Coastcolour bio-optical models and algorithms

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Case 2 Water Inversion Algorithms

Note Case 2 means: > 1 component necessary to describe the variability of water leaving radiance reflectances

- Decomposition technique with a sequence of empirical algorithms using semi-analytical models
- Optimization of the parameters of a forward model to achieve a best fit between the measured and modeled reflectance spectrum
- Look-up table procedure: comparing the measured spectrum with simulated spectra in a look-up table
- Linear Matrix inversion
- Linear combinations from a principle component analysis (based on measured or simulated spectra)
- Neural network inversion with a NN training based on measured or simulated reflectance spectra and corresponeding IOPs
- Classification of water reflectance spectra and determination of a class
- Combination of techniques, e.g. classification and neural networks

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Inversion using a neural network

Pros

- Can be based on simulations using a sophisticated radiative transfer code
- Can include auxiliary information such as angles, temperature, salinity
- Can be constrained (is always constrained)
- Has a clear scope, which is defined by the training data set and its model
- Processing is very fast

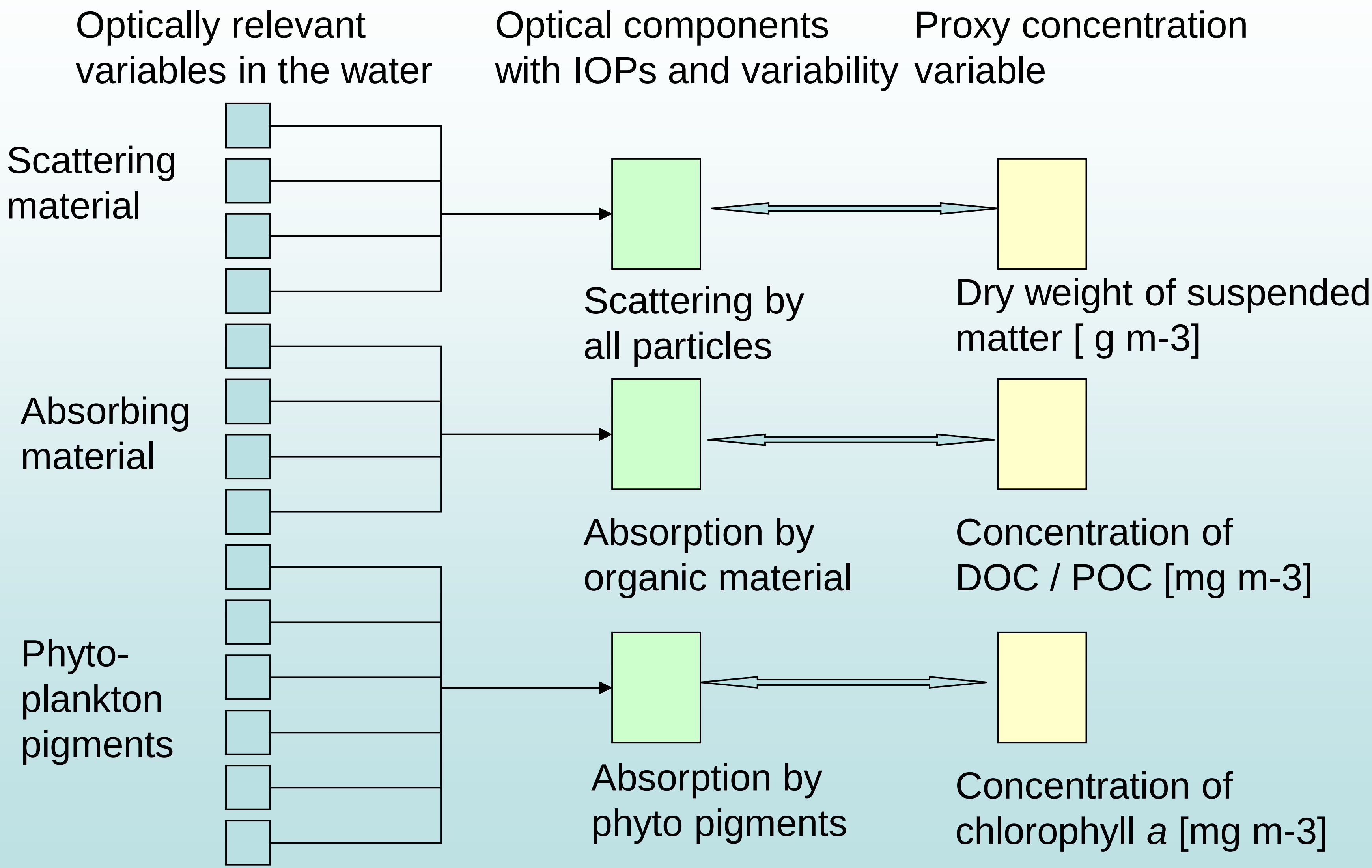
Cons

- Development and changes are time consuming
- Depends not only on the bio-optical / atmosphere model but also very much on the frequency distribution of the variables of the training data set
- The NN is determined by minimization of a mean error of the full training data set, i.e. single cases or certain ranges of cases still might have a large error
- Sensitive to overtraining by too many neurons, so that the interpolation power is lost

Expected uncertainties

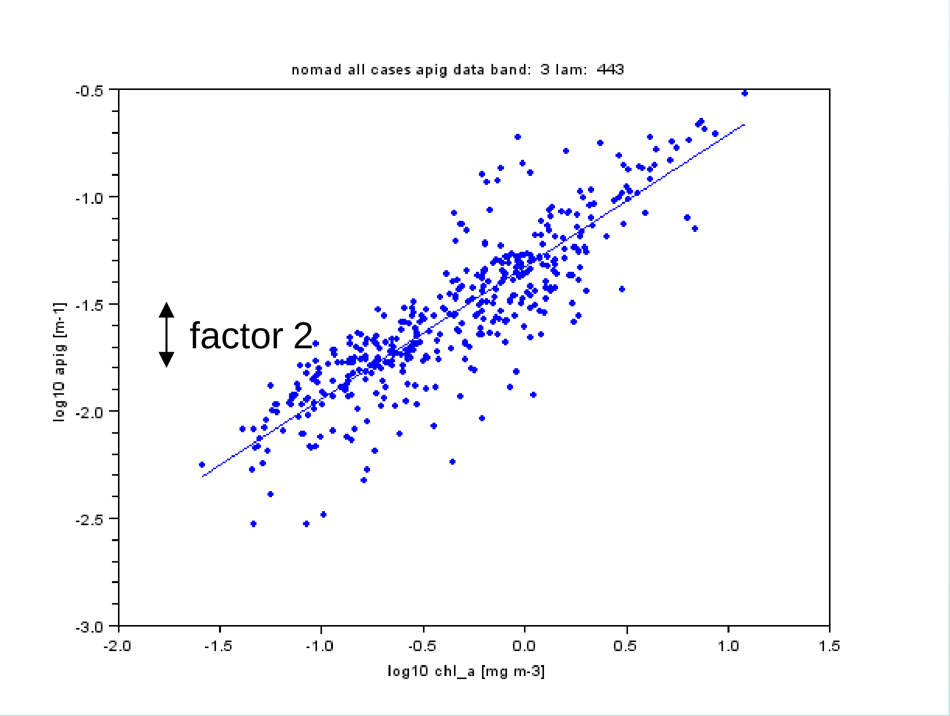
- Limitations by the bio-optical model
- Masking effect, saturation and ambiguities
- Relationship between concentrations and IOPs

Uncertainties due to the bio-optical model



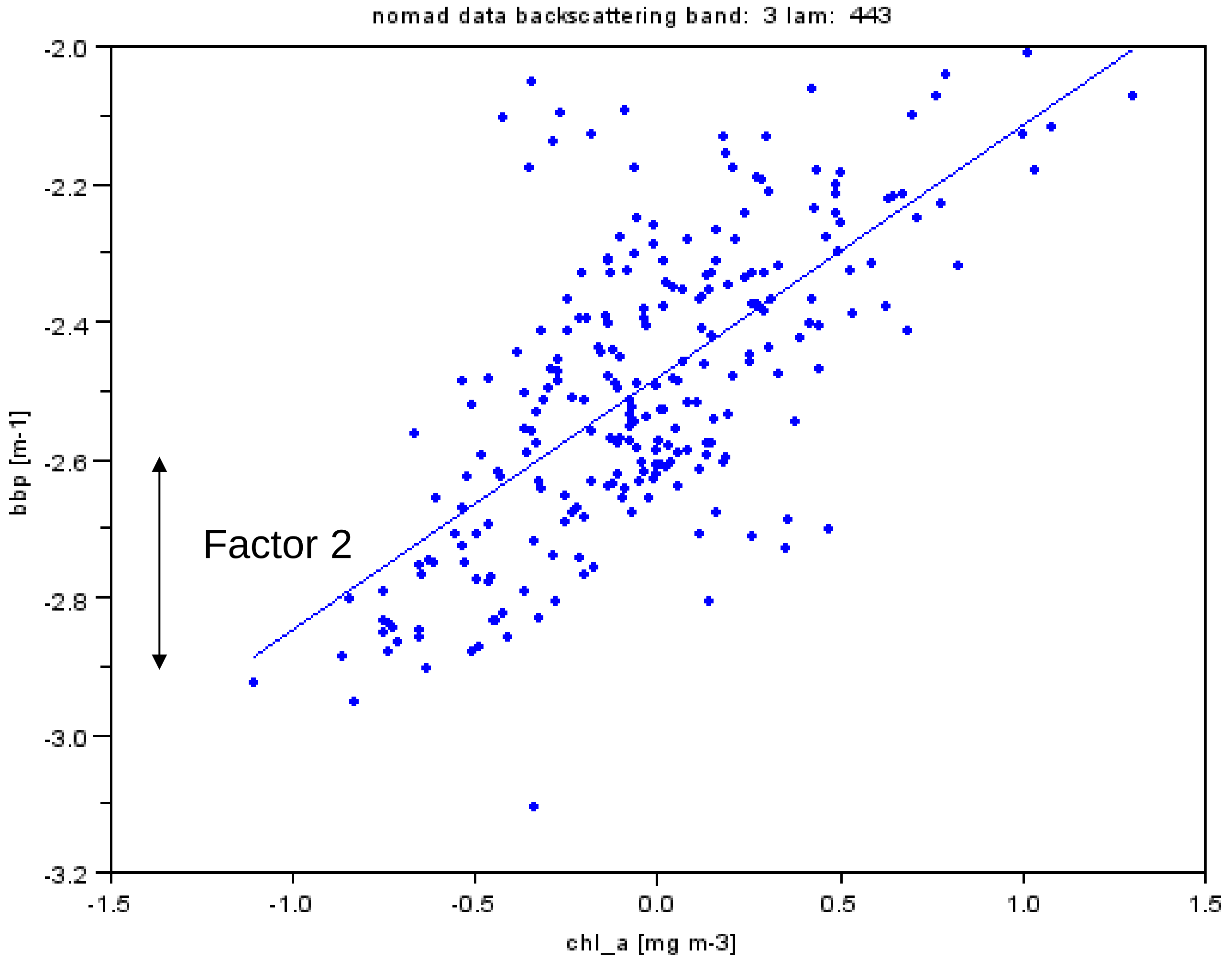
Uncertainty due to optical variability

- 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!



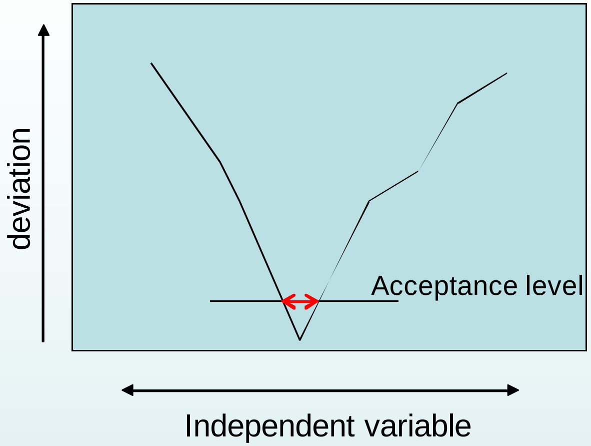
Relationship between log10 of chlorophyll a concentration and log10 of absorption coefficient of phytoplankton pigments

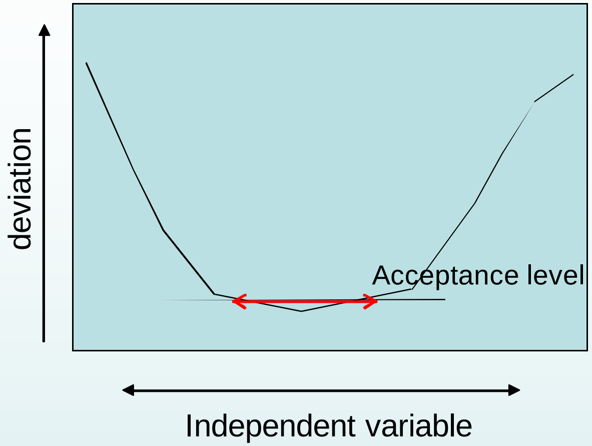
Relationship chl_f and backscattering coefficient



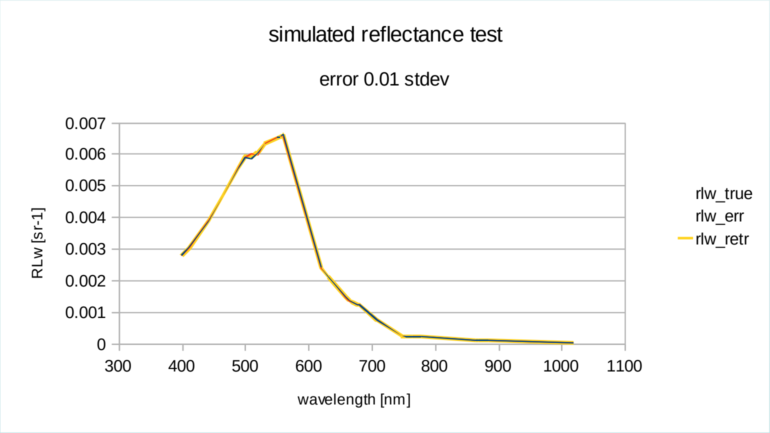
443 nm, 249 samples, log10 scale

Error due to masking and ambiguities





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



- True spectrum simulated
- „measured“ spectrum = true * random error
- Retrieved spectrum when LM has found solution

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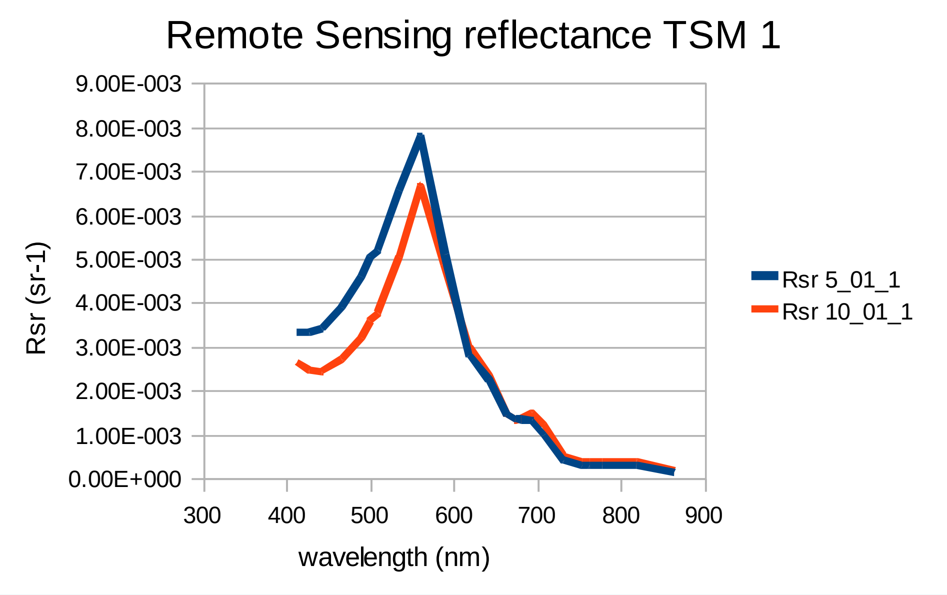
Results and errors of retrieval

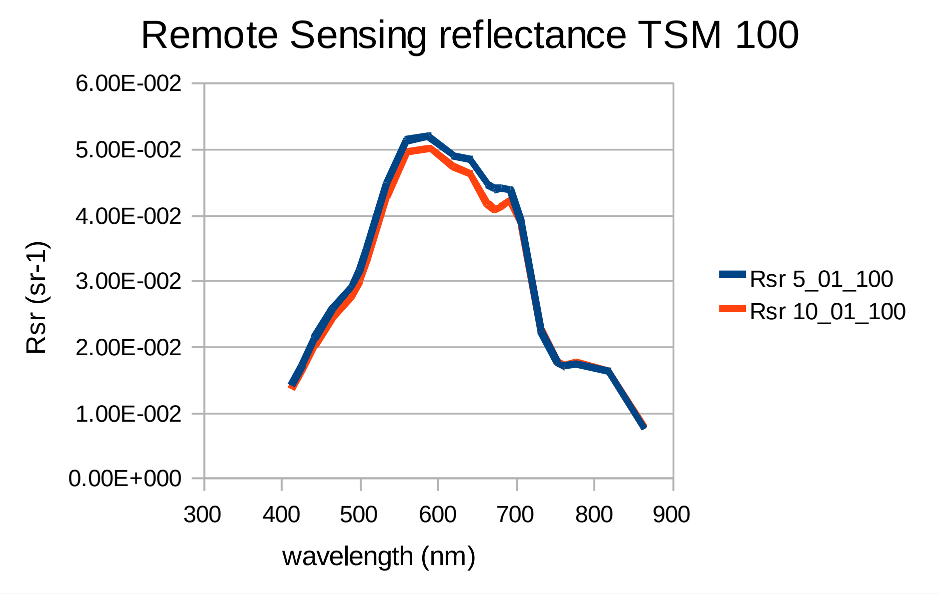
Variable	conc true	conc retr.	stdev of log_conc	err. estimated %	err true %
chlorophyll [mg m-3]	1	0.8337	0.09191	9.626	-19.94
detritus [g m-3]	1	1.152	0.1684	18.34	13.19
gelbstoff a443 [m-1]	0.1	0.1005	0.03566	3.63	0.4842
min. SPM [g m-3]	1	0.9948	0.006498	0.6519	-0.5238

kdmin_true: 0.2096
kdmin_ret: 0.2089
error: - 0.33%

kd490_true: 0.2636
kd490_ret: 0.2609
error: -1.04%

Sensitivity at different concentration ranges and spectral bands

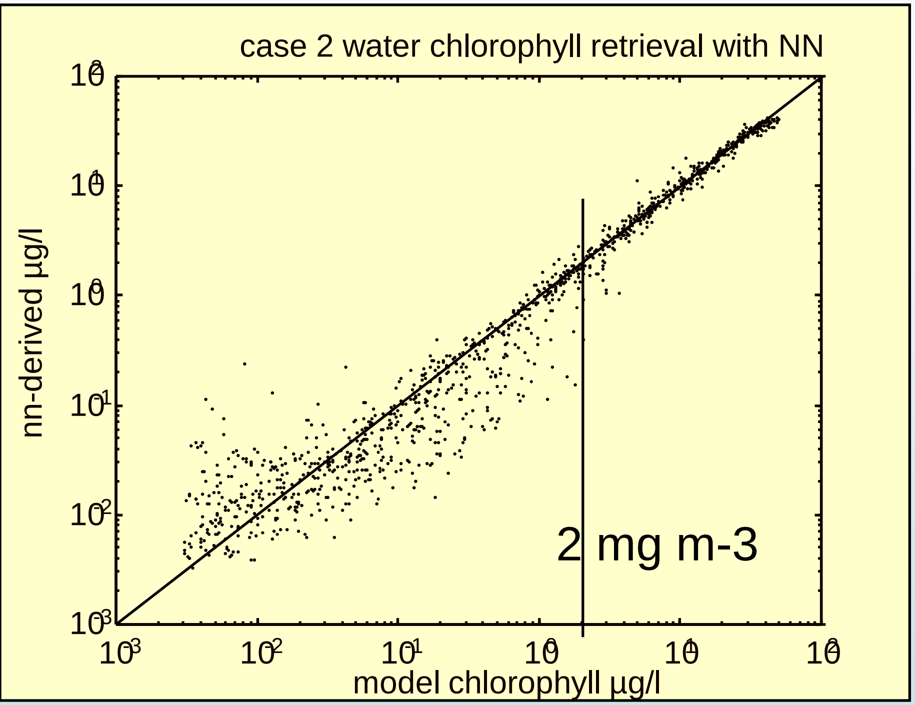


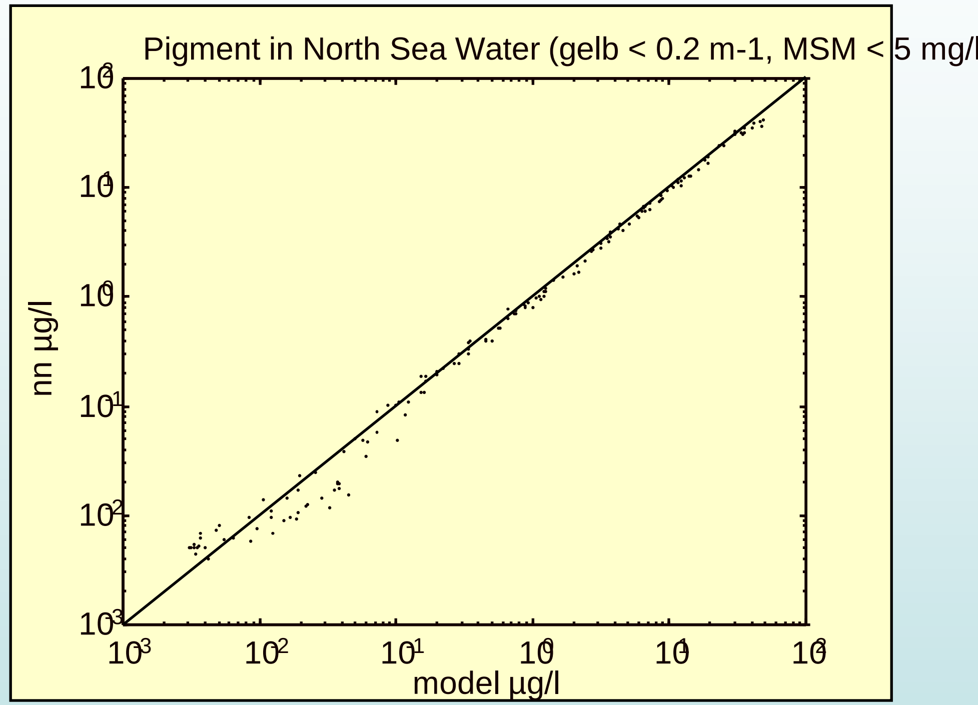


Chl. 5/10 mg m-3
TSM 1 g m-3
aYS(443) 0.1 m-1

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

Uncertainties due to ambiguities for different concentration mixtures

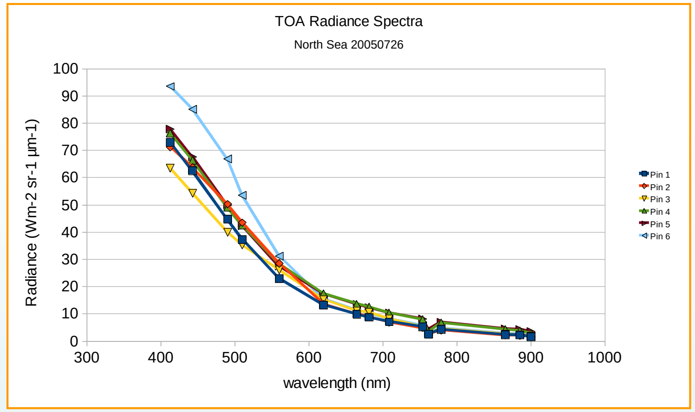




All cases of turbid water

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

What determines the radiance spectrum at TOA



air molecules

different aerosols

thin clouds

contrails

Sky reflectance

Sun glint

foam

floating material

Suspended particles

dissolved organic matter

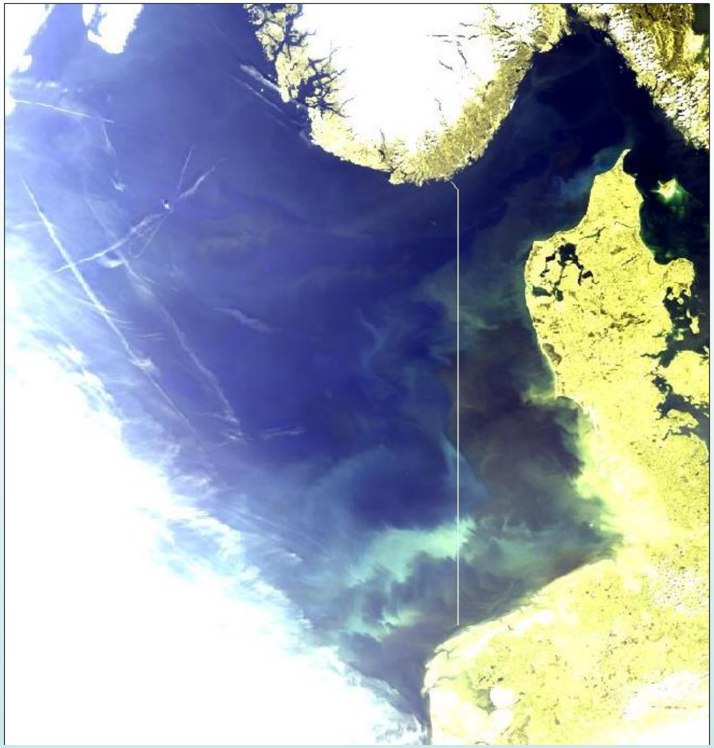
Vertical distribution

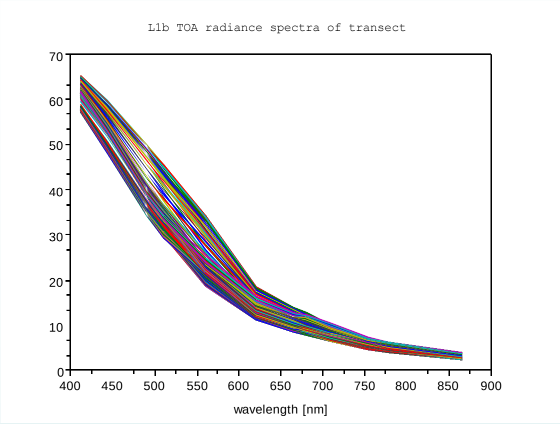
chlorophyll

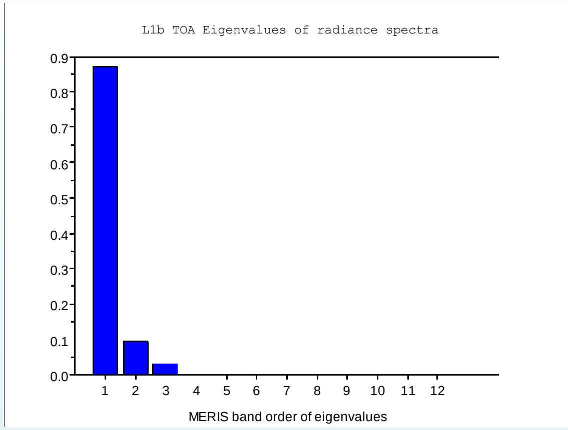
Bottom reflection

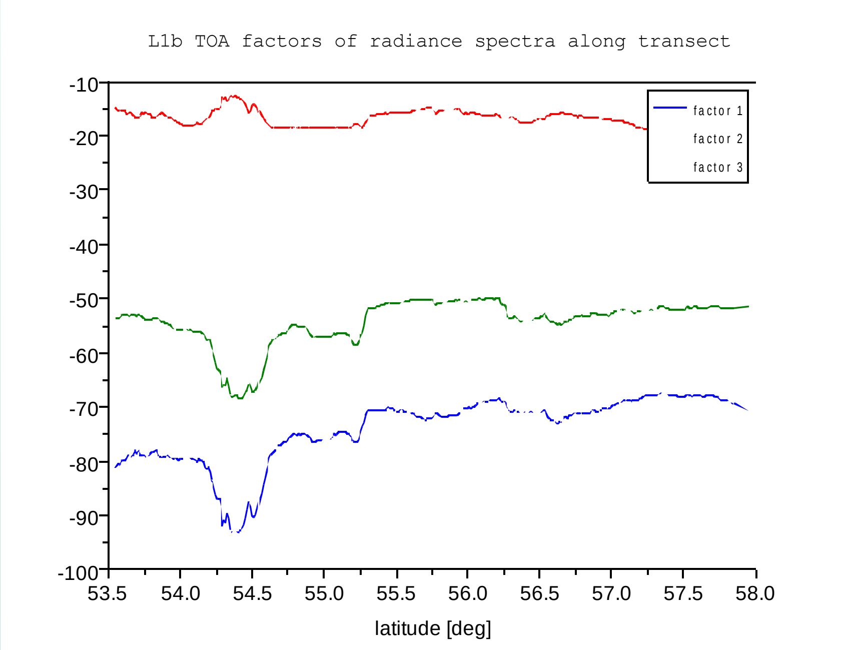
different phytoplankton species

Information content: PCA

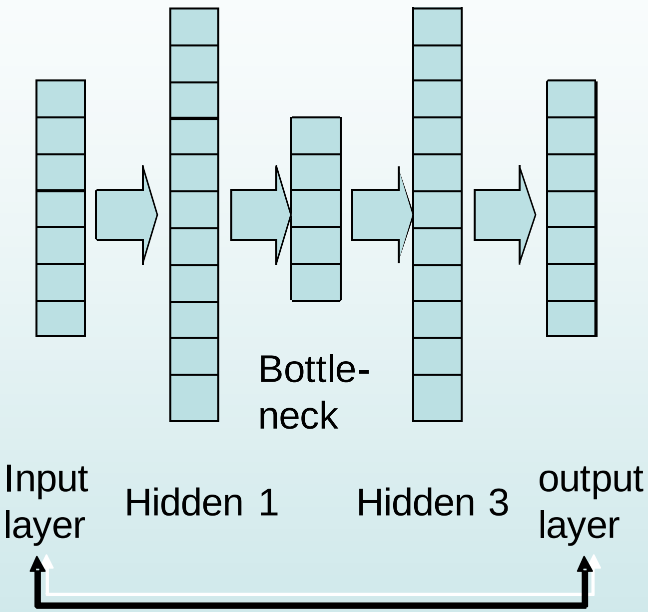




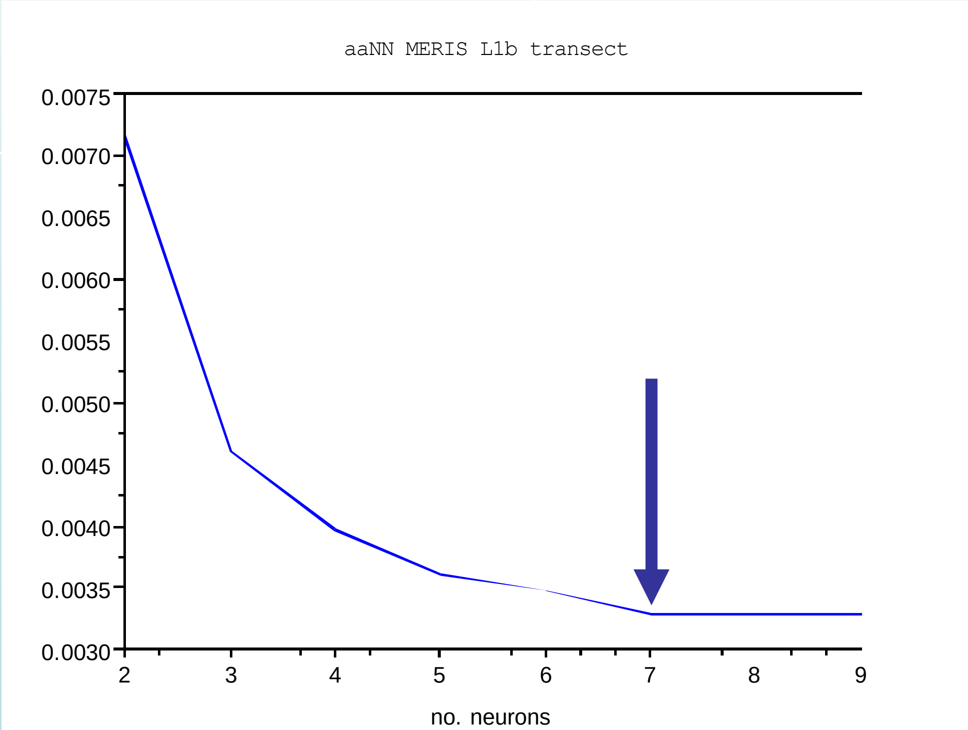




Information content: aaNN



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



The bio-optical model for Coastcolour

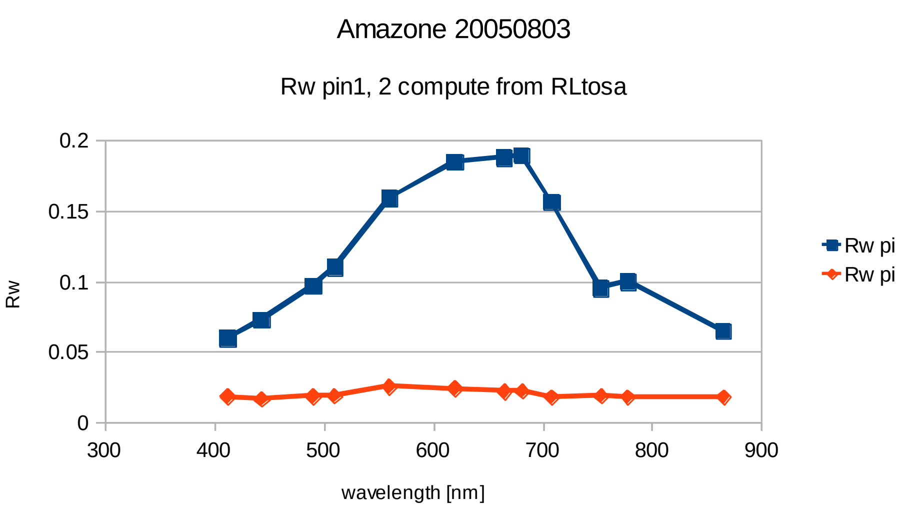
Requirements

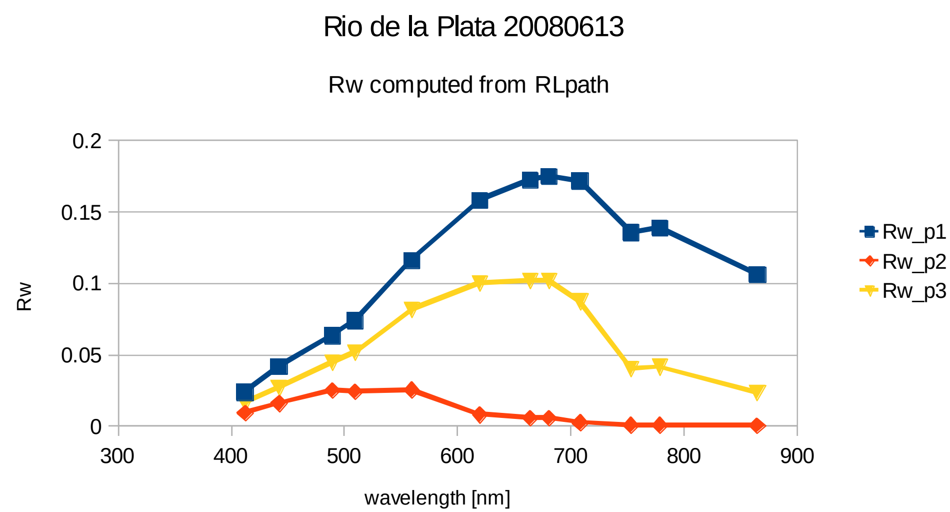
- Shall reproduce NOMAD IOP data set
- Shall reproduce reflectances of MERMAID data set
- Shall include all coastal water cases including
  - areas with extremely high suspended matter concentrations and
  - areas with extremely high concentrations of humic substances
  - Clear ocean water conditions

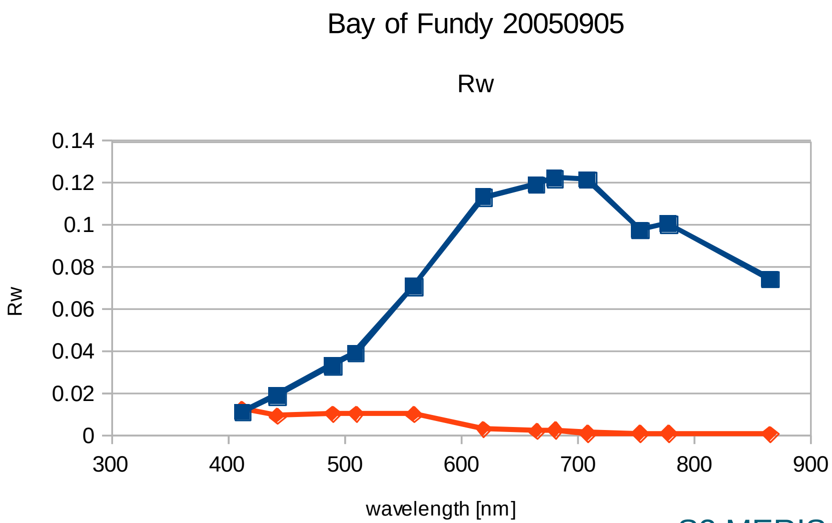
Strategy

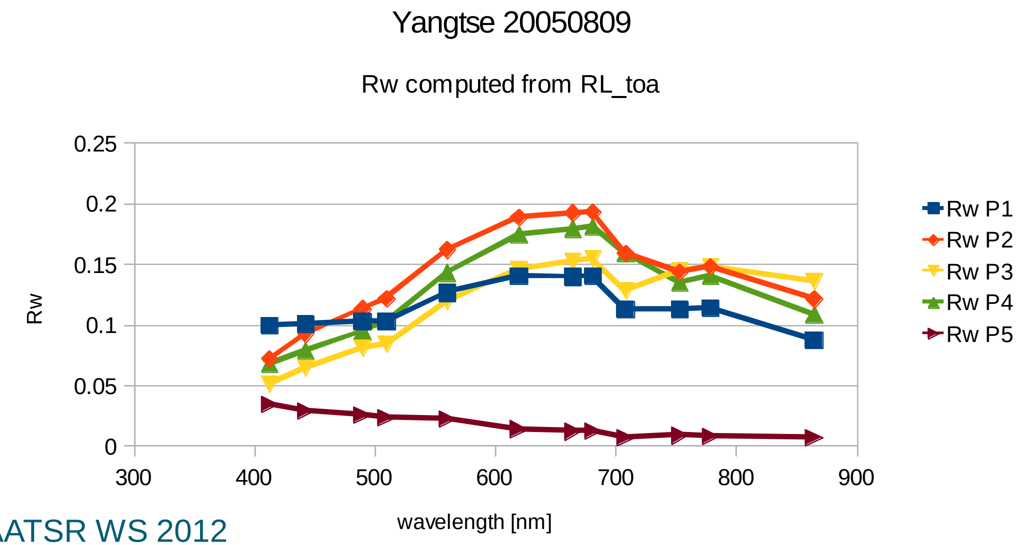
- Define parameters to characterize the frequency distributions of IOPs and reflectance spectra
- Characterize IOPs of NOMAD data set and reflectaces of MERMAID data
- Define and adapt bio-optical model and produce a simulated training data set with ranges and frequency distribution, which meet the parameters of the measured data
- Extend bio-optical model to cover also the extreme cases

Max reflexion spectra in turbid estuaries





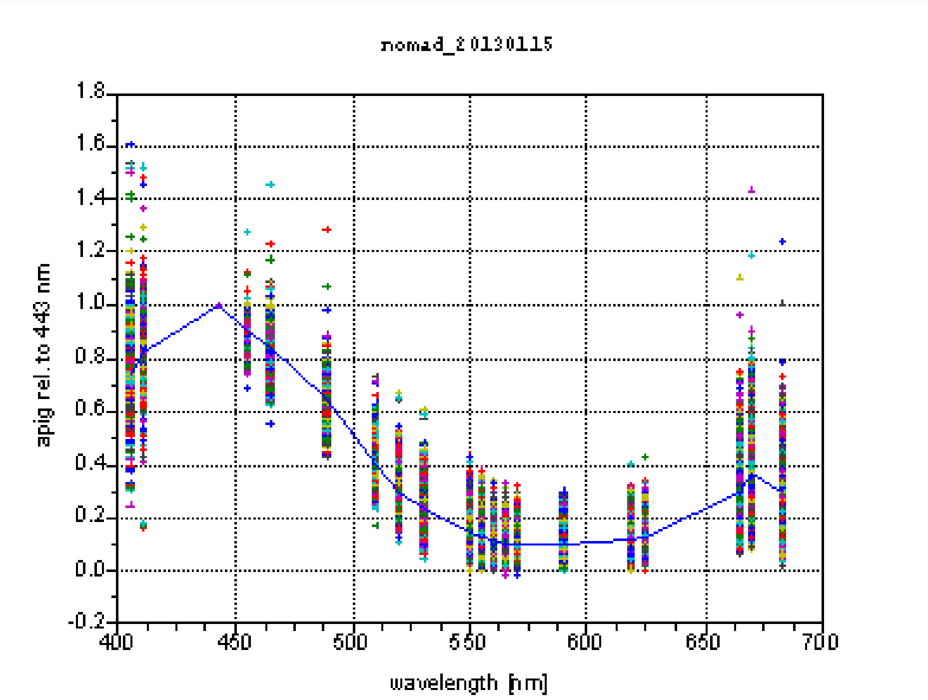




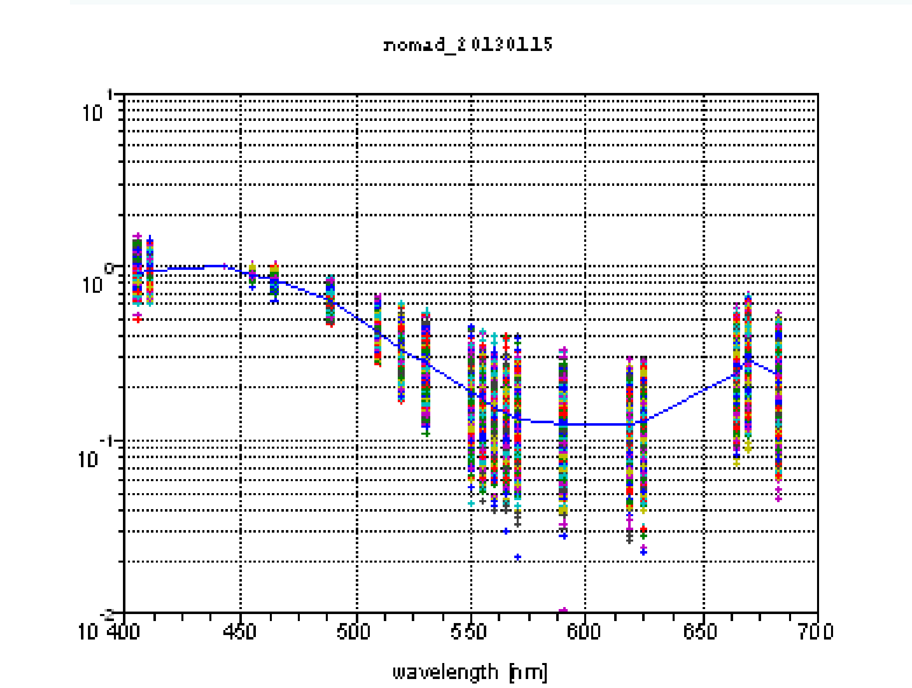
Definition of components

- Coastcolour bio-optical model is based on 5 IOP components
  - Phytoplankton pigment absorption (a_pig)
  - Detritus absorption (a_det)
  - Yellow substance absorption (a_gelb)
  - Particulate matter scattering (b_part)
  - White scatterers (b_wit)
- These 5 IOP components are also reduced to 3 IOP components:
  - A_pig
  - Adg (absorption by a_det + a_gelb)
  - TSM scattering (scattering by b_part + b_wit)
- Spectral optical properties have been derived from NOMAD data set
- Concentration Ranges have been determined
  - to cover water reflectance spectra of NOMAD and MERMAID
  - Extended to include extreme coastal and estuarine water (Rio de La Plata with high scattering , Lena river with high absoption, etc.)

NOMAD pigment absorption spectra

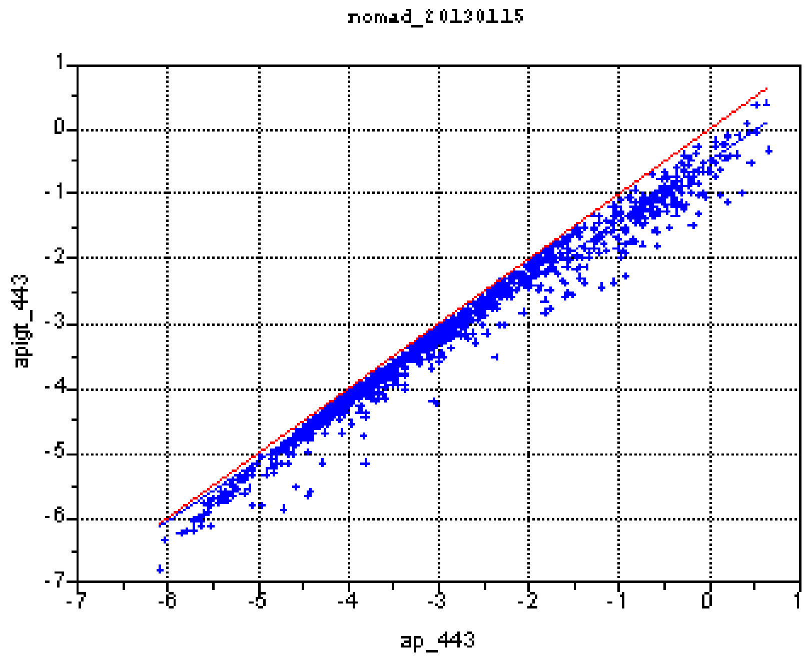


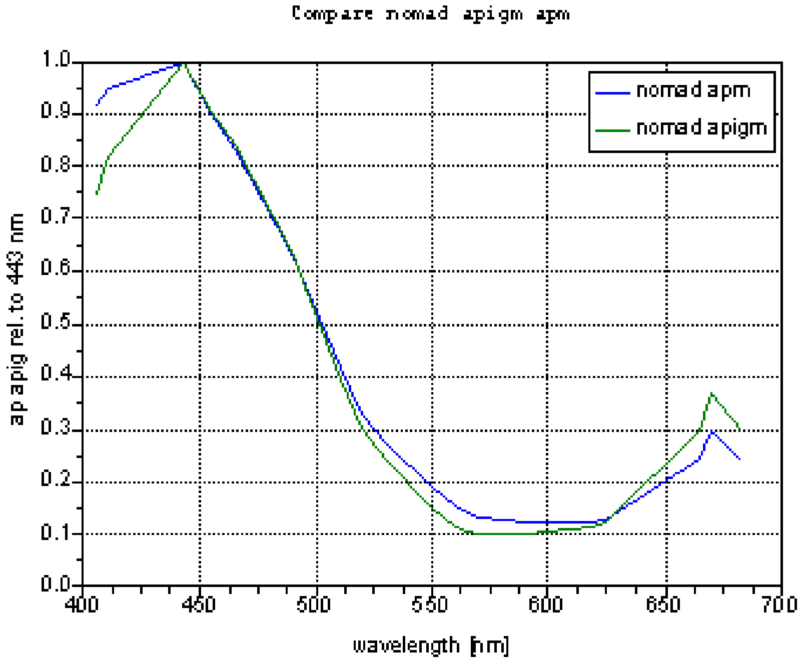
A_pig lin normalized at 443 nm



A_pig log normalized at 443 nm

NOMAD: Relationship between total particle absorption and pigment absorption



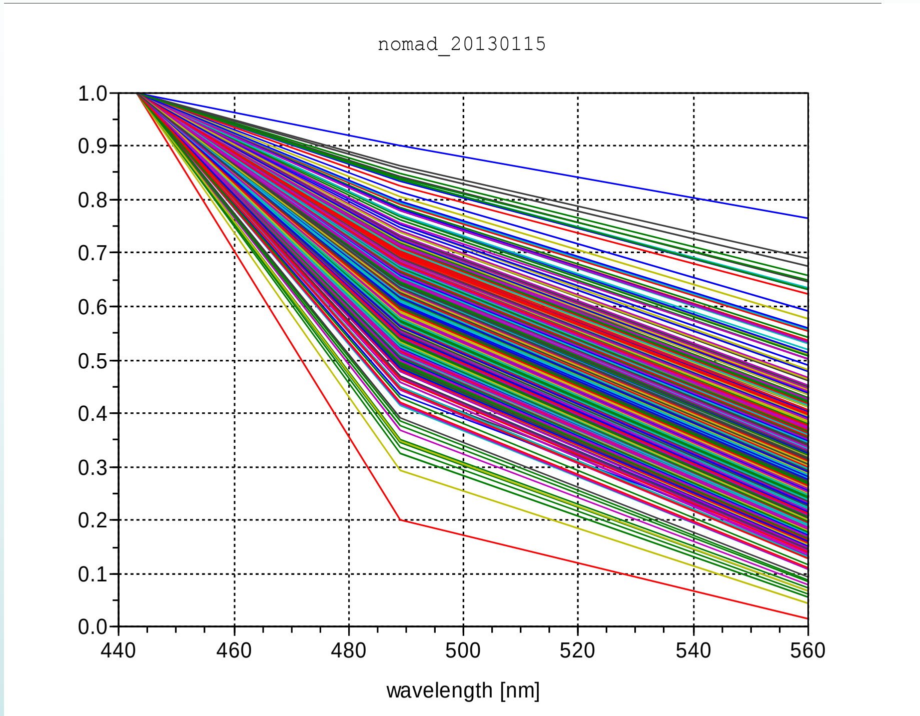


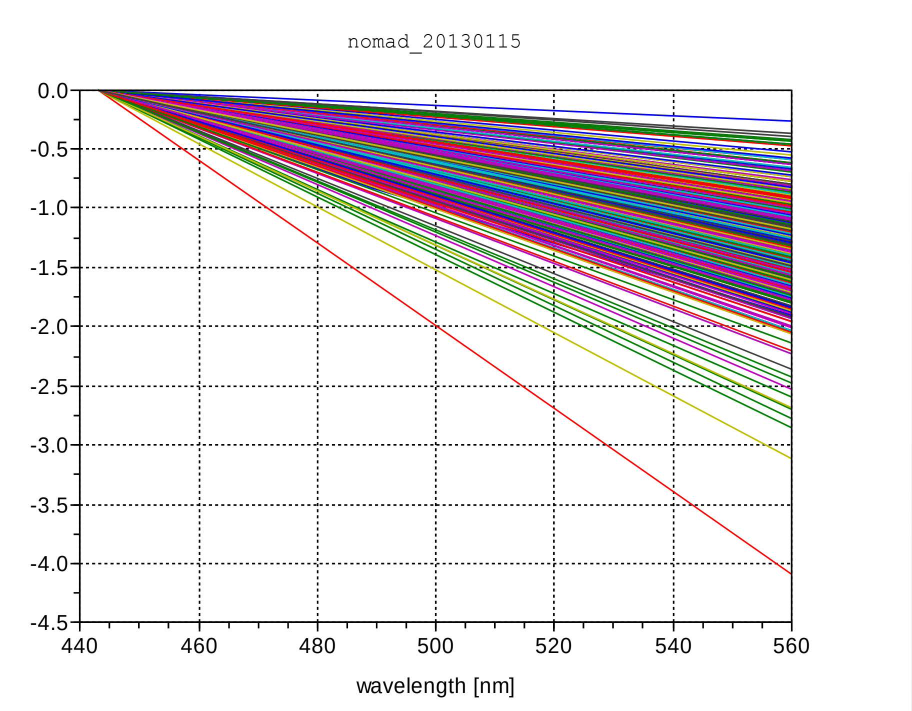
a_pig vs a_p, log scale

Mean absorption spectra of a_pig and a_p

a_pig= exp(log_ap*0.924 - 0.502 - 0.4+rand()*0.8)

NOMAD: wavelength aborption slope of ad





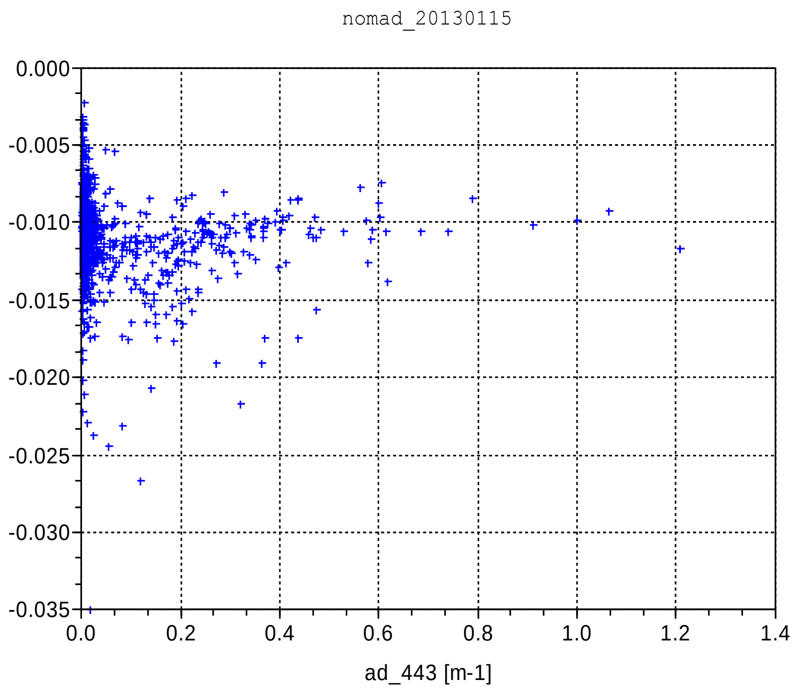
lin

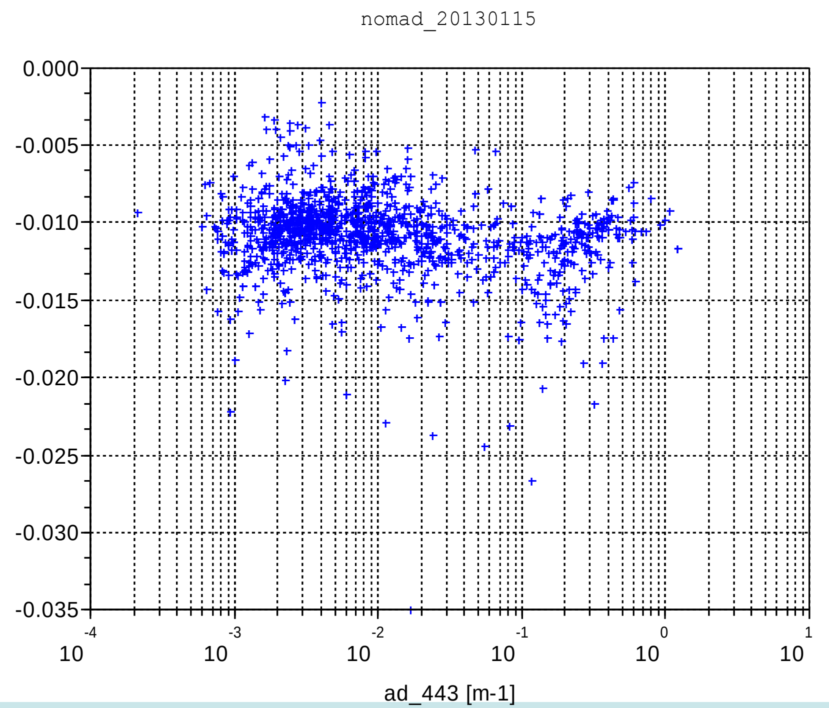
log

slope s, computed from logn(ad560) /(560-443)

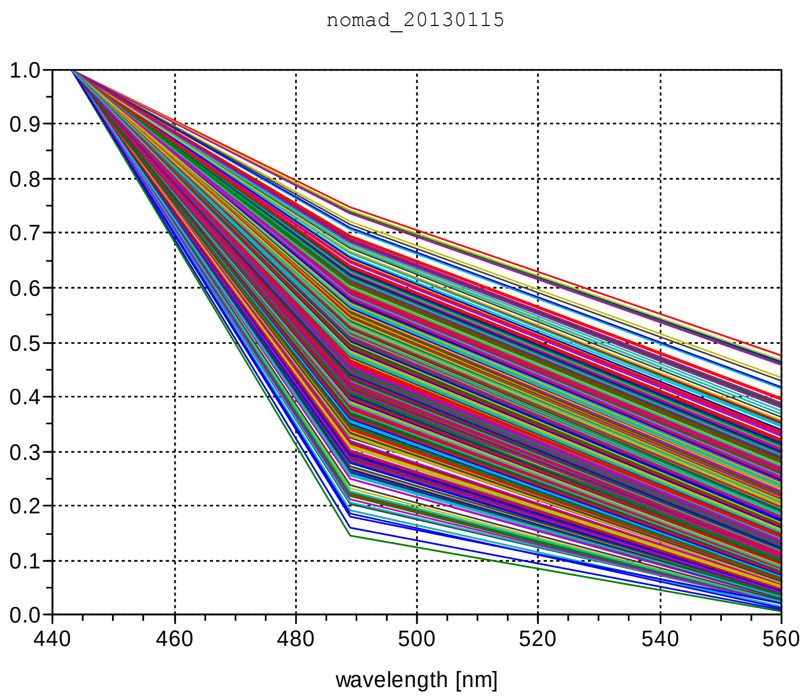
mean s: 0.0108, min s: 0.00228, max s: 0.0349, 5-95% percentile: 0.00738 - 0.015

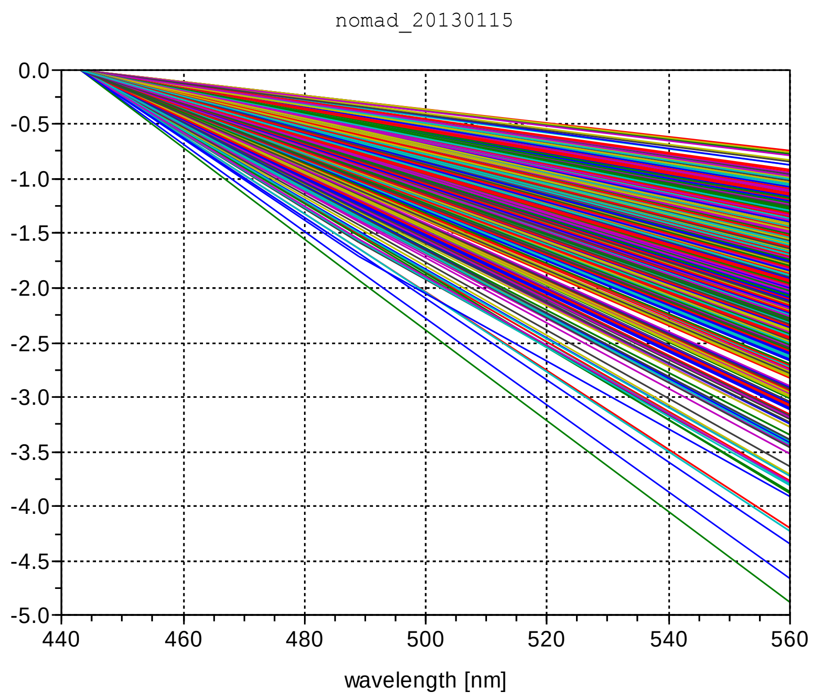
NOMAD: ad wavelength slope as a function of ad_443





NOMAD: wavelength aborption slope s of ag

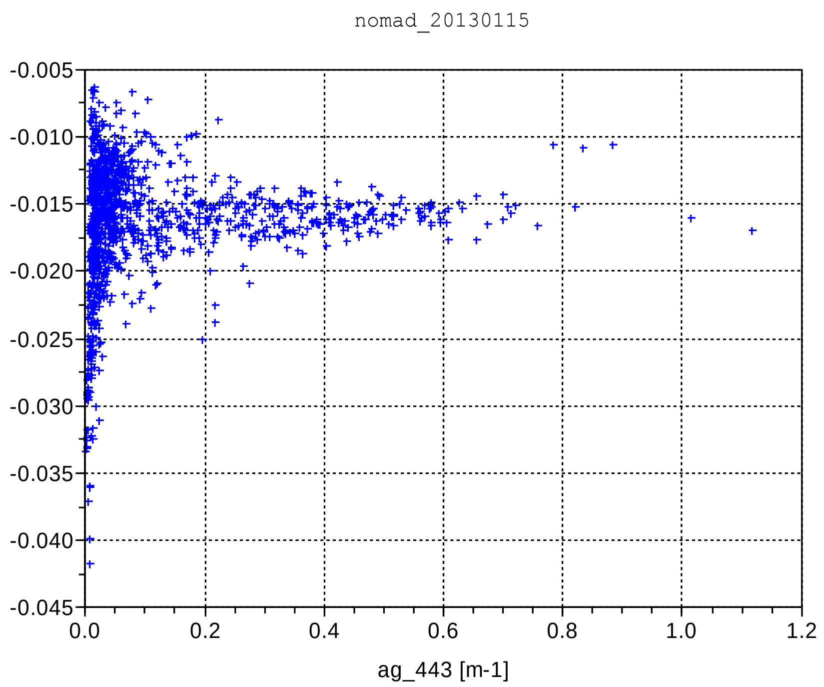


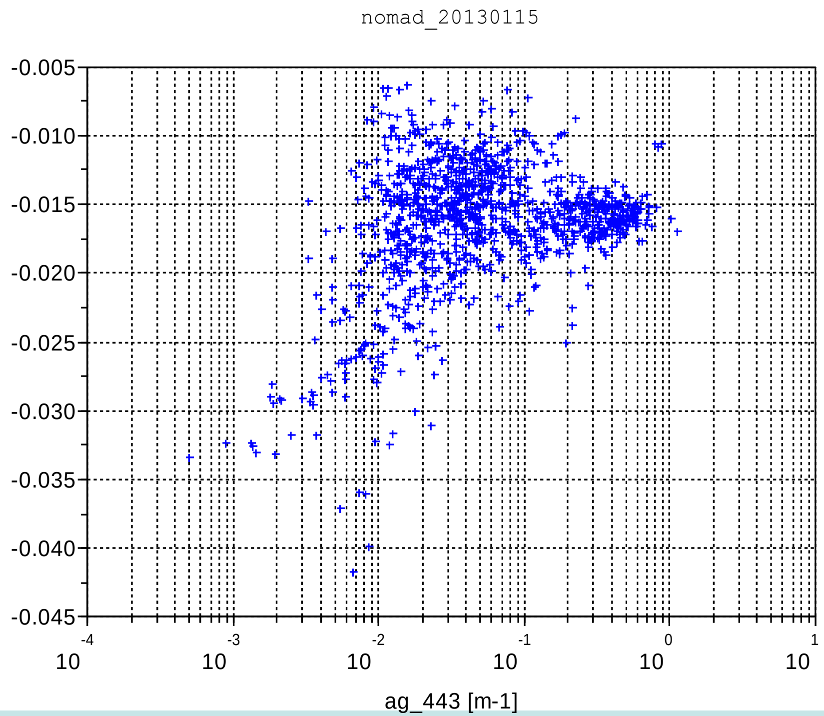


slope s, computed from logn(ag560) /(560-443)

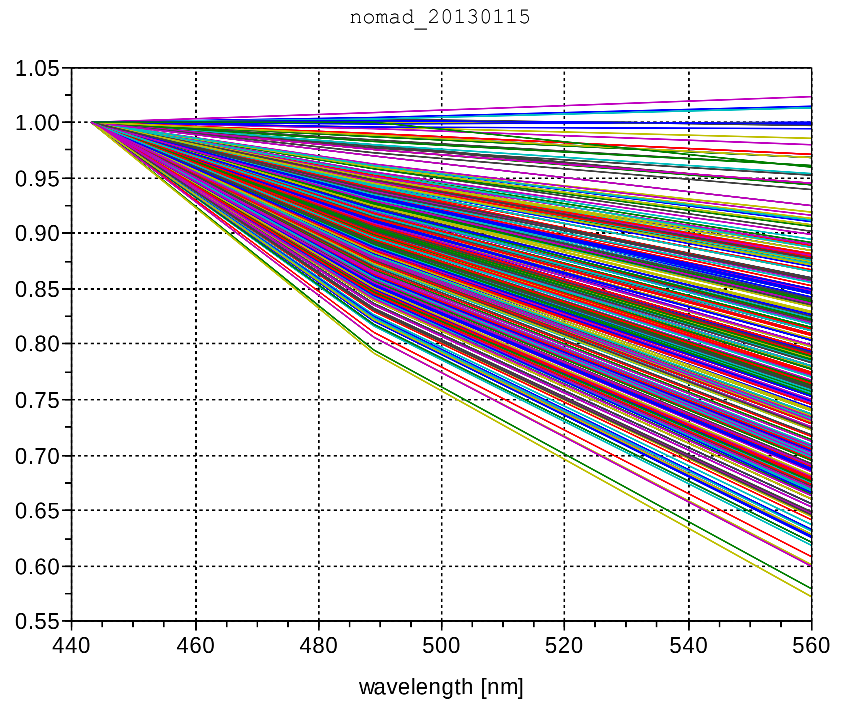
mean s: 0.0163, min s: 0.00635, max s: 0.0417, 5-95% percentile: 0.0105 - 0.025

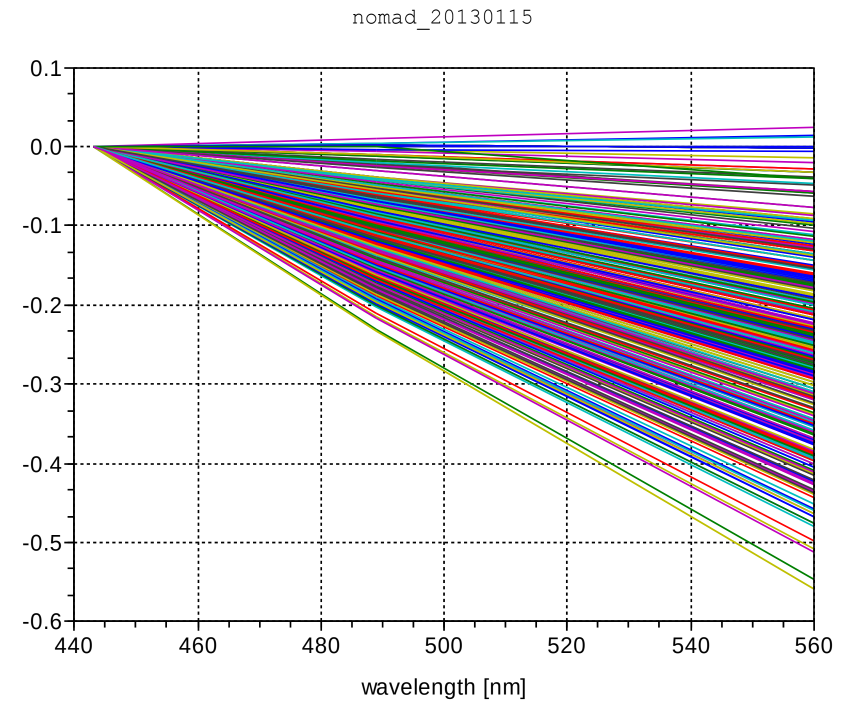
NOMAD: ad wavelength slope as a function of ag_443





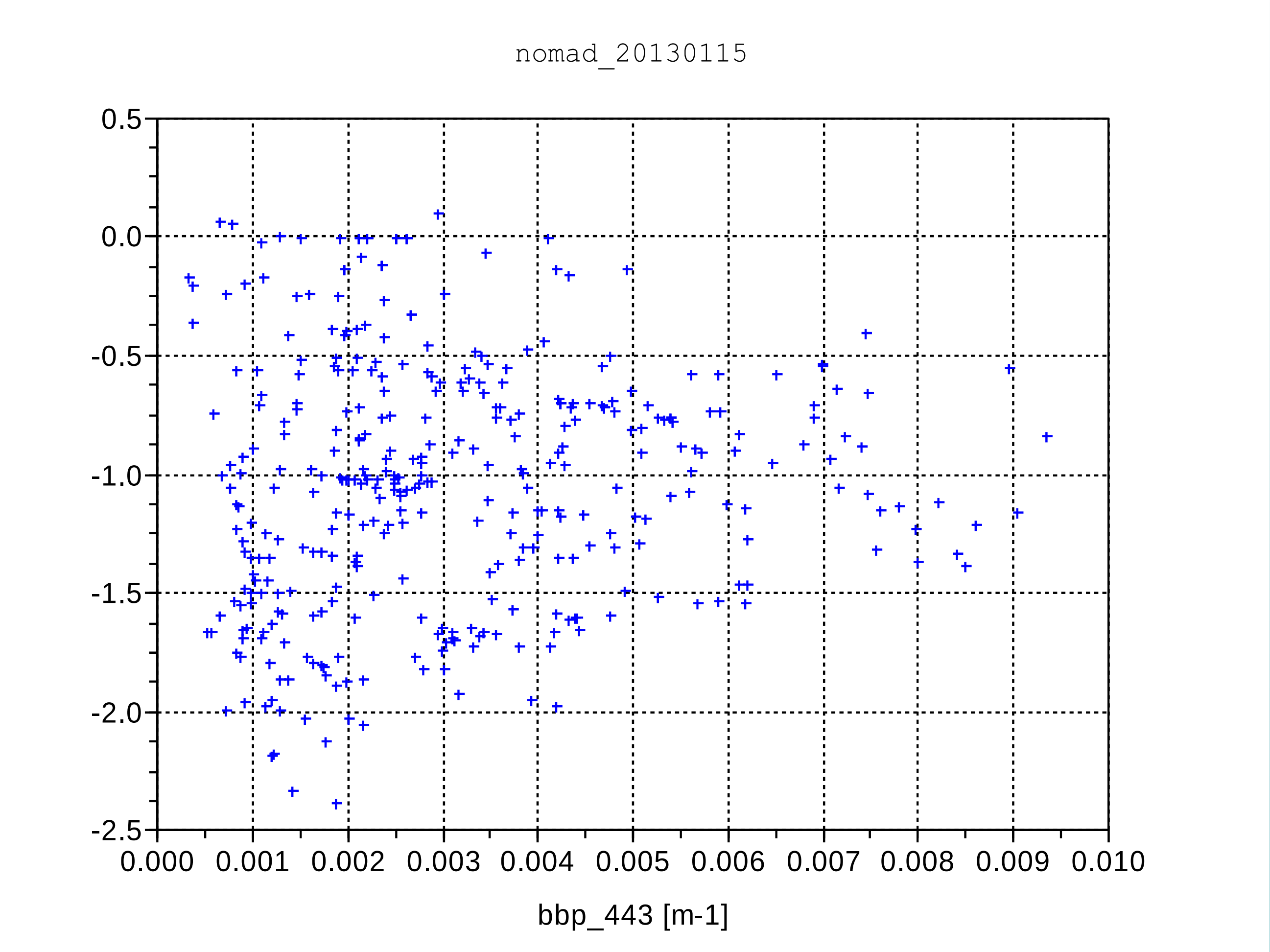
NOMAD: normalized (443 nm) scattering spectra





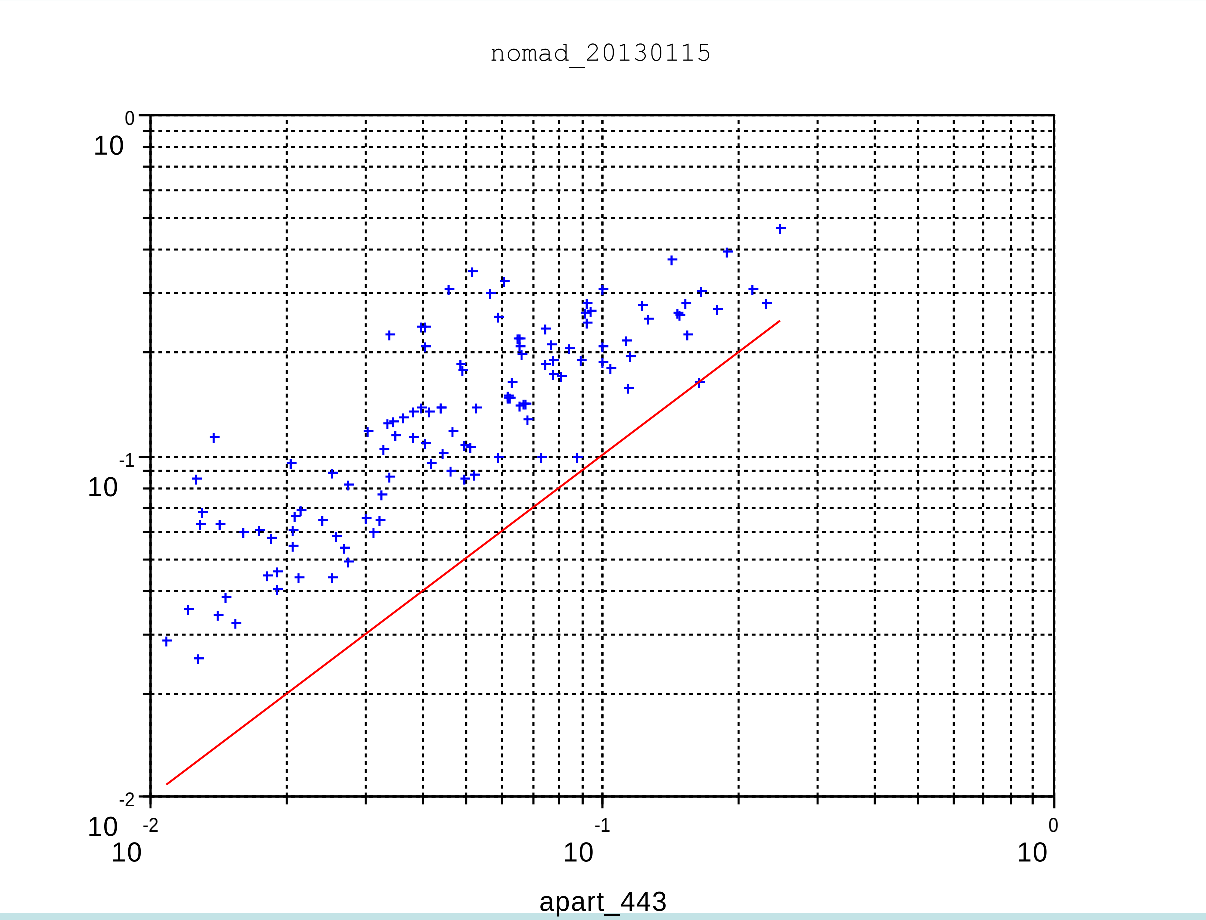
mean s: -1.03, min s: 0.1, max s: -2.4, 5-95% percentile: -0.104 - -1.87

NOMAD: Wavelength exponent of particle backscattering coefficient s

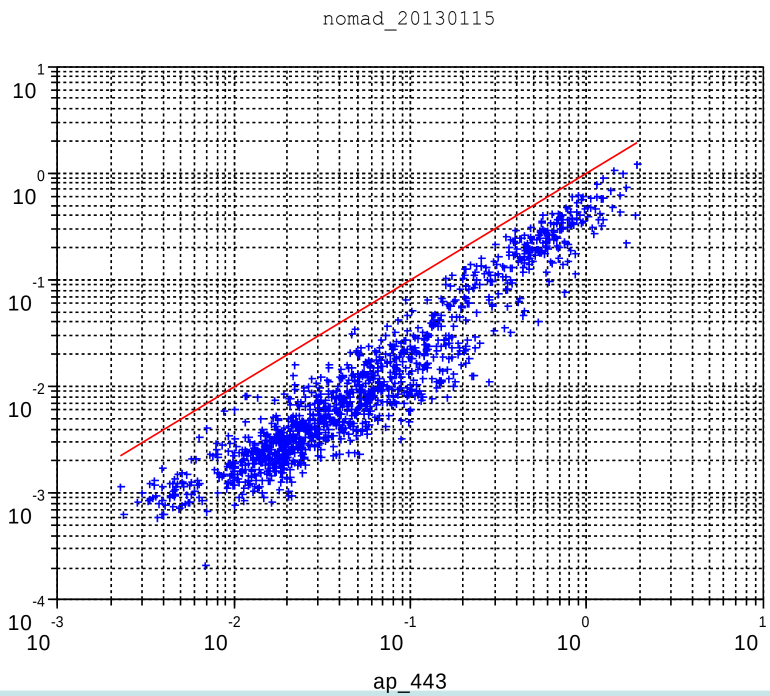


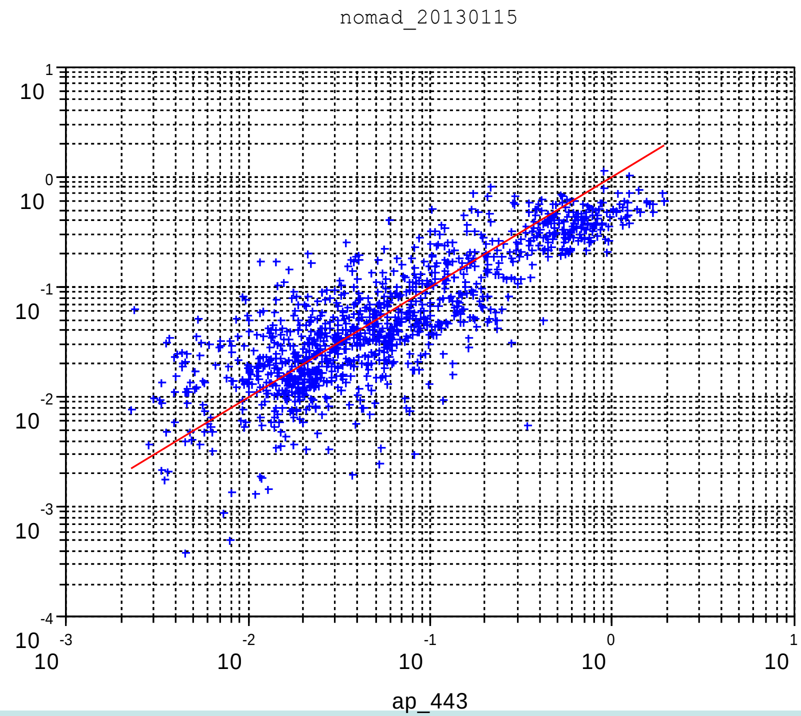
$bbp(\lambda) = bbp(443)*(\lambda/443)^s$

NOMAD: Relationship between bp and ap

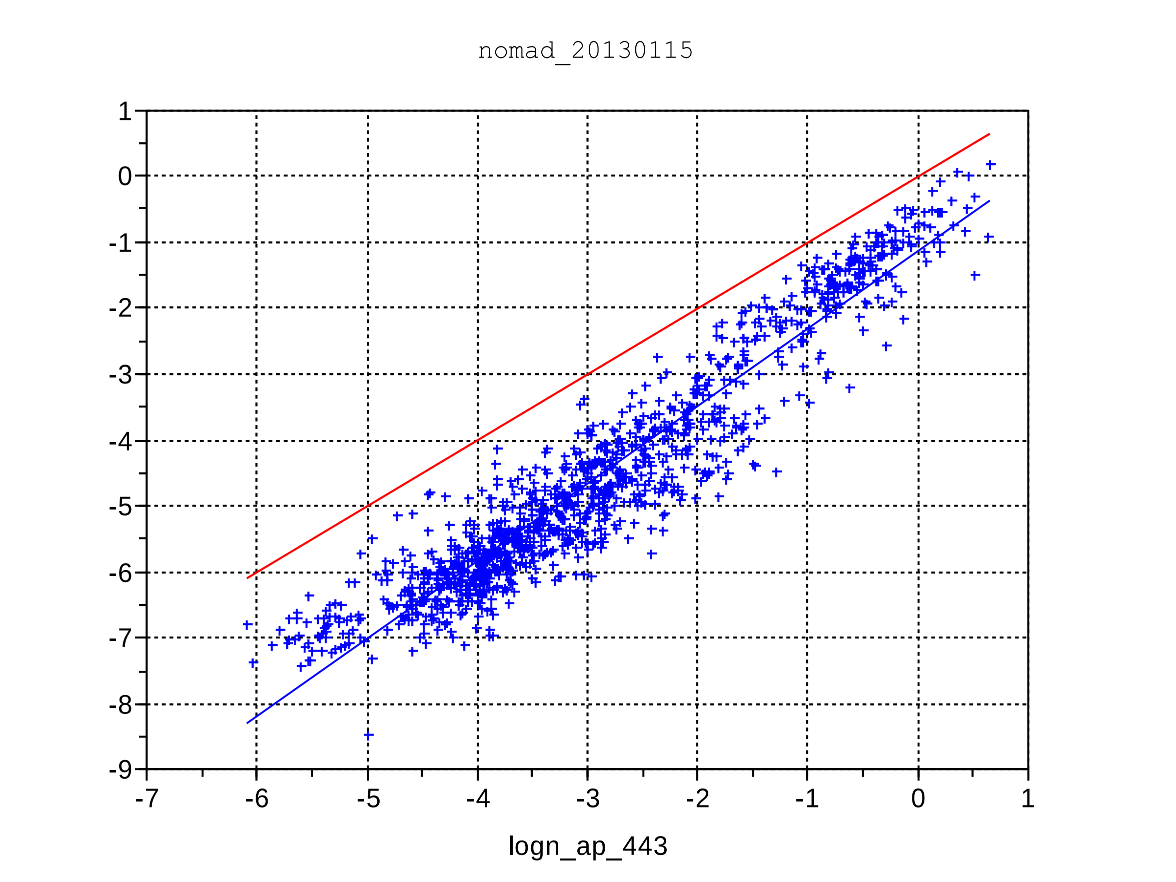


Relationship between ad / ap and ag / ap





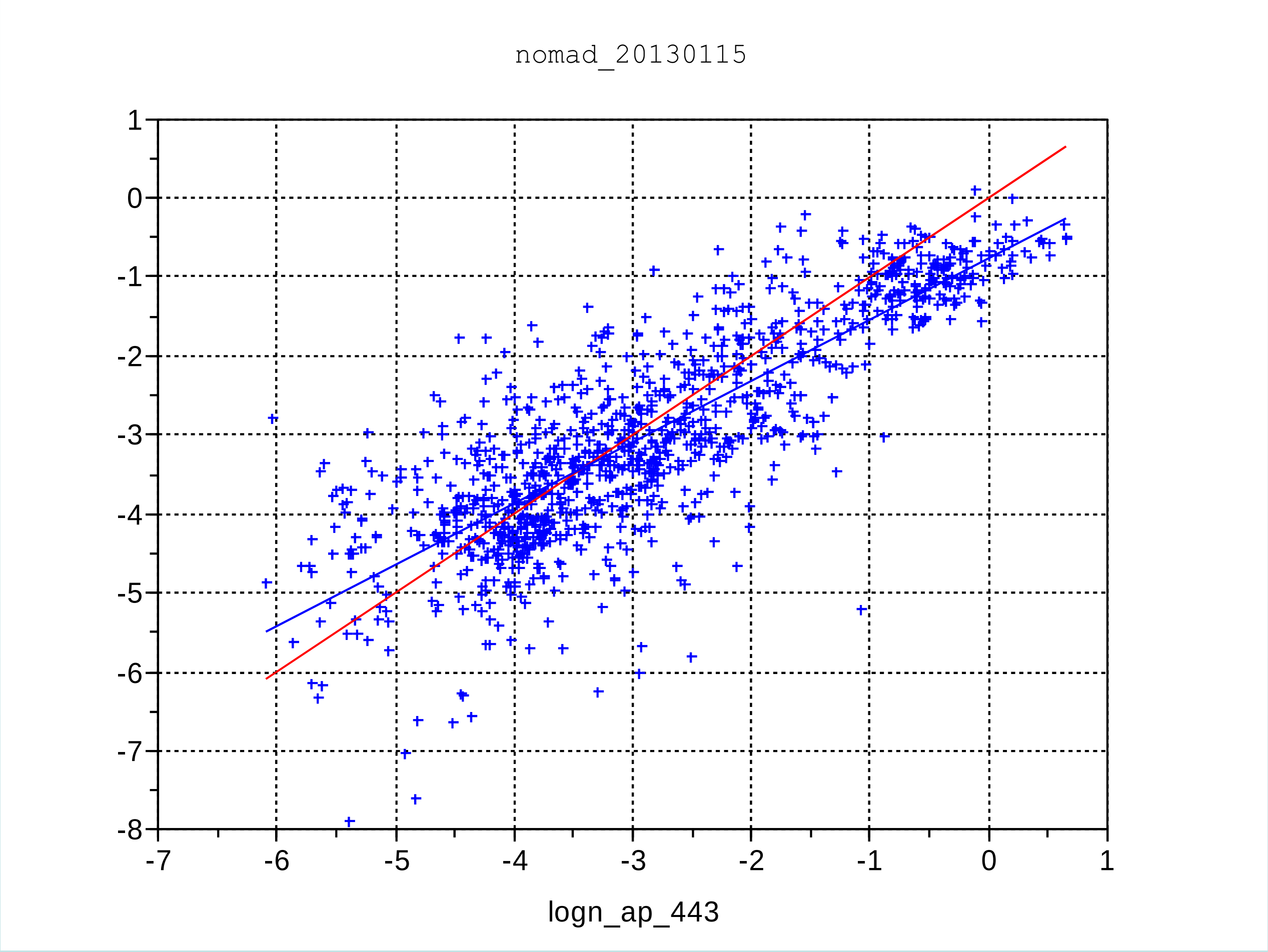
Relationship between ad / ap



logn_ad_443 = logn_ap_443 * 1.172 - 1.152 +- 0.5

ad_443 =exp(logn_ap_443*1.172 -1.152 - 1 + rand()*2.0)

Relationship between ag / ap



a=0.7754, b=- 0.771, sig=0.751

ag_443 = exp(log_ap_443*0.7754 - 0.771 - 1.5 + rand() * 3.0)

Bio-optical model for NOMAD range

- 1. ap particle absorption
  - ap_443 range: 0.002 -2 m-1
- 2. ad Detritus absorption
  - ad_443: 0.0005 - 1 m-1
  - slope: 0.005 - 0.015
- 3. Gelbstoff absorption
  - ag_443: 0.001 -1 m-1
  - slope: 0.01 - 0.025
- 4. Particle Scattering
  - bbp_443: 0.0002 - 0.01, entspricht bp wenn mit 50 multipliziert: bp 0.01 - 0.5, erweitert bis 1.0
  - slope 0.0 - 2.0

NOMAD: Bio-optical model co-variances

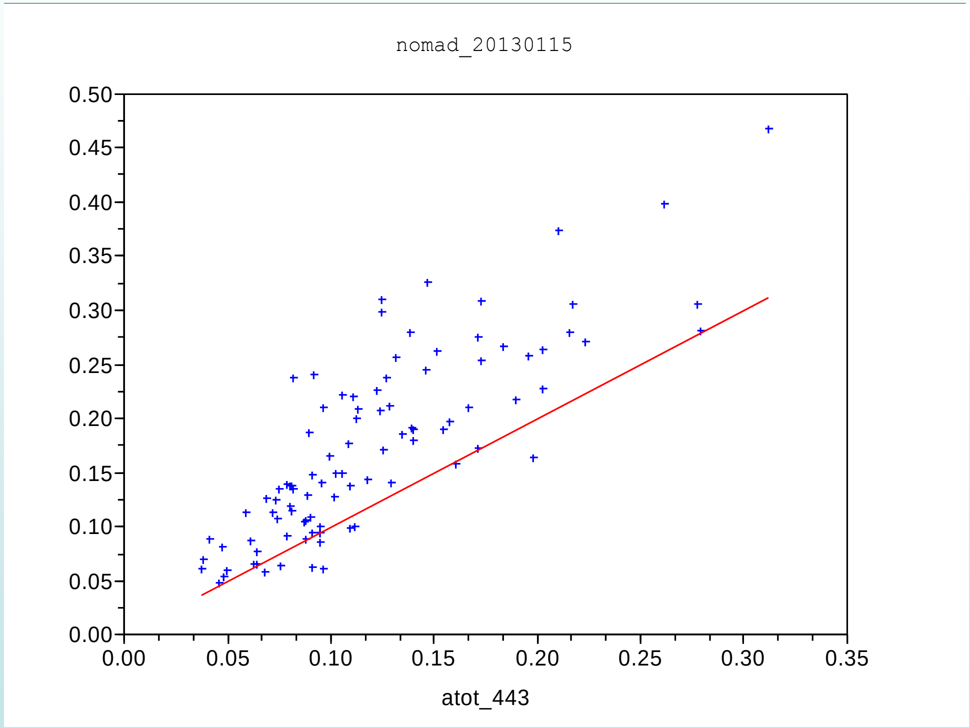
- particle absorption and particle scattering
  - log/bp/ap)= -0.364*log_ap-0.0774, sig = 0.328
  - follows: bp =exp(-0.364*log_ap-0.0774 +- 0.5) *ap
  - bp =exp(-0.364*log_ap - 0.0774 - 0.5+ rand()*1) *ap
-

- detritus absorption
  - log_ad_443=log(ap_443) +- 1.61
  - ad_443 = exp(log(ap_443) -1.61 +rand()*3.22)
  - ad_443 =exp(logn_ap_443*1.172 -1.152 - 1 + rand()*2.0)

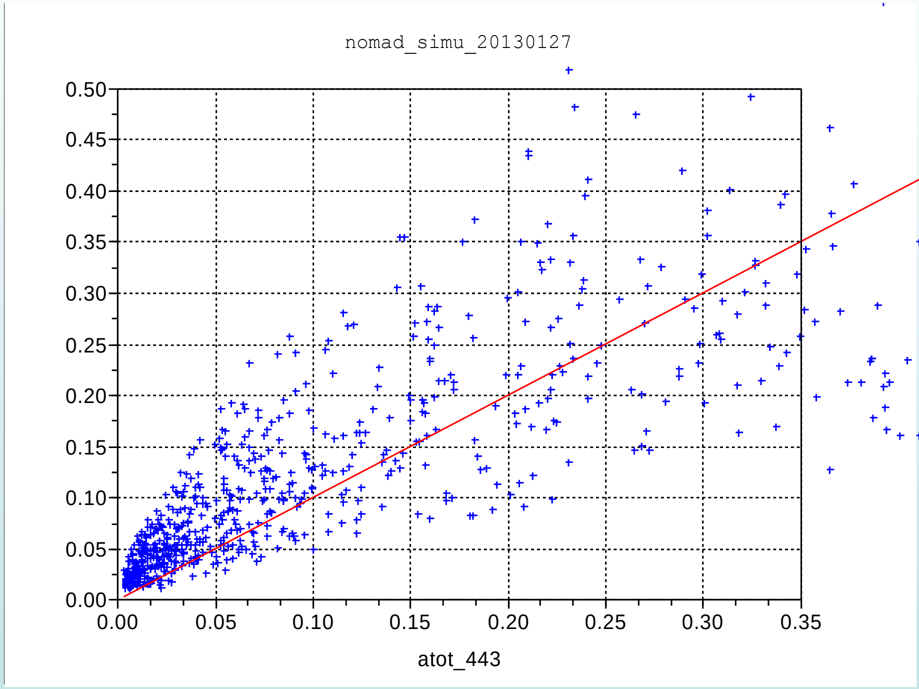
- apig 443 = ap443 - ad_443;
-

- Gelbstoff absorption
  - ag_443 = exp(log_ap_443*0.7754 - 0.771 - 1.5 + rand() * 3.0)

Test of simulated data: btot vs. Atot at 443 nm

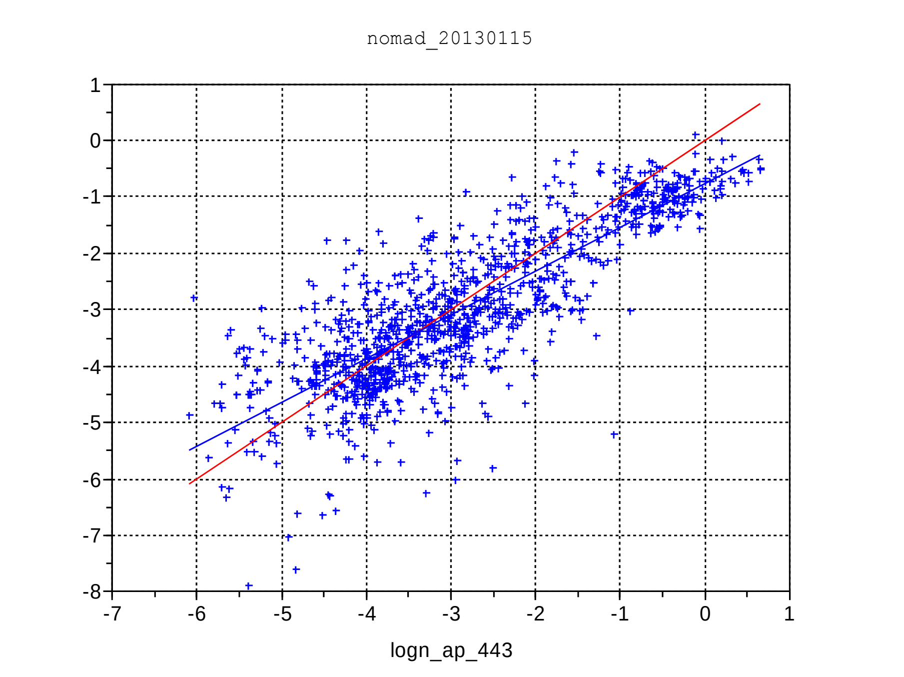


NOMAD

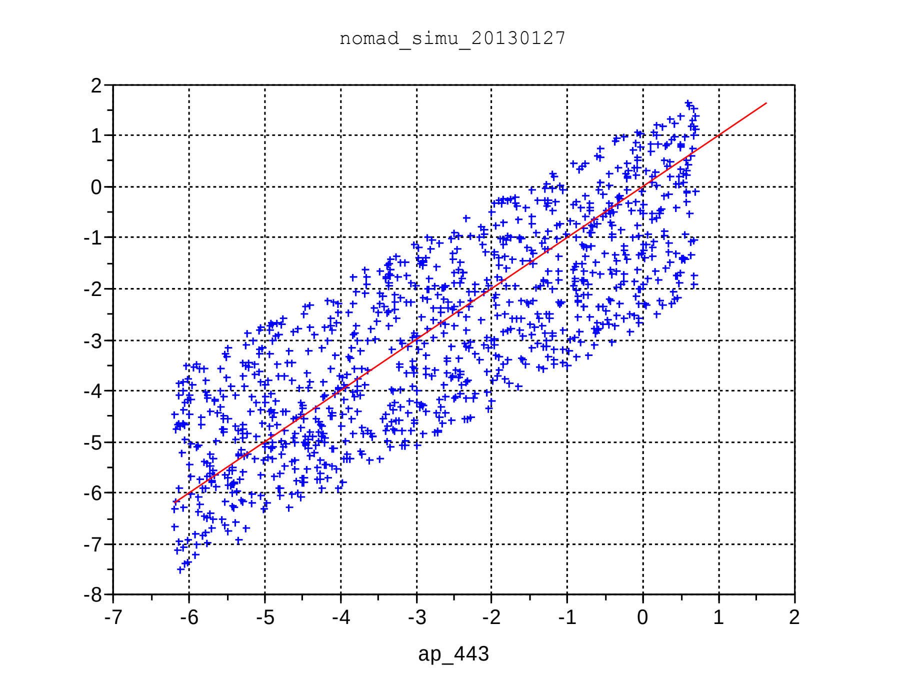


simulated

Compare ag_443 vs. ap_443

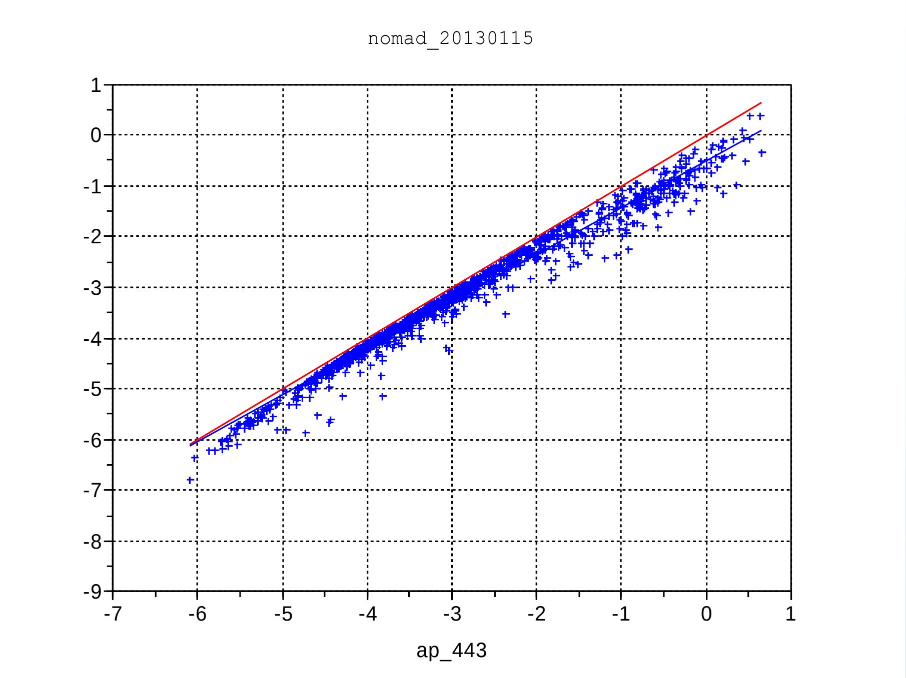


NOMAD

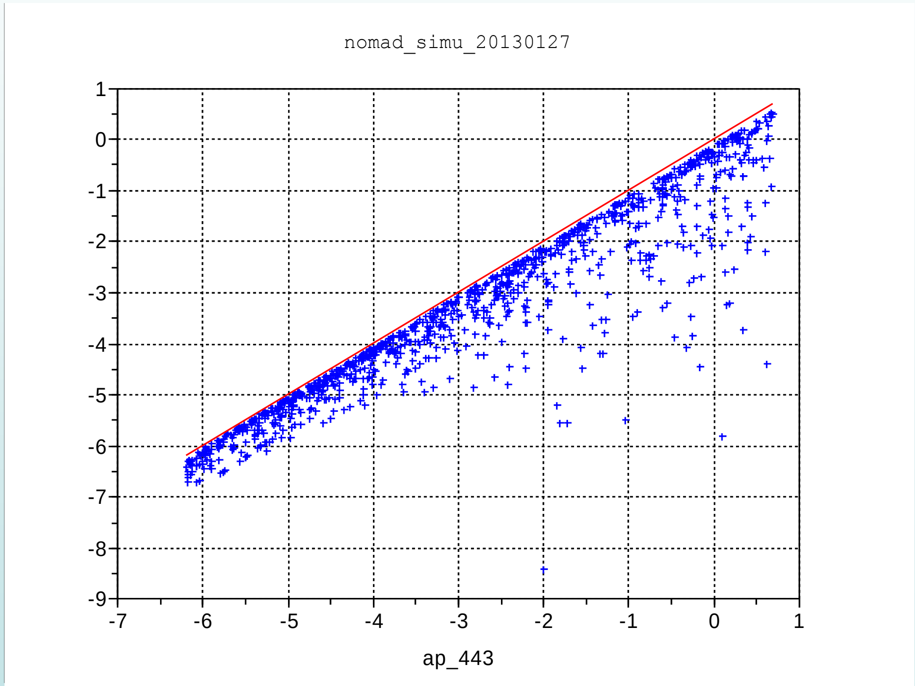


simu

Compare apig_443 vs ap_443

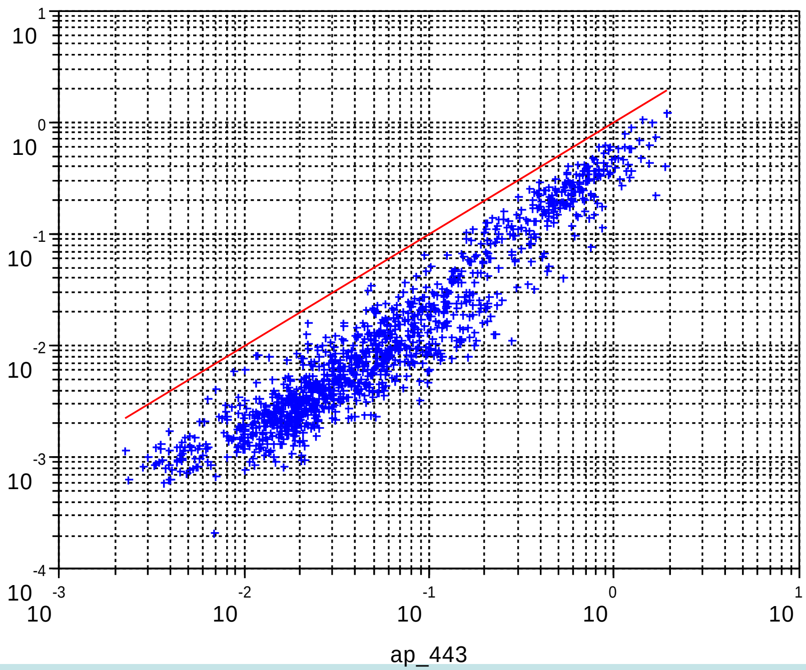


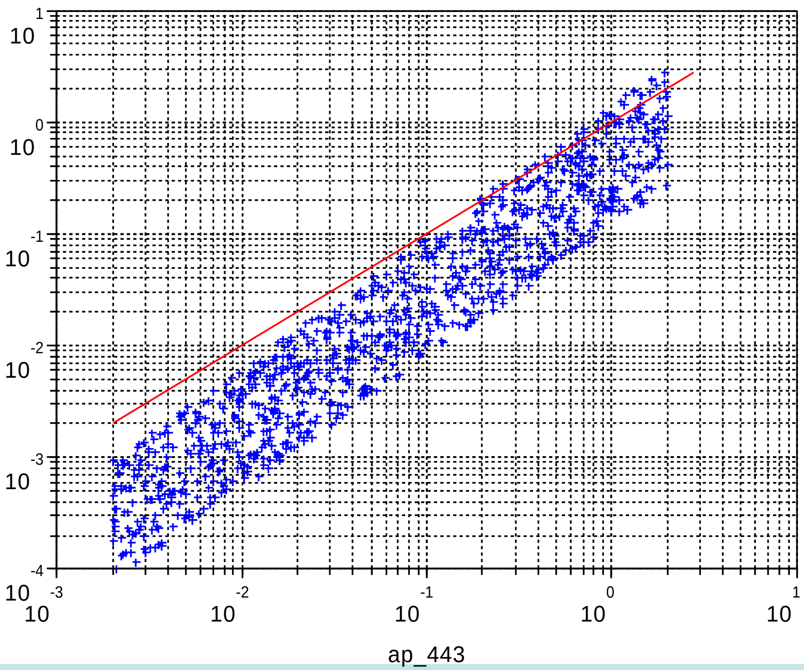
NOMAD



simu

Compare ad_443 vs. Ap_443

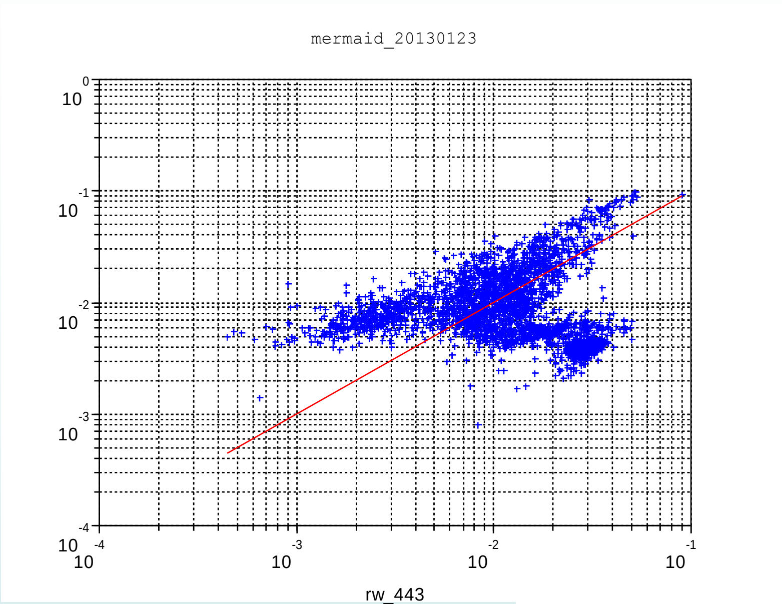




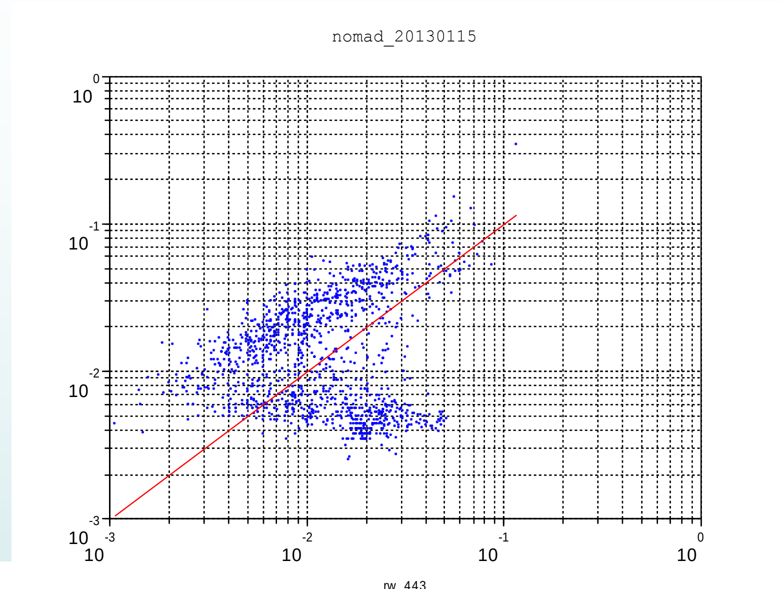
NOMAD

simu

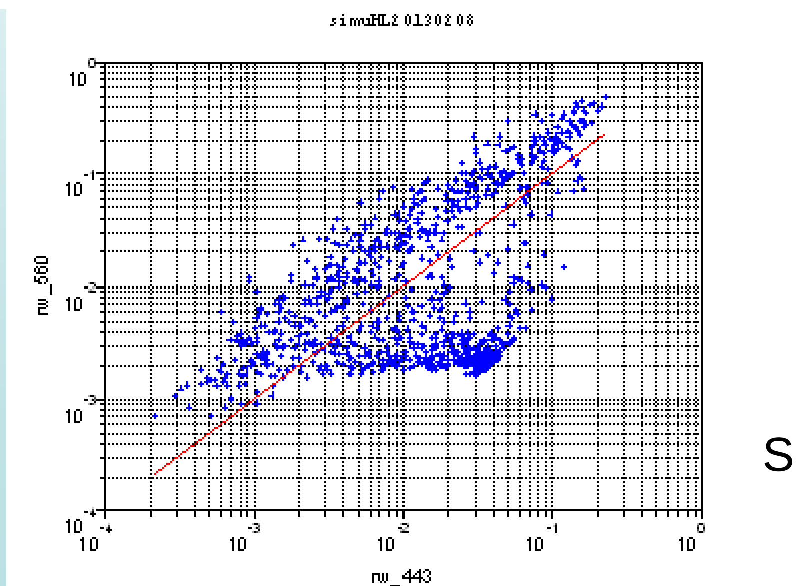
Frequency distribution rw_560 vs. rw_443



MERMAID



NOMAD



SIMU

Model versions

- Spectral slopes
  - ex_agelb =0.025
  - ex_adet =0.0074
  - ex_bpart =1.87
  - ex_bwit =0.0

Min. Ranges reduced Coastcolour	Min. Ranges full Coastcolour
apig: 0.0005 – 1.5	0.0005 – 5.0
agelb: 0.0005 -1.0	0.0005 – 5.0
adet: 0.0005 -1.0	0.0005 – 100.0
bpart: 0.01 – 10.0	0.01 – 100.0
bwit: 0.01 – 10.0	0.01 – 100.0
atot: 0.0005 – 1.5	0.0005 – 5.0
btot: 0.01-10.0	0.01 – 1000.0

Co-variances

- Alternative starting with atot or btot
- atot = exp(log_atot_an + rand()*log_atot_diff)
  - btot_min = atot*0.1
  - btot_min= max(btot_min, btot_an)
  - btot_max = atot*10.0
  - btot_max = min(btot_max, btot_en)
  - btot_diff = btot_max – btot_min
  - btot = exp(log_btot_min + rand()*log_btot_diff)
- btot = exp(log_btot_an + rand()*log_btot_diff)
  - atot_min = atot*00.1
  - atot_min= max(atot_min, atot_an)
  - atot_max = atot*2.0
  - atot_max = min(atot_max, atot_en)
  - atot_diff = atot_max – atot_min
  - atot = exp(log_atot_min + rand()*log_atot_diff)

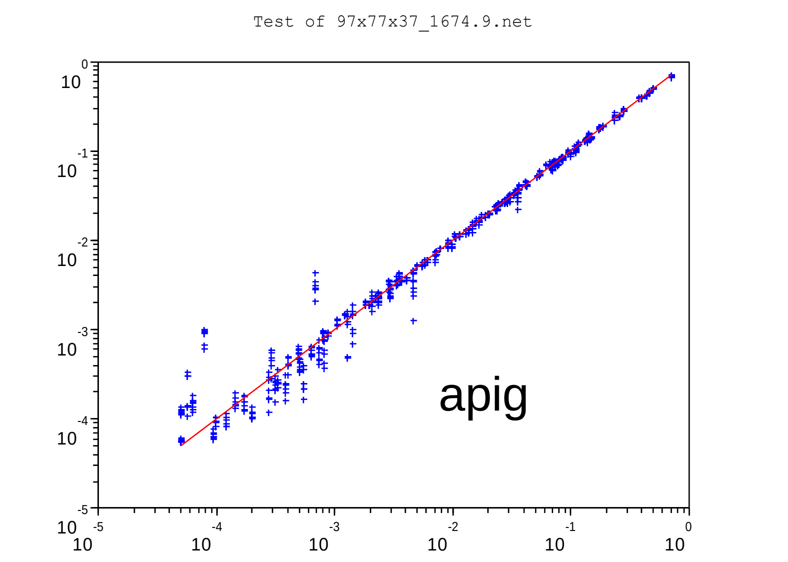
Used values

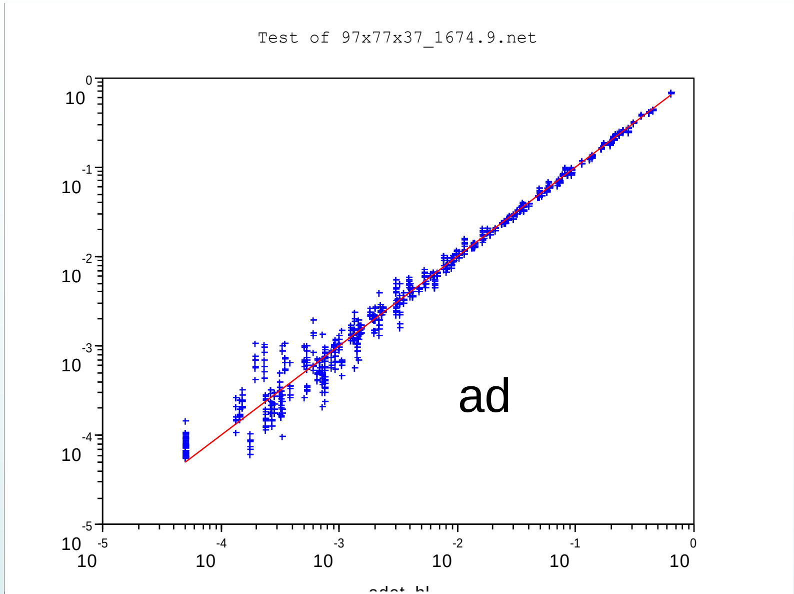
Alternative starting

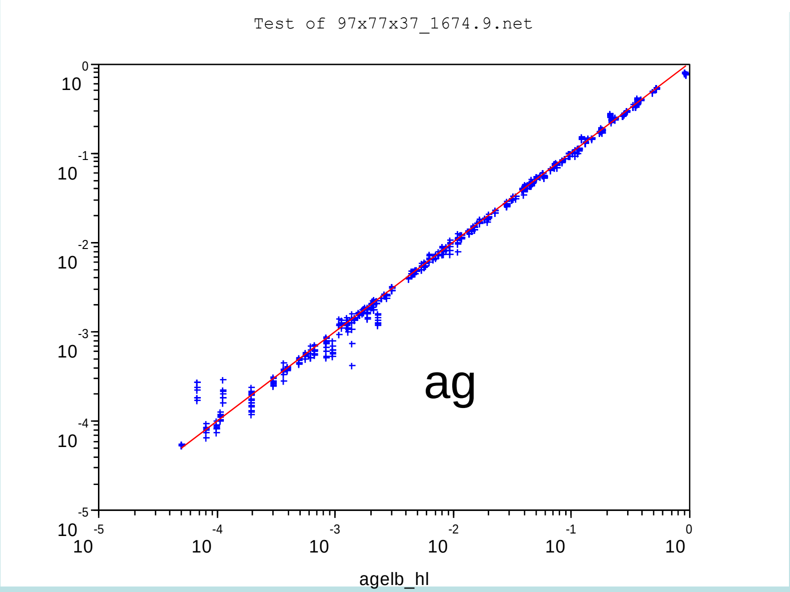
- 1
  - apig= max((rand()*min(apig_en, atot)),(apig_an*0.1))
  - agelb=max((rand()*min(agelb_en,(atot - apig))),(agelb_an*0.1))
  - adet =max((atot-apig-agelb),(adet_an*0.1))
- 2
  - agelb=max((rand()*min(agelb_en,atot)),(agelb_an*0.1))
  - apig= max((rand()*min(apig_en,(atot-agelb))),(apig_an*0.1))
  - adet=max((atot-apig-agelb),(adet_an*0.1))

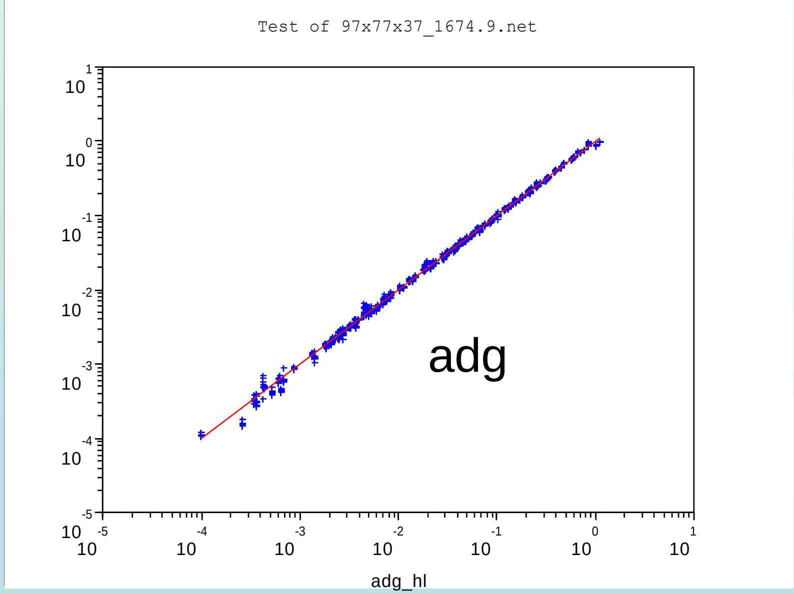
- Simulate 1 Mio. cases within these ranges according to the steps (s. above)

Test of NN with reduced TSM

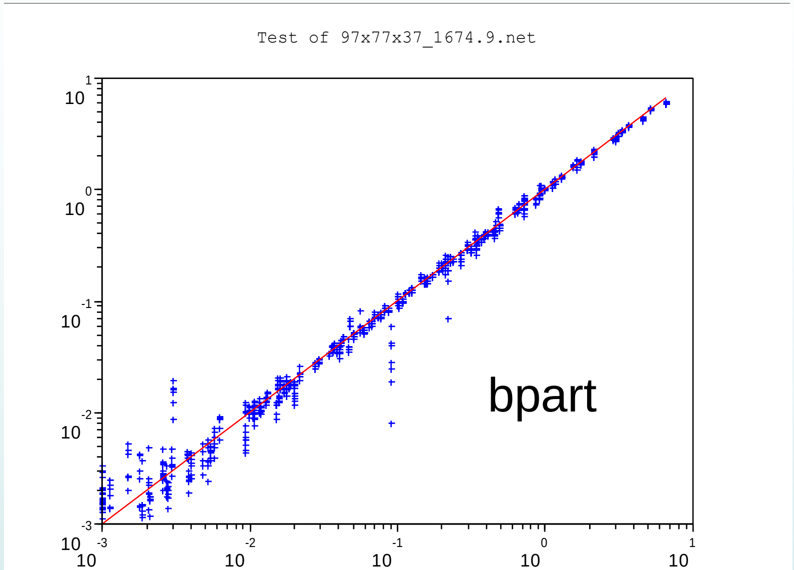


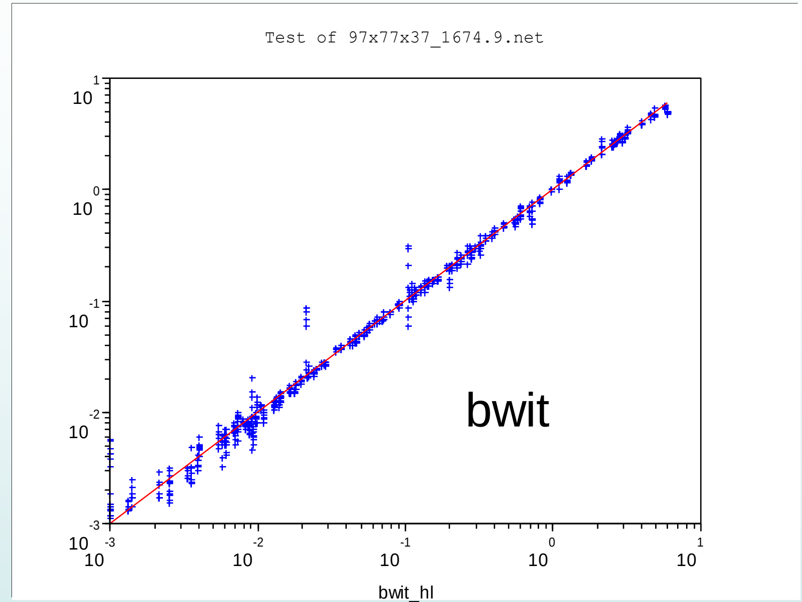


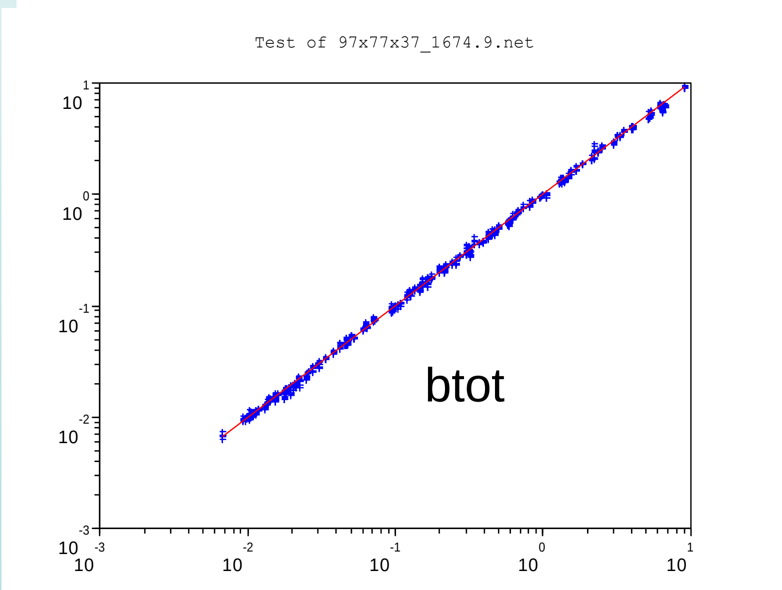


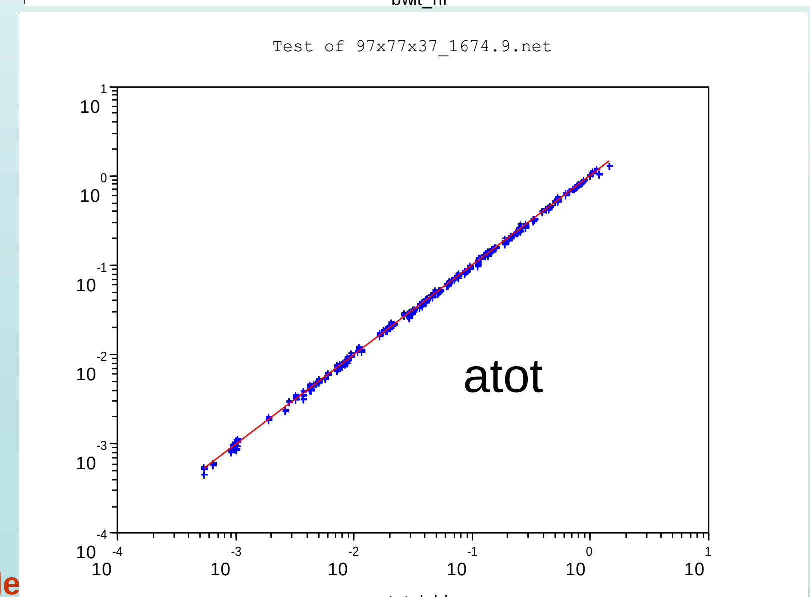


Test of NN with reduced TSM 2









Atmospheric Correction & IOP Retrieval

- Key to success: Atmospheric Correction
  - For Case2 water processing we need an AC which performs over clear, turbid as well as absorbing waters
  - CC-AC emphasis is on turbid waters, even over extreme waters (high reflective as well as highly absorbing) the AC shall not fail
  - Coupled ocean-atmosphere Radiative transfer modelling for AC and IOP retrieval

- Regional IOP retrieval
  - Neural network methodology
    - Global NN & Optical Water Type classification related NNs
    - Strength in turbid waters
  - Quasi Analytical Approach (QAA)
    - Strength in clear waters

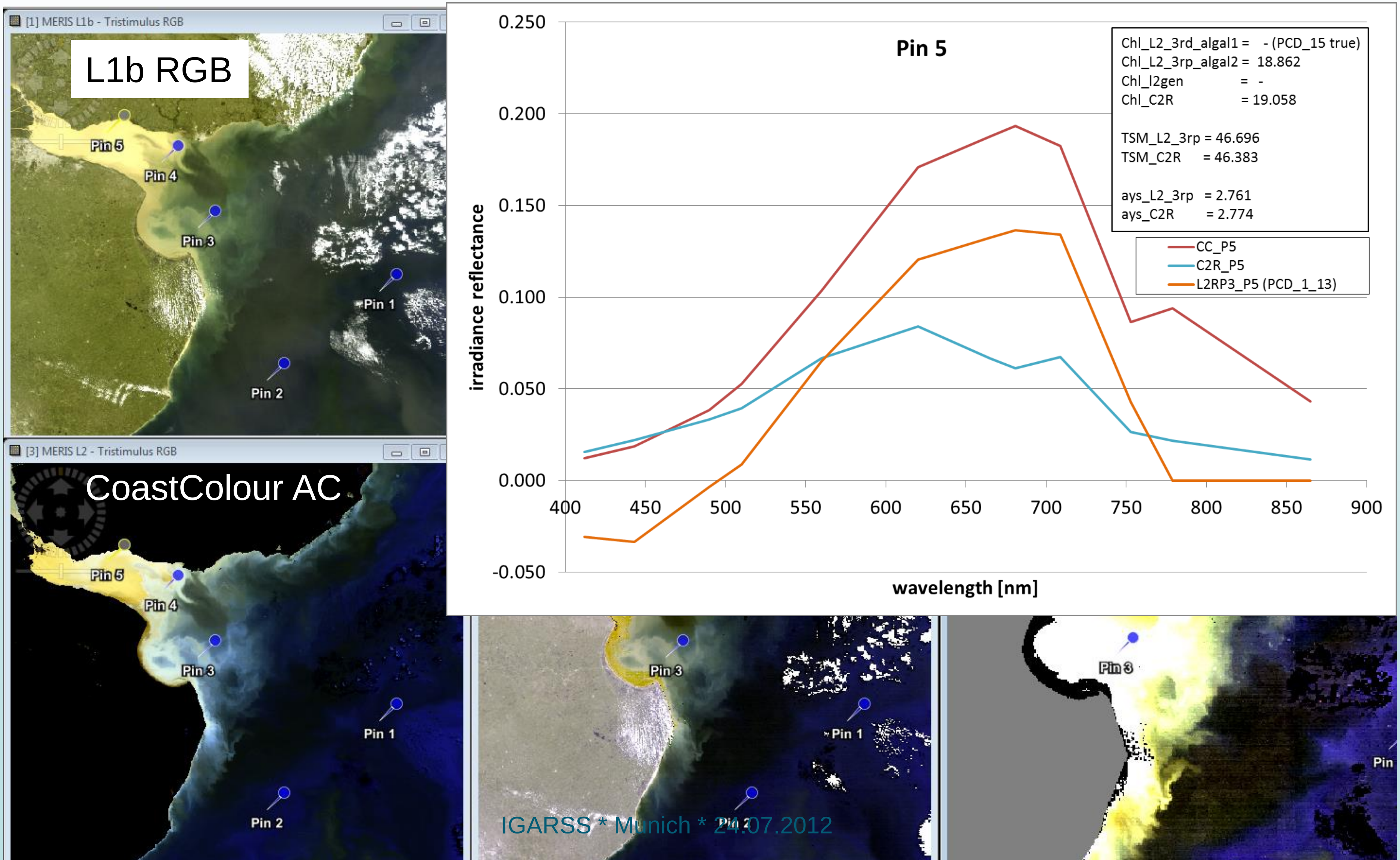
Atmosphere

- Atmosphere
  - Radiative Transfer Model of R. Santer, using Aerosol models based on coastal AERONET measurements
  - Parameters for simulation: AOT 550, angstrom, wind
- All simulations for different sun and viewing angles
- 7 Mio cases with water model simulated

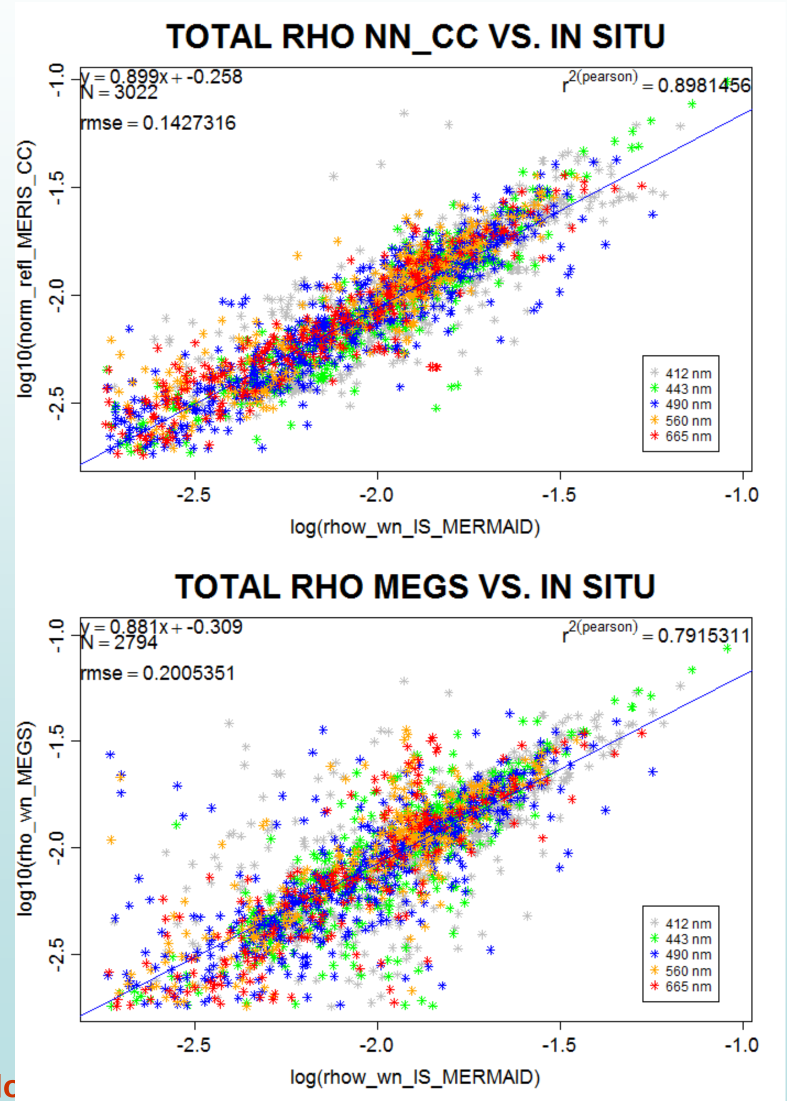
Water

- Analysis of reflectance spectra of extreme cases
- Chlorophyll range 0.01 – 100 mg m^3
- TSM range 0.01 – 1000 mg/l
- Bio-optical model 5 IOP components:
  - a_pig
  - a_detritus (slope 0.0074)
  - a_gelbstoff (slope 0.025)
  - b_particle (slope 1.87)
  - b_white (slope 0.0)
- Balanced frequency distribution
- Temperature: 0 – 36 deg C, salinity: 0 – 42

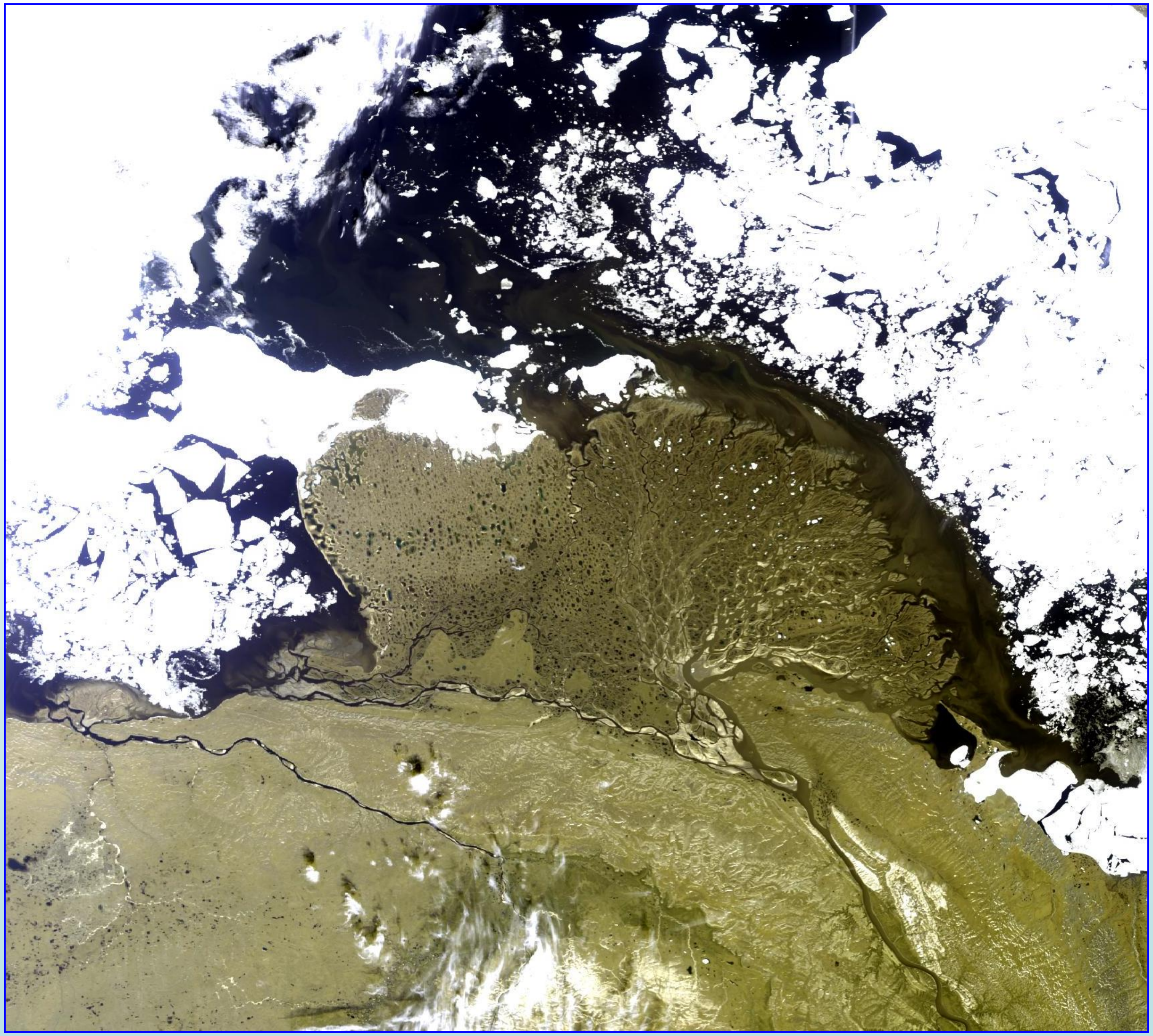
Rio de la Plata



Validation on MERMAID data



Validation of AC and 5 component model: Lena Delta



MERIS FR 20110704

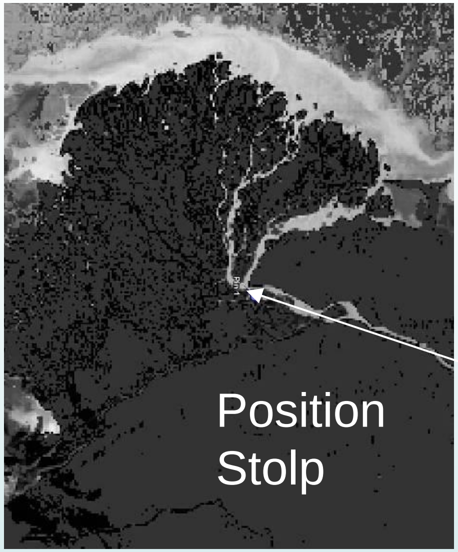
Lena Delta 73 N
Lena > 500 km^3 fresh water, 2nd after Yenesei in the Arctic

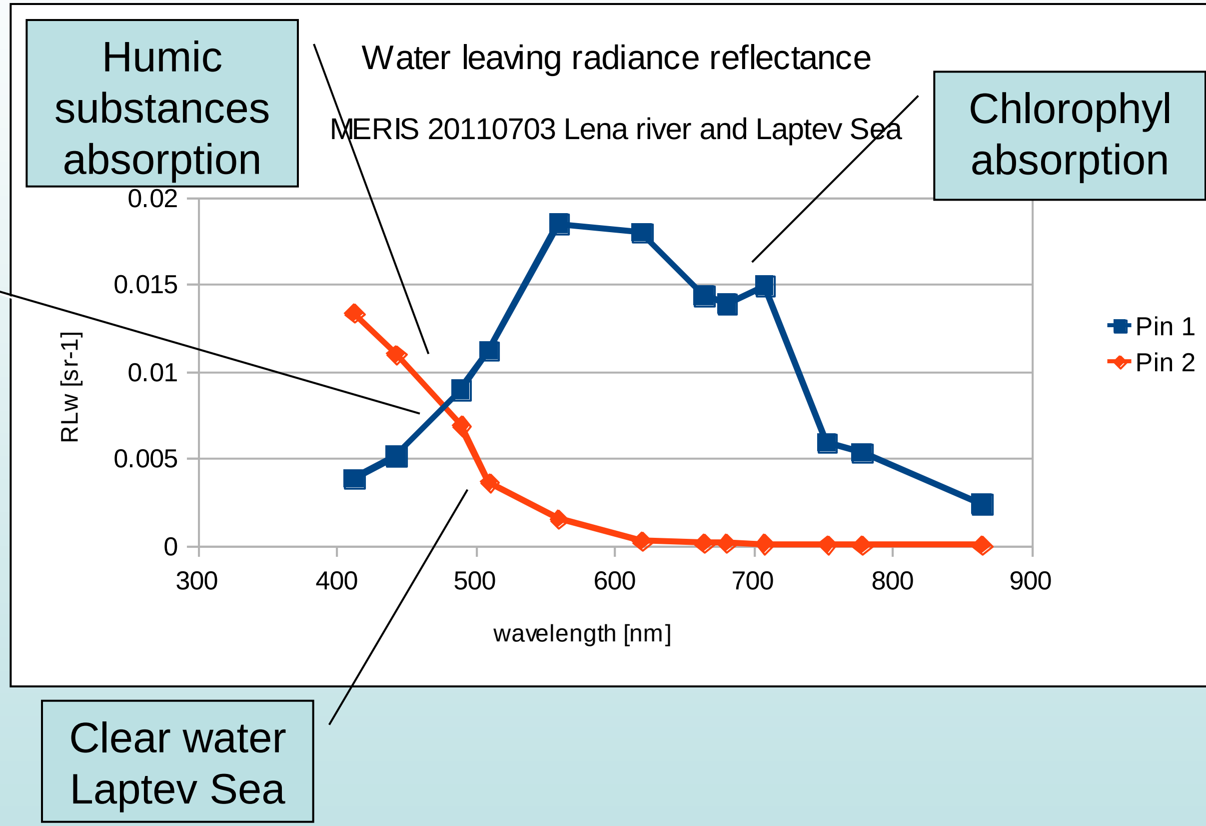
Very high concentration of absorbin substances (Carbon):
adg443 5-8 m^{-1}

Partly very turbid

Bio-optics campaign
June 26 – July 5th 2011

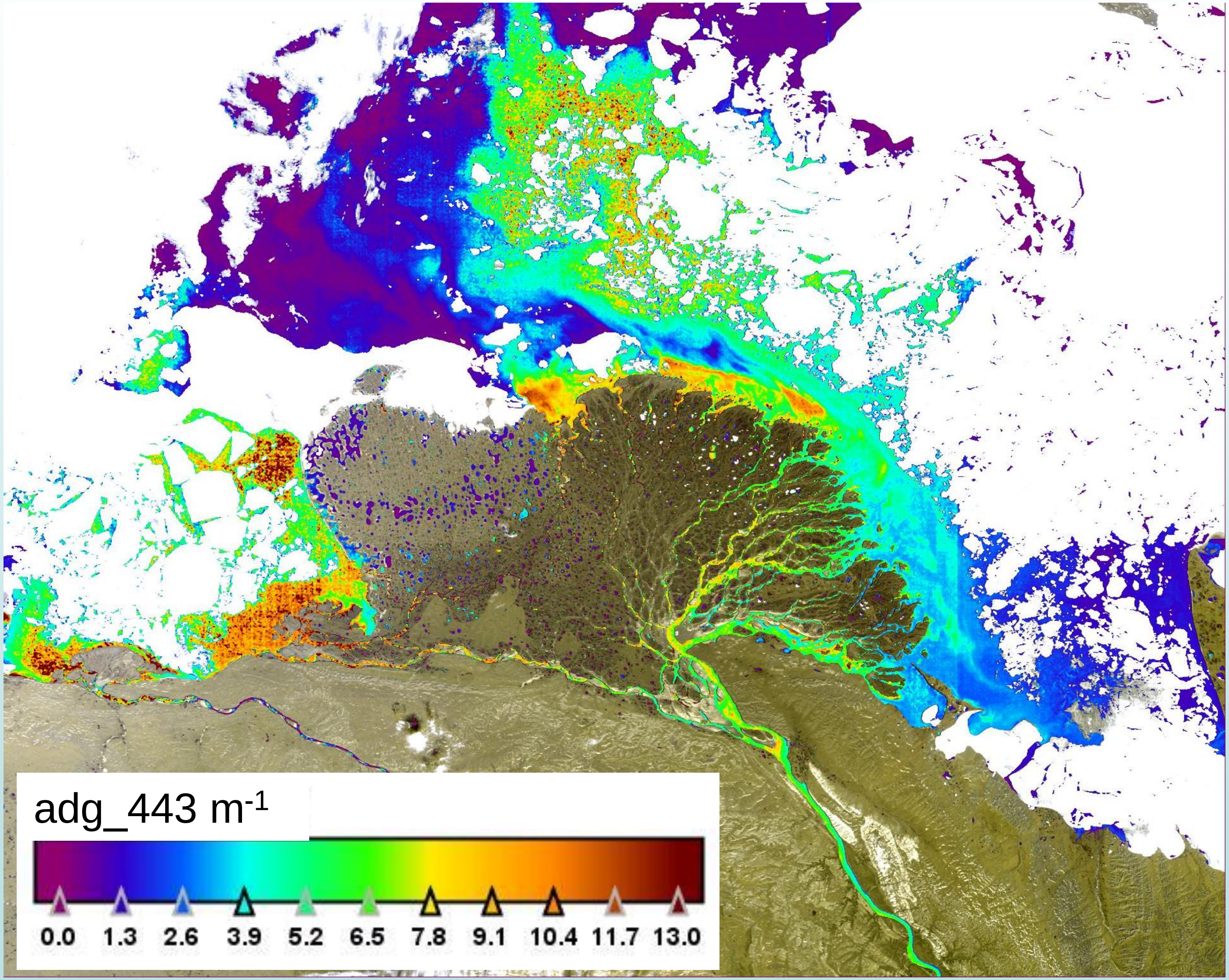
Water leaving radiance reflectance



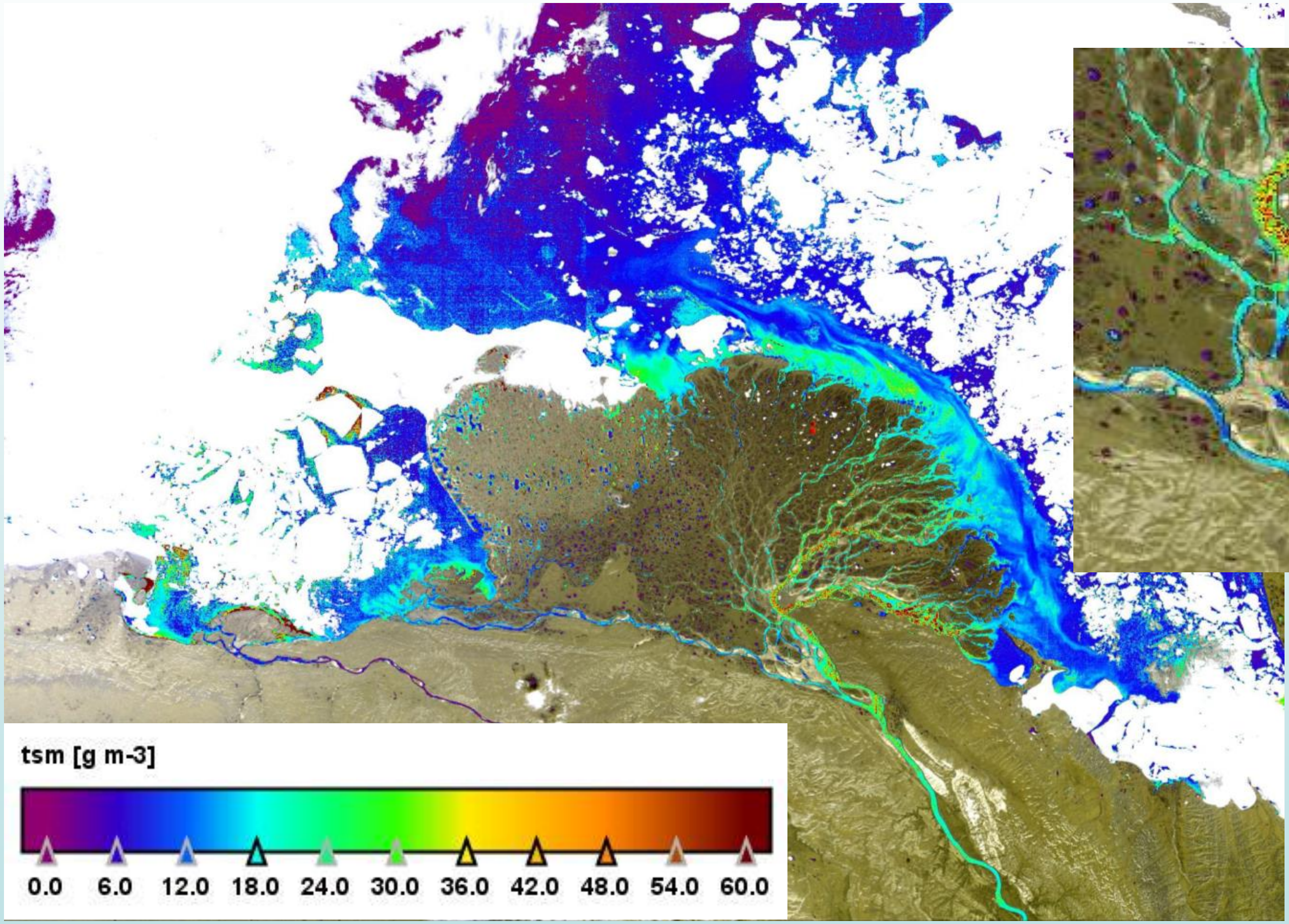


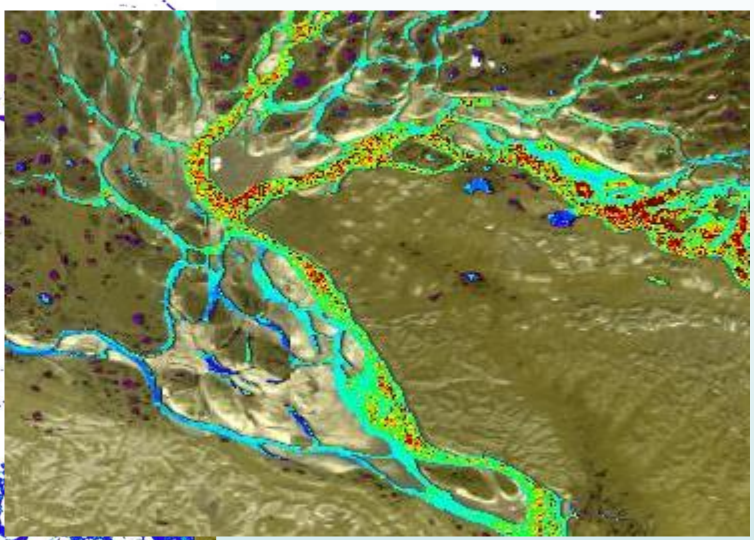
Blue: reflectance at position Stolp
Red: reflectance in clear water Laptev Sea

adg (a_443 of detritus and gelbstoff)



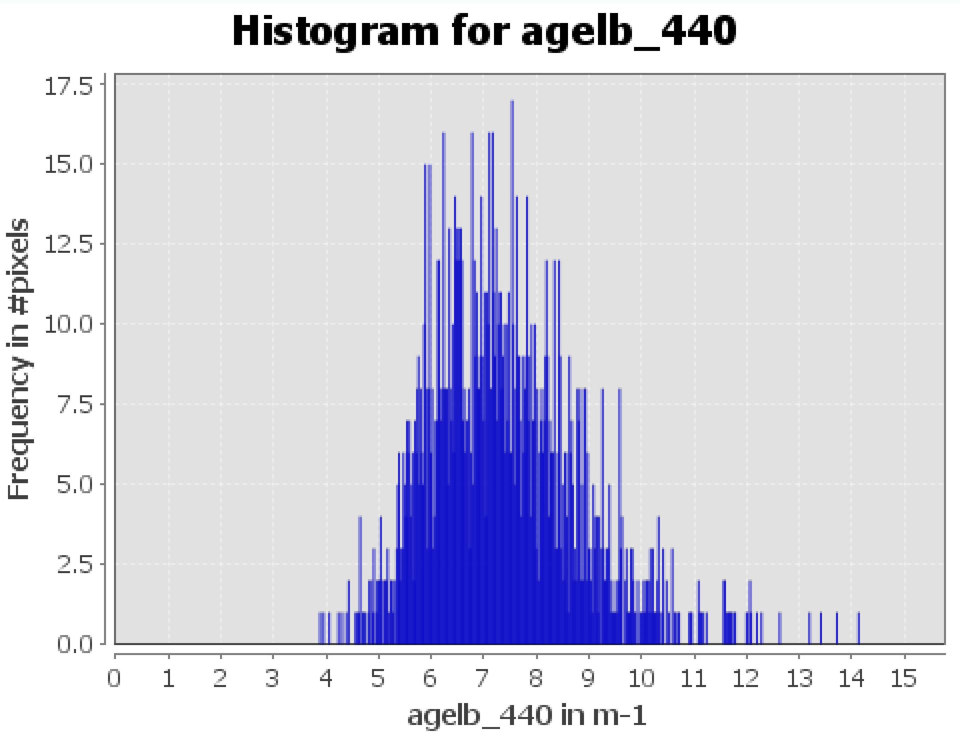
TSM

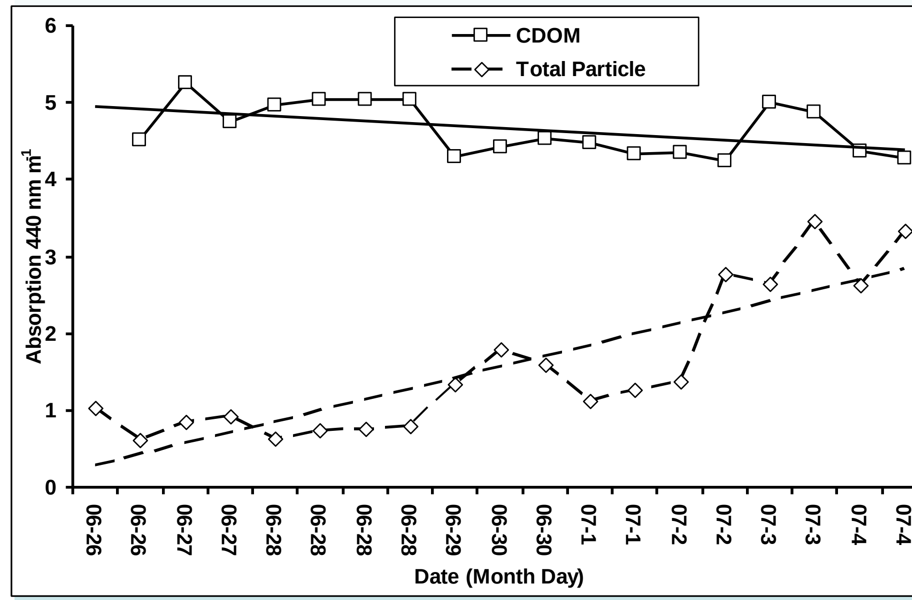




Samples:
8 – 68 g m-3
Mean: 32 +- 20 g m-3

Absorption by CDOM and bleached particles



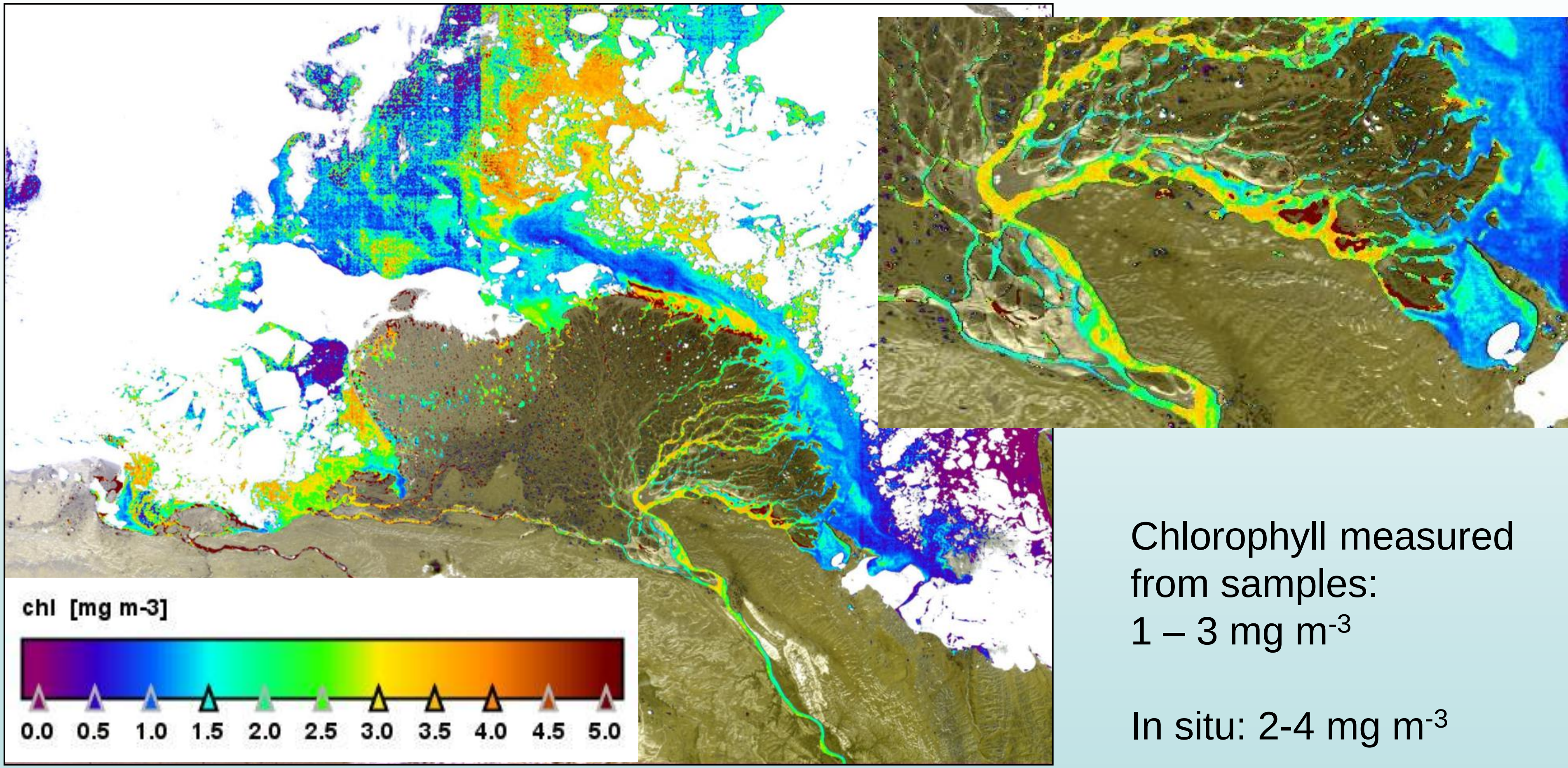


MERIS

In situ

I n s i

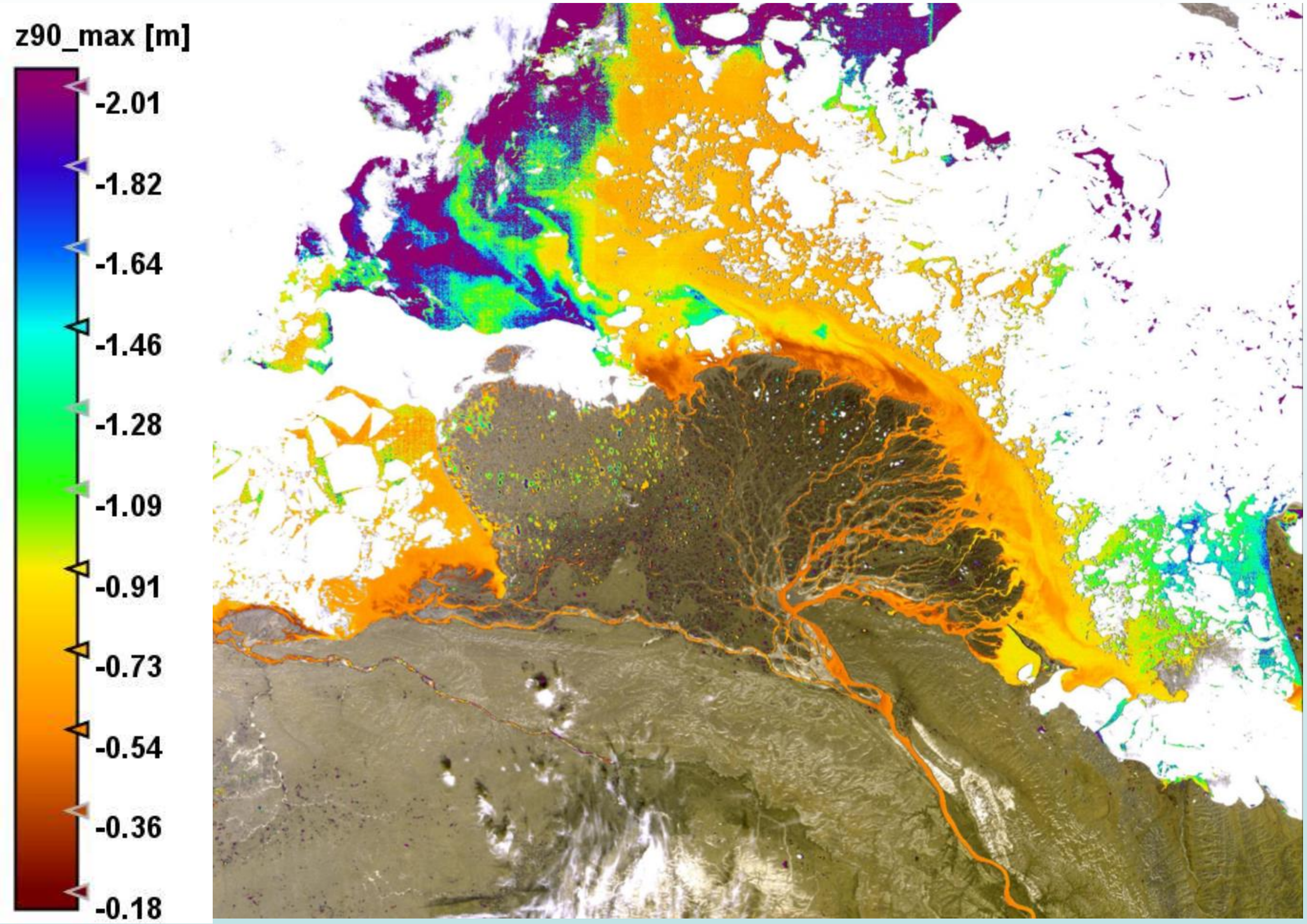
Chlorophyll



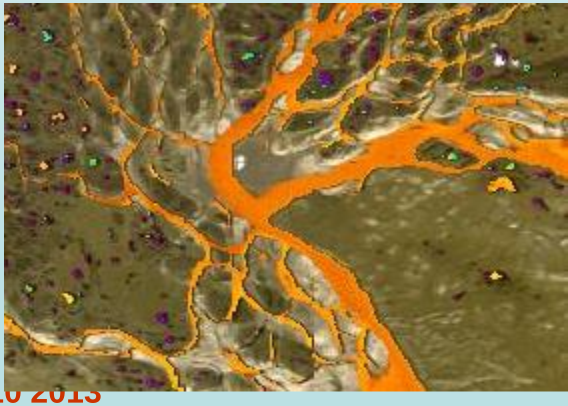
Chlorophyll measured from samples:
1 – 3 mg m^{-3}

In situ: 2-4 mg m^{-3}

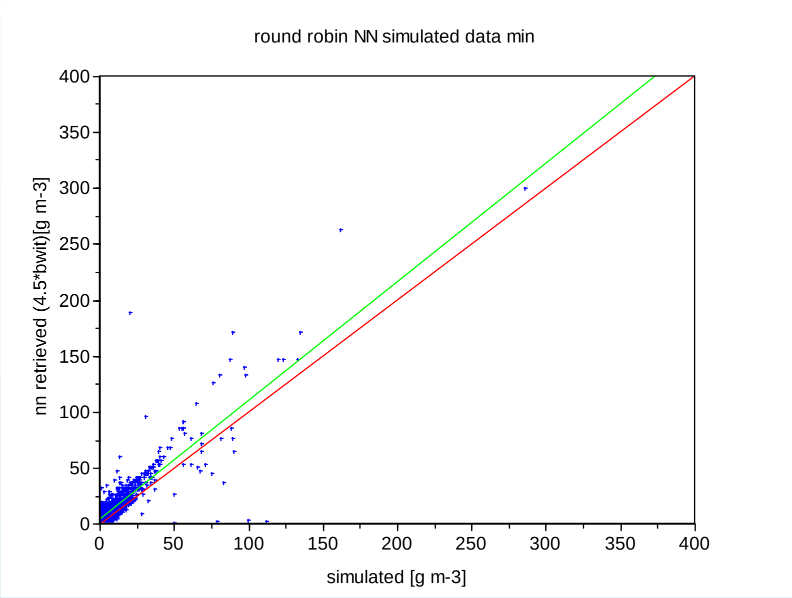
Z90_max



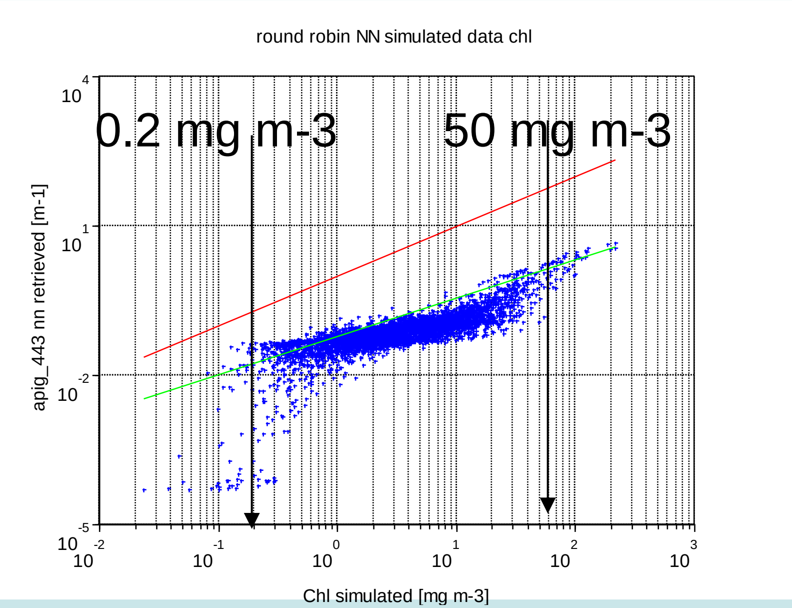
Secchi: 30 – 85 cm



Test with CC-NN of Simulated RR data

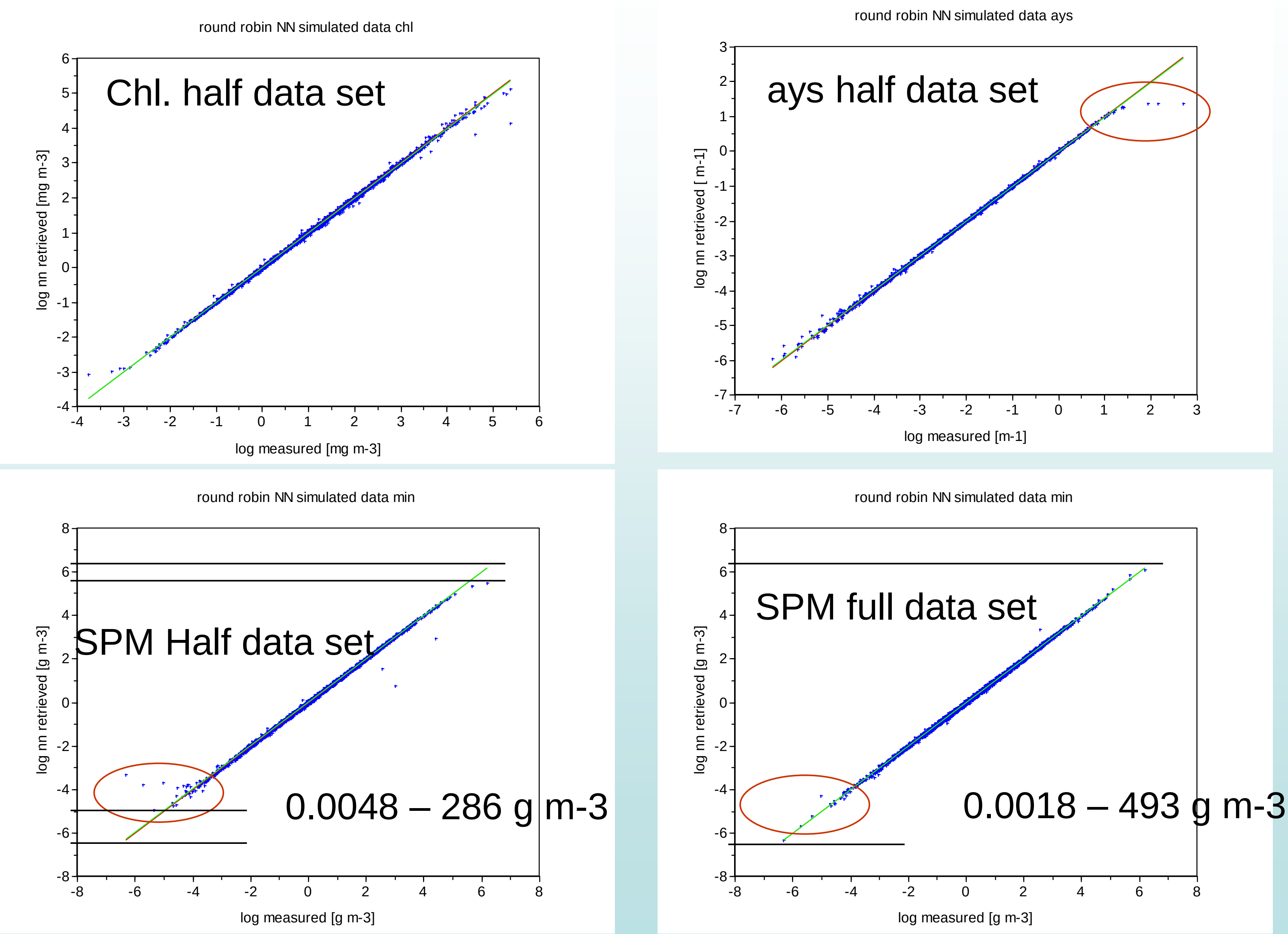


SPM (Min)



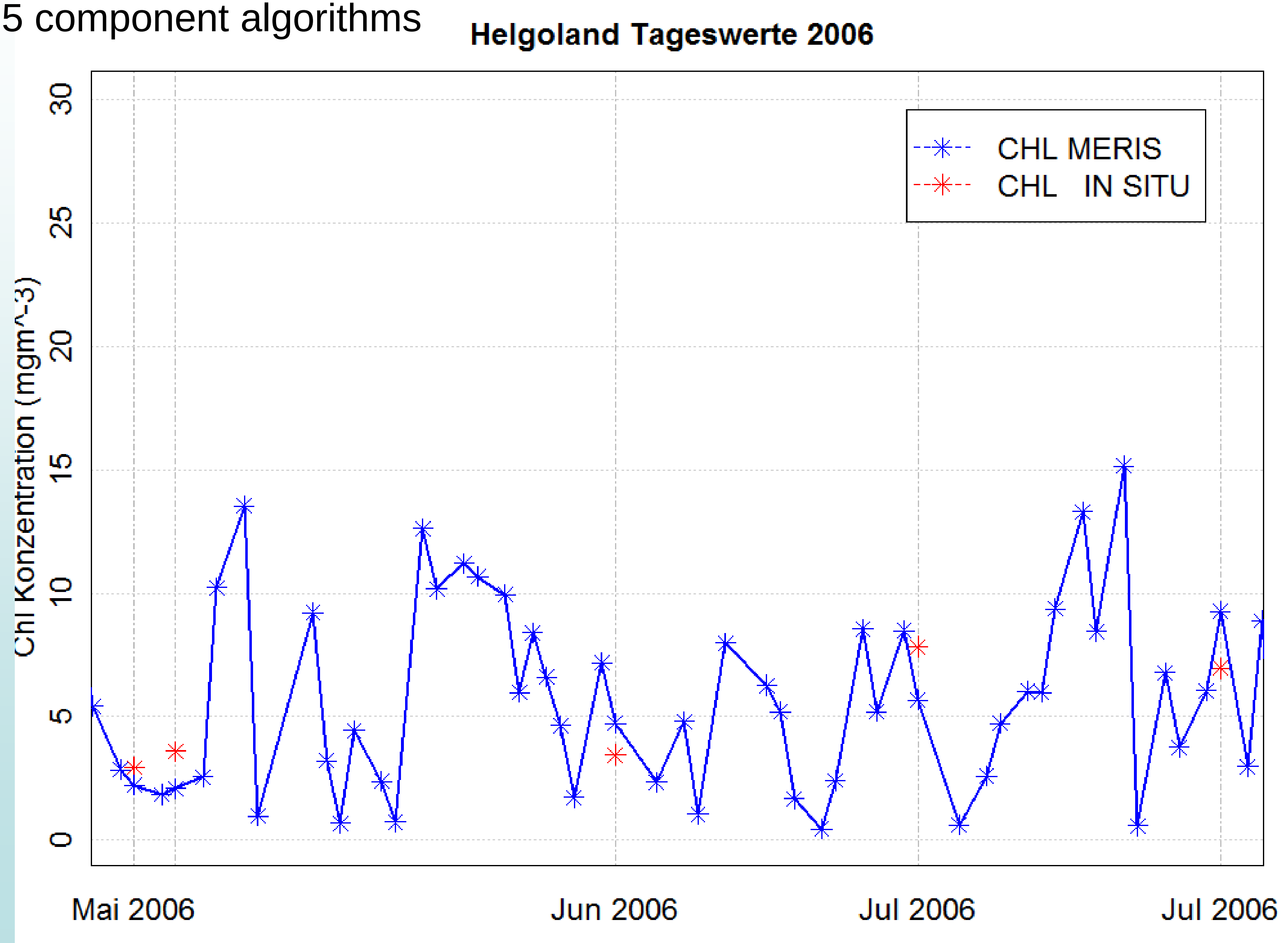
Chlorophyll

Test of simulated RR data set: NN trained on this model

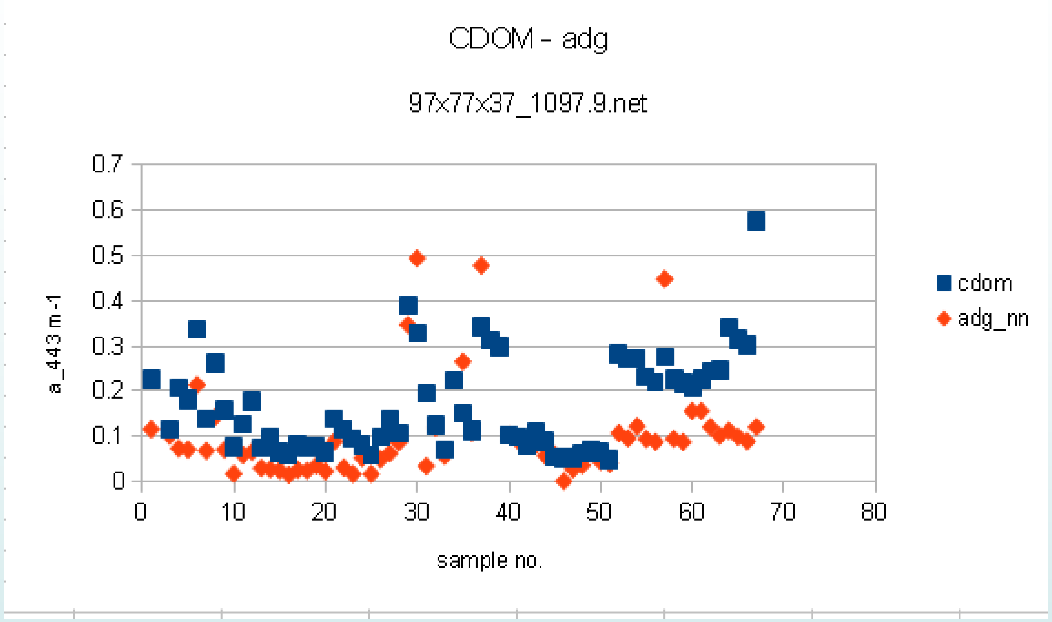


Helgoland Transect

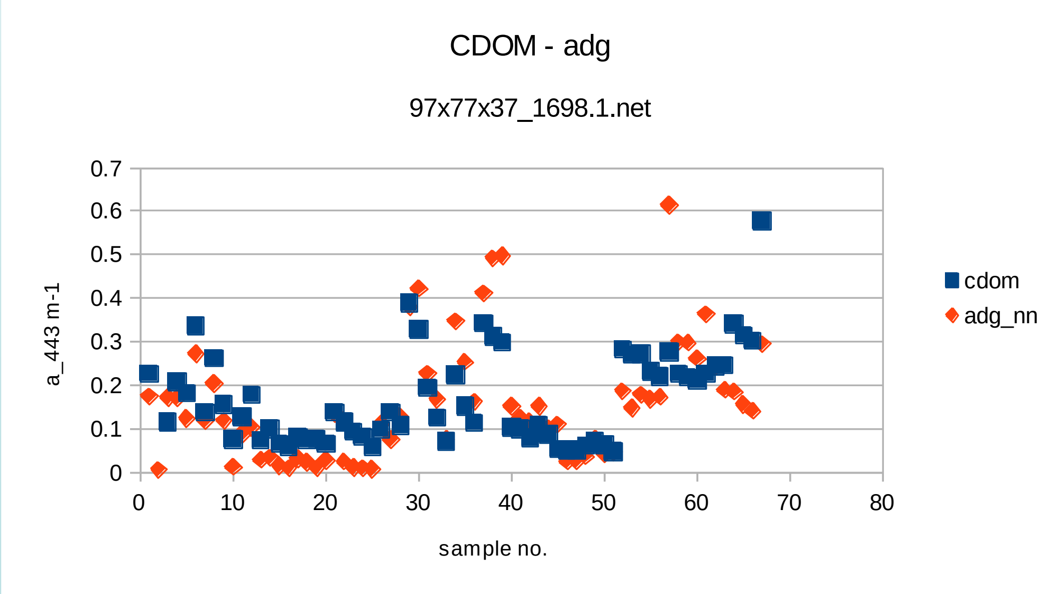
5 component algorithms



Validation NN for CDOM



CC-model with full range

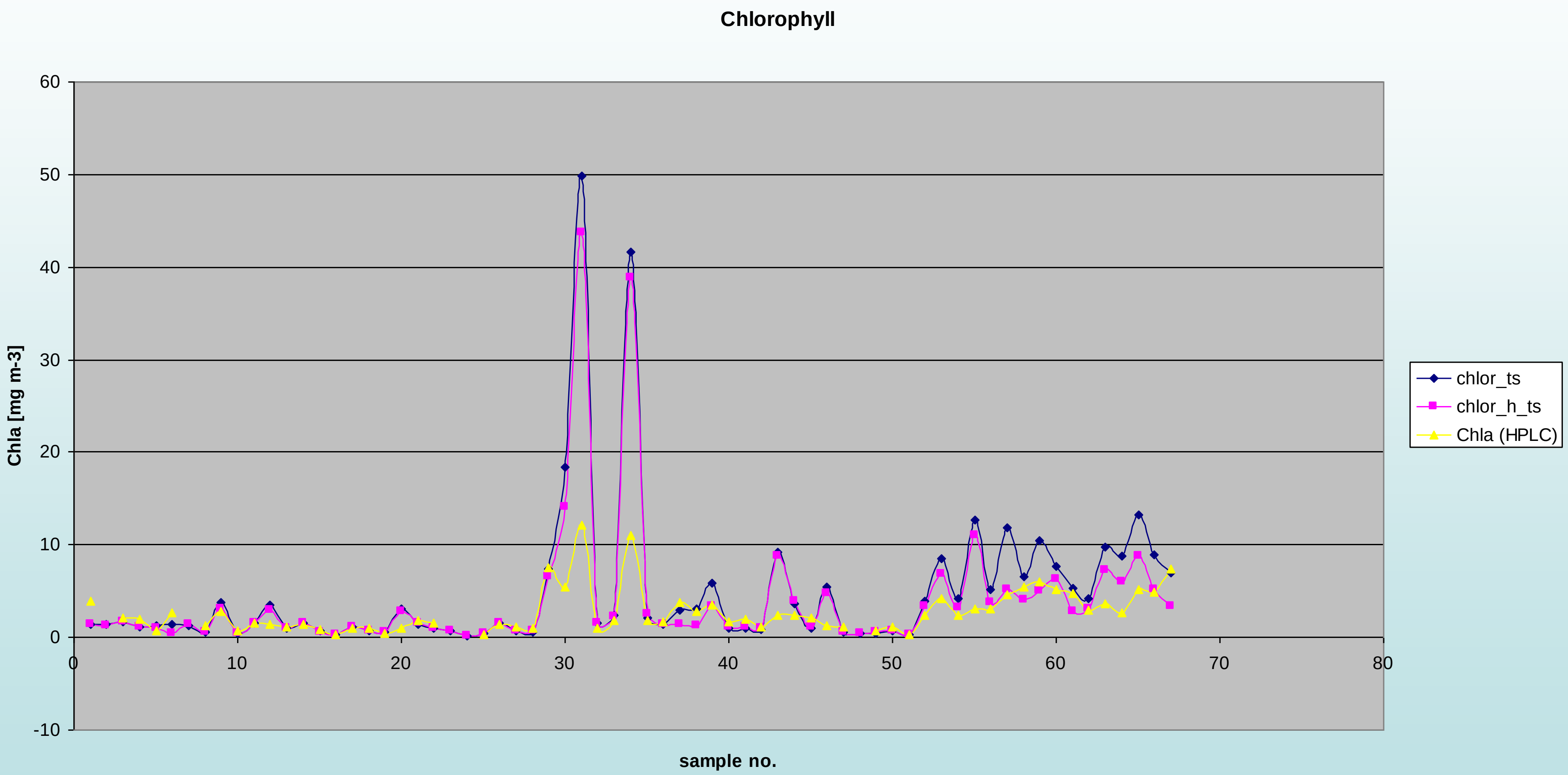


CC-model with limited range

Regional adapted bio-optical model

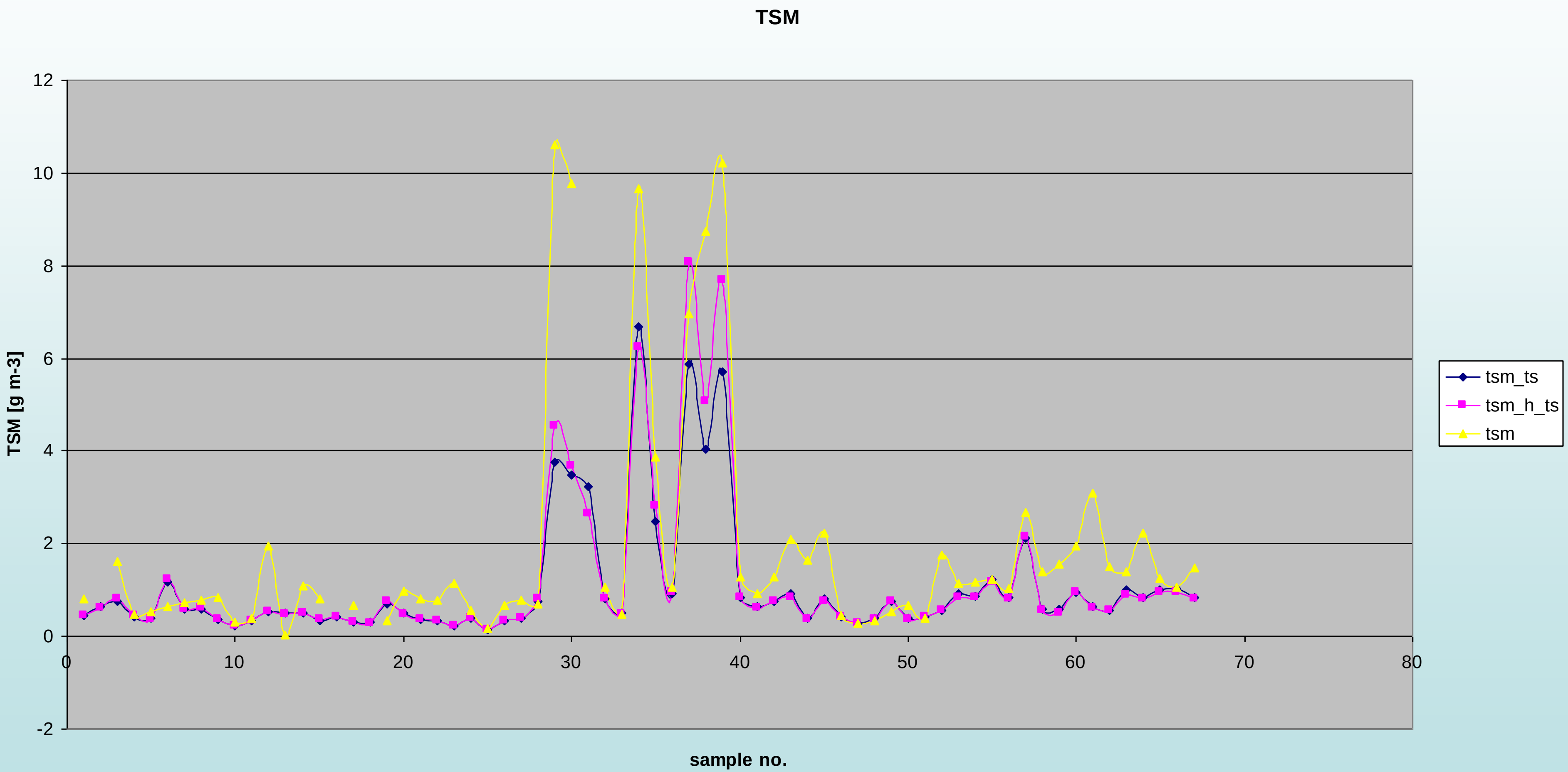
- Based on regional bio-optical model (adapted from T. Schroeder, 2004)
  - North Sea and Baltic Sea (Coastlook project)
  - Ranges of concentrations
  - Ranges of co-variances
  - Phytoplankton absorption: Bricaud et al, 1995
  - Components:
    - Phytoplankton pigment absorption
    - TSM scattering
    - TSM absorption
    - Gelbstoff absorption

Chlorophyll



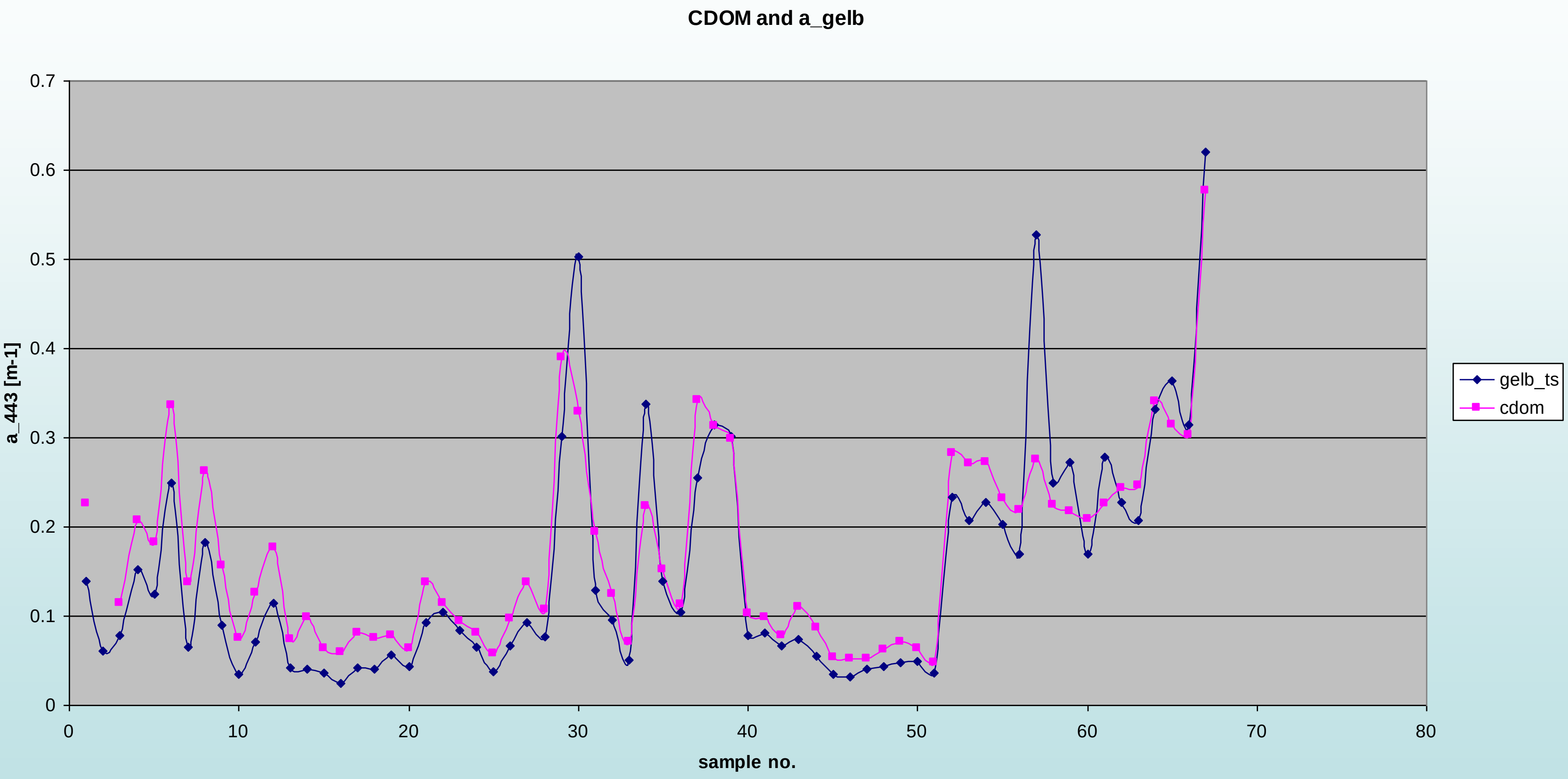
Yellow: chl (HPLC) in situ, blue and red from TRIOS with NN

TSM



Yellow: tsm in situ, blue and red from TRIOS with NN

CDOM Baltic Sea and North Sea



Red: in situ, blue derived from TRIOS using water NN

Summary and Conclusions

- Next steps for second L2 reprocessing
- Merge NN with full and limited TSM / CDMOM range
- Validate results
- Report

Thank you for your attention

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MERIS RGB, Lena Delta, 09. September 2005, orbit: 18438