logoIRD**US-191 "IMAGO" - Direction de l'US191 et la composante océanographique de Bretagne**

User Manual

for

TSGQC

**T**hermo**S**alino**G**raph **Q**uality **C**ontrol

Version 1.5

|  |  |
| --- | --- |
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# Revision History

|  |  |  |  |
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# Software goals

**TSGQC** (**T**hermo**S**alino**G**raph **Q**uality **C**ontrol) software was build to **validate**, **calibrate** and **correct** salinity and temperature measurements from a thermosalinograph on board merchant ships and research vessels:

1. **Validate**: Assign Quality Control codes to every measurement.
2. **Calibrate**: Apply a linear shift to sensor measurements
3. **Correct**: Use external data such as water samples, ARGO, CTD, XCTD measurements to correct the TSG time series.

# Installation

Follow the instructions available on the English page at the following address:

<https://us191.ird.fr/spip.php?article6>3

# Quick Start

The main steps to quality control a **TSG** file are:



Figure 1: TSGQC menus

1. Start **TSGQC** p. 6
2. Open a **TSG file**. Several formats are available p. 11
3. Visually check the data
   1. Compare the measurements to a climatology p. 20
   2. Plot the ship track p. 21
4. Check that every measurement has a position p. **Erreur ! Signet non défini.**
5. Assign a quality code to every measurement p. **Erreur ! Signet non défini.**
6. Save your work p. 16
   1. **NetCDF** format p. 17
   2. **ASCII** format p. 17
7. Open sample files p. 15
8. Adjust the **TSG** data to the sample measurements p. **Erreur ! Signet non défini.**
9. Print figures p. **Erreur ! Signet non défini.**

Secondary **TSGQC** functions:

1. Automatic tests p. 8
2. TSG calibration p. **Erreur ! Signet non défini.**
3. Data processing report p. 36

# Functionalities

## Starting TSGQC

Open a Matlab **'Command Window'**.

The data directory can be chosen in the list-selection dialog box.

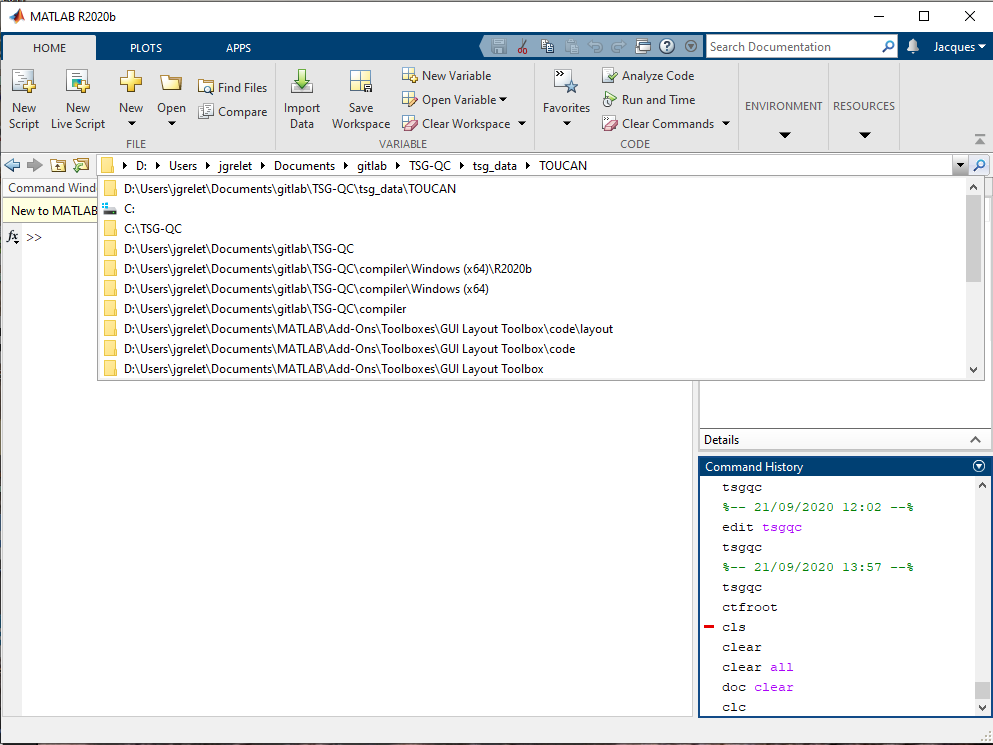


Figure 2: Getting Started

Type the name of the program in the command window:

**>> tsgqc**

The software functionalities can be used once a **TSG** file has been read (p. **Erreur ! Signet non défini.**)

## Main functions



Figure 3: Icon bar

### Toolbar

 Open files p. 11

 Write files in NetCDF p. 16

 Print figures p. **Erreur ! Signet non défini.**

 Zoom in p. 22

 Zoom out p. 22

 Enable and disable pan mode on a plot p. 22

 Quality Control module p. **Erreur ! Signet non défini.**

 Select date limits p. 24

 Vessel track map p. **Erreur ! Signet non défini.**

 Plot climatology p. **Erreur ! Signet non défini.**

 Calibration module p. **Erreur ! Signet non défini.**

 Interpolate missing positions p. **Erreur ! Signet non défini.**

 Correction module p. **Erreur ! Signet non défini.**

 Fill Meta-Data form p. 16

 Write a report file p. 36

### Menus

**FILE menu**

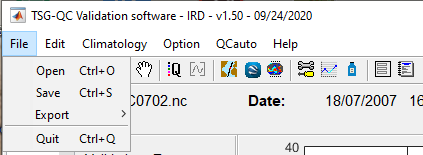


Figure 4: File menu

**Open** Open a file (**TSG**, samples, etc,) p. 11

**Save** Save the data in NetCDF format p. 16

**Export** Save the data in ASCII format p. 17

* + - **TSG** measurements
    - Samples (Water Samples, CTD, ARGO, …)

**Quit** Quit **TSGQC** p. 39

**Edit menu**

This menu is not implemented.

**Climatology menu**

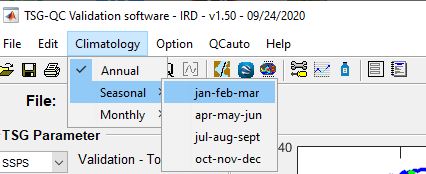


Figure 5: Climatology menu

This menu allows the user to choose the period of the climatology to superimpose on the time series measurements:

1. Annual

2. Seasonal

3. Monthly

The climatology source and its depth can be selected through the **Option - Preferences menu** (see next paragraph)

**Option menu**

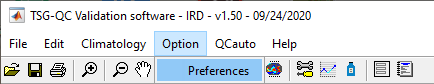


Figure 6: Option menu

The **Option - references** menu is used to set the following preferences:

* Climatology and its depth p. 20
* Calibration coefficient types
* Figures
* Limits for automatic tests to apply with the **QCauto** menu (next paragraph)

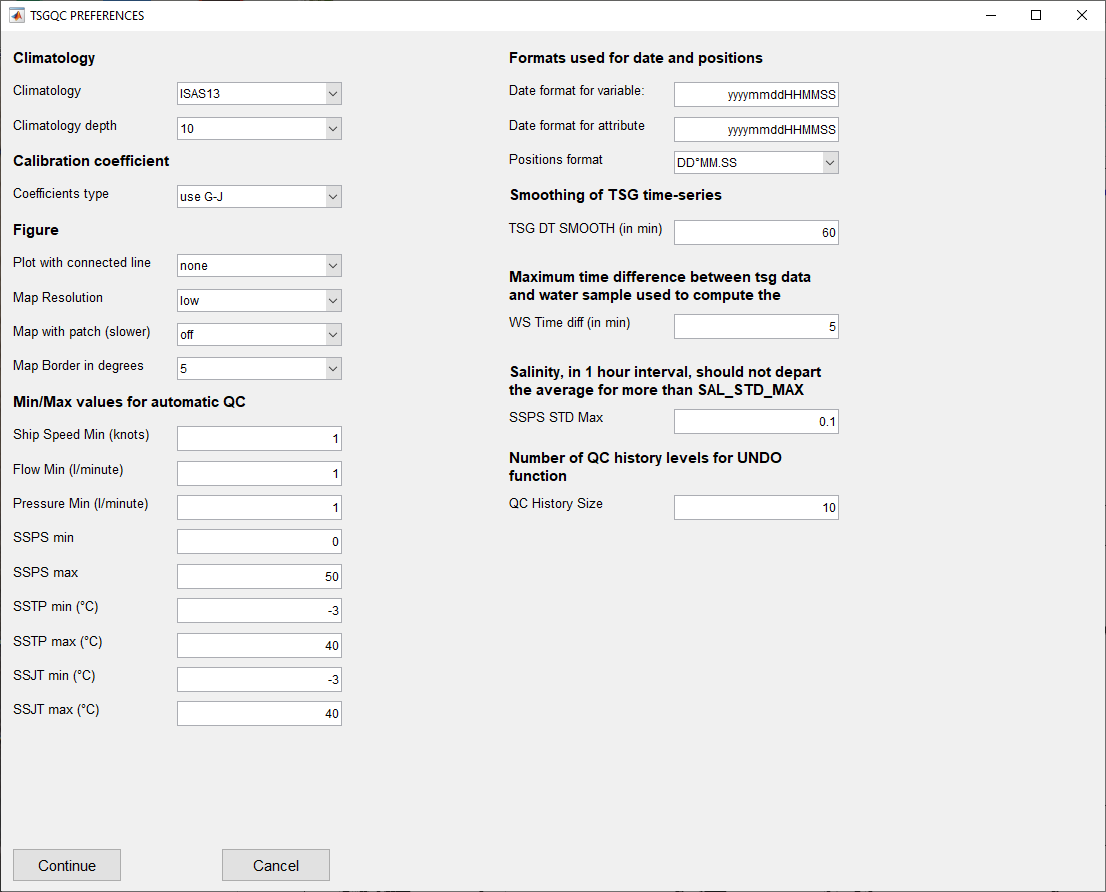


Figure 7:Preferences setting

**QCauto menu**

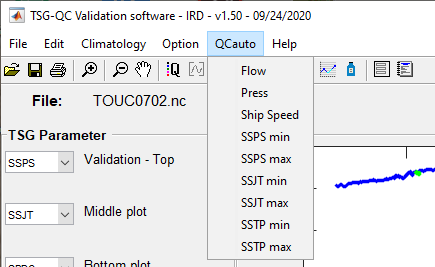


Figure 8: Quality Control menu

**QCauto** allows the user to apply automatic tests to the TSG time series. The tests use limits defined in the “**Option -** **Preferences**” form (see previous paragraph).

A Quality Code “BAD” is applied to measurements outside the limits defined for the test.

**Remarks :**

* There is no Undo function.
* Quality code “HARBOUR” is applied to measurements carried out when the speed of the vessel is below the “Ship Speed Min” value.
* Be careful with automatic tests. For example when a vessel is stopped, measurements can be BAD simply because there is no more water pressure in the TSG. In that case the quality code should be set to “BAD” and not to “HARBOUR”. For research vessels, a null speed in the open ocean is common during stations and should be set to “GOOD”, not to “HARBOUR”.

**Help menu**

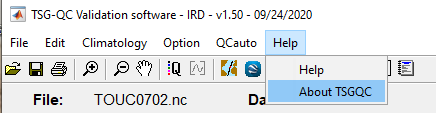


Figure 9: Help menu

The online help is not yet implemented.

About TSGQC displays the SO-SSS logo and some configuration parameters:



Figure 10: Help dialog box

## Opening a File

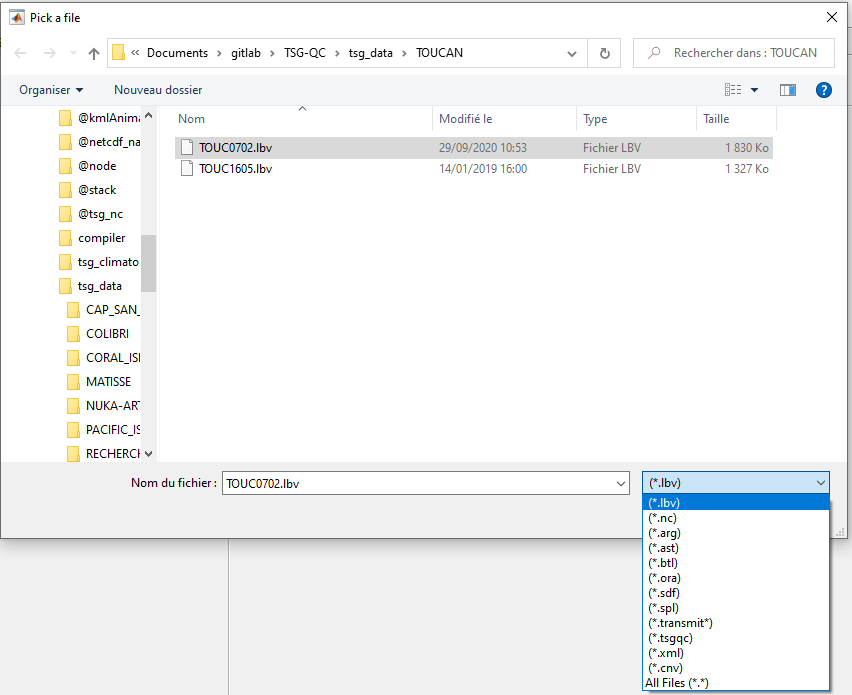


Figure 11: Opening a file



Several file types can be read in TSGQC:

**\*.arg** **ARGO** data file created by G. Reverdin team (UMR LOCEAN) along the ship track

**\*.ast** **TSG** file from the ASTROLABE ship

**\*.btl** Water Sample file (**ASCII** format**)**

**\*.lbv** **TSG** file (**SODA[[4]](#footnote-4)** format) from merchant ships (SOERE SSS)

**\*.nc** **TSG** file (**NetCDF** format**)**

**\*.ora** **TSG** file in **ORACLE** format formerly used by SOERE SSS

**\*.sdf** **TSG** file in **SDF** format formerly used by SOERE SSS

**\*.spl** ‘**Sample**’ files (XBT, CTD, etc. - **ASCII** format)

**\*.transmit** **TSG** file from the merchant ship NUKA ARTICA

**\*.tsgqc** **TSG** file (**ASCII** format)

**\*.xml** XML file in the format used at the US IMAGO for trajectory data.

**\*.cnv** ASCII file in Seabird format from Sbe-processing

Format description can be found page:

**\*.arg** p. 42

**\*.ast** p. 43

**\*.btl** p. 43

**\*.lbv** p. 45

**\*.nc** p. 45

**\*.ora** p. ??

**\*.sdf** p. ??

**\*.spl** p. 43

**\*.transmit** p. 45

**\*.tsgqc** p. 43

**Remark**

A test on double records is performed for:

1. **TSG** measurements: If consecutive identical records are detected the following message box is displayed. The message gives the number of double records and displays the 10 first identical dates. Double records are deleted.

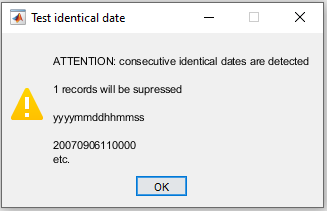


Figure 12: : Test on duplicate recordings

1. **Sample** measurements: The duplicate test is performed on the date and time comparison. No message box is displayed. Double records are deleted.

**Sample** file (**\*.btl**, **\*.spl**, **\*.arg**) cannot be read if no **TSG** file was read. If the user tries to load a 'sample' file, the following window appears:

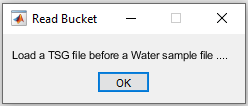


Figure 13: Dialog box, error while reading samples

### Opening a « Merchant Vessel » TSG file (SODA format)

When opening a Merchant Vessel file in the **SODA[[5]](#footnote-5)** format, the following window is displayed:



Figure 14: SODA software, selection of parameters

This window gives a list of the variables found in the header line. **TSGQC** automatically selects the variables essential to its running. The user can modify these choices. For example it is better to choose a GPS date and hour than a PC time.

**sbe21\_raw** variable stores frequency measurements made by the Sea-Bird **TSG**. This information is recorder in NetCDF file.

**sbe21\_ad1** variable stores flow measurements. Data are stored in the NetCDF FLOW variable.

**Remark:**

The vessel speed stored in SODA file (variable SOG) is truncated. It is better to uncheck this variable and let the software compute the ship speed from measurements positions.

### Opening Sample Files (\*.btl, \*.spl, \*argo)

Samples (variable with extension \_EXT in the NetCDF format) can be used to correct the TSG measurements.

It is possible to open and concatenate several sample files. A message box asks if the user wants to replace or concatenate the sample file already loaded in memory.

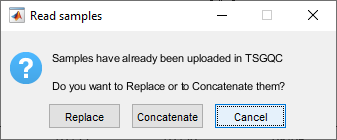


Figure 15: Sample reading dialog box

**Remarque :**

1. If two or more files are concatenated **TSGQC** test for double records. The test is made on the date (year, month, day, hour, minute, second). Double records are deleted. No message box indicating that double records were detected is displayed.
2. **Sample** files (**\*.btl**, **\*.spl**, **\*.arg**) cannot be read if there is no **TSG** file in memory. In that case the following message box is displayed:

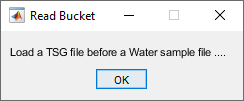


Figure 16: Dialog box, error while reading samples before data

## Saving your work

### NetCDF format

The default-recording format is **NetCDF** (see p. 45). Every information (raw data, calibrated data, adjusted data, sample data, meta-data) is stored in the **NetCDF** file.

Metadata are either read in the original file or the user fills the following input form.

This form is automatically displayed when recording a **NetCDF** file. The form is also available through the shortcut

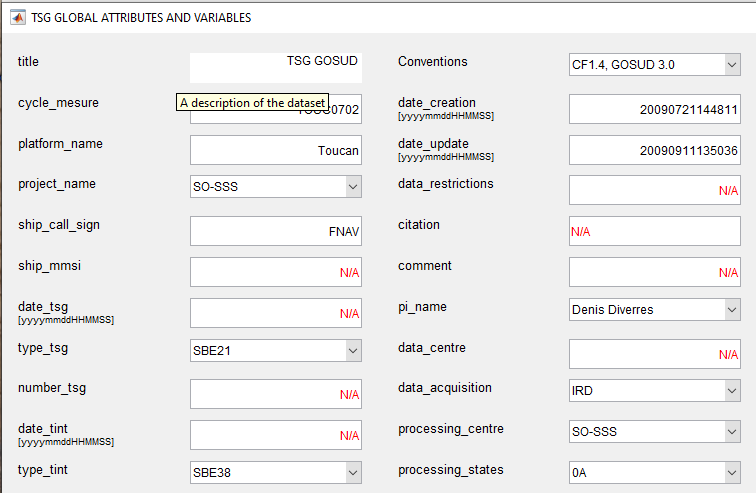


Figure 17: NetCDF Metadata Entry Form

**CYCLE\_MESUR**E and **PLATFORM\_NAME** are the only information necessary to save a file. In general use the ship name in upper-case letters.

For a given **PLATFORM\_NAME** some metadata are saved in an ASCII file. As soon as the user enters a **PLATFORM\_NAME**, **TSGQC** scans the ASCII file to get all the information about this **PLATFORM\_NAME**.

It is recommended to regularly save your work.

### ASCII format

This format can be used for **TSG** and **Sample** measurements. To save data in the ASCII format use the **File - Export** menu.

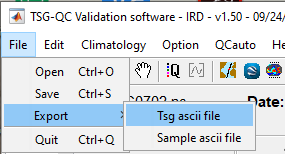


Figure 18: Export in ASCII

The user can export :

* Data **samples (**extension name: **.spl**): A **.spl** file contains all data **samples** loaded in **TSGQC**. **TSGQC** proposes to export the following variables:

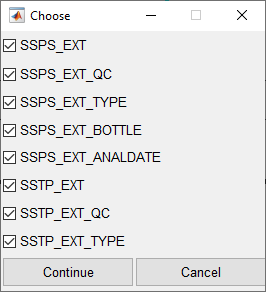


Figure 19: : Choice of parameters exported in ASCII

**Remark:**

For the ARGO file the mean time difference between the TSG and ARGO measurements is added to the ARGO date (column 17 of the **\*.arg** file see p. 42). It is this date, referring to the TSG measurement, which is recorded in the NetCDF and ASCII file.

* **TSG** data (file with extension **.tsgqc)**. **TSGQC** proposes to export the following variables:

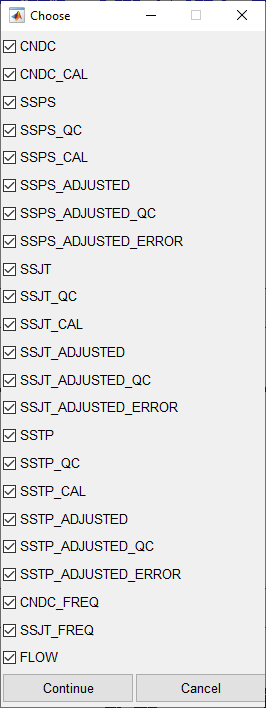


Figure 20: Choice of parameters exported in ASCII

A description of the ASCII format is given p. 43.

## Using TSGQC

### Parameters visualization

Once a **TSG** file has been loaded TSGQC displays 3 figures. The default variables plotted in the figures are:

1. **SSPS**: The salinity in the upper plot. This is also the validation window.
2. **SSJT**: Jacket TSG temperature in the middle plot.
3. **SPDC**: The vessel speed in the bottom plot.

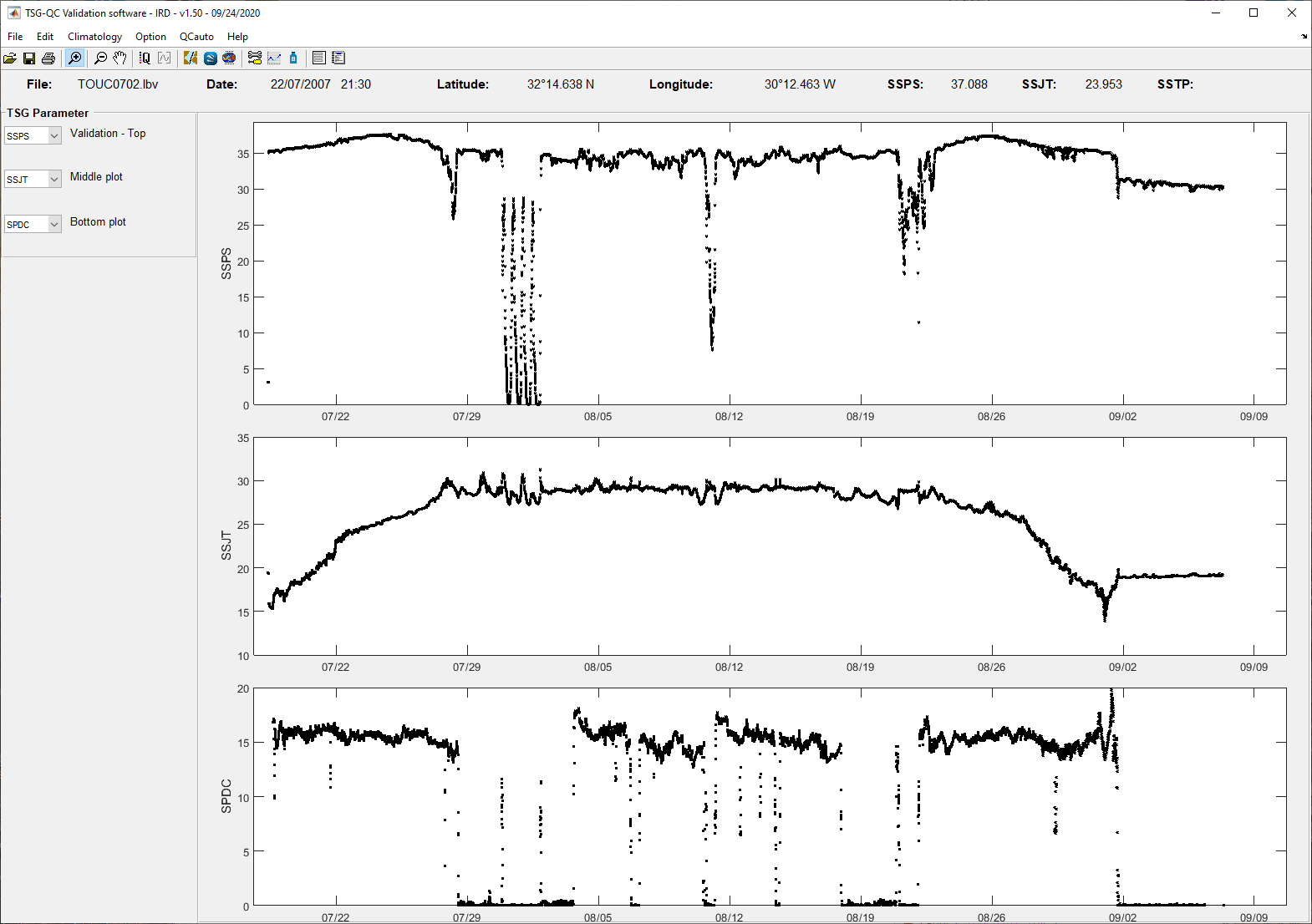


Figure 21:Main graphic window

Y-axis labels correspond to the parameter names in the NetCDF file.

When the user moves the pointer on the TSG curve, information on the date, position, salinity and temperature are displayed in the upper banner



The user can choose the parameters that will be plotted in the three figures. For this, use the three list-selection dialog boxes in the frame box ‘**TSG Parameter’** on the left of the screen.



Figure 22:Secondary Graphic Choice

Figure 23: Main graphic choice

Figure 24: Lower graphic choice

Parameters:

SSPS Salinity measured by the **TSG**.

SSJT Jacket temperature measured by the **TSG**.

SSTP Temperature given by a sensor different from the **TSG** (SBE 38 for example)

SPDC Ship speed.

CNDC Conductivity measured by the **TSG**

SSPS\_STD For average or median **TSG** records this variable gives the standard deviation on the average or median period.

FLOW Sea water flow in the **TSG**.

PRES Water pressure in the **TSG**

LATX Latitude in decimal degree

LONX Longitude in decimal degree

**Remark:**

* If the ship speed is not available in the **TSG** file, it is computed by using **TSG** measurement positions.
* If conductivity CNDC and jacket temperature SSJT from the TSG are available, they are used to compute salinity SSPS.

### Plotting a climatology

The user can choose a climatology file in the **Option - Preferences** menu**.** The only available climatology are Levitus WOA13 and WOA05. Climatology depth can also be modified in this menu. The user can choose between 0 and 10 m.

The mean climatology value (black line) minus/plus 3 times the standard deviation (red lines) is superimposed on the TSG measurement curve (salinity and temperature).

By default, the annual climatology is displayed. The user can display seasonal or monthly climatologies using the '**Climatology**' menu (see p. 8).

The format of the climatology files is described p. 45



Figure 25: Climatology display

### Plotting a Map

Click the following shortcut to get the ship track plotted on a Mercator projection map.

The ship position corresponding to the pointer position on the **TSG** time series (upper plot) is shown as a red circle on the cruise track. This is useful to validate the **TSG** measurements.

The plot is made taking into account the temporal limits of the upper plot: if the user zooms in the **TSG** time series, the map is also zoomed in. The map limits are updated automatically.

The colours associated with the quality codes assigned to the **TSG** measurements are reported on the cruise track.

The map opens in a news MATLAB graphics window. The menus in this window can be used to change the appearance of the map, display the surface climatology in the study area if it is activated in the main window, and print or export the map to a graphic file.

The resolution and type of the coastlines can be selected via the "Map" and "Type" menus respectively. The user should choose a low resolution with the “Type/Patch” mode, otherwise the display will be slowed down when the map is refreshed.

The map can be displayed is several TSGQC modules..

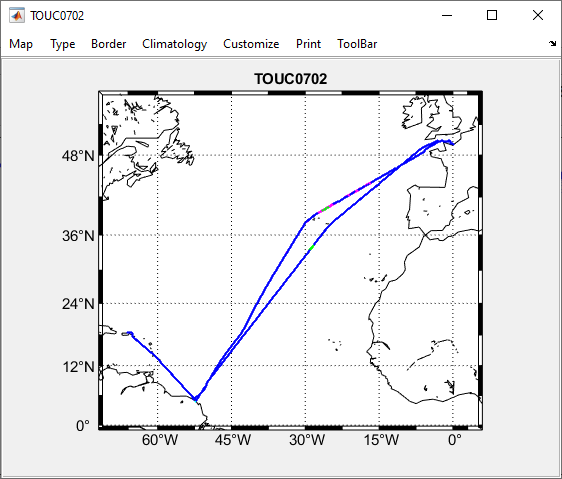


Figure 26: Cartography display with the m\_map toolbox

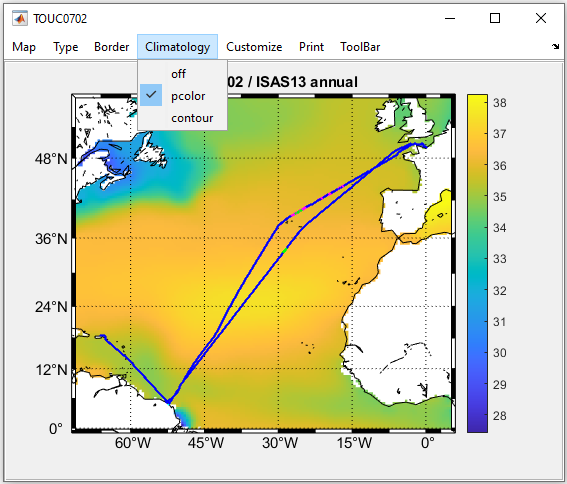


Figure 27:Cartography display with surface climatology, pcolor mode

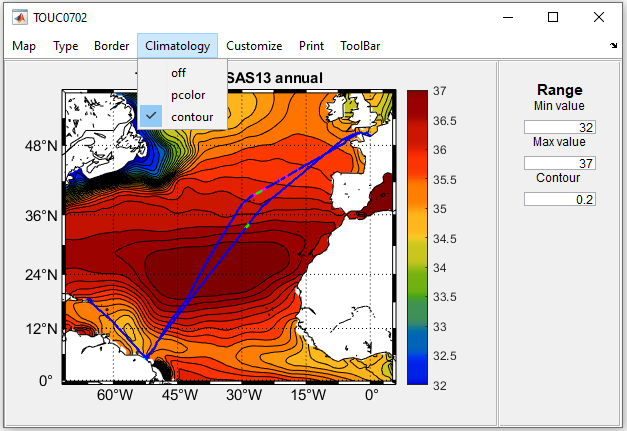


Figure 28: Cartography display with surface climatology, contour mode

### Mapping with Google Earth

By clicking on the Google Earth icon, the trajectory of the ship is displayed on the world map. By zooming in, it is possible to have an extremely precise view of the ship's position. On the other hand, it is not possible to interactively view the associated salinity and temperature measurements.



Figure 29: Displaying Google Earth cartography

### Zoom and Pan functions

**Zoom** tools : The user can increase or decrease part of the time series. Zooming is useful to see greater detail in a small area. When in zoom in mode, the user can draw a rectangle with the pointer around the time series to magnify.

The 3 plots undergo the same change.

You can move your view of a graph up and down as well as left and right with the **Pan** tool. Panning is useful when you have zoomed in on a graph and want to translate the plot to view different portions.

The 3 plots undergo the same displacement.

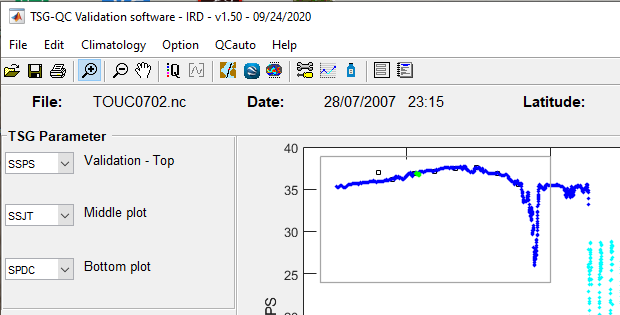


Figure 30: Zoom function

In **Zoom** and **Pan** modes, if you want to reset the graph to its original view, right-click to display the context menu and select **Reset to Original View**.





**Remark :**

When the validation module is active, (see p.26), the ‘**Pan**’ function is directly available when moving the mouse pointer at the bottom of the upper plot.

### Selecting time limits

The user can select part of the time series by setting time limits in the left panel ‘**Date Limits**’. The selection can be made:

* Manually by using the input dialog box of the ‘**Date Limits**’ panel.
* With the mouse, by selecting a portion of the time series. The time limits of the rectangle defined by the pointer are entered automatically in the input dialog box.

This tool can be used in the interpolation and correction modules of TSGQC.

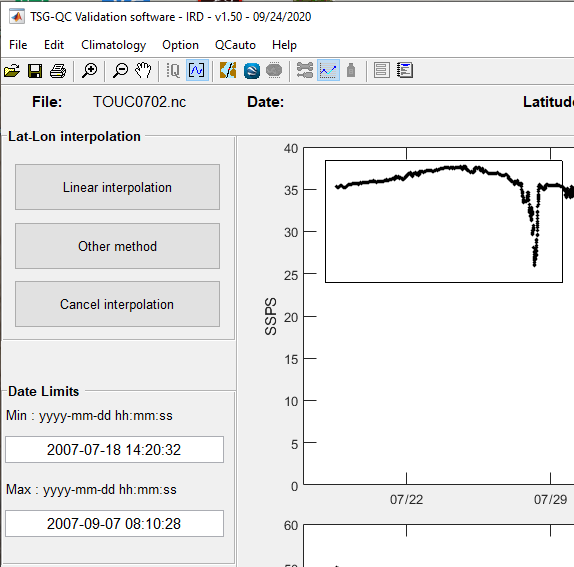


Figure 31: Selection of time limits

### Printing figures

This is a simplified tool to print **TSGQC** plots. Whatever the **TSGQC** module you are working on, you can print the plots displayed on the screen by clicking on the icon .The plots will be drawn inside a Matlab Figure Window.

Then you can use the Matlab menus to print, save or export the plots.

Note that the cruise track is plotted directly in Matlab figure window.

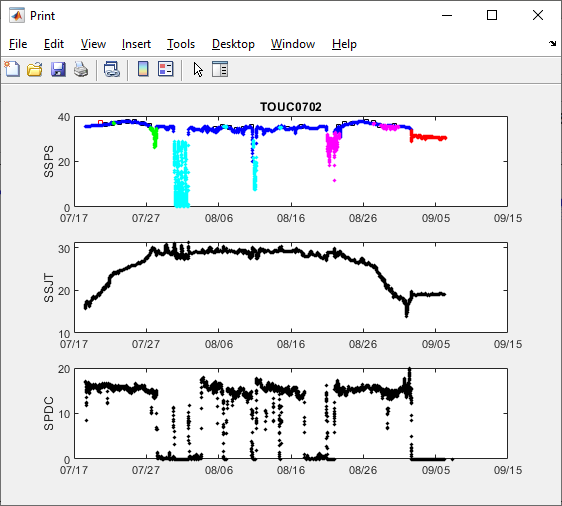


Figure 32: Printing of figures

## Attributing Quality codes to the TSG measurements

The user can assign a quality code only to the measurements of the time series displayed in the upper plot. Quality code can be attributed to the 3 variables **SSPS**, **SSJT**, **and SSTP**. You have to display the variable that you want to assign the quality code (see p. 19). By default the quality code ‘NO CONTROL’ is assigned.

When the validation module is active, quality codes are displayed on the left of the screen, inside the “**Validation Codes”** panel. The number to the right of the radio buttons give the number of measurements assign to a particuliar code (7677 have a quality code GOOD in the example below).

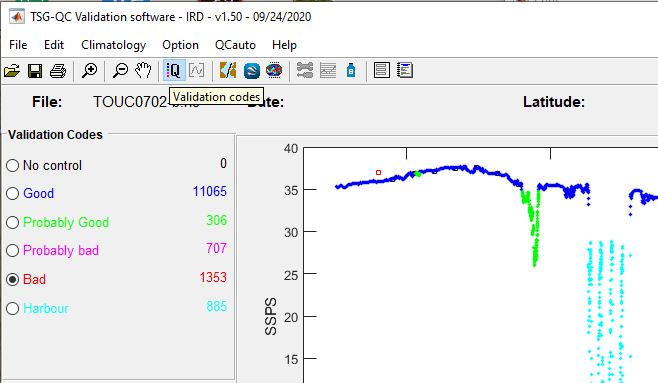


Figure 33: Validation module

To select a part of the time series, move the cross-shape pointer on the time series and click the right mouse button to draw a rectangle which sets the limits of the data measurements whose quality codes will be modified. The code can be chosen with 2 methods:

1. Before the selection, click the mouse button on the chosen code in the “**Validation Codes”** panel.
2. After the selection, right-click to display the following context menu and choose the code:



Selected data get the colour of the chosen code. The HARBOUR code is designed to mark good data taken when the ship is in a port. If the data are not of a good quality, choose another code.

It is of good practice to zoom in the time series, to work with precision.

You can plot a vertical line that spans the three plots to spot particular features:

1. Left-click on the upper plot.
2. Press the Ctrl Key : The vertical line is plotted. Release the key: It disappears. Then move the pointer to another position and press the Ctrl Key.



Figure 34: Display of the vertical selection bar

**Important :**

1. There is a shortcut to **Pan** the figure while you are attributing a quality code to the measurements. The **Pan** function is available when you move the pointer in the bottom part of the upper plot. The pointer shape changes from a cross shape to a hand shape, indicating that the **Pan** function is activated.
2. If the map is displayed when you execute a **Pan** operation, the map is redrawn and takes into account the new limits.
3. When all the quality codes have been attributed it is important to check that the number of **No Control** codes is equal to 0.

## Calibration

You can apply a linear shift (slope and offset) to the conductivity (CNDC) and jacket temperature (SSJT) time series (or part of).

Enter the slope and offset in the input dialog box in the **Calibration** panel for:

1. The conductivity
2. The jacket temperature (temperature measured by the TSG)
3. Precise Temperature if a sensor exists.

Once these data are entered click on the ‘**Calibrate’** button. Calibrated data are kept in variables with **CAL** extension: **SSPS\_CAL**, **SSJT\_CAL**...

Non-calibrated data are plotted in black, calibrated data in red.

Use the ‘**Cancel Calibration**’ button to cancel the corrections.

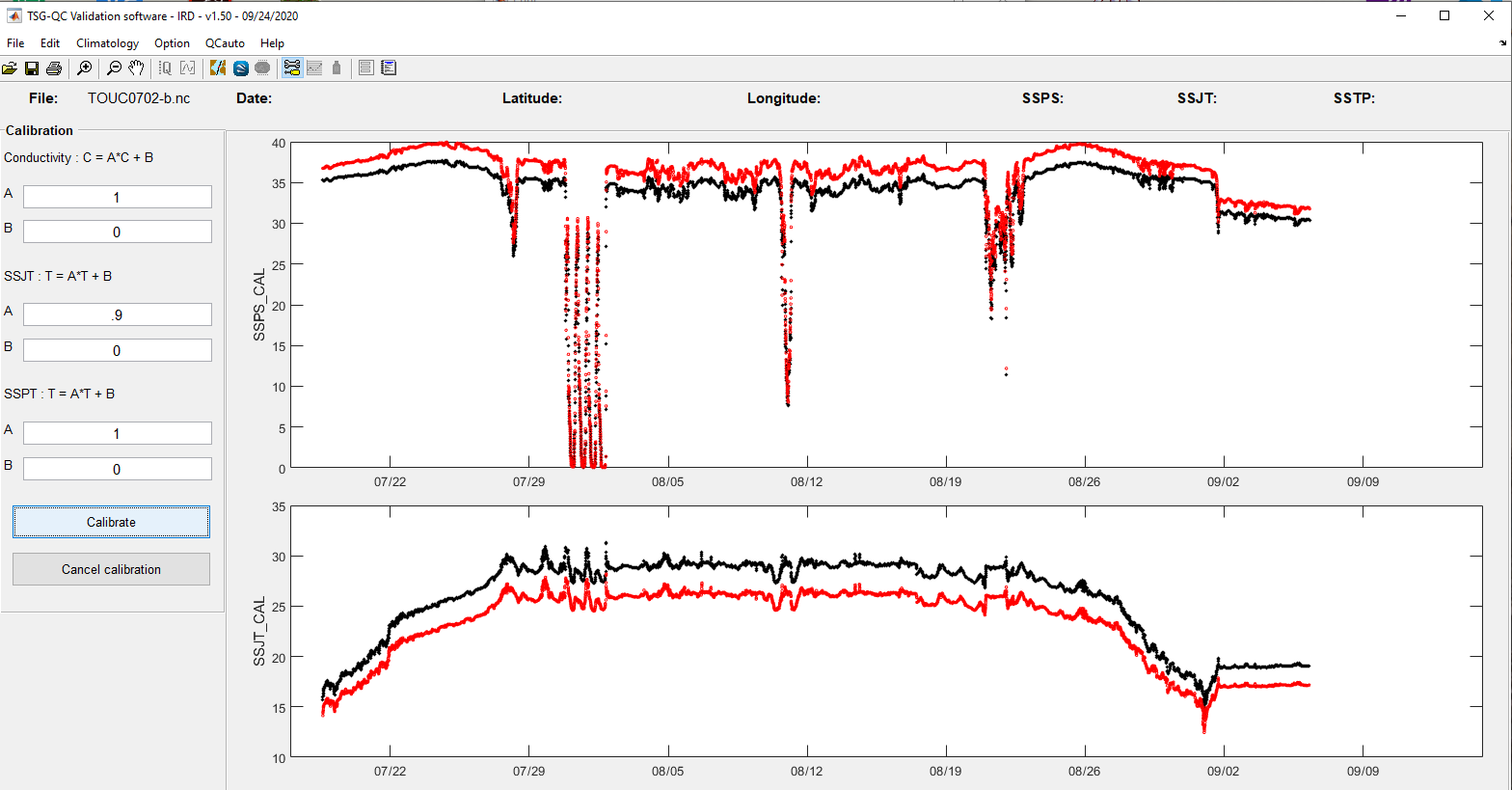


Figure 35: Calibration module display

**Remark:**

That function is not frequently used. It is better to use Samples to correct/Adjust the data.

## Interpolating latitudes and longitudes

Disruption of GPS acquisition can lead to get salinity and temperature measurements without any position (but referenced in time from the PC for example).

A latitude and longitude can be assigned to this measurement using a linear interpolation between known positions. This is a crude method which supposes that the ship has a constant velocity and a straight trajectory. However the method is satisfactory in the cases when periods without positions are small. The interpolation figure window is the following:

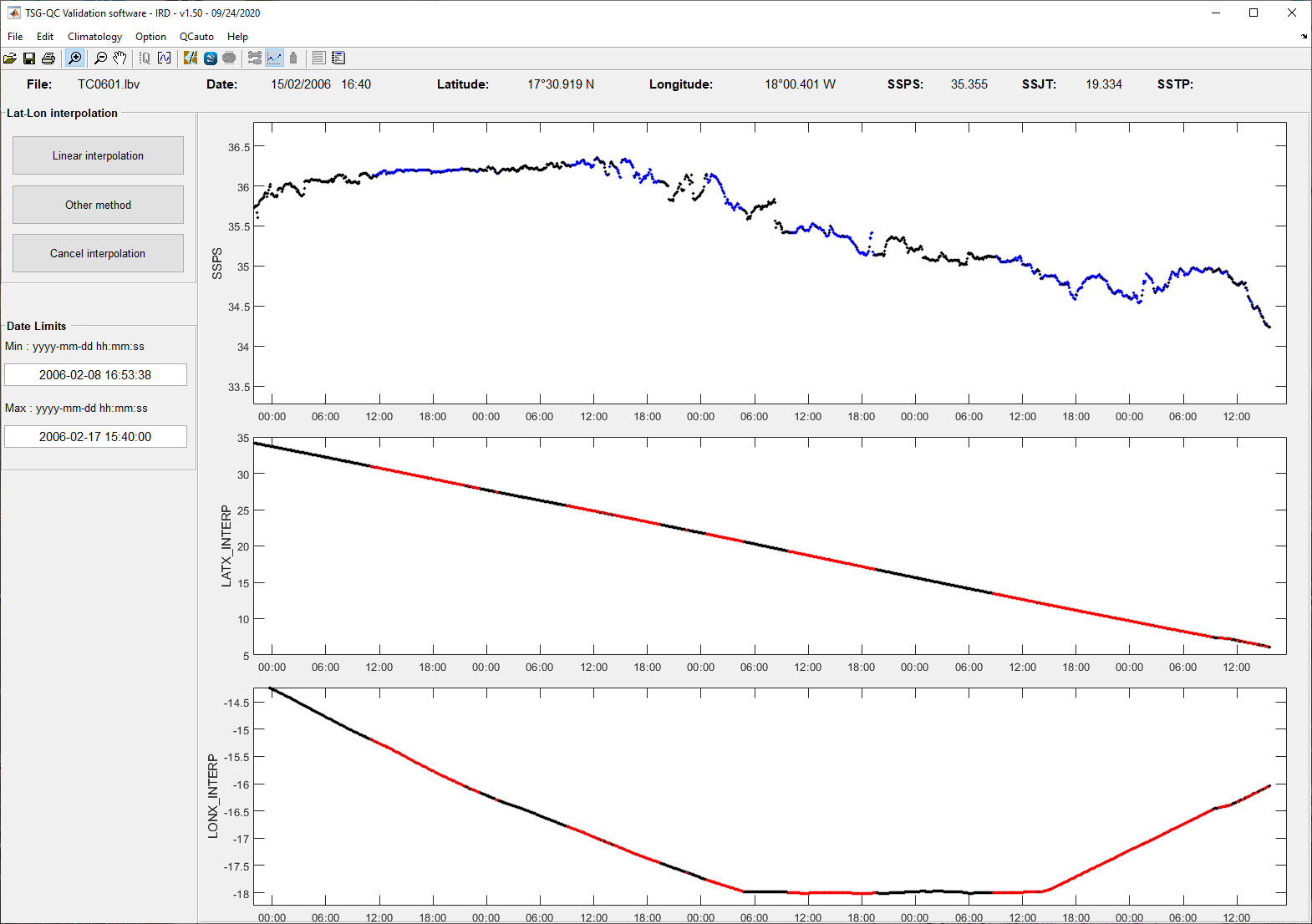


Figure 36: Position interpolation module

The upper plot displays the salinity time series. Blue points indicate measurements without position. The middle plot display the latitude of the measurements and the bottom plot the longitudes.

Once the user has clicked on the **Linear Interpolation** button, interpolated latitudes and longitudes are drawn in red (plots 2 and 3). To check the validity of the interpolation it is better to zoom in. The quality code of the latitude and longitude (**POSITION\_QC)** is set to 8 (code: **Interpolated value)**.



You can make the interpolation only on some section of the ship track. In that case use the Date Limits tools to select the temporal limits (see p 24).

## Correcting the data

TSG data can be corrected by comparison with discrete samples (Water Sample, CTD, XCTD, ARGO...).

The parameter (**SSPS**, **SSTP**...) that will be corrected must first be displayed in the upper plot of the calibration window of **TSGQC** (see p. 19 ).

Data corrected are stored in variables with the extension **\_ADJUSTED: SSPS\_ADJUSTED, SSTP\_ADJUSTED, ....** The raw data are not modified.

If corrections are not applied to the entire time series but only to some part of the measurements, the \_**ADJUSTED** variables only contain corrected data.The other elements of the **\_ADJUSTED** variables are set toNaN (Not a Number).

An error is assigned to every corrected measure (see the algorithms p. 35). Error values are stored in variables with the extension **\_ADJUSTED\_ERROR**.

The quality code of the adjusted data, **\_ADJUSTED\_QC,** is identical to the quality code assigned to the raw variable (\_**QC**)**.**

The correction module window looks like this:

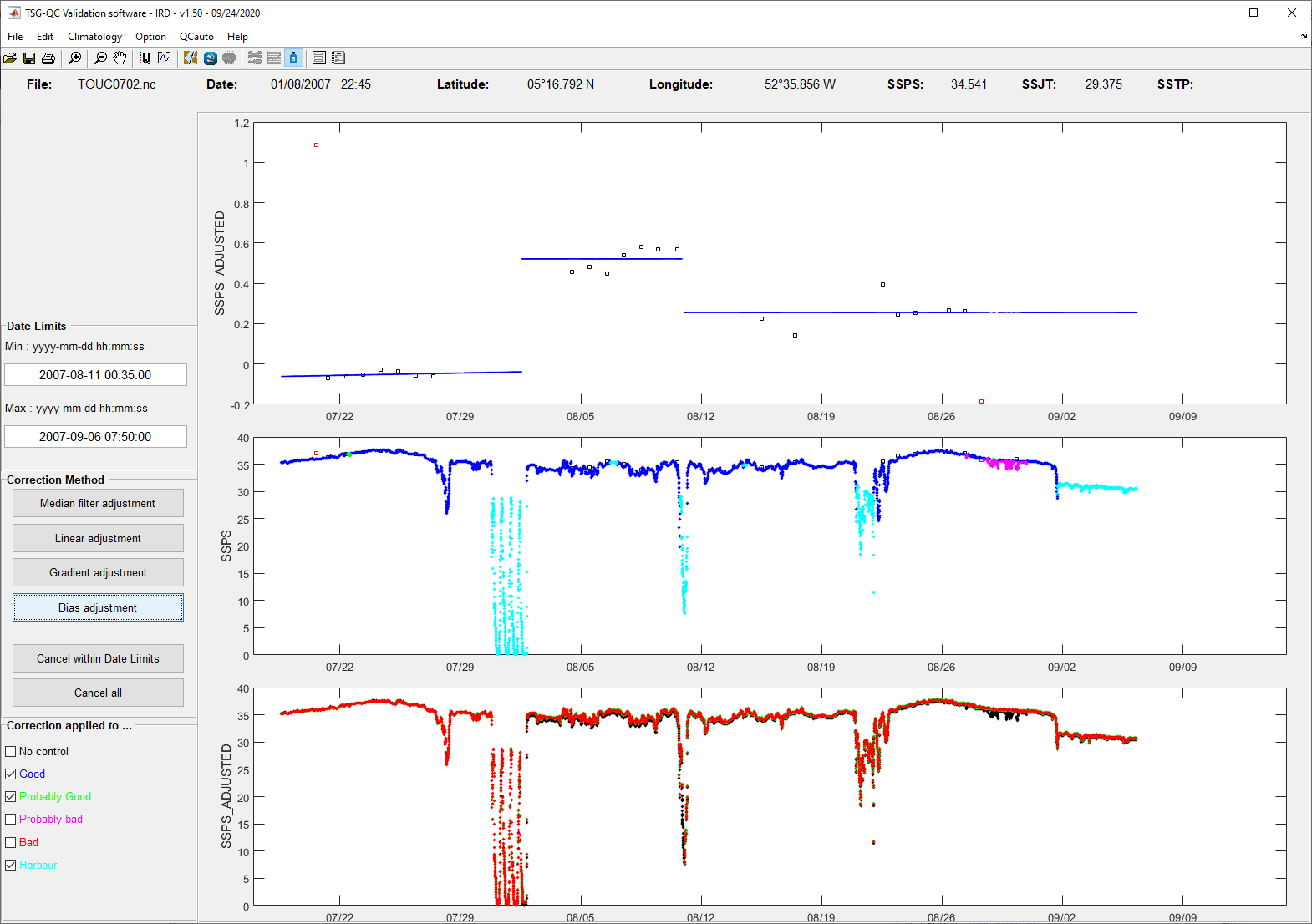


Figure 37: Correction module

### Description

*Upper plot*

Differences between discrete **samples** and **TSG** data are drawn in the upper plot.

Square markers are used to plot Water samples collected on board merchant ship (identified by a **SSPS\_EXT\_TYPE** value set to **WS** in **\*.btl** files). Circle markers are used for the other samples (ARGO, CTD ... in files with extension **\*.spl**, **\*.arg**).

The blue curve is the correction that will be applied to the TSG data. The correction can be made in several parts and is not necessary applied on the entire time series.

Quality codes can be attributed to **samples** with the same method than for the **TSG** time series (see p. 26).

**Remark:**

If for some **samples** there is no **TSG** measurements close in time or if the **TSG** measurements have quality code sets to **Probably Bad** or **Bad** the differences are not drawn in the upper plot.

*Middle plot*

The raw **TSG** time series colored with its quality codes is drawn in this figure.

*Bottom plot*

In this figure the following elements are drawn :



1. In black, the raw TSG time series
2. In red, the adjusted TSG time series.
   1. Either after being calibrated.
   2. Or after correction with discrete samples. Adjusted data from comparison with discrete samples replace calibrated data. If this correction is cancelled, the calibrated time series reappears.
3. In green, the error on the adjusted TSG time series.

### Functionalities

*Quality codes of discrete* ***samples***

Quality codes can be attributed to **samples** with the same method than for the **TSG** time series (see p. 26).

Only discrete samples with quality codes set to **NO\_CONTROL**, **GOOD**, and **PROBABLY\_GOOD** are used to compute the correction applied to the **TSG** time series.

*Choice of date limits*



Figure 38: Choice of a time limit



The correction can be applied on the entire time series or to parts of it. This is done using the time selection tool (see p 24).

*Correction depending on the quality code*

Correction is applied to the raw TSG time series depending on the quality codes. To select the quality codes that will determine which part of the time series will be adjusted, click the check boxes in the panel figure **Correction applied to**....

In the following example the correction will be applied only to TSG measurements with a **Good** and **Probably Good** quality code.



Figure 39: Choice of correction according to QC

*Correction Methods*

Four different methods of correction can be applied to the **TSG** time series (or part of). Different methods of corrections can be applied on different parts of the time series.

Corrections or part of them can be cancelled.



Figure 40: : Sélection du type de correction



Running median filter. See the algorithm p. 35

Detail of the algorithm is described in the following document:

G. Reverdin, F. Gaillard, S. Contardo, D. Mathias, Y. Gouriou, D. Dagorne, *Réseau bleu Coriolis : Qualification des mesures navires/ Salinité de surface*, Coriolis, pp 60, septembre 2006.



Linear adjustment, to correct instrumental drift mainly due to biofouling of the sensor.

See the algorithm p. 36



Gradient adjustment, to smoothly correct TSG time series in regions of strong salinity/temperature gradient where the TSG/sample difference shifts sharply across the gradient

See the algorithm p. **Erreur ! Signet non défini.**



Bias adjustment, to apply a constant correction estimated from a climatology or other trips, when no sample is available.

Enter the bias in the following input dialog box:

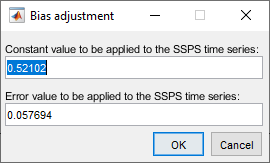


Figure 41: Bias input dialog box



The push-button ‘**Cancel within Date Limits**’ can be used to cancel the correction applied on sections of the **TSG** time series. The section is defined by its time limits (panel ‘**Date Limits**’).



The time-limits selection is made using the **Date limits** tool (see p 24).



The push-button ‘**Cancel all**’ cancels all the corrections applied to the time series.

### Algorithms

#### Median filter correction

The method, defined in function corTsgMedian.m, is composed of several steps :

*Step 1: Difference between discrete samples and TSG data*

1. Data are collocated in time. **TSGQC** selects the **TSG** measurements which are the closest to the **sample**. Function: diffTsgSample.m.
2. The sample data are not compared to the collocated **TSG** measurements but to a mean of **TSG** measurement around the collocated **TSG** data. Function: tsg\_average.m.
   1. The **TSG** average is computed with measurements with a quality code: **NO\_CONTROL**, **GOOD**, **and PROBABLY\_GOOD**.
   2. The window used to calculate the average is given by the variable tsg.cst.TSG\_DT\_SMOOTH. This variable is defined in the tsg\_initialisation.m function. The window is equal to 1 hour.
   3. A rejection test of the **TSG** data, based on the standard deviation, is performed to exclude **TSG** data with too much dispersion. TSG data which deviate more than STD\_MAX from the average are excluded. This value is defined in the tsg\_initialisation.m function. It is equal to 0.1 for salinity and 1°C for temperature.
3. -Sample-**TSG** difference is computed as soon as the 2 measurements are not more distant in time than TSG\_WS\_TIMEDIFF. This value is defined in the tsg\_initialisation.m function. It is equal to 5 minutes.



Figure 42: Median filter correction parameters

Surface salinity is a quantity that can vary quickly; the comparison of TSG data with water samples, whose dating is not always very precise, is complicated by the presence of salinity peaks, even if they are real. That is why **TSG** data are smoothed over 1 hour time period. We thus avoid comparing water samples to outlying salinity measurements (not representative) and then to produce a bad estimation of the correction to be applied to the TSG salinities.

*Step 2: Correction*

1. Only samples with a quality code equal to: **NO\_CONTROL**, **GOOD**, **and PROBABLY\_GOOD** are taken into account.
2. For each point of comparison **TSGQC** computes the mean value and the standard deviation of the differences **Samples** minus **TSG** in a COR\_TIME\_WINDOWS window. This value is defined in the tsg\_initialisation.m function. It is equal to 10 days. Samples deviating more than 3 times the standard deviation from the average are eliminated. Their quality code is set to **BAD**.
3. For each comparison point **TSGQC** computes the median value of the differences **Samples** -**TSG** in the window COR\_TIME\_WINDOWS.
4. The median values of the differences are then linearly interpolated at the date of the **TSG** measurements and the correction is added to the raw **TSG** data.

*Step 3: Error calculation*

An estimated correction error is then computed for each TSG measurement. The error is a function of the number of point of comparison (= N) used to compute the correction value:

• if N < 4 : error = 1.

• if N ≥ 4: error = standard deviation (sample - TSG) / √(N-1) )

In no case the error cannot be less than 0.01. If lower errors are computed they are put to 0.01.

#### Linear adjustment

The method, defined in function corTsgLinear.m, is composed of several steps :

*Step 1: Difference between discrete sample and TSG data*

Cf. paragraph a) Median filter correction p. 35

*Step 2 : Correction*

TSGQC uses the Matlab function polyfit to find the line best-fitting (least squares) the sample – TSG differences. The linear adjustment is made with at minimum 3 samples.

If there are only 2 samples, TSGQC computes a mean difference.

*Step 3: Error calculation*

The error of the linear adjustment is computed using the Matlab function polyval and corresponds to the uncertainty on the slope of the best-fitting line.

In the case of there are only 2 samples, the error is equal to the mean difference divided by 2.

In no case the error cannot be less than the sensor accuracy (computed in tsg\_accuracy.m), which is around of the order of 0.01. If lower errors are computed they are set to the sensor accuracy.

#### Gradient adjustment

*Step 1: Difference between discrete sample and TSG data*

Cf. paragraph a) Median filter correction p. 35

*Step 2: Correction*

Between two consecutive samples in the correction window where TSG-sample differences are D1 and D2, the correction value D varies from D1 to D2 as a linear function of the salinity (or temperature) variations of the TSG.

*Step 3: Error calculation*

The default error value is half the correction value. If the error computed this way is smaller than the sensor accuracy (about 0.01), then the later is used as the error value.

## Data processing report

Click this icon to get a simplified report on the processing of the TSG.

The report file has the following format:

TSGQC REPORT

03-Aug-2010 10:06:08

TSG file : D:\svn\tsg-qc\tsg\_data\touc0702.nc

No water sample file used during this session

No external sample file used during this session

14684 total number of records

0 records have interpolated position

0 records have been deleted because they have no date

0 records deleted because their date are not increasing

0 records deleted because of velocity > 50 knots

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* CNDC PARAMETER \*\*\*\*\*\*\*\*\*\*\*\*\*\*

Time series not calibrated

Number of measurements : 14684

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* SSPS PARAMETER \*\*\*\*\*\*\*\*\*\*\*\*\*\*

Time series not calibrated

Number of measurements : 14684

43 - 0.29 % NO\_CONTROL code

11445 - 77.94 % GOOD code

355 - 2.42 % PROBABLY\_GOOD code

433 - 2.95 % PROBABLY\_BAD code

1633 - 11.12 % BAD code

0 - 0.00 % VALUE\_CHANGED code

754 - 5.13 % HARBOUR code

0 - 0.00 % NOT\_USED code

0 - 0.00 % INTERPOLATED\_VALUE code

21 - 0.14 % MISSING\_VALUE code

6504 - 44.29 % records have been corrected

9 ARGO samples in the file

24 WS samples in the file

No CTD sample

No XBT sample

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* SSJT PARAMETER \*\*\*\*\*\*\*\*\*\*\*\*\*\*

Time series not calibrated

Number of measurements : 14684

14663 - 99.86 % NO\_CONTROL code

0 - 0.00 % GOOD code

0 - 0.00 % PROBABLY\_GOOD code

0 - 0.00 % PROBABLY\_BAD code

0 - 0.00 % BAD code

0 - 0.00 % VALUE\_CHANGED code

0 - 0.00 % HARBOUR code

0 - 0.00 % NOT\_USED code

0 - 0.00 % INTERPOLATED\_VALUE code

21 - 0.14 % MISSING\_VALUE code

No records have been adjusted

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* SSTP PARAMETER \*\*\*\*\*\*\*\*\*\*\*\*\*\*

no time series

## Exit TSGQC

If the **TSG** measurements have been modified (quality codes, adjustment, etc.) and if the file has not been saved the following message box is displayed:

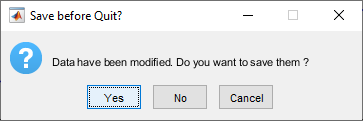


Figure 43: Save before exit dialog box

# Data Format

## Name of the variables

The variable names used in **TSGQC** follow the ROSCOP Parameter Code. All the variables are described in the **CORTSG\_format\_gosud.doc** document.

The same variable names are used to write and read the header of the ASCII files.

**TSGQC** makes a distinction between high resolution **TSG** data (< 5 minutes) and discrete **sample** data (Water samples, CTD, ARGO, XBT, XCTD, etc.).

### Main variables used for TSG data

The main variables used to describe the **TSG** data are:

DATE Date (string ‘YYYYMMDDHHMMSS’)

DAYD Julian day

LATX Latitude in decimal degree

LONX Longitude in decimal degree

CNDC Conductivity measured by the **TSG**

SSPS Salinity computed by using CNDC and SSJT

SSJT Temperature measured by the **TSG**

SSTP Temperature measured with a precise sensor (SBE 38 for example)

SPDC Speed ship (in knots).

FLOW Flow of pipe that feeds the **TSG**

PRES Water pressure in the **TSG**

Secondary variables based on these main variables are built. Some example for the SSPS variable:

SSPS\_QC Quality code assigned to SSPS

SSPS\_CAL Calibrated SSPS time series

SSPS\_ADJUSTED Adjusted SSPS time series

SSPS\_ADJUSTED\_QC Quality code assigned to SSPS

SSPS\_ADJUSTED\_ERROR Error assigned to adjusted SSPS time series

*Note on the differences between XXXX, XXXX****\_CAL****, XXXX****\_ADJUSTED*** *where XXXX = SSPS, SSJT, SSTP*

XXXX is the raw data (SSJT, SSTP) or is computed (SSPS).

A quality code can be assigned to this data: variable XXXX\_QC.

Raw data variable are neither modified nor deleted. If a modification is applied a new variable is created.

Calibrated data: XXXX\_CAL.

If a calibration is made the variable XXXX.CAL is created but there is no XXXX\_CAL\_QC variable. The user must use the quality code of the raw variable: XXXX\_QC

Adjusted data: XXXX\_ADJUSTED

If a correction is made to the time series the variable XXXX.ADJUSTED is created. This variable only contains corrected measurements. If part of the time series is not corrected those measurements are not stored in the adjusted variable, their value is set to NaN (Not a Number).

An error estimation is assigned to the adjusted data. It is stored in the XXXX\_ADJUSTED\_ERROR variable.

The quality code, XXXX\_ADJUSTED\_QC, assigned to the XXXX\_ADJUSTED variable is equal to the quality code assigned to the raw data.

To summarize, when you want work with TSG data you must check the existence of the following variables, in that order:

1 – XXXX\_ADJUSTED.

If the variable exists and is not empty, correction has been applied to the raw data. An error is given by the XXXX\_ADJUSTED\_ERROR variable and the quality code by the XXXX\_ADJUSTED\_QC variable.

2 – If the XXXX\_ADJUSTED variable is empty you must check if XXXX\_CAL exists

In that case a calibration was performed. Use then the XXXX\_QC variable to get the quality codes assigned to the measurements.

3 – At least if there is no XXXX\_ADJUSTED and XXXX\_CAL variables, use the XXXX and XXXX\_QC variables.

**Remark:**

During the same trip, the availability of these different variables may change over time. Thus, the variable XXXX\_ADJUSTED will only be defined for the sections of the trip where external data are available, while the variable XXXX alone may be available and usable elsewhere.

### Discrete sample

Discrete sample variables have the extension \_EXT.

DATE\_EXT Date (string ‘YYYYMMDDHHMMSS’)

DAYD\_EXT Julian day

LATX\_EXT Latitude in decimal degree

LONX\_EXT Longitude in decimal degree

SSPS\_EXT Salinity

SSTP\_EXT Temperature

The SSJT time series can be corrected by using SSTP\_EXT data.

Derived variables are:

SSPS\_EXT\_QC SSPS Quality codes

SSTP\_EXT\_QC SSTP Qualitiy codes

SSPS\_EXT\_TYPE Instrument used to get the samples (4 digits):

ARGO ARGO measurements

CTD CTD measurements

UNKN Unknown

WS (**W**ater **S**ample) Water sample analysed in laboratory

etc.

SSTP\_EXT\_TYPE Instrument used to get the samples (4 digits):

ARGO ARGO measurements

CTD CTD measurements

UNKN Unknown

etc.

SSPS\_EXT\_BOTTLE number or reference of the water sample bottle (WS)

## Input files

**TSGQC** can read data files with the following format:

1. ARGO p. 42
2. ASCII p. 43
3. ASTROLABE p. 43
4. Merchant ship (Logiciel SODA - SOERE SSS) p. 45
5. NetCDF GOSUD p. 45
6. ORACLE p. ??
7. SDF p. ??
8. NUKA ARCTICA p. ??

Filename extensions are:

TSG data

ASCII **.tsgqc**

ASTROLABE **.ast**

NetCDF **.nc**

SOERE SSS **.lbv (formerly.ora or .sdf)**

NUKA ARCTICA **.transmit\***

Sample data

ASCII **.btl** for water sample.

**.spl** for every type of discrete measurements (CTD ...)

ARGO **.arg** ARGO data in LOCEAN format.

## Output files

**TSGQC** can write data files with the following format:

1. NetCDF GOSUD - see **CORTSG\_format\_gosud.doc**

NetCDF files allows the user to keep all the information about the TSG measurements: meta-data, TSG time series, sample data.

This is the default output format

1. ASCII

This format can be used for TSG time series and discrete sample. The format is the same for input and output files.

A description of the format is available p. 43

## ARGO Format (\*.arg)

Nicolas Martin (Engineer at LOCEAN) developed a software that collocates ARGO floats position and ship track. The collocation is made for **TSG** data managed by the Coriolis data center. ARGO measurements are kept if they are found at the surface at less than 50 km and 5 days of the ship trajectory.

The internet address of the collocalisation ARGO-TSG site is:

<http://www.locean-ipsl.upmc.fr/~TSG-ARGO/>

The site is daily updated.

In the ARGO file there is one line per ARGO collocalisation.

1-6 Date of the ARGO profile: YYYY-MM-DD HH:MI:SS

7 Longitude of the ARGO profile

8 Latitude of the ARGO profile

9 Profiler number

10 Cycle number

11 Pressure of the ARGO measurement (\*)

12 Pressure quality

13 ARGO salinity

14 Salinity quality code

15 ARGO temperature

16 Temperature quality code

17 Mean time difference between the ARGO et TSG measurements (\*\*)

18 Mean distance between the ARGO et TSG measurements

19 Number of TSG salinity

20 Average of TSG salinity

21 Standard deviation of TSG salinity

22 Number of TSG temperature

23 Average of TSG temperature

24 Standard deviation of TSG temperature

(\*) By default it is the pressure the closest to 5 m, between 0 and 10 m and with quality code of ‘1’ or '2'

(\*\*) Less than R km and at +/-J days (by default R = 50 km and J = 5 days)

**Important**

**TSGQC** adds the mean time difference between the **ARGO** and **TSG** measurements (column n°17) to the date of the ARGO profile. It is that date which is stored in **NetCDF** and **\*.spl** files.

## ASTROLABE Format (\*.ast)

This format has been created for the ASTROLABE ship **TSG** by Elodie Kestenare (UMR LEGOS).

**Example :**

**%HEADER DDMMYY hh mi ss LATX LONX T\_canisterRaw T\_remoteRaw SSSraw SSJT SSTP SSPS SSPS\_ADJUSTED PRES**

**211009 0 0 0 -42.8824 147.3407 12.9442 12.8127 33.1911 -99.0000 -99.0000 -99.0000 -99.0000 1.73**

**211009 0 1 0 -42.8824 147.3407 12.9442 12.8133 33.1935 -99.0000 -99.0000 -99.0000 -99.0000 1.75**

**211009 0 2 0 -42.8824 147.3407 12.9442 12.8150 33.1950 -99.0000 -99.0000 -99.0000 -99.0000 1.75**

**211009 0 3 0 -42.8824 147.3407 12.9449 12.8152 33.1971 -99.0000 -99.0000 -99.0000 -99.0000 1.75**

**211009 0 4 0 -42.8824 147.3407 12.9462 12.8171 33.2006 -99.0000 -99.0000 -99.0000 -99.0000 1.75**

**211009 0 5 0 -42.8824 147.3407 12.9471 12.8213 33.2028 -99.0000 -99.0000 -99.0000 -99.0000 1.75**

**211009 0 6 0 -42.8824 147.3408 12.9484 12.8229 33.2043 -99.0000 -99.0000 -99.0000 -99.0000 1.74**

## ASCII Format (\*.btl, \*.spl, \*.tsgqc)

Files with ASCII format have the same structure for **TSG (\*.tsgqc)** and sample files **(\*.btl, \*.spl**):

**TSG** data

%PLATFORM\_NAME TOUCAN

%HEADER YEAR MNTH DAYX hh mi ss LATX LONX SSPS SSPS\_QC SSJT SSJT\_QC SSTP SSTP\_QC

2007 07 18 14 20 32 49.9168510 -3.0475171 35.300 0 15.702 0 NaN 9

2007 07 18 14 25 32 49.9076500 -3.0808330 35.290 0 16.028 0 NaN 9

2007 07 18 14 30 32 49.8984489 -3.1142170 35.281 0 15.997 0 NaN 9

2007 07 18 14 35 32 49.8893013 -3.1478500 35.273 0 16.130 0 NaN 9

2007 07 18 14 40 32 49.8801155 -3.1815331 35.260 0 16.170 0 NaN 9

2007 07 18 14 45 32 49.8716011 -3.2158000 35.262 0 16.296 0 NaN 9

There can be one or more header line. They must begin with the ‘%’ character. Metadata can be written in the header lines. In that case you must first indicate the variable name listed in the NetCDF format (see **CORTSG\_format\_gosud.doc)**

The header line beginning with %HEADER is absolutely necessary. This line describes the variables available in the file.

The 6 first variables are necessary (in that order):

* year YEAR
* month MNTH
* day DAYX
* hour hh
* minutes mi
* seconds ss

Then the order of the NetCDF variables is not imposed. In the preceding example the file contains the following variables:

LATX Latitude

LONX Longitude

SSPS TSG salinity

SSPS\_QC Salinity quality code

SSJT TSG temperature

SSJT\_QC TSG temperature quality code

SSTP Temperature sensor

SSTP\_QC Temperature sensor quality code

In the preceding example the name of the ship where the TSG is installed is assigned to the **NetCDF** variable **'PLATFORM\_NAME'**.

**Warning**

**\*.spl** files can be used:

1. to load discrete samples
2. to export in a unique file discrete samples data.

**TSGQC** adds the mean time difference between the **ARGO** and **TSG** measurements (column n°17) to the date of the ARGO profile. It is that date which is stored in **NetCDF** and **\*.spl** files.

## NetCDF format (\*.nc)

**NetCDF** files allows the user to keep all the information about the **TSG** measurements: meta-data, **TSG** time series, sample data..

The format is described in the document [**CORTSG\_format\_gosud.pdf**](https://git.outils-is.ird.fr/grelet/TSG-QC/-/blob/master/tsg_doc/CORTSG_format_gosud.pdf)

## SODA format (\*.lbv)

This format is used for the acquisition of **TSG** data onboard merchant ships managed by the SOERE SSS.

The acquisition software **SODA[[6]](#footnote-6)** is developed under LabView by David Varillon (IRD - US191 ‘IMAGO’ - Nouméa). The software documentation: **SODA\_User\_manual.pdf** is available on demand..

## NUKA ARTICA format (\*.transmit\*)

This format has been created for the Nuka Arctica ship TSG by Gilles Reverdin (UMR LOCEAN).

Example :

46 NUK 2001 7 7 1741 59.40 -0.05 13.29 34.846

46 NUK 2001 7 7 1746 59.40 -0.10 13.23 34.932

46 NUK 2001 7 7 1751 59.42 -0.13 13.16 34.959

46 NUK 2001 7 7 1756 59.42 -0.18 13.16 34.954

46 NUK 2001 7 7 18 1 59.43 -0.22 13.17 34.970

46 NUK 2001 7 7 18 6 59.43 -0.27 13.10 34.983

46 NUK 2001 7 7 1811 59.45 -0.30 13.04 34.984

46 NUK 2001 7 7 1816 59.45 -0.35 12.99 34.986

46 NUK 2001 7 7 1821 59.47 -0.38 12.92 34.984

46 NUK 2001 7 7 1826 59.48 -0.43 12.92 34.981

## Format des fichiers ORACLE (\*.ora)

This format was formerly used for the **TSG** data of merchant ships managed by the SOERE SSS.

## Format des fichiers SDF (\*.sdf)

This format was formerly used for the **TSG** data of merchant ships managed by the SOERE SSS.

## Configuration file format (\*.ini)

The \*.ini files are used for the configuration of the SODA acquisition software. When reading \*.lbv or \*.tsgqc files, if an .ini file is present in the directory with the same name, it will be read by TSGQC and the meta-data will be automatically imported.

Example file CSLO1604.INI :

[GLOBAL]

PLATFORM\_NAME = "Cap San Lorenzo"

SHIP\_CALL\_SIGN = "LXSQ"

SHIP\_MMSI = "253126000"

PROJECT\_NAME = "ORE-SSS"

CYCLE\_MESURE = "CSLO1604"

DATA\_TYPE = "TRAJECTORY"

DATA\_MODE = "D"

PI\_NAME = "DIVERRES"

DATA\_CENTRE = "IRD-BREST"

DATA\_ACQUISITION = "ORE-SSS"

WS\_TYPE = "OSIL"

TYPE\_TSG = "SBE21"

TYPE\_TINT = "NA"

SAMPLING\_PERIOD = "300"

Example of reading and displaying a .tsgqc file and the .ini file if present in the same directory. To display the contents of an .ini file in the Matlab console, the TSGQC software must be launched in "debug" mode with the following command:

>> tsgqc('debug','true')

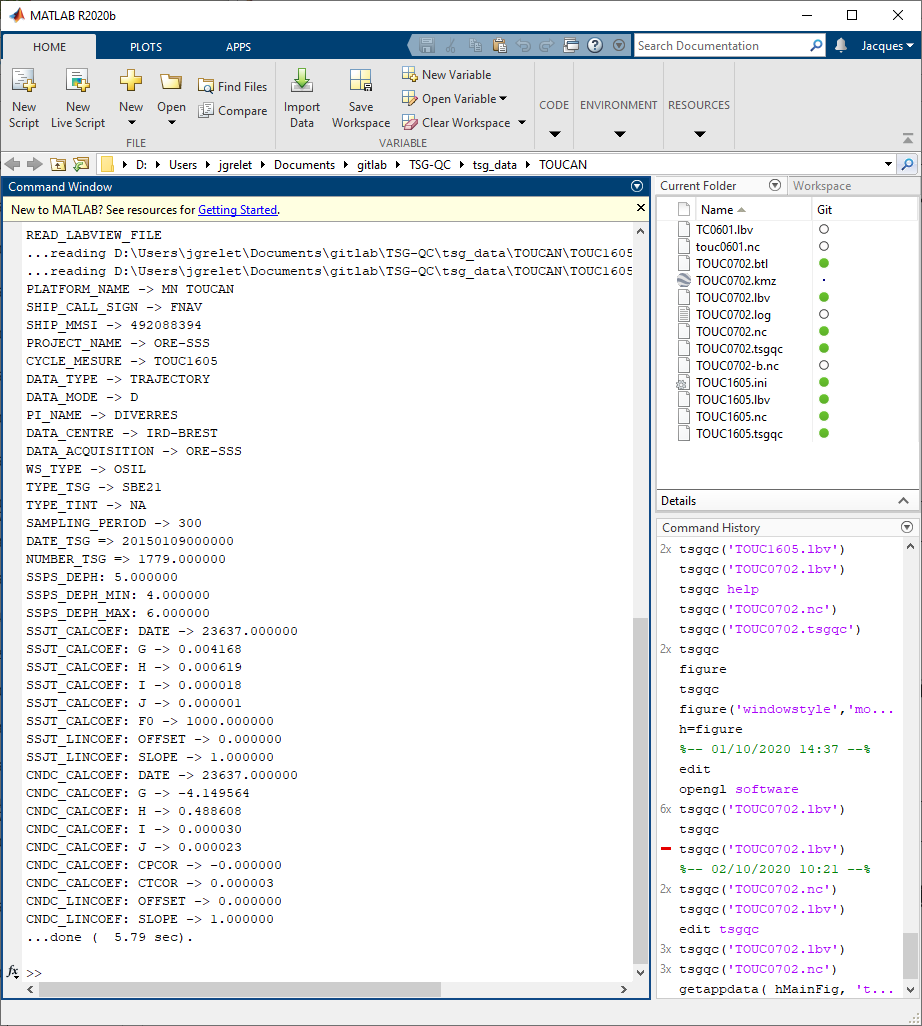


Figure 44: Matlab console for displaying an .ini parameter file

## Climatology file format

The climatology files used by TSGQC are in NetCDF format and extracted from :

* the WOA05 and WOA13 atlas (WORLD OCEAN ATLAS 2005 and 2013): <https://www.nodc.noaa.gov/OC5/woa13/>
* the climatology of the LOPS (IFREMER) ISAS13 and ISAS15: <https://www.seanoe.org/data/00412/52367/>

**TSGQC** uses reduced **NetCDF** files containing only the climatology at 0 and 5 m.

Data are available in 3 files: annual, seasonal, monthly

The available variables are :

WOA\_MEAN\_SSTP: temperature

WOA\_MEAN\_SSPS: salinity

WOA\_MEAN\_DOX: oxygen

with the standard deviation (WOA\_STD\_SSTP) and the number of observations used to build the climatology (WOA\_OBS\_SSTP).

In these NetCDF files, the dimension WOA\_TIME will take the following values for:

WOA\_TIME = 1 for the annual file

WOA\_TIME = 4 for the seasonal file

WOA\_TIME = 12 for the monthly file

Example of seasonal file structure with the ncdump command :

$ ncdump -h woa13\_annual\_surf.nc

NetCDF woa13\_annual\_surf {

dimensions:

WOA\_TIME = 1 ;

WOA\_DEPH = 2 ;

WOA\_LONX = 1440 ;

WOA\_LATX = 720 ;

variables:

float WOA\_TIME(WOA\_TIME) ;

float WOA\_DEPH(WOA\_DEPH) ;

WOA\_DEPH:units = "Depth" ;

WOA\_DEPH:long\_name = "meters" ;

WOA\_DEPH:\_FillValue = -99.9999f ;

float WOA\_LATX(WOA\_LATX) ;

WOA\_LATX:units = "Latitude" ;

WOA\_LATX:long\_name = "degree\_north" ;

WOA\_LATX:\_FillValue = -99.9999f ;

float WOA\_LONX(WOA\_LONX) ;

WOA\_LONX:units = "Longitude" ;

WOA\_LONX:long\_name = "degree\_east" ;

WOA\_LONX:\_FillValue = -99.9999f ;

float WOA\_MEAN\_SSTP(WOA\_TIME, WOA\_DEPH, WOA\_LATX, WOA\_LONX) ;

WOA\_MEAN\_SSTP:units = "Sea Surface Temperature mean" ;

WOA\_MEAN\_SSTP:long\_name = "degre Celcius" ;

WOA\_MEAN\_SSTP:\_FillValue = -99.9999f ;

float WOA\_MEAN\_SSPS(WOA\_TIME, WOA\_DEPH, WOA\_LATX, WOA\_LONX) ;

WOA\_MEAN\_SSPS:units = "Sea Surface Salinity mean" ;

WOA\_MEAN\_SSPS:long\_name = "PSU" ;

WOA\_MEAN\_SSPS:\_FillValue = -99.9999f ;

float WOA\_STD\_SSTP(WOA\_TIME, WOA\_DEPH, WOA\_LATX, WOA\_LONX) ;

WOA\_STD\_SSTP:units = "Sea Surface Temperature standard deviation" ;

WOA\_STD\_SSTP:long\_name = "degre Celcius" ;

WOA\_STD\_SSTP:\_FillValue = -99.9999f ;

float WOA\_STD\_SSPS(WOA\_TIME, WOA\_DEPH, WOA\_LATX, WOA\_LONX) ;

WOA\_STD\_SSPS:units = "Sea Surface Salinity standard deviation" ;

WOA\_STD\_SSPS:long\_name = "PSU" ;

WOA\_STD\_SSPS:\_FillValue = -99.9999f ;

short WOA\_OBS\_SSTP(WOA\_TIME, WOA\_DEPH, WOA\_LATX, WOA\_LONX) ;

WOA\_OBS\_SSTP:units = "Sea Surface Temperature number observation" ;

WOA\_OBS\_SSTP:long\_name = "none" ;

WOA\_OBS\_SSTP:\_FillValue = -100s ;

short WOA\_OBS\_SSPS(WOA\_TIME, WOA\_DEPH, WOA\_LATX, WOA\_LONX) ;

WOA\_OBS\_SSPS:units = "Sea Surface Salinity number observation" ;

WOA\_OBS\_SSPS:long\_name = "none" ;

WOA\_OBS\_SSPS:\_FillValue = -100s ;

// global attributes:

:description = "WOA13 CLIMATOLOGY Surface temperature salinity annual" ;

:author = "J Grelet IRD US191 Brest" ;

:date = "03 Jul 2018" ;

## Glossary

GOSUD **G**lobal **O**cean **S**urface **U**nderway **D**ata

[www.ifremer.fr/gosud/](http://www.ifremer.fr/gosud/)

NetCDF Network Common Data Form

[https://www.unidata.ucar.edu/software/NetCDF/](https://www.unidata.ucar.edu/software/netcdf/)

ROSCOP **R**eport of **O**bservations/**S**amples **C**ollected by **O**ceanographic **P**rogrammes

<http://www.ices.dk/Ocean/roscop/index.asp>

SOERE SSS **S**ystèmes d’**O**bservation et d’**E**xpérimentation pour la **R**echerche en **E**nvironnement **S**ea **S**urface **S**alinity

http://www.legos.obs-mip.fr/fr/observations/sss/

WOA WORLD OCEAN ATLAS

<https://www.nodc.noaa.gov/OC5/woa18/>

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