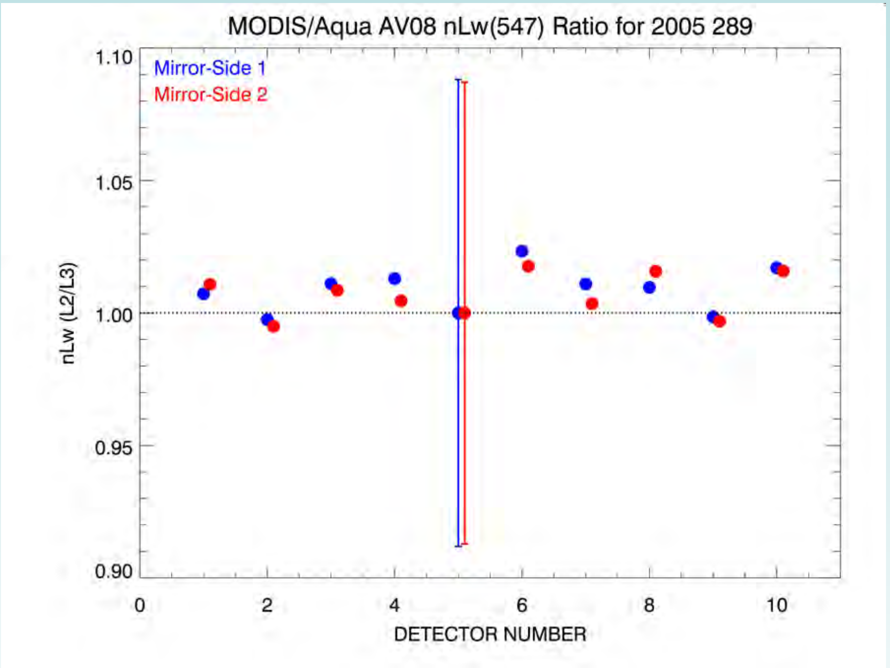




Example of scan-angle-dependent residuals in MODIS/Aqua normalized water-leaving radiances. Data is from a recent test processing for day 289 o5 2005. Red and blue symbols are mean Level-2 to Level-3 ratios witin each scan pixel, stratified by scan mirror side. The dashed line shows one standard deviation on the mean.

Detector dependent uncertainties





Example of detector-dependent residuals in MODIS/Aqua normalized water-leaving radiances. Data is from a recent test processing for day 289 o5 2005. Red and blue symbols are mean Level-2 to Level-3 ratios witin each detector of the respective waveband, stratified by scan mirror side. The error-bars show one standard deviation on the mean.

Uncertainties related to comparison with in situ data

- Error in method and handling, e.g. HPLC for chlorophyll determination
- Sample not representative for water volume of pixel
- Vertical distribution: water comes from a certain depth, e.g. 4 m for FerryBox
- Temporal difference between sample and satellite overpass
- Sub-pixel patchiness
- Scatter in bio-optical data, e.g. relationship between concentration and IOPs

Strategies to determine uncertainties for coastal water: Solutions

- **Out of scope detection**
  - Check of auxilary variabels, e.g. windspeed -> whitecaps
  - Check of reflectance in particular bands: NIR reflectance for floating material
  - Auto-associative neural network
  - Combination of backward and forward neural network (standard MERIS processing)
  - Convergence of optimization procedure on high deviation level
- **Ambiguities in bio-optical / reflectance model**
  - Analysis of simulated data using the bio-optical model
- **Uncertainties on a pixel by pixel basis**
  - Empirical from observations
  - Variations in optimization procedure
  - Determination using variations of simulated data set -> look up table, NN

Summary and Conclusion: uncertainties

- There are a lot of factors, which determine top of atmosphere radiance spectra
- Vice versa the information content of TOA spectra is much too low to determine all of these factors independently
- In complex water the signal can be very low in the blue spectral range
- Atmospheric correction then extremely critical
- In complex water the dominant component might mask the effect of all other components
- In this case the uncertainty range for the subdominant components increases significantly
- Saturation effects limit the accuracy and may cause a shift in the importance of bands
- There are constellations of atmosphere / water which leads to failure in the algorithms
- These out of scope conditions have to be detected and marked per pixel using flags and uncertainty indicators
- Expected errors can be determined by sensitivity studies
- Of high importance is a continuous validation using in situ observations of high quality

Colour Remote Sensing of complex water is possible!

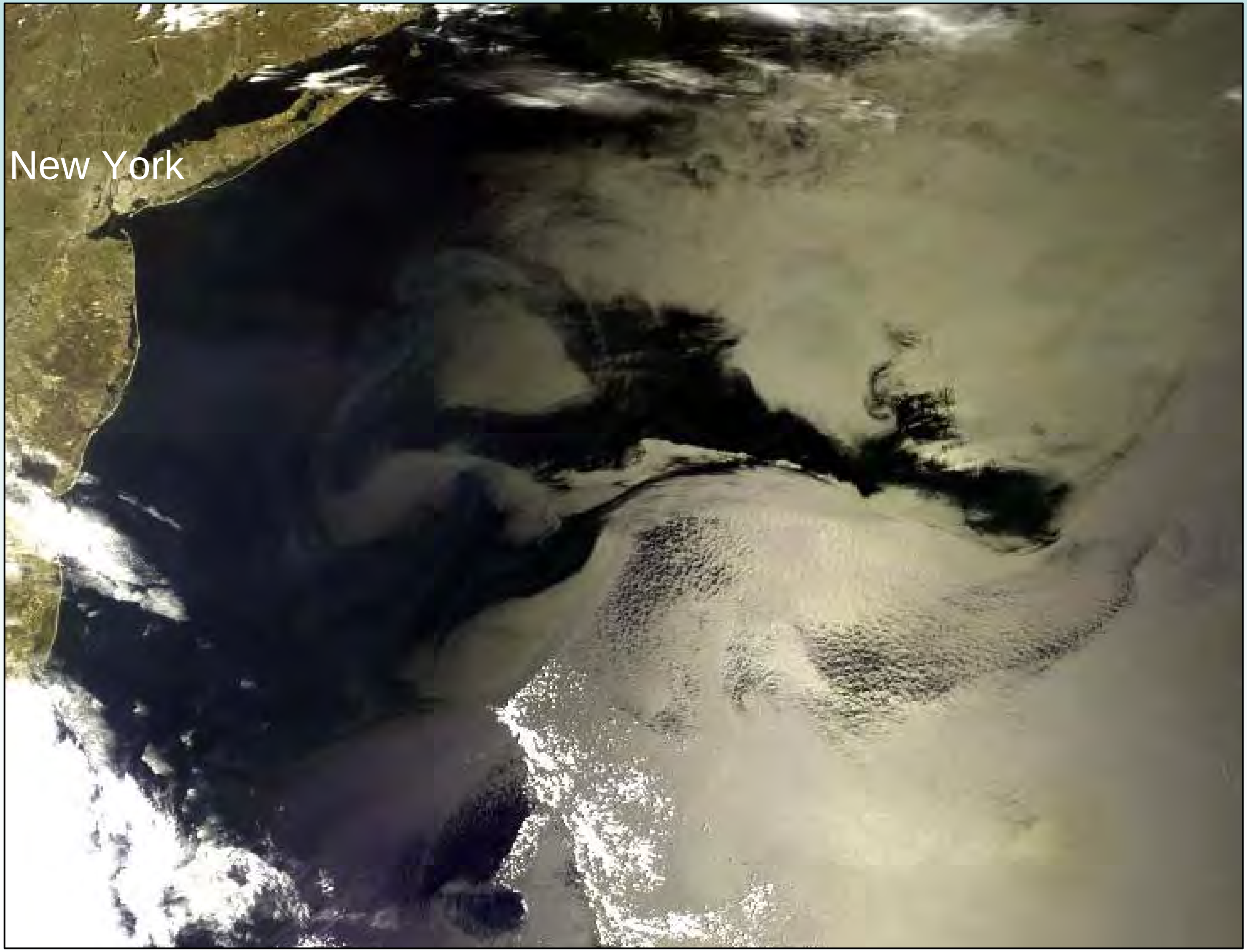
But:

- Restrict to a small number of components with similar optical properties
- Detection of special cases such as red tides, cyanobacteria
  - Exclude or develop special algorithms
- General knowledge about vertical distribution at different seasons
- Bathymetry to estimate possible bottom effects
- Determine penetration depth / z90 depth
- Determine scope of algorithm
- Develop algorithm to determine / flag out of scope conditions
- Determine uncertainties for each product

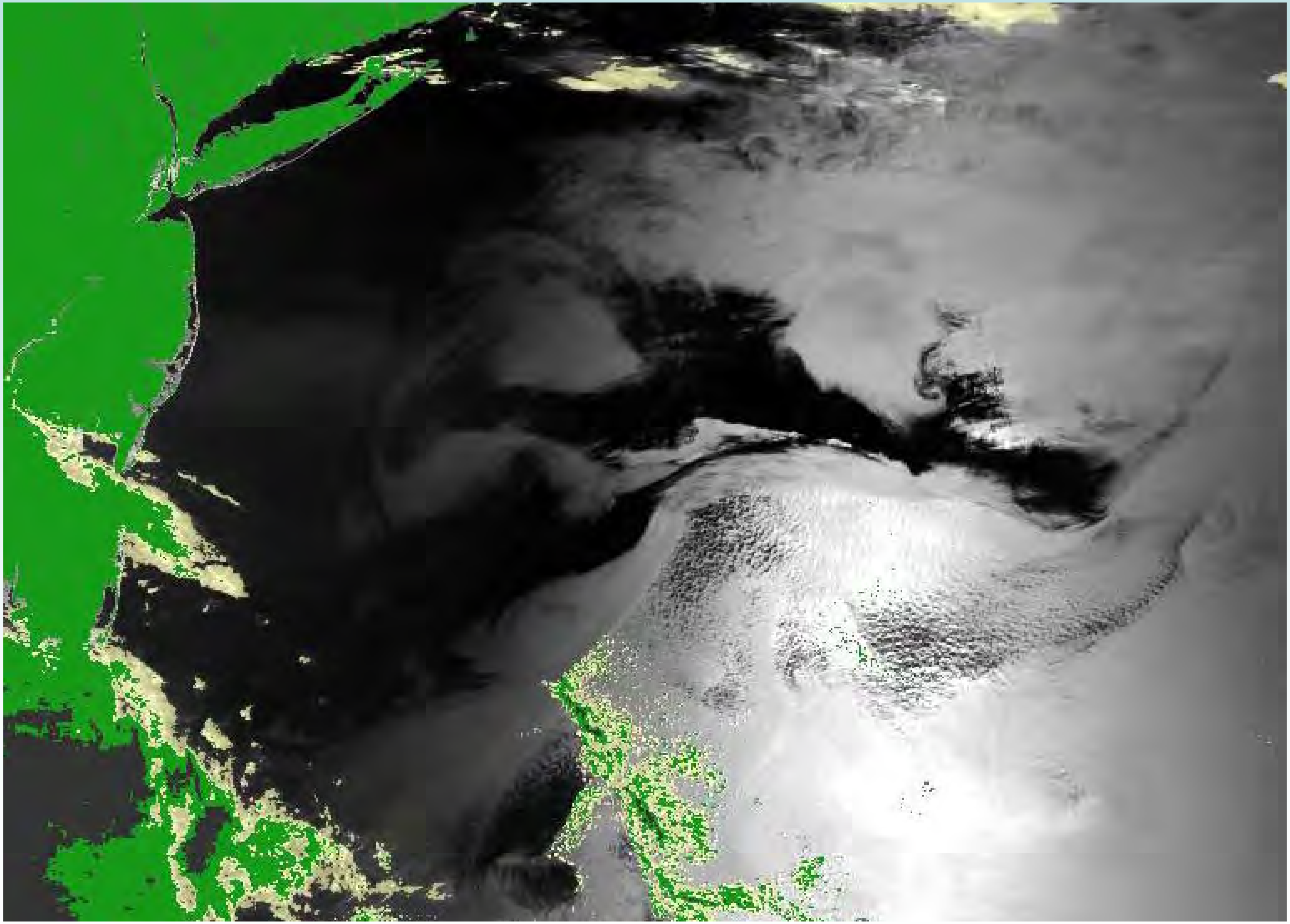
Atmospheric correction most challenging issue

- Develop special procedures for atmospheric correction over complex waters
- Problems: adjacency effects, floating material
- Determine conditions when AC leads to too large uncertainties

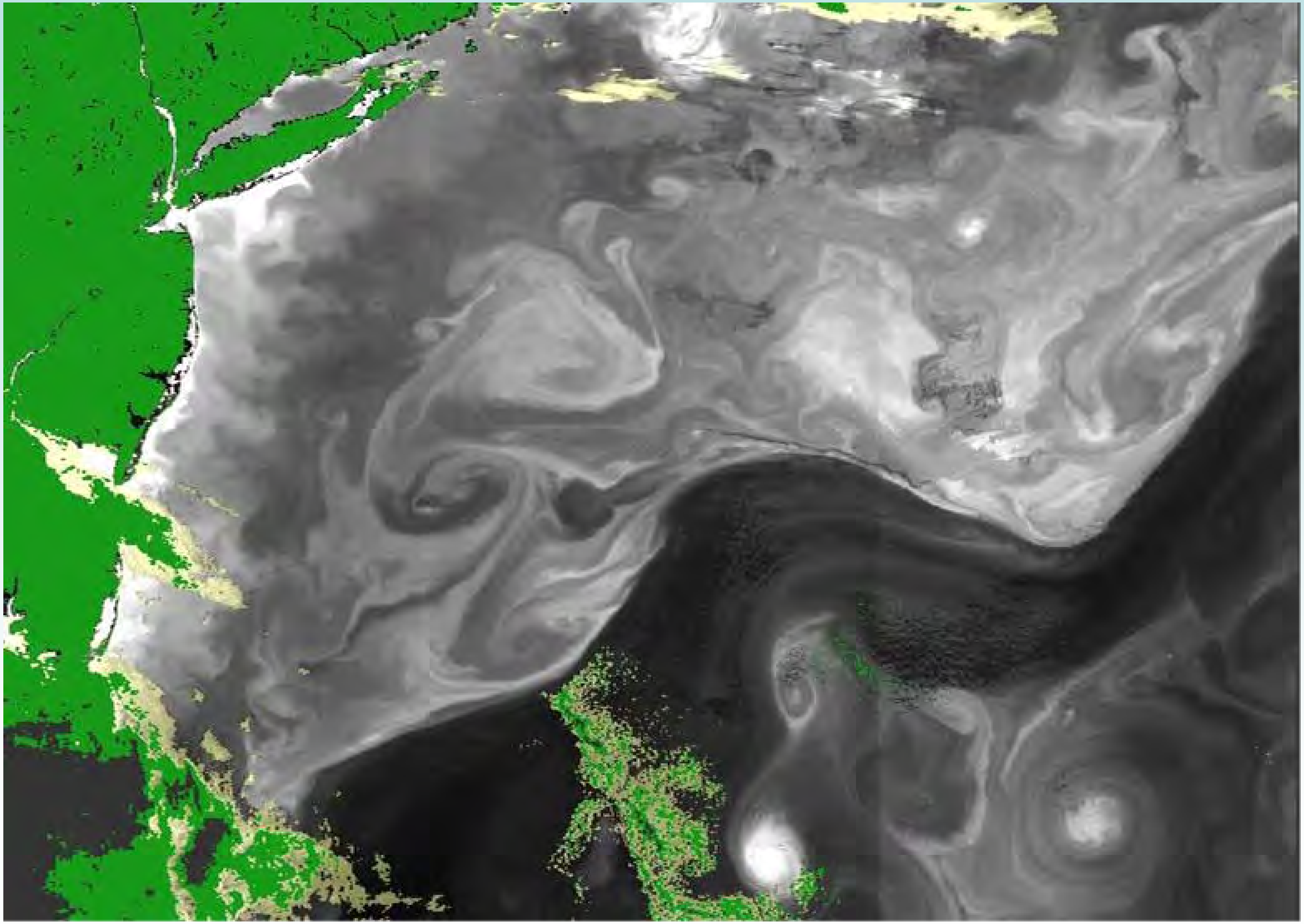
MERIS 20070505
Top of atmosphere radiance reflectance RLtoa RGB



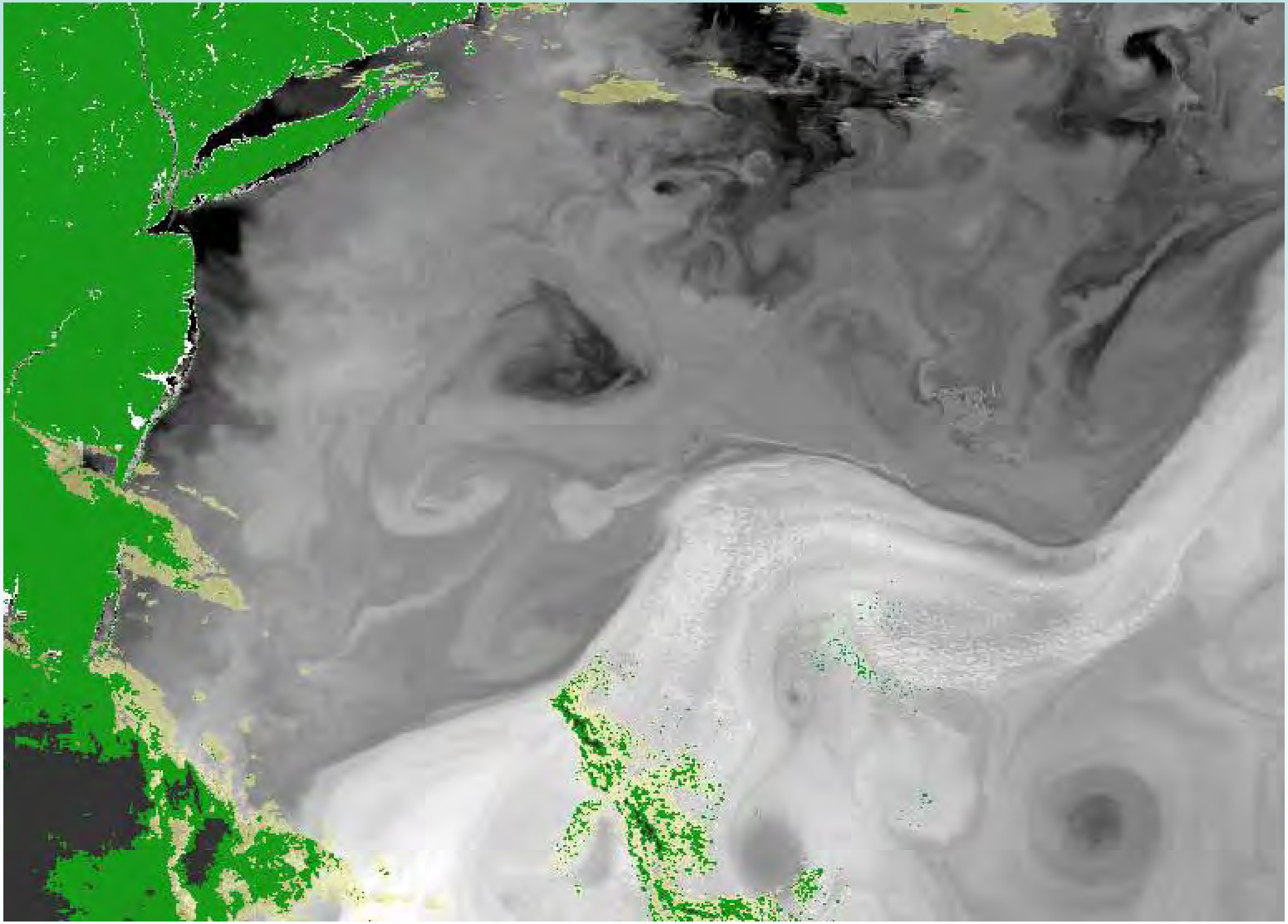
Path radiance+ Fresnel reflectance RLpath MERIS band 5 (560 nm)



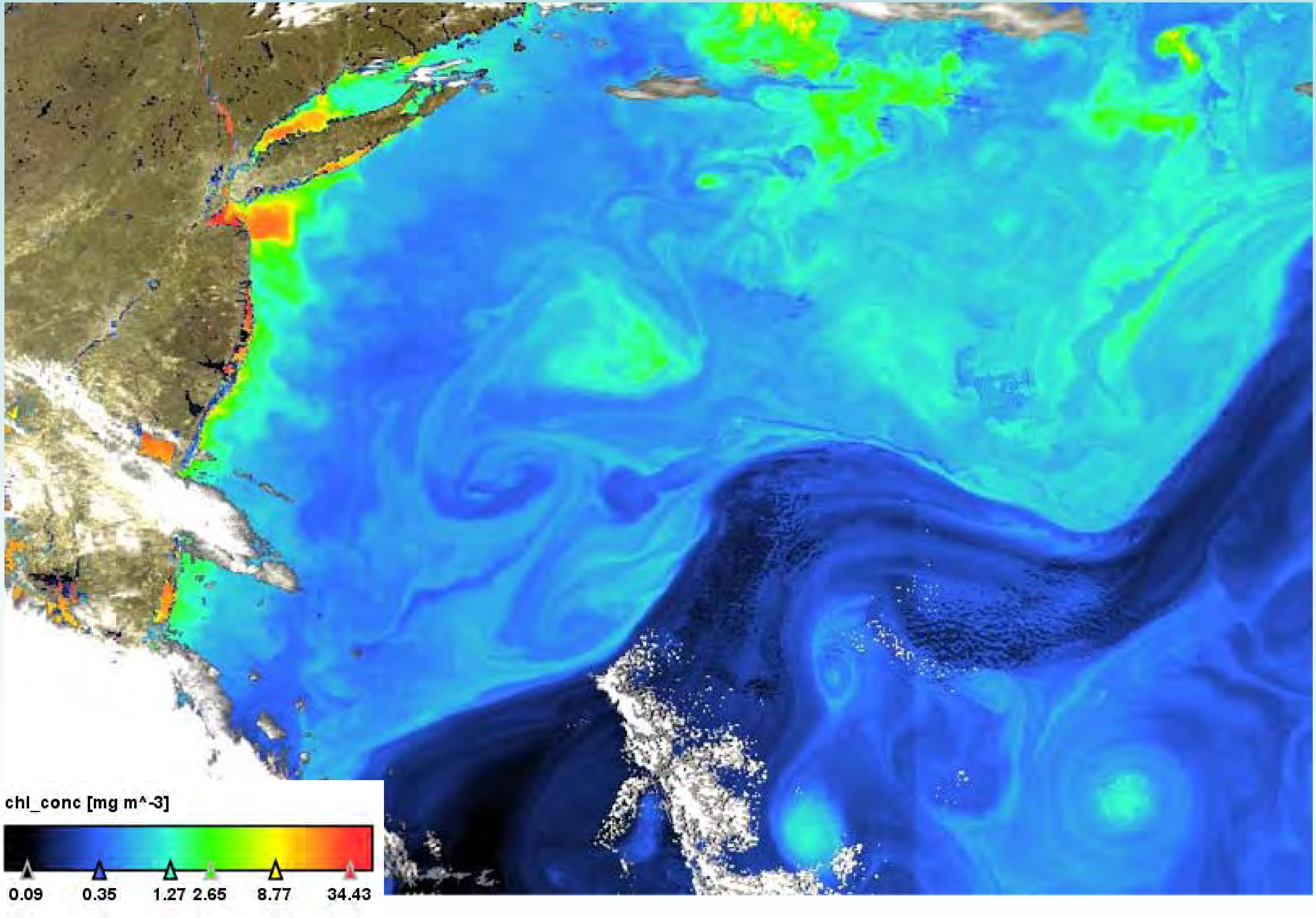
Water leaving radiance reflectance RLw MERIS band 5 (560 nm)



Water leaving radiance reflectance RLw MERIS band 2 (443 nm)



Chlorophyll



Acknowledgemets

- Supported by various projects
  - ESA Case 2 Water Regional Algorithm
  - ESA Glint correction
  - ESA Water radiance
  - ESA CoastColour
  - ESA Dragon
  - DLR DeMarine
- Neural Network Training software H. Schiller, GKSS
- MERIS data provided by ESA
- Implementation of C2R and Glint correction in BEAM: M. , Brockmann-Consult

Summary and conclusions

- Uncertainty in coastal water products can be large due to the large number of factors in atmosphere and water, which determine the reflectance spectrum
- Conditions where algorithms (AC & water) fail
- Prerequisite for a successful retrieval are optical models of the atmosphere and the water, which meet the actual conditions
  - Regional models might be necessary
- Reflectance spectra have to be tested if they are within the scope of these models
  - Out of scope spectra have to be flagged, treated with special algorithms or excluded from further processing
- Limited sensitivity of reflectance spectrum and ambiguities lead to an uncertainty even for spectra, which are in scope
  - Uncertainties have to be quantified on a pixel-by-pixel basis
- Validation in coastal waters by match up in situ samples can be difficult due to patchiness and fast changes
  - Uncertainties in in situ match up data have to be quantified
  - Validation should be complemented by statistical analysis of larger areas, transects and time series