Project	AtlantOS – 633211
Deliverable number	D7.11
Deliverable title	Interior Carbon EOV Report
Description	Interior carbon syntheses and impact of AtlantOS observations
Work Package number	7
Work Package title	Data flow and data integration
Lead beneficiary	GEOMAR
Lead authors	Toste Tanhua, Nico Lange
Contributors	WP7 partners
Submission data	12 November 2018
Due date	31 July 2018
Comments	D7.11 is delayed as a relevant progress has been made over the last few months. At the end of September, the team had a 3-day face-to-face meeting with the GLODAP group to finalize the adjustments to the cruises, and the publication of GLODAPv2.2018 the will follow by the end of the year.

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Last updated: 15 November 2018

Stakeholder engagement <u>relating to this task</u>*

WHO are your most important stakeholders?	☐ Private company If yes, is it an SME ☐ or a large company ☐? X National governmental body X International organization ☐ NGO ☐ others Please give the name(s) of the stakeholder(s): …
WHERE is/are the company(ies) or organization(s) from?	☐ Your own country ☐ Another country in the EU ☐ Another country outside the EU Please name the country(ies): …
Is this deliverable a success story? If yes, why? **If not, why?**	X Yes, because GLODAP is a very valuable ocean data product that is now being updated, and is closer to a routine publication on a regular basis ☐ No, because …..
Will this deliverable be used? **If yes, who will use it?** **If not, why will it not be used?**	X Yes, by marine biogeochemist, modellers and observers. ☐ No, because …..

NOTE: This information is being collected for the following purposes:

1. To make a list of all companies/organizations with which AtlantOS partners have had contact. This is important to demonstrate the extent of industry and public-sector collaboration in the obs community. Please note that we will only publish one aggregated list of companies and not mention specific partnerships.
2. To better report success stories from the AtlantOS community on how observing delivers concrete value to society.

*For ideas about relations with stakeholders you are invited to consult <u>D10.5</u> Best Practices in Stakeholder Engagement, Data Dissemination and Exploitation.

1 Executive summary/ Abstract

The distribution of biogeochemical variables in the interior ocean can be determined to high precision and accuracy from water samples collected on research vessels. It has been shown that the amount of inorganic carbon is increasing and that the amount of oxygen is decreasing in the ocean over time, although with significant regional variability. Similar changes are likely happening for other biogeochemical essential ocean variables (EOVs), such as nutrients. In order to quantify these trends, often over multi-decadal time-scales, highly accurate observations are needed. Although the methods to determine the concentration of biogeochemical variables in seawater samples are well established and high precision can be expected, there are still challenges with the accuracy, i.e. systematic biases in the data. The reason for biases vary widely between variables and instrumentation, and can to some extent be over-come with the use of certified reference materials (CRMs). However, CRMs are not used consequently enough by the community.

In order to solve the issue of possibly biased interior ocean biogeochemical data, a method of secondary quality control (i.e. bias correction) has been developed and applied to an internally consistent data product, GLODAPv2 (Olsen et al., 2016). This product has been developed through a few different project the last two decades and is now reaching a more mature readiness state. GLODAPv2 that contains data from close to one million water samples was released in 2016 after several years of work by the GLODAP community. We are now working towards a system where this data product can be updated on an annual time-scale. AtlantOS work is going towards creating the procedures and routines needed for these regular updates and will release a new version of the data product by the end of 2018, GLODAPv2.2018.

GLODAPv2.2018 will include interior ocean carbon relevant data from at least 32 new cruises (this number will likely increase slightly) in the Atlantic Ocean. The data from these cruises has gone through a stringent quality control to qualify for GLODAP standards and the addition of these data to the data product will be essential for: Quantifying interior ocean storage of anthropogenic carbon; quantifying and understanding ocean deoxygenation; detecting changes in nutrient distribution, and a range of other relevant questions. The GLODAPv2 data has, at this point in time, been utilized in more than 70 scientific peer reviewed papers since its release in 2016 (see the GLODAP home page; https://www.glodap.info/).

2 Introduction

This task is focused on integrating interior-ocean biogeochemical, including carbon, data to a uniform data product. This is done in the context of an update of the existing data product GLODAPv2 (Olsen et al., 2016), that was published in 2016. The GLODAPv2 product is, in turn, an update of the data products GLODAPv1.2 (Key et al., 2004), the CARINA (Key et al., 2010) and PACIFICA (Suzuki et al., 2013) that were merged together and updated with a large amount of new cruises. This resulted in the extensive product GLODAPv2 that in essence is an internally consistent data product including interior ocean carbon relevant data from discrete samples from CTD casts. It is the most complete and consistent data product of interior ocean carbon available. The term "carbon relevant" means that only cruises with inorganic carbon data or transient tracer data have been included in the product, but that all data measured on those water samples are included in the product. GLODAPv2 contains data from 724 cruises, close to 1 million individual water samples.

The data in GLODAP has gone through a rigorous quality control (QC) procedure. This process includes a "primary QC" (1st QC) that is focused on the precision of the data, i.e. it involves detecting, and flagging, outliers in addition to standard checks on format, units, and the realistic value of the data. For each individual cruise in the product this has been performed in a consistent way, involving numerous Q/A with the data originators and reading of cruise reports. The secondary QC focuses on the accuracy of the data, i.e. detection of, and correction of, any systematic biases in the data. A range of software tools to accommodate the QC process has been developed (Tanhua et al., 2010) and are continued to be developed. For instance, a software package to facilitate 1st QC of "bottle data" has been developed in the AtlantOS project (WP2.2) and has been used for completing this task, providing valuable feedback between developers of the software package and the users within the same project.

The first versions of GLODAP and the associated data products as described above have so far been released irregularly and seldom. The work in AtlantOS is part of a process that will allow updated versions of GLODAP to be published regularly, i.e. annually. GLODAP can be found at NCEI https://www.nodc.noaa.gov/ocads/oceans/GLODAPv2/ and at the designated GLODAP website https://www.glodap.info/ where we plan to post regular updates, Figure 1.

The data that goes into GLODAPv2, and currently the only way of acquiring high accuracy data to detect decadal change of interior ocean inorganic carbon, are coming from water samples from research vessels – there is a close link to WP2.1 in AtlantOS that has been instrumental in coordinating and supporting the research vessel program in the Atlantic. The data delivery from RVs, particularly the repeat hydrography program, to data portals and finally to the data product GLODAP has benefited from work on data harmonization and data flow of WPs 7.1 and 7.2 in AtlantOS. This level of update of GLODAP, and the road towards a more seamless data delivery would not have been possible without the work of WP2.1, Wp7.1 and WP7.2 in particular.

The internally consistent, i.e. accurate, data in GLODAP is critical for biogeochemical observations carried out and supported by WP3 on autonomous observing networks; biogeochemical sensors do need calibration and validation from reference quality measurements by research vessels and are reliant on the consistent data in GLODAP. The result in this task thus support work also in WP3 of AtlantOS.

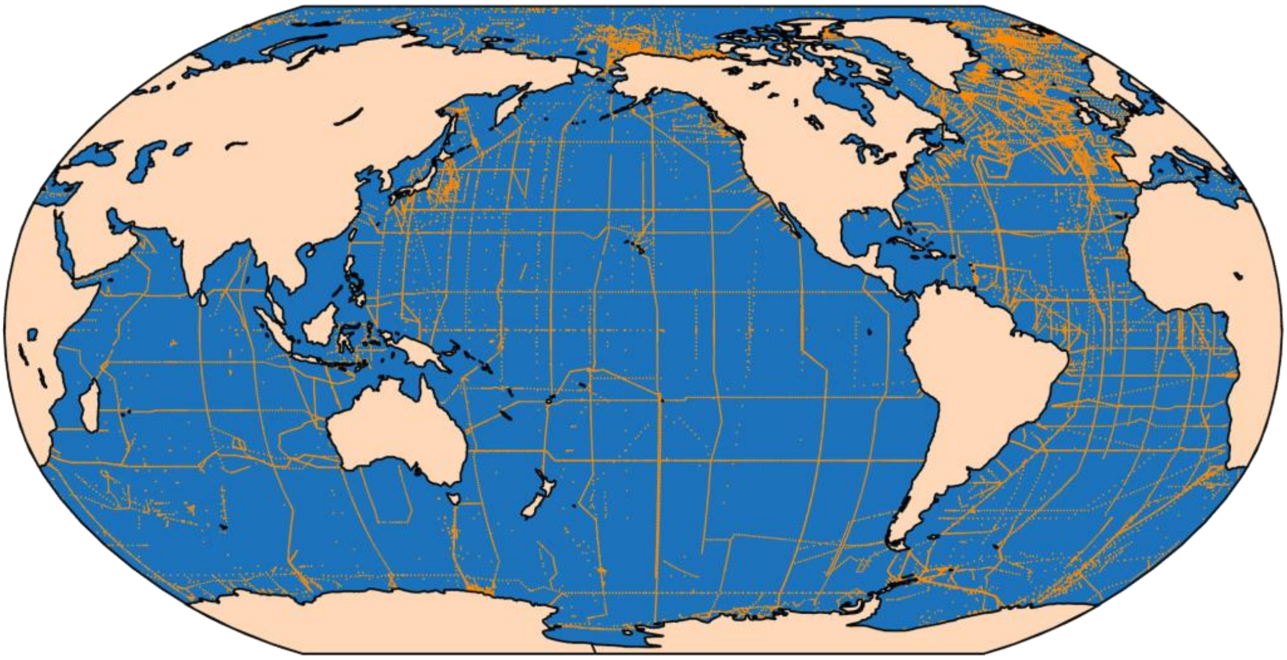

Figure 1: *Map of stations in GLODAPv2 published in 2016.*

The variables contained in the GLODAP data product include "all variables measured from a water sample", i.e. for some cruises we get a set of "exotic" (not commonly measured) variables that are included in the product. However, the 2nd QC process (i.e. the bias control) is only carried out on a set of "core variables"; salinity, DIC, TA, pH, nitrate, phosphate, silicate, oxygen and the transient tracers (CFC11, CFC12, CFC113 and CCl4).

3 GLODAPv2.2018

The main (but not only) provider of interior ocean carbon relevant data is the global repeat hydrography program GO-SHIP (www.go-ship.org). This program focuses on repeating a number of long ship "sections" with regular, deep, CTD stations on a decadal scale (although some lines are repeated more frequently). The first repeat of all lines was completed during the WOCE project, mainly during the 1990's, and the second repeat cycle was completed in 2015. GLODAP is striving to align to this cycle by publishing a full update of GLODAP after each GO-SHIP repeat cycle is completed, i.e. GLODAPv3 will be published in 2025. In the interim time we strive for annual updates of the product, the one to be published this year will be GLODAPv2.2018. The difference between the full update and an interim update is the way the data are treated: For the full update all cruises in the product will be used for the 2nd QC without any adjustments to any variables, and all adjustments will be assessed "from scratch", although guided from previous assessments of adjustments. This is a very tedious work and can only be motivated on decadal scales. For this work 2nd QC procedures as reported by Tanhua et al. (2010) are used. For the annual, interim, updates new, i.e. not previously included, cruises will be added to the product. The internal consistencies of the reported values for these cruises are checked vs. the last full update in a procedure that do not foresee any changes of the adjustments in the existing data product in a process described by Lauvset and Tanhua (2015).

The new cruises for GLODAPv2.2018 have gone through a rigorous quality control, both primary and secondary. For the secondary QC the suggested adjustments and supporting material, such as plots and comments, have been uploaded to the adjustment table hosted at GEOMAR, https://glodapv2.geomar.de/adjustments/list, Figure 2. This list is for GLODAPv2 and is publically available, the list of additional cruises for GLODAPv2.2018 is password protected but as soon as the product will be released a "non-editable" version of the adjustment table will be published. The adjustment table has been produced by the data management team at GEOMAR in Kiel; support, updates and maintenance to the table is one of the tasks of the data management team at GEOMAR that is supported by AtlantOS. This table has been, and continues to be, an invaluable tool for the secondary QC process, and an essential documentation accompanying the data product explaining in detail, with plenty of plots, why a particular adjustment was applied, or not.

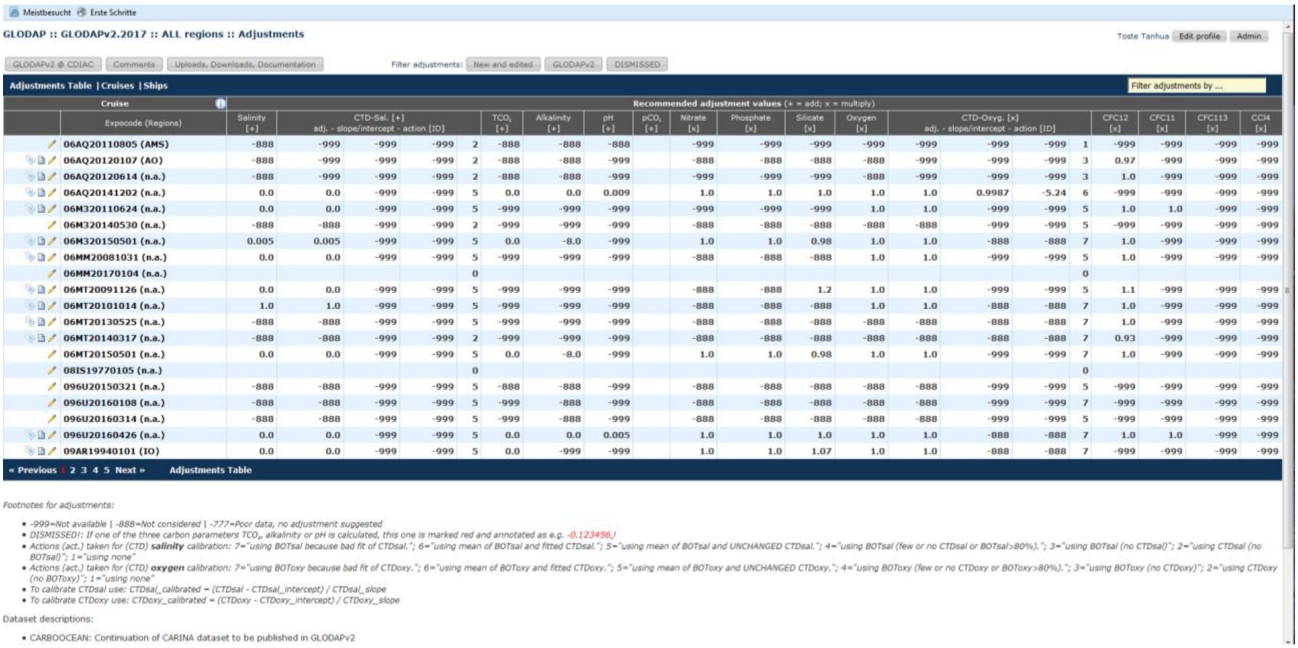

Figure 2: *Screenshot of the GLODAPv2.2018 adjustment table.*

The secondary QC process is mostly based on a process known as cross-over analysis: Whenever the cruise track of two cruises cross one can compare the measured values of the two cruises. For the deep water - on most locations - there are only very small changes to be expected so that any systematic difference is indicative of a bias for one of the cruises. If this bias is repeatedly found for a number of crossovers with different cruises, it is likely that the measurements of that cruise are biased and that an adjustment is motivated. The result of such a crossover is illustrated in Figure 3 where the crossover of one "new" cruise is checked vs. cruises in the GLODAPv2 data product.

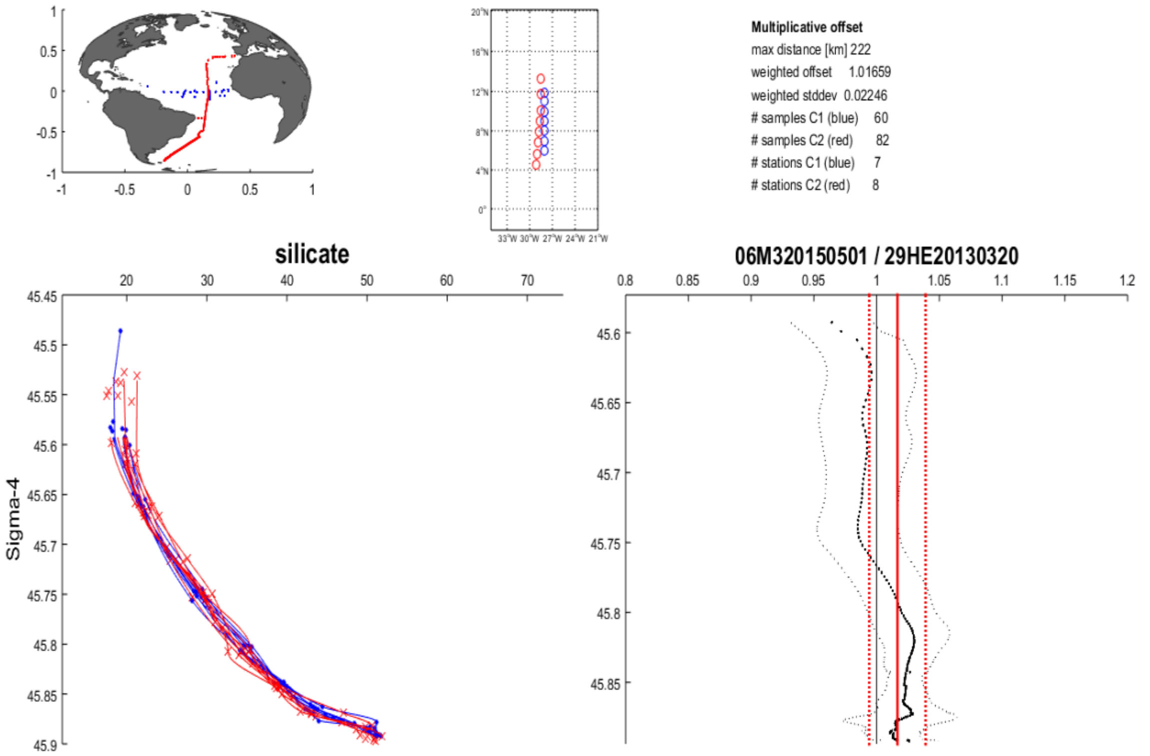

Figure 3: *Example of a crossover for a cruise in the tropical Atlantic, the cruise in blue is a new cruise that is compared to a cruise from GLODAPv2 (in red).*

A collection of such crossovers will give an indication whether or not an adjustment is needed. This can be illustrated in Figure 4, where the weighted mean of a number of crossovers for one cruise vs GLODAPv2 is shown.

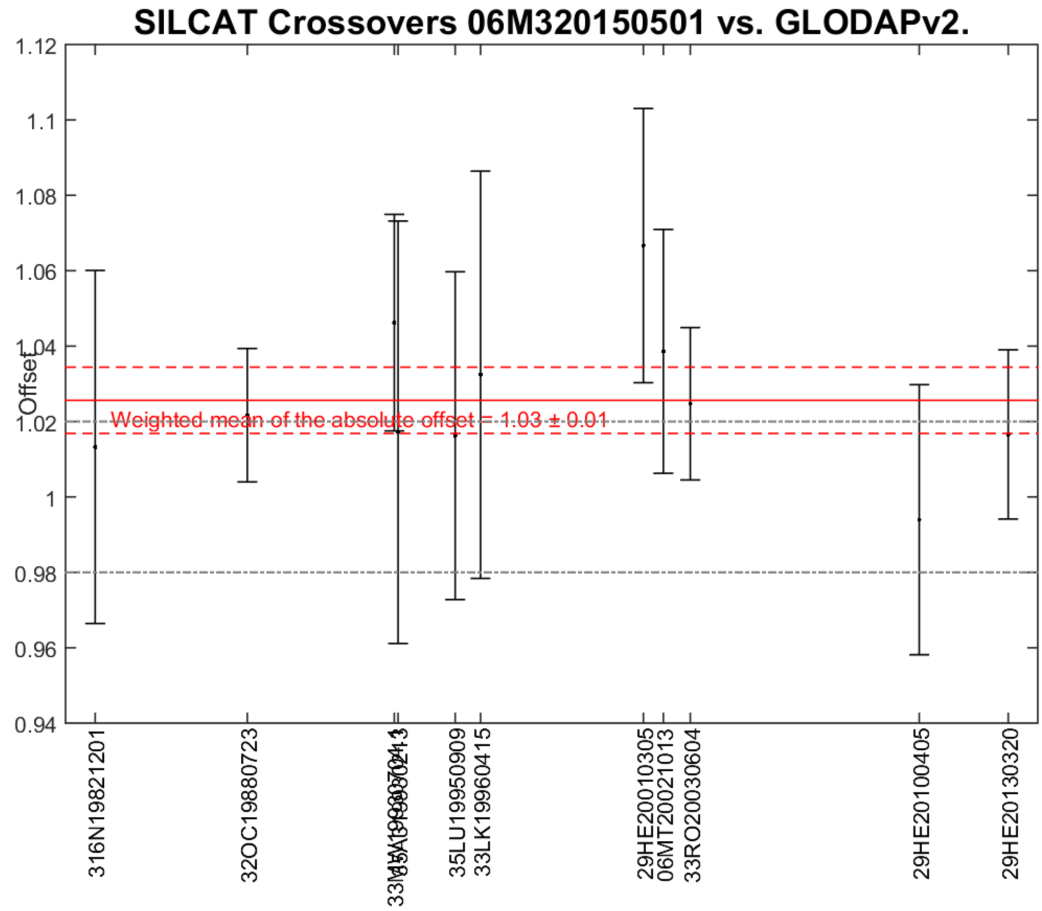

Figure 4: *This figure shows the collected results for all crossovers for silicate for cruise 06M320150501 vs. GLODAPv2. The generally high values (i.e. above 1) indicate that a downward adjustment for silicate could be necessary.*

In addition to the crossover analysis three further methods are used to detect biases. Quantities of transient tracers strongly depend on time, but temporal trends generally hinder the possibility to draw conclusions from crossovers. Following the procedures described Steinfeldt et al. (2010), the CFC surface equilibrium saturations in combination with CFC ratios are thus analysed as an alternative. Further, if for a particular cruise not enough crossovers for a robust decision are present, multi-linear-regressions of the nearby area/basin help to identify suspicious parameters (e.g. Jutterström et al., 2010)This method was especially beneficial in poorly accessible areas(i.e. with few cruises) such as the Arctic ocean. Lastly, as a consequence of the sparse pH data, additional carbonate interconsistency checks (TA, DIC and pH) are performed to analyse its accuracy (Olsen et al., 2016).

Several of these processes are manual at this stage (although the secondary QC scripts in matlab runs autonomously) and require user input. Progress is being made at this stage on making these processes more automatic (although some user input will likely be needed also in the future), this is in cooperation with the EU project RINGO and the ICOS OTC.

The final decisions on adjustments are taken by the GLODAP reference group – a group of chemical oceanographers with extensive experience in both data analysis and data acquisition. This group will meet by end of September for 3 days and carefully wet all suggested adjustments, or lack thereof.

GLODAPv2.2018 is planned for release by the end of 2018. For this interim update we have quality controlled and processed data from 32 new (i.e. cruises not previously included in GLODAPv2) cruises for the Atlantic Ocean containing >54.000 data points, see Table 1 and Figure 5. In addition we have conducted updates to 24 cruises already in GLODAPv2 – mostly this comprises of adding variables previously not available (variables measured after the cruise, such as tritium and He-3, tends to be delayed in the reporting), but on some occasions we have received updated data sets from PIs (mostly recalibrated data).

Expocode	No. of samples	Expocode	No. of samples
New cruises		Updated cruises	
06AQ20120107	3742	06MT19960910	1850
06AQ20141202	1215	29CS19930510	1081
06M320110624	2549	29GD19821110	439
06M320140530	1037	29GD19840218	635
06M320150501	1774	29GD19840711	1656
06MM20081031	4610	29GD19860904	927
06MT20091126	2554	29HE19980730	985
06MT20101014	2349	29HE20030408	132
06MT20130525	4278	316N19970717	2497
06MT20140317	3388	316N19970815	2117
18HU20130507	1099	33AT20120324	2651
18HU20140502	1411	33AT20120419	2554
18HU20150504	842	33LK19960415	2055
18MF20120601	655	35LU19890509	587
29AH20110128	3714	35LU19950909	1854
29AH20120623	2447	35TH19990712	2311
316N20070207	1580	35TH20040604	2529
316N20111106	802	49NZ20031106	3908
33RO20131223	2660	67SL19881117	1635
35PK20140515	1803	74AB19910501	1338
64PE20110724	395	74DI19900612	111
74DI20110520	908	74DI19970807	3025
74DI20110606	610	90MS19811009	305
74DI20120731	427	320620070203	1551
74EQ20151206	3035		
74JC19990315	2442		
74JC20001121	396		
74JC20071231	348		
74JC20150110	305		
74JC20151217	347		
74JC20161110	333		

Table 1: *The cruises and number of samples from the Atlantic Ocean that have been added (left columns) or updated (right columns) to GLODAPv2.018. Note that this is a preliminary table as we might be able to add a few more cruise before we close submission in mid-September 2018.*

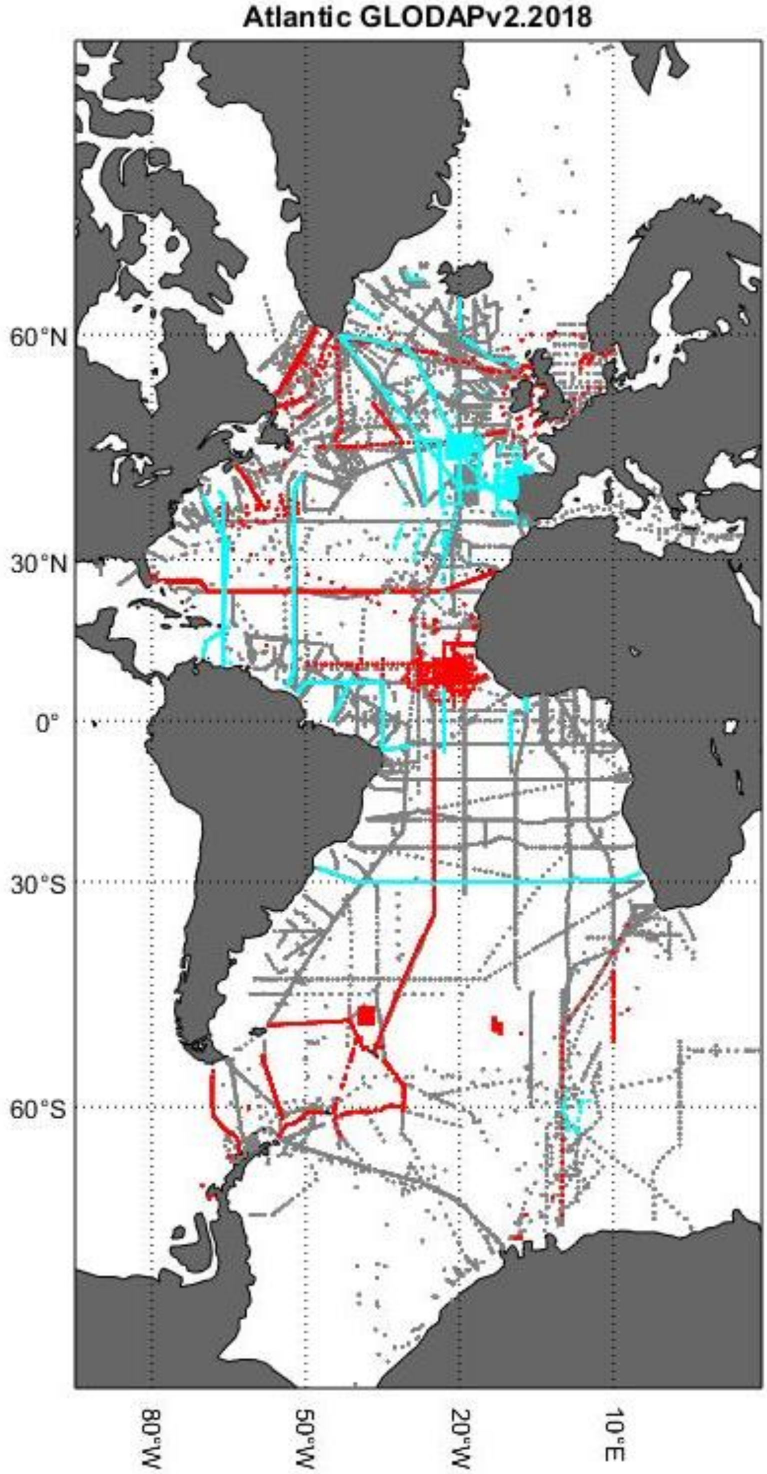

Figure 5: *Map of the Atlantic Ocean data in GLODAPv2 (grey dots) and the new stations that are included in GLODAPv2.2018 (red dots). The blue dots denote stations where updates have been carried out.*

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