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SAGEO$_2$-*Argo*

SOCCOM **A**ssessment and **G**raphical **E**valuation for **O**xygen

Modified for use with International Biogeochemical Argo Floats

Software User Manual
V1

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“Software was developed and made freely available by the Monterey Bay Aquarium Research Institute in support of the Southern Ocean Carbon Climate Observations and Modeling (SOCCOM) project.”

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1. Context

It has been shown that Aanderaa oxygen optodes (in widespread use on board biogeochemical Argo profiling floats) suffer from pre-deployment storage drift and can under-estimate oxygen concentration by up to 20% once deployed (Takeshita et al, 2013; Johnson et al., 2015; Bittig et al., 2018). Many floats are now capable of taking in-air measurements while at the surface which allow for post-deployment calibration of the oxygen optode, bringing data accuracy closer to 1% (Johnson et al., 2015; Bittig et al., 2018). While this is the preferred correction method, post-deployment optode calibration can also be performed using the World Ocean Atlas (WOA) climatology (Takeshita et al., 2013) or by comparing float data to high-quality shipboard measurements.

However, currently the amount of adjusted oxygen data available on the Argo GDACs is limited, with the U.S. serving the majority of the Argo Bfiles containing corrected oxygen data. Increasing the amount of science-quality oxygen data available to users in real-time requires simple and consistent correction methods that can be adopted globally across DACs for operational implementation. SageO_2 is a MATLAB Graphical User Interface (GUI) developed at MBARI to assist in deriving oxygen optode gain corrections for use in real-time processing. In this version of the software, oxygen concentrations are corrected using a multiplicative gain factor, G:

$$[O_2]_{corr} = G \times [O_2]_{raw} \tag{1}$$

Details related to the calculation of G using different reference datasets follow Johnson et al. (2015) and are described in section 3.2. The code library used to support GUI functionality and calculate optode gain was initially built as part of the Southern Ocean Carbon Climate Observations and Modeling (SOCCOM) float processing workflow at MBARI. The original version utilized raw incoming *.msg files from SOCCOM APEX and NAVIS floats. Modifications to the GUI were recently made to support its use for other float types within the Argo float Global Data Assembly Centers (GDACs) and at other research institutions.

The SageO2-Argo software is now available here and can be used to visualize float oxygen data from Argo netCDF files in comparison to WOA climatology and NCEP reanalysis products (used to estimate atmospheric oxygen partial pressure along a float track) in order to derive float-specific gain correction values. These correction factors can then be integrated into the DAC processing stream and used to populate the adjusted oxygen parameter (DOXY_ADJUSTED) within Argo Bfiles. Please note that the software in its current state has undergone limited external testing, is provided as-is, and may require modification to suit the needs of each DAC employing its use. Part of this limitation is due to the inconsistencies in how in-air oxygen data is stored within *BRtraj.nc files across the GDAC database. Additionally, visualizing comparisons to bottle data is highly dependent on the structure of supporting shipboard data files at respective DACs. It is our hope that open access to the software will allow for further testing and improvements to the GUI. Additionally, we hope that the sharing of these tools will help improve the accuracy of the global BGC Argo oxygen dataset and bring the global BGC Argo community closer to maintaining internal consistency with regards to the quality control adjustments of float oxygen data served on the Argo GDACs.

2. GUI Setup

2.1 System requirements

The SageO_2-Argo GUI was written using the MATLAB programming platform for Windows, release R2015b. Be aware that backwards compatibility and performance on other platforms (Linux, Mac) has not been fully tested. MATLAB must be properly installed and licensed on your machine before proceeding.

2.2 Toolbox requirements

There are two freely-available external MATLAB toolboxes that must be downloaded prior to GUI use. The GUI itself was built within the framework of MATLAB's "GUI Layout Toolbox" which supports the construction of complex layouts with graceful resizing capabilities. Links to download/install information for each required toolbox are listed in Table 1 below. *BE SURE TOOLBOX DIRECTORIES AND FUNCTIONS ARE PERMANENTLY ADDED TO YOUR MATLAB PATH.*

Table 1: External Toolboxes Required for SageO_2-Argo

Toolbox	Download	Notes
GUI Layout Toolbox	https://www.mathworks.com/matlabcentral/fileexchange/47982-gui-layout-toolbox	Note the two separate download options for MATLAB versions before and after R2014b.
Nctoolbox-1.1.3	https://github.com/nctoolbox/nctoolbox	Be sure to permanently add the toolbox setup to your startup.m file. See notes under "setup" at the download link location.

The MATLAB NaNsuite, m_map1.4, and SEAWATER functions are also called within the software, but these toolboxes have been included within the code repository under
…\ARGO_PROCESSING\MFILES\nansuite\
…\ARGO_PROCESSING\MFILES\m_map1.4\ and
…\ARGO_PROCESSING\MFILES\MISC\, respectively.

2.3 Your float data repository

2.3.1 Setting up your float data repository

The SageO_2-Argo GUI was built to access specific netCDF and text files, namely the Argo formatted *.BRtraj.nc, *meta.nc, and *Mprof.nc files found on the Argo

GDACs, as well as a textfile conversion of the *Mprof.nc file (ODV*.TXT, produced by the user, see section 2.3.2). Whether you intend to use the GUI to visualize incoming data from a single float, or multiple floats, you will want to have all files organized in a single repository on your local machine or network (this will be your “DATAdir”). Figure 1 provides an example of a local data repository containing a number of Coriolis floats. Each subfolder in the repository is float-specific and holds all float files necessary for data visualization (see Figure 2).

Figure 1: Screenshot of an example float data repository on a Windows system

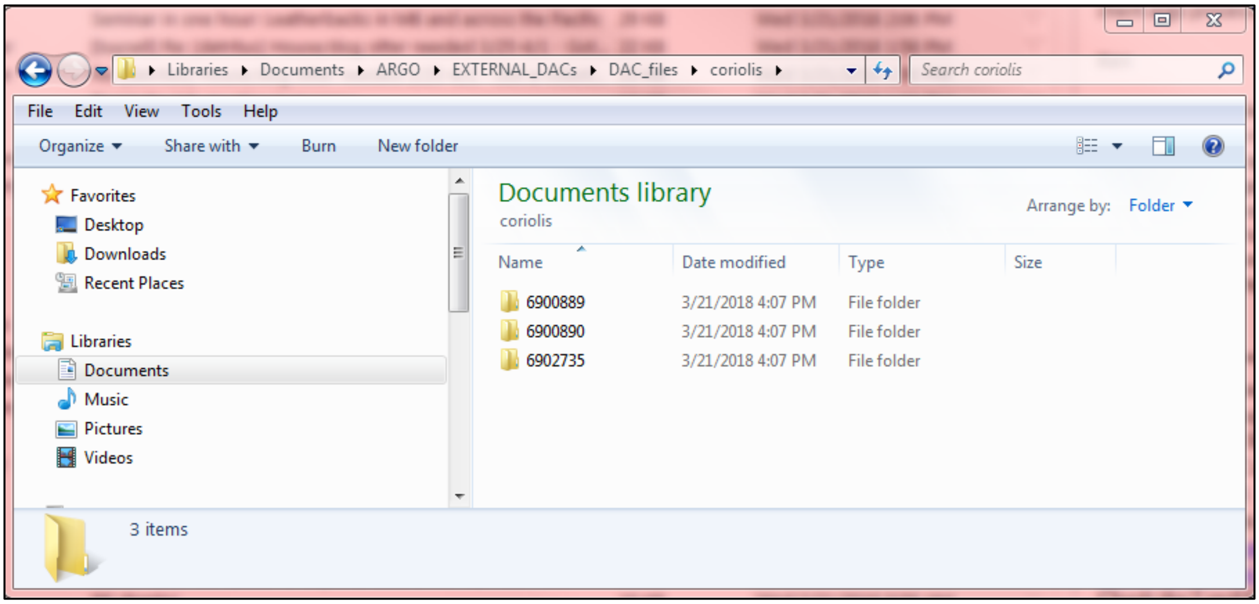
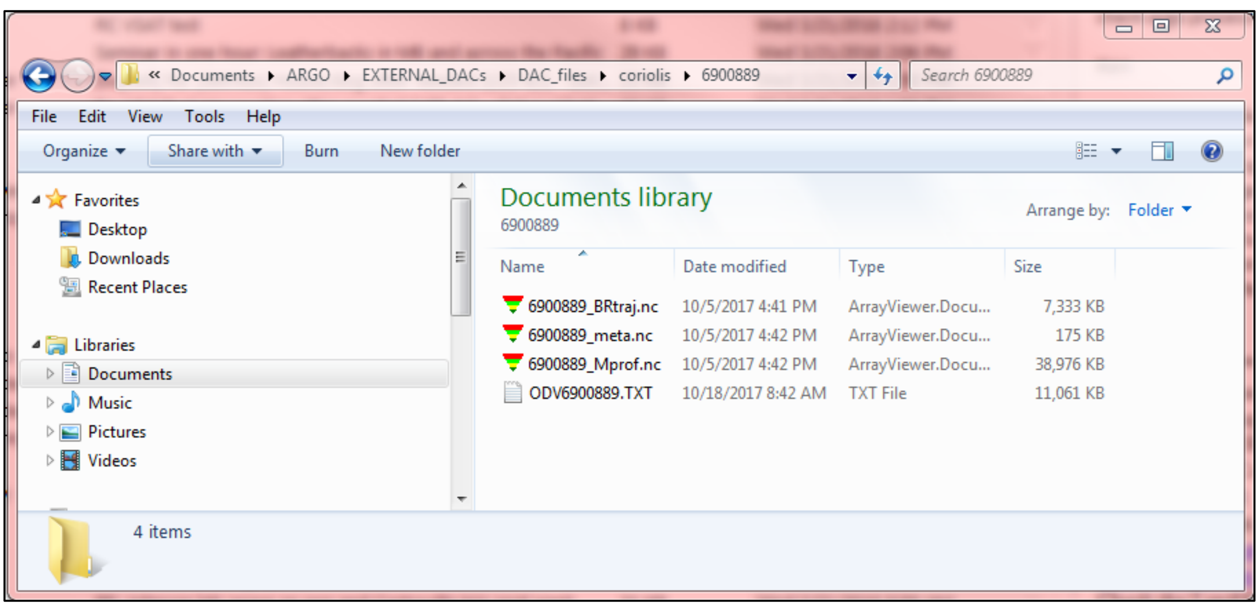


Figure 2: Screenshot showing the contents of a single float subdirectory within the float data repository in Figure 1.



2.3.2 Routines to support file acquisition

Within the code library there are routines to assist you in organizing your input files. If you do not already have the Argo NetCDF formatted files on your local machine for your floats of interest, you can (a) download them manually from the Argo GDAC (note that at the present moment only the ifremer GDAC is supplying merged Mprof files), or (b) use the MATLAB function "get_ARGOifremer_files.m" located in …/ARGO_PROCESSING/MFILES/GUIS/SAGE_O2Argo/ for automated file retrieval.

Additionally, you will need to generate the ODV*.TXT file using "mprofmat2ODV.m" located in …/ARGO_PROCESSING/MFILES/GUIS/SAGE_O2Argo/. This part of the setup is necessary in order to convert profile data within the Mprof file into the format used in SageO2-Argo. Currently, the merged Mprof files available on the ifremer GDAC are not user-friendly (they include large amounts of fill-space and BGC parameters are not necessarily linked to the same pressure axis. For example, PROVOR floats don't always have T & S data collocated with O_2). The ODV*.TXT file assists in aligning parameter data. Improving the format of the Mprof data files was an action item stemming from ADMT18 and is currently being investigated. Note that future improvements to the Mprof data structure in the future may require modifications to GUI setup and code.

2.4 GUI install

Once you have verified your system requirements, have downloaded and installed the necessary toolboxes, and have set up your data repository, it is time to install the GUI software. This step defines and adds all necessary paths, and also downloads NCEP and WOA files to local repositories. If you haven't done so already, clone the GUI repository "ARGO_PROCESSING" from github here: https://github.com/SOCCOM-BGCArgo/ARGO_PROCESSING and place it somewhere on your local machine (for example C:\Users\USER\Documents\MATLAB\, where USER is the username of the machine). Install steps are as follows:

1) Open MATLAB
2) Navigate to …\ARGO_PROCESSING\MFILES\GUIS\SAGE_O2Argo\ (in other words, change your MATLAB "current folder" to this location).
3) At the command-line, define your data repository and install all paths as shown in Figure 3 (first two lines are entered by the user).

Figure 3: Screenshot of MATLAB command line after successful GUI install.

```
>> DATAdir ='C:\Users\tmaurer\Documents\ARGO\EXTERNAL_DACs\DAC_files\'

DATAdir =

C:\Users\tmaurer\Documents\ARGO\EXTERNAL_DACs\DAC_files\

>> INSTALL_sageO2Argo(DATAdir)
INSTALLING "ARGO_PROCESSING\MFILE" PATHS...
INSTALLING "ARGO_PROCESSING\DATA" PATHS...
CHECKING FOR LOCAL WOA2013 FILES...
WOA files were found:

woafiles =

woa13_all_O00_01.nc
woa13_all_O01_01.nc
woa13_all_O02_01.nc
woa13_all_O03_01.nc
woa13_all_O04_01.nc
woa13_all_O05_01.nc
woa13_all_O06_01.nc
woa13_all_O07_01.nc
woa13_all_O08_01.nc
woa13_all_O09_01.nc
woa13_all_O10_01.nc
woa13_all_O11_01.nc
woa13_all_O12_01.nc
woa13_all_O13_01.nc
woa13_all_O14_01.nc
woa13_all_O15_01.nc
woa13_all_O16_01.nc

CHECKING FOR LOCAL NCEP FILES...
NCEP files were found:

ncepfiles =

pres.sfc.gauss.2011.nc
pres.sfc.gauss.2012.nc
pres.sfc.gauss.2013.nc
pres.sfc.gauss.2014.nc
pres.sfc.gauss.2015.nc
pres.sfc.gauss.2016.nc
pres.sfc.gauss.2017.nc
pres.sfc.gauss.2018.nc

INSTALL COMPLETE.
```

4) You should now be able to launch the GUI by typing:
   >> sageO2Argo

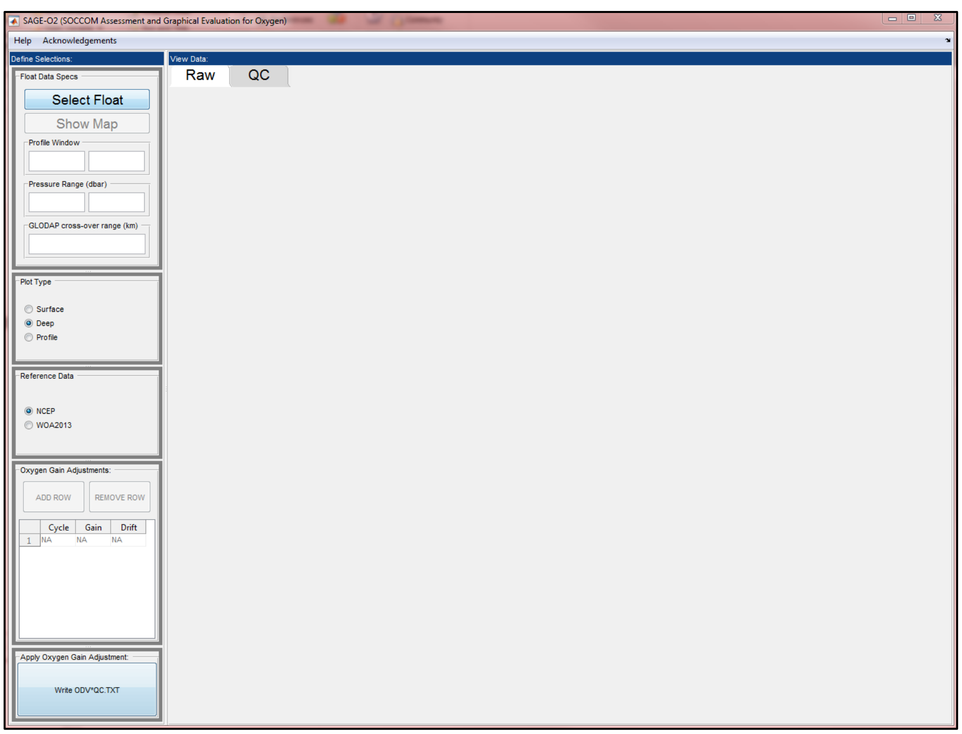
3. Running the GUI

3.1 File Selection

Upon typing "sageO2Argo" at the MATLAB command prompt, you should see the empty GUI interface as shown in Figure 4 below. The left-most column of panels is where the user can select options and actions while the right panel (including "RAW and "QC" tabs) will display the results of these actions. Note that both the main window and each individual input panel can be resized to more easily fit your screen by selecting and dragging panel edges with your mouse.

Once here, click on the "Select Float" button near the top left of the interface. This should open a directory dialog box pointing to the location you designated as your data repository during the install process. From here, you can highlight the float subdirectory of interest and click "select folder". Note that it may take a number of seconds before input data begins to load, depending on the speed of your machine. You may watch the MATLAB command prompt for progress updates.

Figure 4: The SageO2-Argo GUI interface.



3.2 Visualization preferences

Figure 5 shows an example of the GUI screen once your float data is loaded. The first input panel in the left panel column, titled, "Float Data Specs" will allow you to view your float's trajectory on a map (see Figure 6), and change the range of profiles, range of pressures, or threshold distance for crossovers comparisons with high quality shipboard oxygen measurements. Here, we use the GLODAPv2 data set as the shipboard reference (Olsen et al., 2016).

Within the second input panel, titled, "Plot Type", the user is able to toggle between different data views. The "Surface" and "Deep" buttons refer to the data shown in the bottom two time series panels. This is useful for visualizing the oxygen, temperature and salinity time series in relation to your calibration data, represented in the top two time series panels. You can also toggle the "Profile" button. This is where profile data (depth on bottom axis) can be viewed in reference to GLODAPv2, and is where bottle data, if available and implemented into the GUI, would be visualized.

The third input panel, titled "Reference Data", is where the user can toggle between different reference data sets. Section 3.3 describes these options in more detail.

The fourth input panel, titled "Oxygen Gain Adjustments", has been left disabled in the current software version. Within the SOCCOM project, we currently use a single gain correction factor (G in equation (1)) for post-deployment correction of oxygen data, calculated as the average gain computed over the lifetime of the float (shown in blue on the interface, to the right of the second panel in Figure 5). This input panel potentially allows for automatic computation of drifts in gains among user-assigned breakpoints (designated by Cycle number). If the user wishes to develop this functionality further for DAC implementation, see the discussion in section 4.2.

The last input panel, titled "Apply Oxygen Gain Adjustment" allows you to apply the mean gain value (shown in blue to the right of the second subplot) to the data. The pushbutton generates a ODV*QC.TXT file within your float directory which includes the corrected oxygen data.

Note that the example shown in Figure 5 is for Coriolis float 6900889. For this float, the DOXY_ADJUSTED variable is already populated within its respective Mprof file. If interested in float data managed by other DACs, we always recommend using the adjusted data provided by the DAC, as they hold the most knowledge with respect to floats under their management, and may employ more sophisticated oxygen adjustment methods (ie, as outlined in Bittig et al., 2018).

Figure 5: The SageO2-Argo GUI interface showing Coriolis float 6900889. (a) oxygen data (pO_2 or %sat) and select reference data (NCEP pO_2 is the default), (b) gain values derived from the top panel (mean gain over the lifetime of the float is shown in blue to the right), (c) oxygen data (umol/kg) from within designated depth and profile range, and (d) temperature and salinity data from within designated depth and profile range.

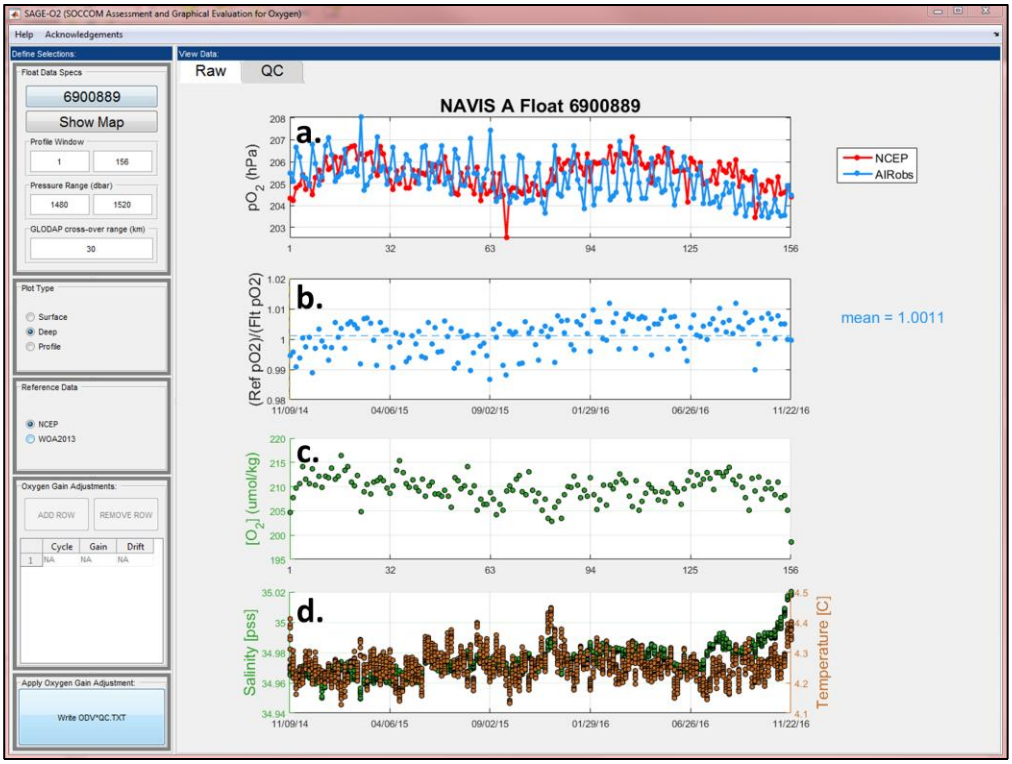
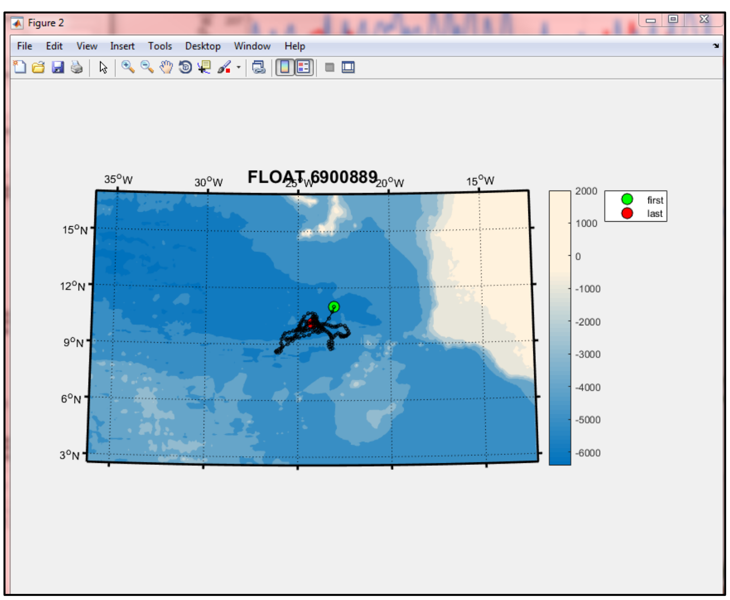


Figure 6: Map window display for Coriolis float 6900889



3.3 Gain computation using reference datasets

There are two options for reference datasets within the GUI with which to compare float data and derive gain corrections: (1) NCEP reanalysis surface pressure (converted to oxygen partial pressure), and (2) World Ocean Atlas (WOA) 2013 surface water percent saturation. Either reference can be used for visualizing or computing gain factors at each cycle, although NCEP is the preferred method, assuming your float has in-air measurement capabilities, because it is independent of ocean climatology. Details and relevant equations used in the computation of gain factors specific to each reference dataset are described below.

3.3.1 Gain computation using NCEP reanalysis

The preferred product for oxygen gain computation within the SageO2-Argo software is NCEP/NCAR Reanalysis-1 six-hourly surface pressure (https://www.esrl.noaa.gov/psd/data/gridded/data.ncep.reanalysis.surface.html; Kalnay et al., 1996). This is a Gaussian gridded product with units of Pascals, which are converted to hectopascals (millibar equivalent) prior to proceeding. Within the GUI, NCEP atmospheric surface pressure (P_{NCEP}) values are then converted to oxygen partial pressure based on the assumption that water vapor is 100% saturated at the sea surface. The calculation follows equation (2) below. The water vapor pressure (p_{H_2O}, in hPa) is calculated using equation (3), where T represents optode temperature in degrees Celsius (Argo parameter TEMP_DOXY) (Aanderaa Operating Manual TD269, 2009).

$$p_{O_2} = \left(P_{NCEP} - p_{H_2O}\right) \times 0.20946 \qquad (2)$$

$$p_{H_2O} = e^{\left[52.57 - \left(\frac{6690.9}{T+273.15}\right) - 4.681 \times ln(T+273.15)\right]} \qquad (3)$$

The sensor gain that is estimated from air oxygen for each individual profile, *i*, is then computed using equation (4), as outlined in Johnson et al. (2015):

$$g_i = p_{O_2NCEP} / p_{O_2FLOAT} \qquad (4)$$

where p_{O_2NCEP} follows from equation (1) and p_{O_2FLOAT} comes directly from the PPOX_DOXY parameter (reported in millibars) within the float's BRtraj file. In this version of the software the overall gain factor, G, used is then the mean of the n individual g values (equation (5)). Bittig et al. (2018) has described a more complex calculation that can correct for seawater carryover on the sensor during optode sampling while in air. However, at this point in time relatively few floats make the series of measurements required to apply this correction. Implementation of the Bittig protocol has not yet been incorporated into this version of the software, but could be at some future date.

$$G = \frac{\sum_{i=1}^{n} g_i}{n} \tag{5}$$

Be aware that the GUI is designed to retrieve NCEP data off of the web for the most up-to-date products. However, if internet connectivity is slow or unavailable, you may modify the target assignment in the function …/ARGO_PROCESSING/MFILES/FLOATS/getNCEP.m (see lines 96-98) to point to a local directory. We have included pre-downloaded data within the GUI repository (see …/ARGO_PROCESSING/DATA/NCEP_TEMPORARY), although the pres.sfc.gauss.2018.nc file would need to be downloaded to reflect the current date.

3.3.2 Gain computation using WOA2013

If your float is incapable of taking in-air optode measurements, an optode gain correction factor can be derived within the SageO2-Argo GUI using WOA percent saturation. Within the software repository, percent saturation WOA 2013 monthly climatology data (1 degree spatial resolution) are stored for comparison against float data. Percent saturation from the float is calculated following equation (6) below, where the solubility of oxygen (O_{2Sol}) is computed as a function of temperature and salinity following Garcia & Gordon (1992) and using solubility constants from Benson and Krause (1984) (see equation 8 and Table 1 in Garcia & Gordon, 1992). Individual gain values, g_i, are then computed using equation (7), where $\%Sat_{WOA}$ and $\%Sat_{Float}$ represent the mean WOA and mean float percent saturation values for the upper 25 m of the profile, respectively.

$$\%Sat = [O_2]/[O_{2Sol}] \times 100 \tag{6}$$

$$g_i = \%Sat_{WOA}/\%Sat_{Float} \tag{7}$$

Again, in this version of the software the overall gain factor, G, used is then the mean of the individual g values found at each cycle (equation (5)).

4. Modifying the GUI to suit your needs

4.1 Variable input file types

As previously mentioned, this GUI was designed to read profiling float data stored within Argo *.nc files. However, depending on the data manager's needs, one might wish to modify the GUI to read directly from a float's incoming msg files. This is how the SageO2 GUI was originally set up for processing and adjusting data for the SOCCOM fleet, and SOCCOM's "internal" version of the GUI software (managed by data managers at MBARI) can be made available upon request. The mfile

…/ARGO_PROCESSING/MFILES/GUIS/SAGE_O2Argo/getall_floatdata_sO2Argo.m is one of the main files requiring modification when switching to alternative input files.

4.2 Average versus drifting gain

Assessment of post-deployment optode stability has given rise to variable results within the literature (Johnson et al., 2015; Bushinsky et al., 2016; Bittig and Kortzinger, 2015; Bittig and Kortzinger, 2017). A recent paper by Bittig et al. (2018) provides a thorough review on this topic, and also presents more recent analysis suggesting that individual optodes may exhibit significant post-deployment drift within +/- 0.6%/yr, while at the same time suggesting the need for further research on the subject.

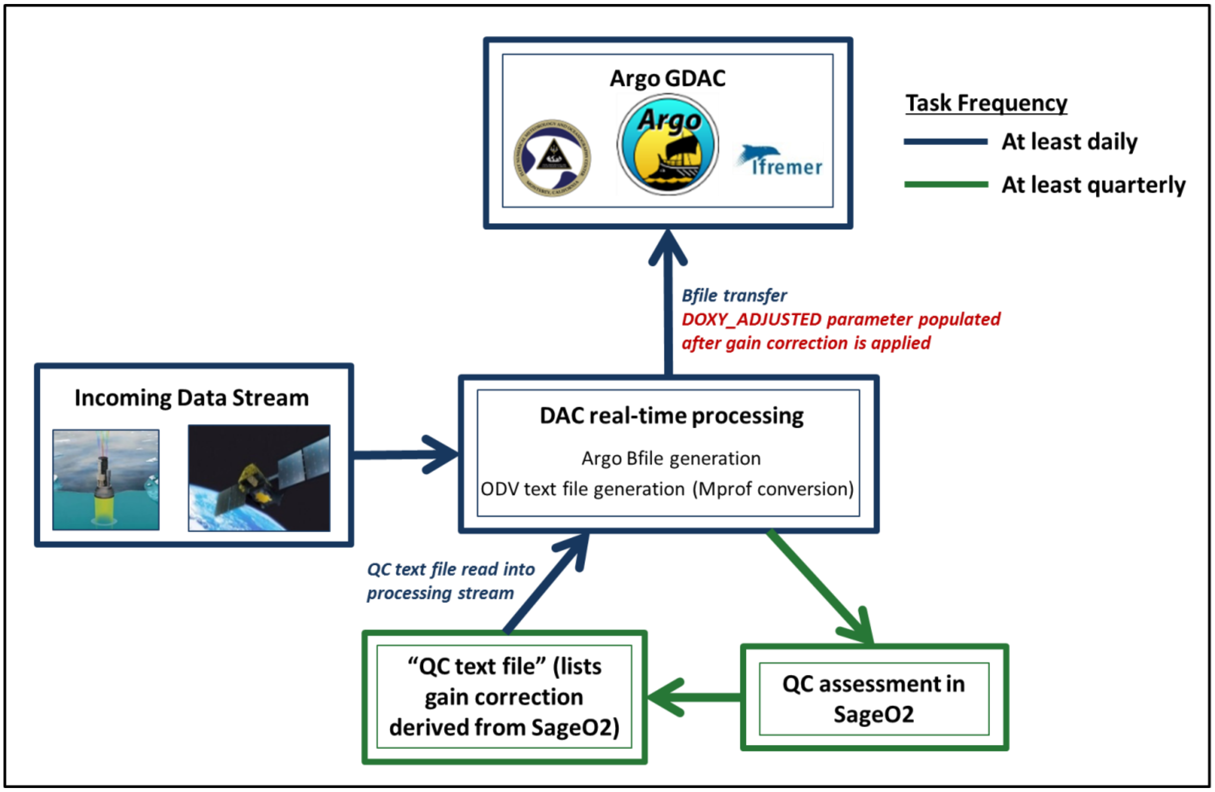
In light of these mixed findings, the operational simplicity of utilizing a single average gain correction in the real-time adjustment of optode data has lent itself as the primary method of optode correction for the SOCCOM fleet (to date). However, characterizing the amount of optode drift between user-defined change points is currently possible within the SageO2 GUI. To enable and/or further develop this feature, review the code and associated callbacks for "Control Box 4: Oxygen Gain Adjustments" within …/ARGO_PROCESSING/MFILES/GUIS/SAGE_O2Argo/sageO2Argo.m

4.3 Exporting gain values for use in DAC processing – suggested workflow

Oxygen gain correction values derived using the SageO2-Argo GUI should be applied to raw incoming oxygen data from the float using equation 1 to generate the DOXY_ADJUSTED parameter, and the resulting adjusted data should be submitted to the GDAC within a float's B-files. For newly deployed floats, a gain correction value can be derived as early as the fifth cycle, and then applied to subsequent incoming cycles in near real-time, although for such floats it is suggested that gains be revisited periodically throughout the float's life.

Currently, the GUI allows the user to apply the derived gain to the oxygen data and store it within a "corrected" ODV*QC.TXT file. However, automatically exporting average optode gain values outside of the GUI for incorporation into Argo netCDF files is not currently part of the GUI functionality; this task has been left to the user, as each DAC manages a unique processing workflow. However, the schematic in Figure 7 provides an example of the type of workflow employed at MBARI. The use of float-specific "QC text files", which store current and historical QC adjustment values for each sensor, are read into the processing stream so that adjusted data parameters get populated in near real-time. Depending on the user's needs, initializing and appending gain adjustment values to such a file could easily be performed within the GUI with the addition of a pushbutton and associated callback function.

Figure 7: Schematic of potential workflow for incorporating optode adjustments into Argo data files.



4.4 Incorporating shipboard reference data

If bottle data from deployment casts are available for your floats and you are interested in incorporating this data into the GUI, you will need to review the functions …/ARGO_PROCESSING/MFILES/FLOATS/get_shipboard_data.m as well as .../ARGO_PROCESSING/MFILES/GUIS/SAGE_O2Argo/redraw_PROF_sageO2Argo .m

These functions were built in reference to shipboard data in WOCE Hydrographic Program (WHP) Exchange format, used by CCHDO: https://exchange-format.readthedocs.io/en/latest/introduction.html
and key off of specific associated parameter names, as defined here: https://exchange-format.readthedocs.io/en/latest/parameters.html.
The easiest approach to incorporating your bottle data into the GUI (requiring the smallest number of code modifications) would be to follow the same parameter naming conventions and formatting as is used in the WHP Exchange format.

4.5 A note on in-air data storage in Argo *BRtraj files

As mentioned, the preferred method for deriving oxygen gain correction values involves comparing in-air optode measurements with NCEP reanalysis. Current BGC Argo guidelines suggest storing in-air optode data (as partial pressure of oxygen, in millibars) within BRtraj files as PPOX_DOXY, identified by the general measurement code (MC) 1100 for in-air oxygen measurements (relative measurement codes also apply, see Scanderbeg et al., 2015, Annex F). However, this scheme is not sufficient for programmatically identifying "true" in-air data due to the variability in measurement acquisition among platforms. Table 2 lists examples of various operational "in-air" optode sampling schemes, all of which are currently identified by either MC 1090 or 1099. However, you will notice that some of these measurements are taken in surface water and are not "true" in-air samples.

Table 2: Examples of various operational "in-air" optode sampling schemes

Example float	Platform	In-Air Sample Scheme*	MC used in BRtraj file
Coriolis 6902740	Provor CTS4	Unpumped near-surface data (optode mounted on a stick, so some samples taken in air)	1100-10 = 1090
Coriolis 6900889	NAVIS	"Surface sequence" (5 samples in surface water followed by 10 samples in air)	1100-10 = 1090
AOML 5904693	APEX	"Surface sequence" (4 samples in surface water followed by 8 samples in air)	1100-10 = 1090
AOML 5904662	APEX	Single in-air reading during float telemetry phase	1100-1 = 1099

*Specific example for float listed (in other words, not necessarily consistent within listed platform type)

In the current version of SageO2-Argo, we have imposed a pressure threshold of 0.1 dbar associated with PPOX_DOXY measurements (MC=1090 or 1099) as a potential method to identify "true" in-air data. Users may be interested in modifying this approach, based on more thorough knowledge of their float's behavior. Additionally, at ADMT18 it was suggested that the measurement codes used to identify in-air oxygen data within the BRtraj files become more explicit to better represent the activity of the float during in-air measurement acquisition (for example, separate MC for in-water versus in-air surface sequence samples). Thus, be aware that future changes to in-air MCs within the BRtraj files would require code updates.

5. Concluding remarks

The SageO2 GUI has been used successfully at MBARI for managing oxygen gain adjustments for over 100 operational floats. It is our hope that the recent modifications to the software for application to Argo floats can assist external DACs in either deriving oxygen gain factors directly, or in developing similar tools to support their respective workflows, ultimately increasing the amount of adjusted oxygen data submitted to the GDAC in real time. We welcome any comments, questions, or suggestions. Additionally, if you would like to help us improve the software by contributing to the code repository on github please let us know!

6. References

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