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E-AIMS

Euro-Argo Improvements for the GMES Marine Service

Ocean colour: Impact study results and recommendations

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1. Introduction and context

In the past two decades, thanks to the advent of satellite ocean-color radiometry (OCR), biogeochemical processes at the ocean surface have begun to be observed at a regular spatial and temporal resolution. These observation techniques are however limited due the fact that they "only" measure the upper part of the marine water column and that the biological information at the sea surface are derived thanks to application of bio-optical models (which have their own limitations and validation range). Therefore, it is necessary to increase the in situ observation density associated with measurements from space.

The profiling floats of the Argo array were initially designed for physical oceanography and hydrography. They now also represent a promising technology for future observations in ocean biogeochemistry and bio-optics.
The availability of bio-profilers measurements is intended to be used to make the connection between the 2D-horizontal picture derived from Ocean Colour and the 1-D vertical information provided by floats. However, several issues appear to perform this connection i) the "common" products that would be derived from these two techniques are principally the Chlorophyll-a concentration and the diffuse attenuation coefficient (Kd). Both of them are indirect measurements from Ocean Colour (i.e. making use of semi-empirical model from direct measurements of backscattered light at the sea surface) and the measurement from the float is also an indirect measurement of the Chlorophyll (through fluorescence). The direct comparison between the two sources of "indirect" observation might therefore allow pointing toward weakness (or strength) on measurements from both origins as well as on their transformations.
Apart from issues above described, the bio-Argo availability shall be used in addition to ocean colour observations for cross Cal/Val activities of both techniques. This availability is also essential for refining bio-optical algorithms, implementing new and explorative strategies in marine biogeochemistry, as well as supporting biogeochemical-modelling activities (in association with the development of biogeochemical data assimilation techniques).

This deliverable has been realized in order to present the impacts of bio-Argo observations for three purposes:

1. The validation of satellite observations and for joint in- situ/satellite analysis applied for ocean color parameters,
2. The improved knowledge of marine biology thanks to availability of surface AND vertical information (and impact on bioregions definition),
3. The assimilation of profilers data into biogeochemical modelling

The goal is to assess what should be the appropriate upper ocean sampling to enhance each of the three purposes above, and to provide a set of recommendations to help define the new phase of Argo automatic profilers.

2. Applicable documents

DA-1: Annex 1 to the grant agreement N0 312642: "Description of work", date 24 April 2012

3. Complementarity between Ocean Colour and bio-floats

It is intended to use the bio-Argo in addition to ocean color observations for cross Cal/Val activities of both techniques. This availability is also essential for refining bio-optical algorithms, implementing new and explorative strategies in marine biogeochemistry, as well as supporting biogeochemical-modelling activities (in association with the development of biogeochemical data assimilation techniques).

More specifically, this availability of bio-floats products are particularly relevant in the perspective of OLCI on board Sentinel 3 planned to be launched in 2015. There is a real need to interface the bio-Argo component with the ESA Mermaid Cal/Val facility.

3.1. The challenge of the cross validation

The problematic of cross-validation is to master the uncertainties of the two elements we compare. “Master the uncertainties” does not mean that we can change it but, principally that we know them.

On the following figure are indicated the uncertainties decomposition for the bio floats and for the observation from satellite (the example here is focused on Chlorophyll-a).

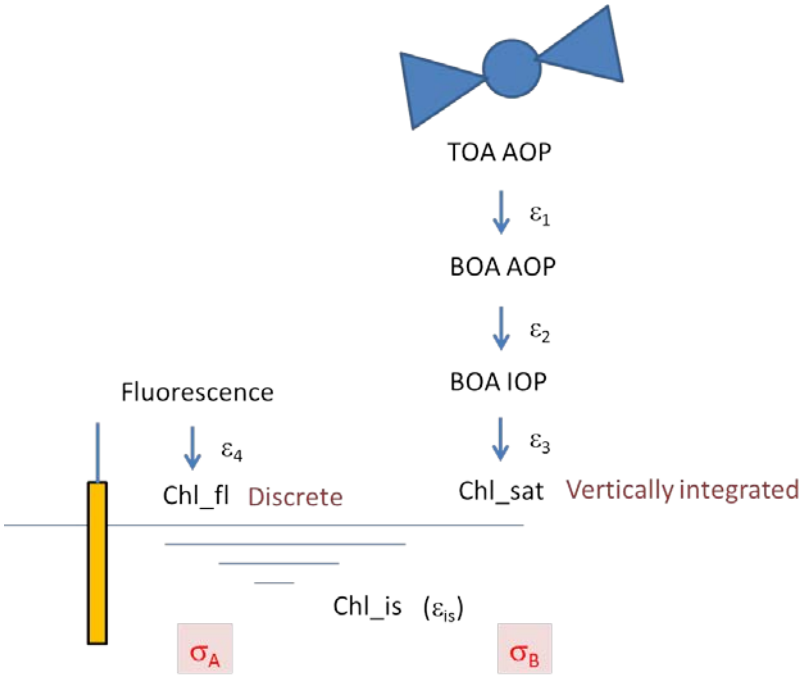


Figure 1 – error budget for the bio-float (σA) and for the remote sensing (σB)

3.2. Uncertainty, accuracy, precision and errors

In order to be sure of the measurement quality, it is important to take into account the measurements protocol and recommendations defined in the **G**uide of **U**ncertainty in **M**easurements (JCGM 100:2008, GUM 1995 ; http://kcdb.bipm.org/default.asp).

Uncertainty of measurement is a parameter, associated with the result of a measurement that characterizes the dispersion of the values that could reasonably be attributed to the measurand.

Uncertainties are data products, they are assessed quantitatively and are beginning to be part of the data management structure (for instance, these uncertainties will be included into upcoming Sentinel 3-OLCI missions products and will cover the ε1, ε2, ε3 displayed on figure 1) and are still largely studied and documented in the today's literature (e.g. IOCCG report on uncertainties). The GlobColour project supported by ESA-DUE has allowed has allowed to develop and operate an operational system merging L2 Ocean Colour products acquired by MERIS, MODIS-A and SeaWiFS at global scale and with a 4 km spatial resolution. This service supports a continuously increasing user's community needs (long time series of ocean colour products including uncertainties estimates). The service is based on a strong system approach and on the development of efficient tools and architecture fit for the purpose. [*http://globcolour.info*; *http://hermes.acri.fr*] and is used for ocean colour validation (and accounting for uncertainties).

Accuracy is a qualitative concept regarding the closeness of the agreement between the result of a measurement and the true value of the measurand.
The required accuracy of the measurement is necessary to determine the specification and definition for the measurand; it should be defined with sufficient completeness so that for all practical purposes its value is unique.

Precision is a qualitative concept regarding self-consistency of the results of a measurement.

Error of the result of a measurement and the true value of the measurand are both unknowable.
There are 2 mean types of errors:

- *random error*: from unpredictable variations, given rise to variability in the results of repeated measurements. It is the result of a measurement minus the mean that would result from an infinite number of measurements of the same measurand carried out under repeatability conditions.
- *systematic error*: cannot be eliminated but it often can be reduced by eliminating systematic effects.

Thanks to the large number of bio-floats, the random error on the observations can be assessed by statistical analysis of the observations from the same floats. The real difficulty comes from the detection and estimation of the systematic error. This could be further complicated due to temporal drift that can affect the observation (as it is the case for nitrates measurements).

3.3. Qualification of the observations from the bio-floats.

This qualification (in fact the estimation of random and systematic parts of σ_A) is still subject of research. Nevertheless several elements are currently used to support this qualification.

For a given biological stable area, the number of sampling should offer enough samplings to derive the precision of the measurement under the form of the repetability of the observation. By doing this it is expected to catch the *precision* of the sensor in term of dispersion (only) around a common value ; possible bias should be detected and corrected for by other means (e.g. biological consideration such as no Chlorophyll at very large depths). Bioregional classification proposed by D'Ortenzio and d'Alcalà (2009) and seasonal cycles will be performed to constrain and refine the sampling design. Apart from these considerations, we describe here below, present means to detect and quantify random and systematic error on bio-profilers observations.

3.3.1. *Random error*

The *noise* on observed profile is currently assessed through simple (but careful) filtering techniques. The figure below shows the evolution in time of such noise level. However, this "error" is more related to the detection noise than to the whole random error.

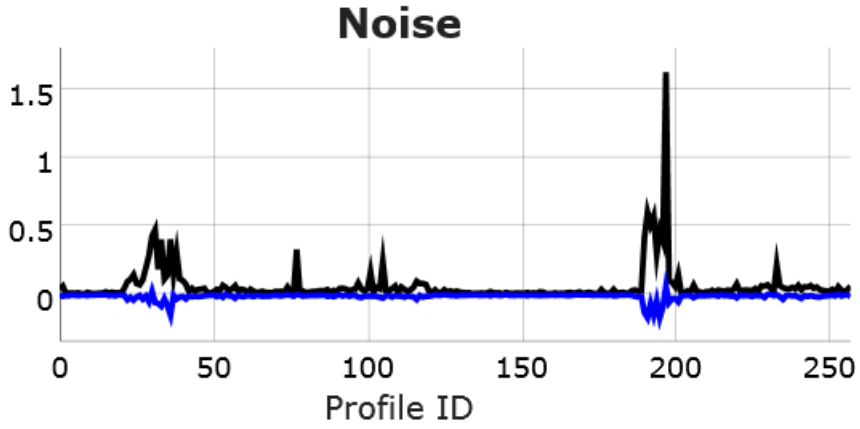


Figure 2 – Temporal evolution of random noise on Chlorophyll profile observed by the same float

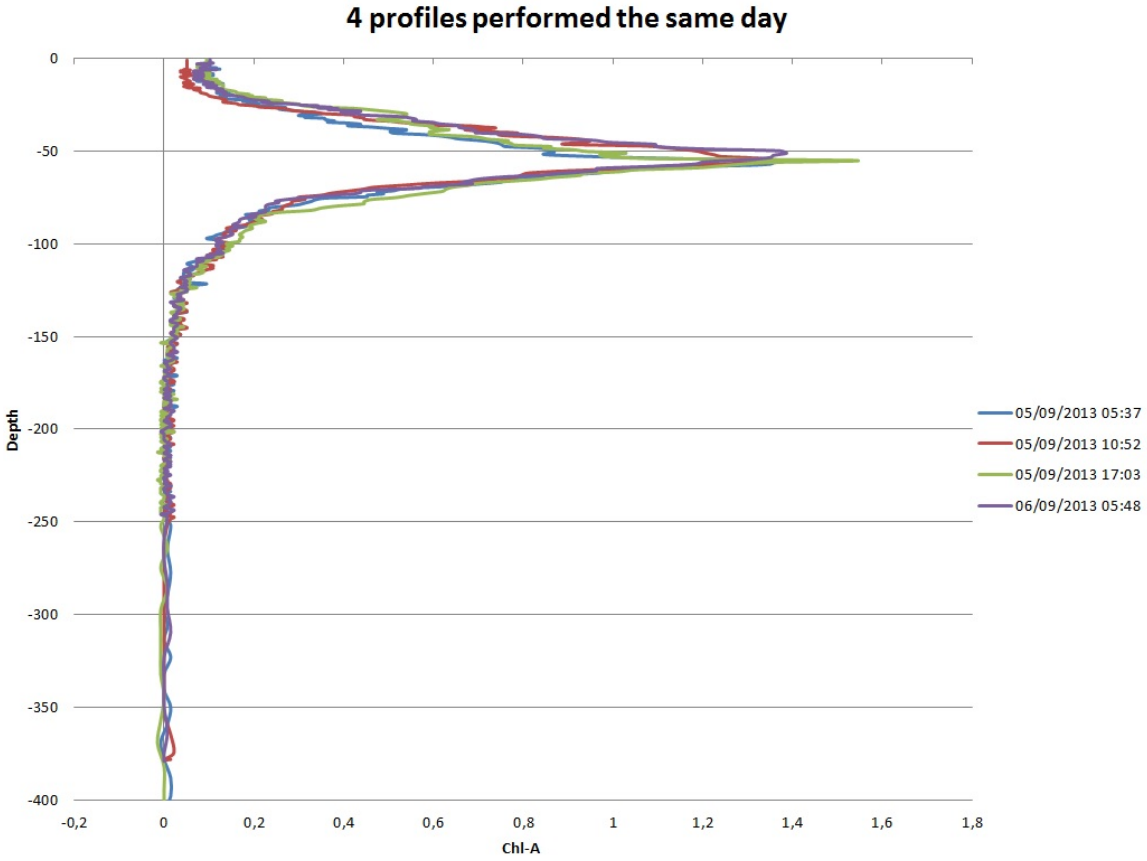


Figure 3a – Four consecutives observations of Chlorophyll at 6 hours interval each

Another metric which is investigated today is the *stability* of the measurements. This is estimated by using high frequency profiling (every 6 hours or every 24 hours) and make the comparison between two consecutive profiles. The low frequency variation could be attributed to a change in the biology or biomass advection while the high frequency is most likely due to random uncertainties say ε_F. On figure below, one can appreciate the overall stability over the day (note the quenching effect lowering the retrieved value of the Chlorophyll).

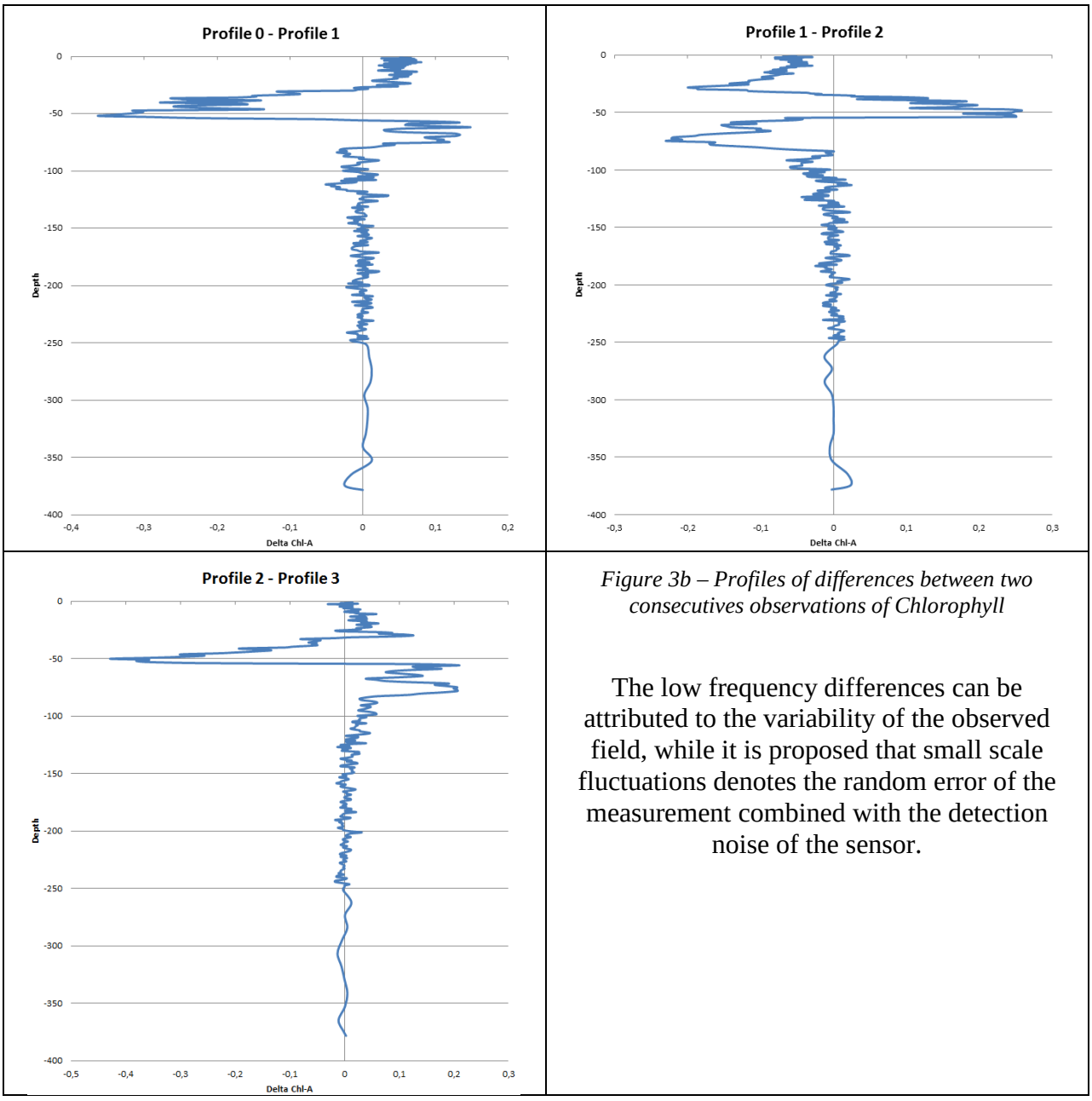


Figure 3b – Profiles of differences between two consecutives observations of Chlorophyll

The low frequency differences can be attributed to the variability of the observed field, while it is proposed that small scale fluctuations denotes the random error of the measurement combined with the detection noise of the sensor.

The final random uncertainties for a given profile should therefore be a combination of the detection noise and the random part ε_F.

3.3.2. *Systematic error*

The systematic error could be assessed by three means (this is the present status but other means could be identified in the next future).

Dark signal – for several types of measurements, it is known the measured parameters shall be close to zero at large depth. The dark value is the value of the measurement at large depth. Its drift and fluctuation from one profile to another is a mean to estimate the quality of the measurements (it is used for QC) but also to qualify it. For instance, herebelow is presented the evolution of dark value for Nitrates measurements that clearly shows the temporal and regular drift.

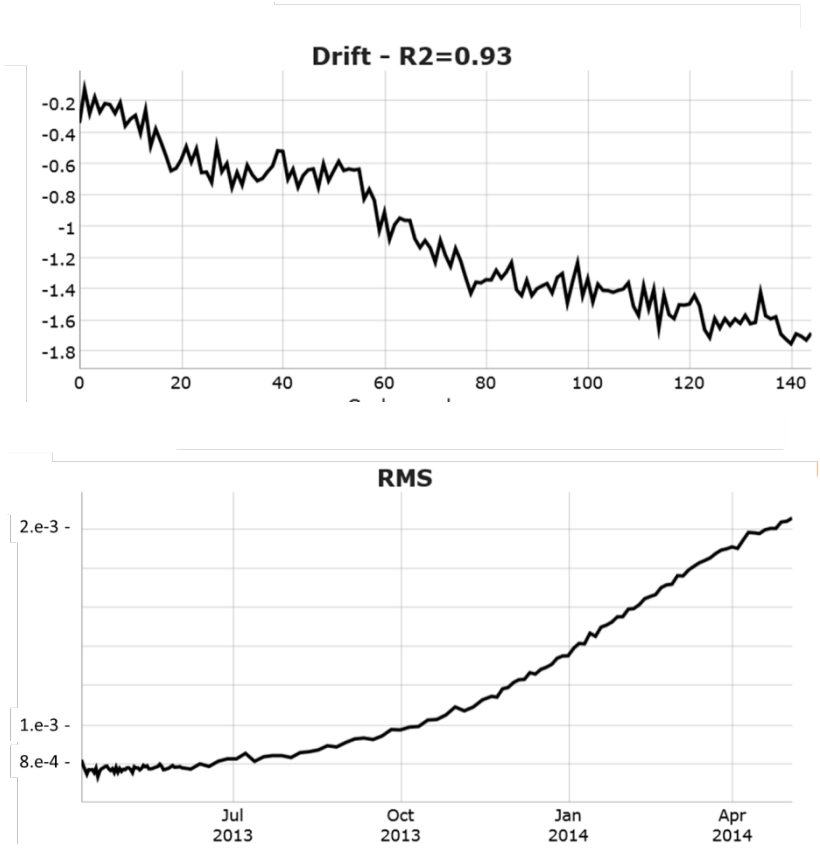


Figure 4 – Temporal evolution of the dark value (top) and of the noise on the profile of NO3 (bottom). The dark value follows a linear trend (high determination factor for a linear fit)

Inter-comparison of profiles - Thanks to concomitant deployment of 7 floats in North Atlantic is it possible for a restricted time window to inter-compare measurements made by different floats in similar waters. The figure below indicates the trajectories of each float from the deployment point. It is clear that 3 routes are followed (the branch by #20 and #38; the one by #13 and #22, and the one by #23, #25 and #29). The 21st of April 2013, 5 floats are very close and so it is possible to perform a cross-comparison, assuming that the observed waters are similar in an area of less than 2 km of radius. The result is presented on figure 6.

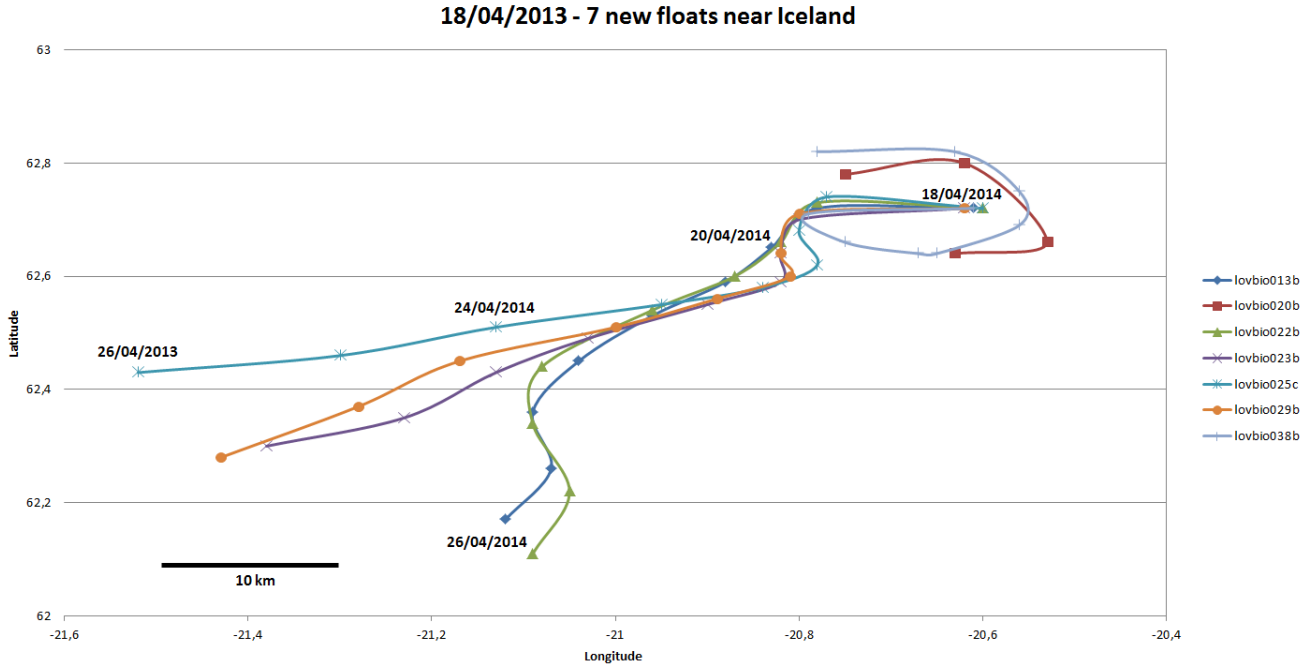


Figure 5 – Trajectories of 7 bio-floats deployed at the same location and the same date (18/04/2013)

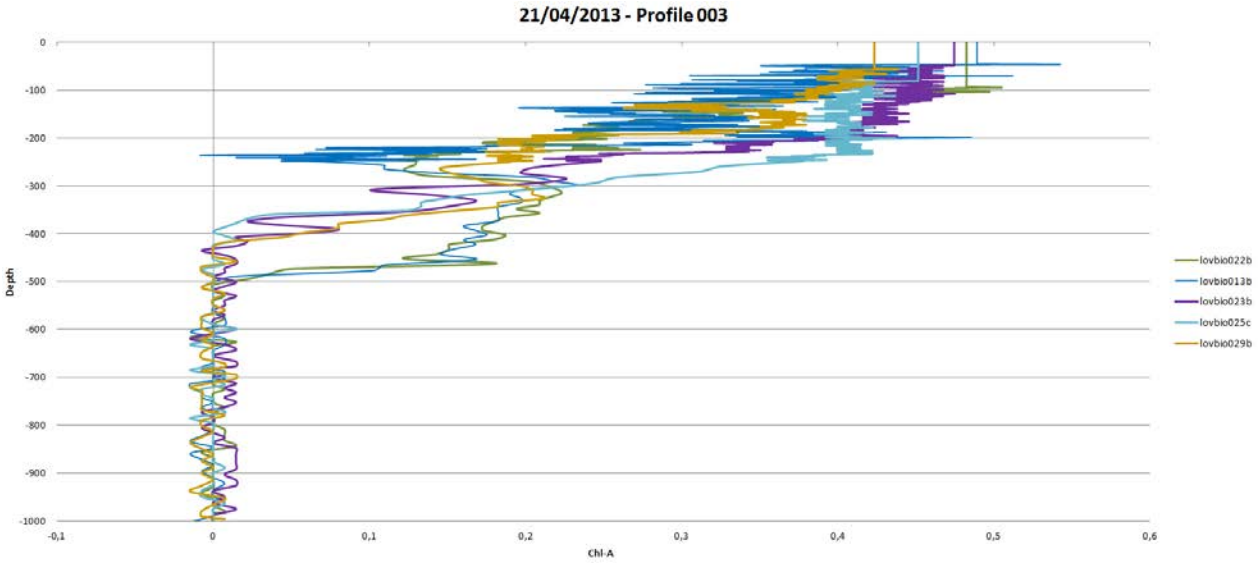


Figure 6 – Cross comparison of floats assumed to sample the same waters – Clearly floats 13 and 22 are crossing water type different from the one sampled by floats 23, 25, 29.

The results on figure 6 provide an estimate (that is to be further analyzed) of the what could be a systematic error between different sensors.

Proval – The Laboratoire d'Océanographie de Villefranche sur Mer has developed a bio-float (Proval) dedicated to very fine measurements to be used for sensor calibration. The float presented on figure below is a new Provor CTS5 (NKE) with a high speed, bidirectional Iridium telemetry. The payload is constituted with 2 sensors one for E_d at 380, 412, 443, 490, 510, 560, 665 nm + PAR; and one for Lu at 380, 412, 443, 490, 510, 560, 665 nm. Additional sensors can be added (Chla, backscattering, …). The Proval can be deployed in parallel to biofloat in order to provide a reference at the beginning of the biofloat cruise. The Proval is recovered after

operations. Its geometry allows avoidance of self-shading and part of its payload is redundant. It is an excellent means for pre-qualification of biofloats at sea.

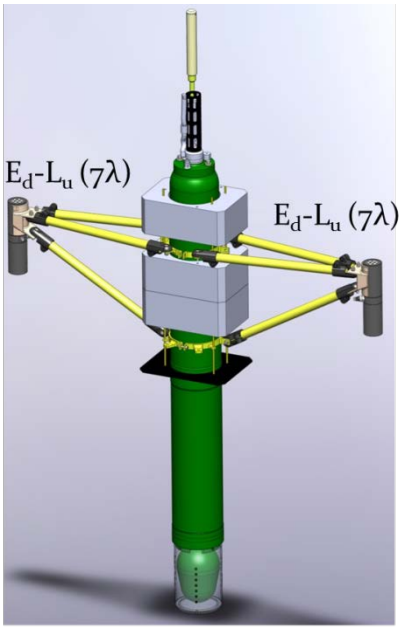


Figure 7– ProVal float developped by Laboratoire d'Océanographie de Villefranche-sur-Mer

3.4. Algorithmic approach

On top of these error estimates that would allow the validation of ocean colour, three complementary approaches, based on the available algorithms could also be put in place to reinforce the data quality and validity assessment.

1. First approach is to reproduce the technique proposed by Xing et al, (2011), that is to say the interpolation method to retrieve Chlorophyll and to put it against satellite observation to assess bio-profilers and satellite stability (and therefore *uncertainty*).
2. Second is to establish a bio-profiler calibration using Boss et al. (2008) method and compare it stability with satellite observations (here the Ocean Colour is used as reference, further to Boss et al. paper we will introduce the documented *precision*)
3. Lastly correlations between bbp and Chla profiler measurements will be carried out, based on the four formulas proposed by Boss (2008) to underlined the inherent data quality. This last step is however more proposed as an extra quality check analysis to optionally flag data or suspisous reccurent behavior of one of the two observations. At this stage available empiral (or semi-) expressions will be used to check consistencies with all measurements from the profiler (in principle, Fluorescence of Chlorophyll-a, bbp532, bbp770, Ed (at 380, 412 and 490 nm) and Photosynthetically Available Radiation).

3.5. Recommendations

Support to satellite ocean colour validation by bio-floats is to be understood as a reciprocal exercise. Both means of observations have to be seen as complementary. The level of use for a mutual benefit is strongly depending on the characterization of uncertainties and error of the bio-

floats observations. If we know this uncertainty we can compare to satellite and even go towards a reciprocal validation. Without this knowledge the bio-profilers could support the ocean colour from space to be used for verification and quality control.

We propose to take advantage of the statistical independence of both observations (ocean colour and bioprofilers) to make use of classical statistical analysis to combine all the information; values of the Chlorophyll-a from different sources with associated accuracies and precision (this technique is similar to the ensemble-like approach used to derive the SST from several sensors). The main assumption is that the possible bias component has been removed prior to this combination – this should be the result of the QC DM operations.

We have described means to master the uncertainties of the bio-profilers observations. These means still have to be widely put to test and validate before specifying a robust and systematic methodology.

The first set of recommendations for validation could be;

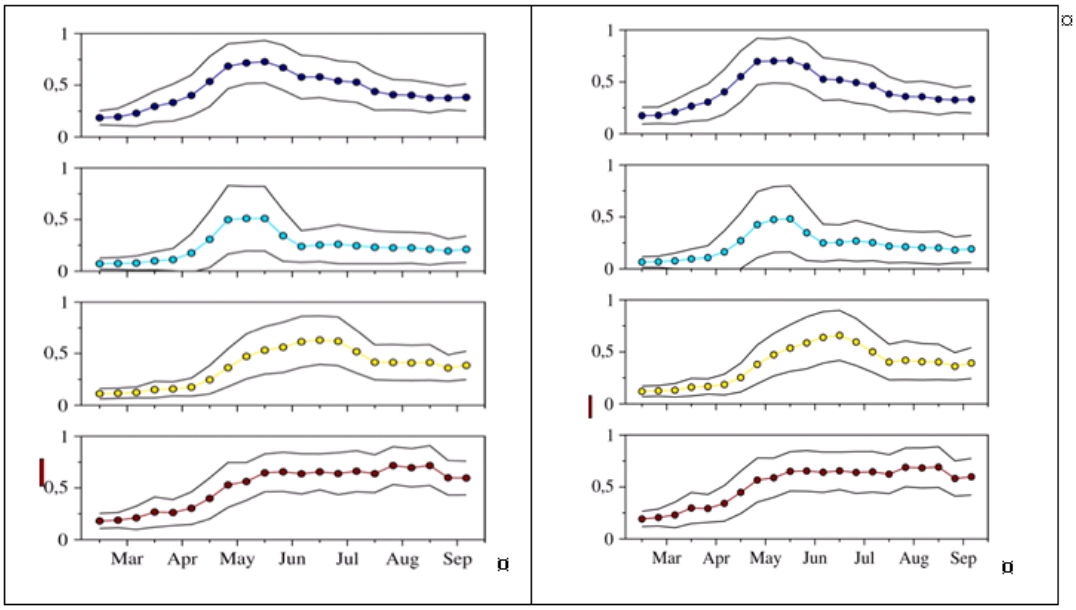
- Optimise the matchup strategy (ie. program the biofloats to raise the ocean surface at the time of an OLCI path)
- Focus on the validation of IOP instead of AOP; e.g. the validation is preferably to be done on reflectances and Kd and, in a second step to Chlorophyll in order to be less dependant of fluorescence efficiency.
- Program high frequency cycle of profiling for each floats when it is located in a biological stable area.
- Make use of Proval to perform parallel sampling during the launch of each biofloats.
- When bio float is recovered, perform same type of analysis (to check the validity of uncertainties estimates),
- Pursue research works for characterization of σ_A

4. Research – bioregions

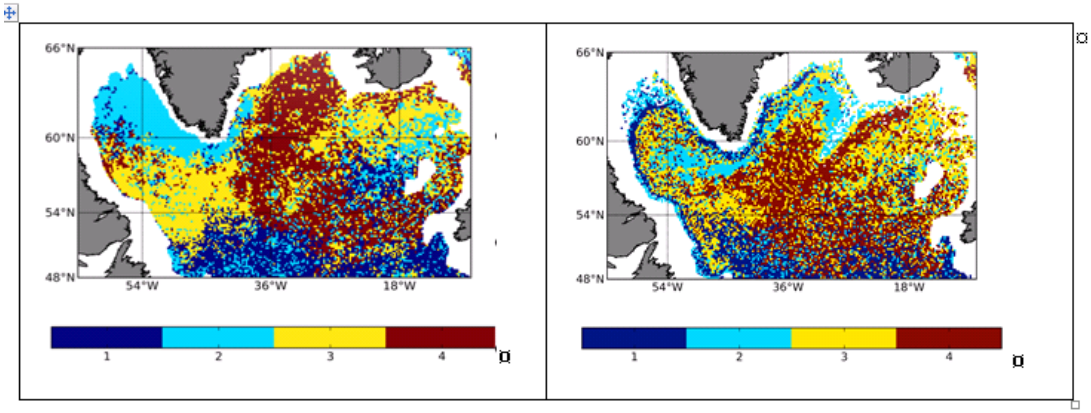
In parallel to ocean colour exploitation, impact studies based on the bioregional classification proposed by D'Ortenzio and d'Alcalà (2009) and seasonal cycles has been performed to constrain and refine the sampling design and to check whether it could be used for QC DM.

4.1. Optimisation of the sampling design and deployment strategy

This part of the work benefits from and adopts the methodologies tested and recommended by the OSS2015 project, funded by the EU Seventh Framework Programme (FP7) – Space 2011. The testing area was the north Atlantic for which "traditional" bioregionalisation based on exploitation of satellite imagery (thus with an Eulerian representation) has been compared to a bioregionalisation derived from what is "seen" by profilers (thus with a Lagrangian representation).



Centroids for the 2 bio-regionalisation of the NA. Left panel "Eulerian" bio-regionalisation; right panel: "Lagrangian" bio-regionalisation



Spatial distribution of the membership for the NA bio-regionalisation. Left panel "Eulerian" bio-regionalisation; right panel: "Lagrangian" bio-regionalisation. Colours are the same as above

Figure 8 – Bioregions in NA derived from eulerian representation (left) and from Lagrangian representation (right) (from OSS2015)

The exploitation of this cluster approach is very simple, it says that any bioprofilers launched at a given time in one cluster would see the same biological story (see by example, the four types of seasonal evolution on figure 8 (top panel). In turn, and if validated, it could strongly orientate the sampling strategy by proposing a limited number of float launch per bioregions.

4.2. Use of bio-floats to validate the bioregions approach

A bioregion might be defined as a homogeneous area in which the seasonality of biology cycle is rather stable (this does not mean that the level of biological life is the same – only the seasonality). A dedicated tool has been put in place to check this assumption (see below screen shot of the seasiderendezvous.eu). Research works are underway to try to validate the bioregions developed in OSS2015 (either based on pure-satellite information or by modelling the drift of a virtual constellation of bio-floats and using satellite data as in situ truth).

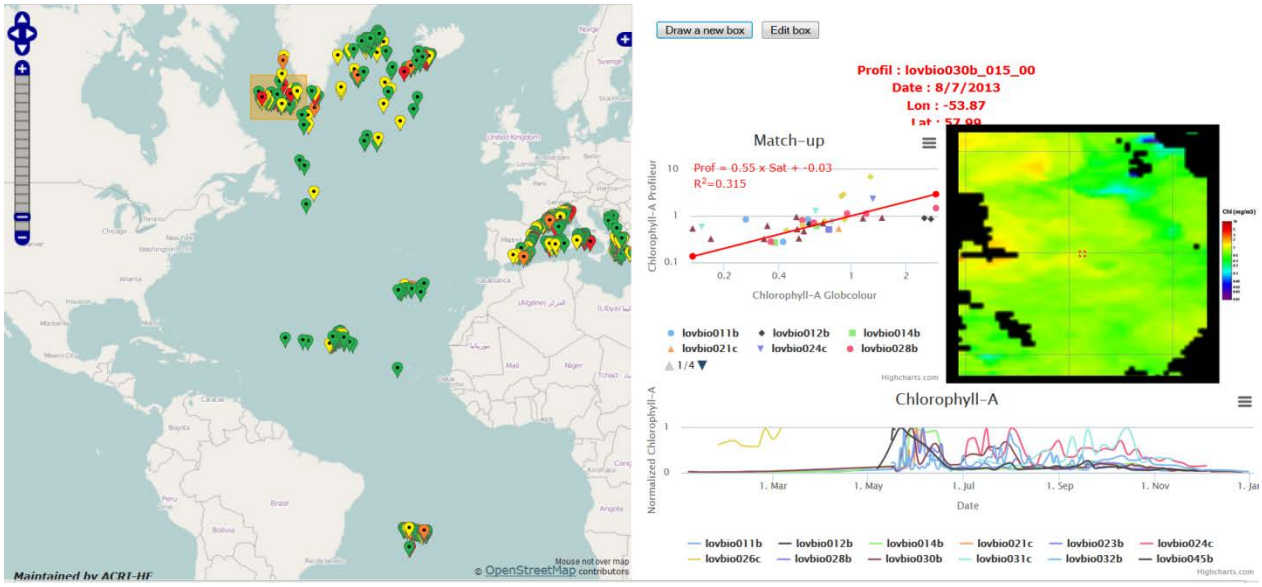


Figure 9 – screenshot of seasiderendezvous.eu – on the left panel is the matchup with GlobColour data and on the left bottom part is the normalized temporal evolution of all Chlorophyll observations that are available in the selected box (orange box that has been selected by the users on the global map)

4.3. Recommendations

The analysis of the bioregions and the potential for validation supported by the bio-float observation could constitute a major step in the setting up of a reliable climatology. For this, it is recommended to pursue the validation through the exploitation of all available profiles. In particular, computation of correlation spatial scales by region could be a very valuable input to this analysis.

5. Assimilation

As the number of bio-profilers in operation is increasing, the assimilation into BGC model appears to be the natural next step for the exploitation of biofloats observations in order to merge

the 2D view from Ocean Colour and their 1D-vertical view. Although the assimilation in BGC model is not really in the scope of E-aims, it is also important to keep this component in mind as modelling shall become a large user of this type of network (as it is for Argo floats). Therefore an appropriated and adjusted deployment strategy should be defined.

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