

User Manual

for

TSGQC

ThermoSalinoGraph Quality Control

Version 1.5

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|------------------|--|--------------------|--|
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| Fonction : | | Fonction : | |

1. Revision History

| Dates | Versions | Chapitres concernés | Commentaires et modifications |
|--------------|-----------------|----------------------------|--------------------------------------|
| August 2010 | 1.5 | Creation | English version |
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3. Software goals

TSGQC (ThermoSalinoGraph Quality Control) 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.

4. Quick Start

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

1. Start **TSGQC** p. 6
2. Open a **TSG file**. Several formats are available p. 11
3. Visually check the data

a. Compare the measurements to a climatology p. 20
b. 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

a. **netCDF** format p. 16
b. **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:

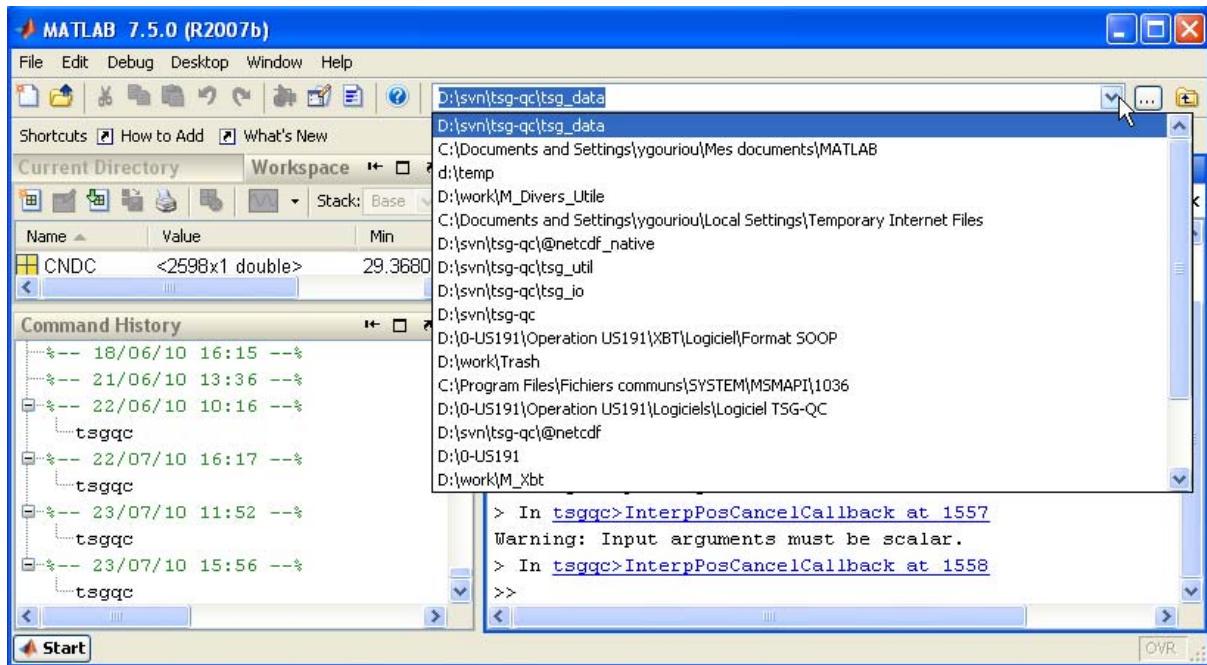
1. Automatic tests p. 8
2. TSG calibration p.
Erreur ! Signet non défini.
3. Data processing report p. 36

5. Functionalities

A. Starting TSGQC

Open a MATLAB 'Command Window'.

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

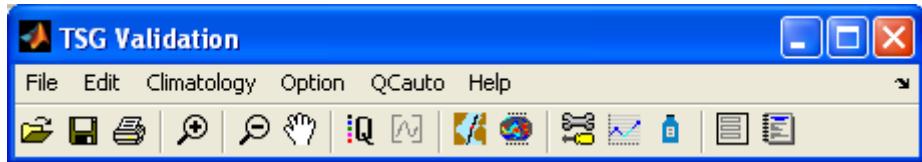


Type the name of the program in the command window:

```
>> tsgqc
```

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

B. Main functions

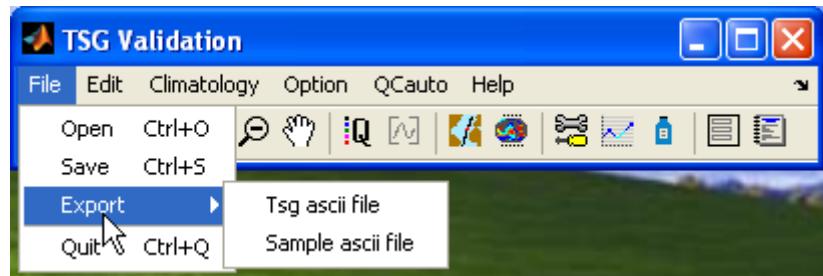


1. Toolbar

| | | |
|------------------------------------|---------------------------------------|-------|
| | 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 |

2. Menus

FILE menu

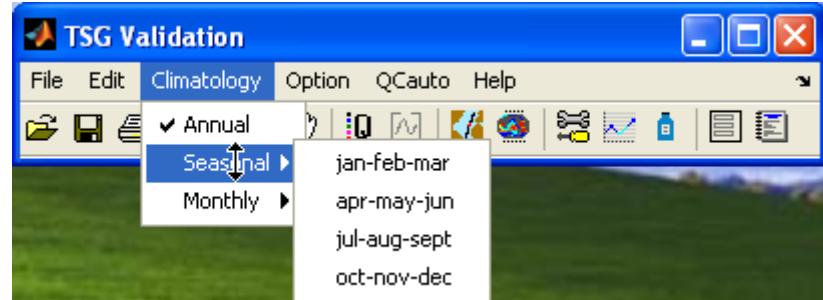


| | | |
|---------------|---|-------|
| Open | Open a file (TSG , samples, etc,) | p. 11 |
| Save | Save the data in NetCDF format | p. 16 |
| Export | Save the data in ASCII format <ul style="list-style-type: none">▪ TSG measurements▪ Samples (Water Samples, CTD, ARGO, ...) | p. 17 |
| Quit | Quit TSGQC | p. 39 |

Edit menu

This menu is not implemented.

Climatology menu

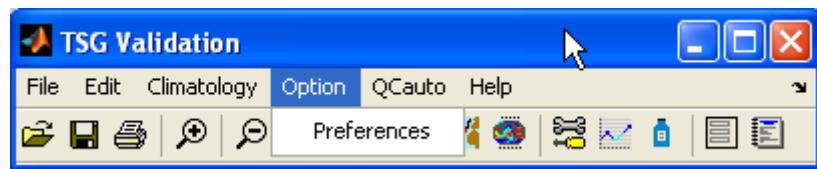


This menu allows the user to choose the period of the climatology to superimpose on the time series measurements:

1. Annual
2. Seasonal
3. Monthly

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

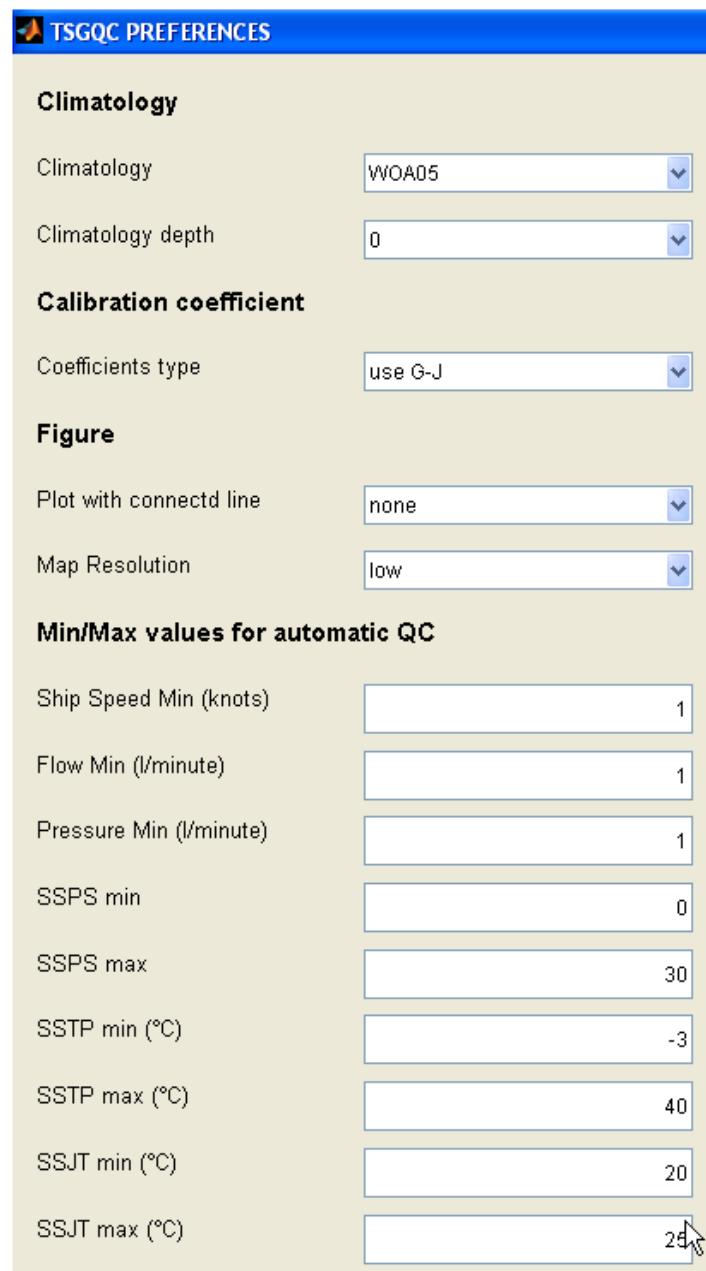
Option menu



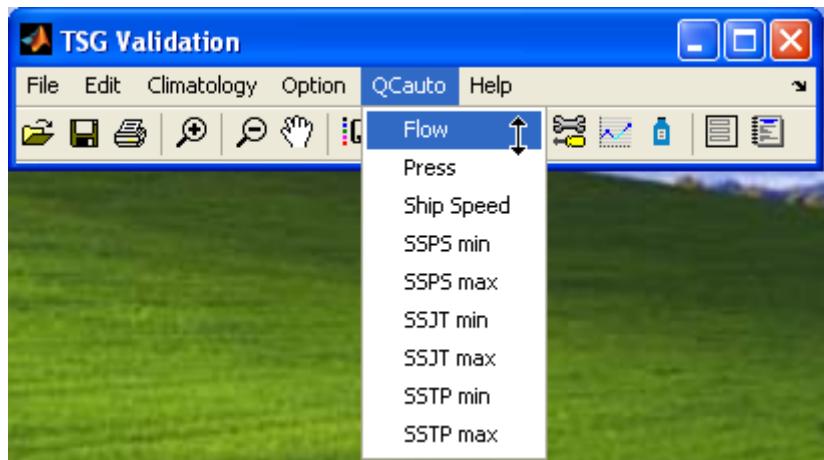
The **Option - references** menu is used to set the following preferences:

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

p. 20



QCauto menu



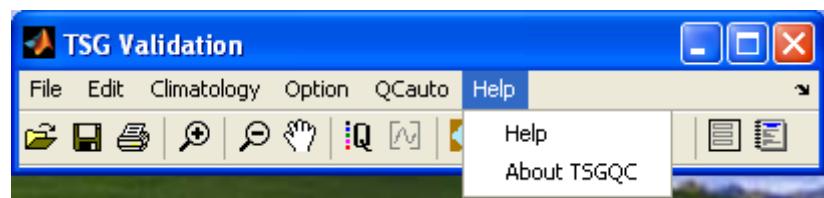
QCauto allows the user to apply automatic tests to the TSG time series. The tests use limits defined in the “Option - Preferences” form (see previous paragraph).

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

Remarks

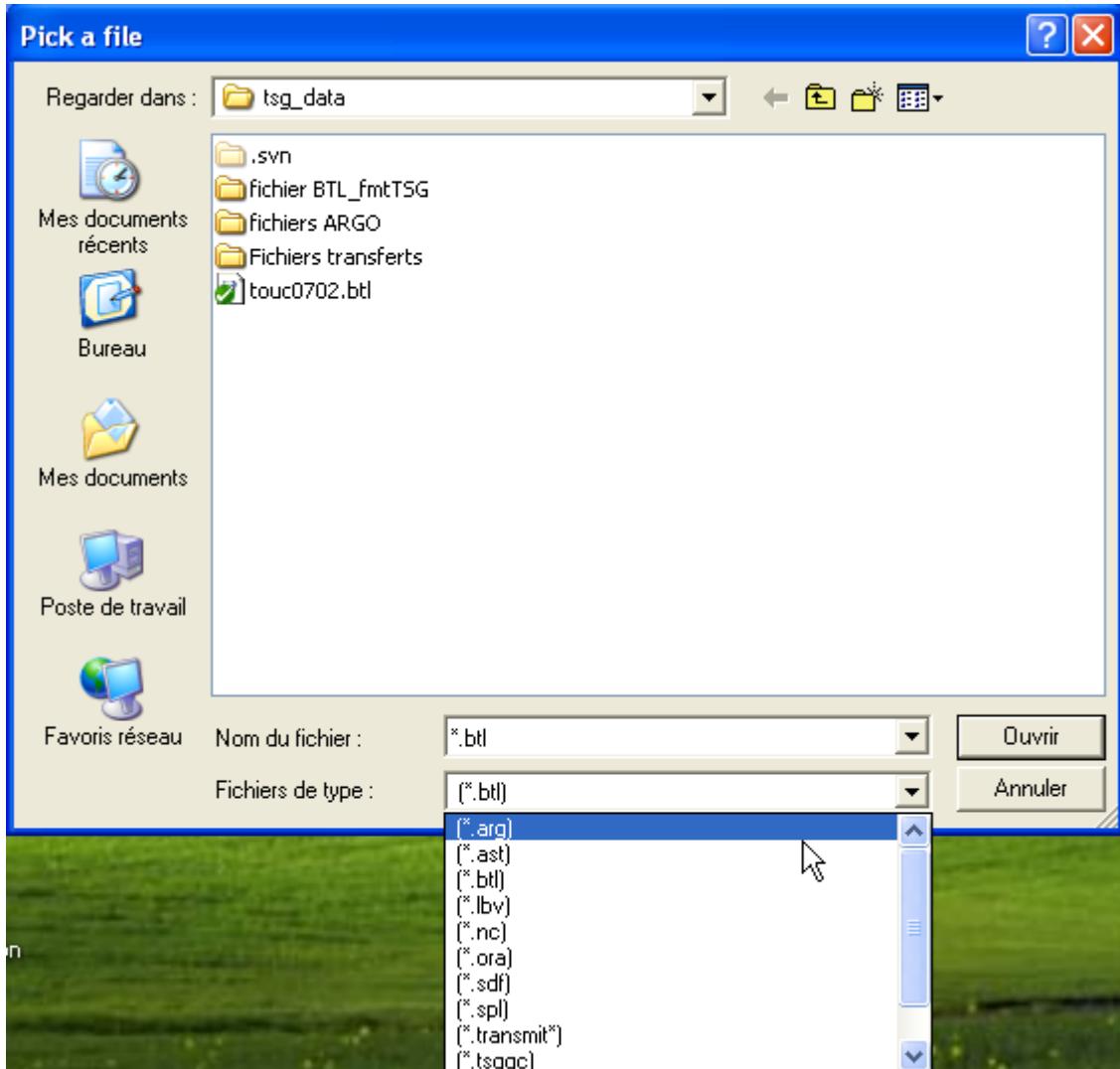
- ✓ There is no Undo function.
- ✓ Quality code “HARBOUR” is applied to measurements carried out when the speed of the vessel is below the “Ship Speed Min” value.
- ✓ Be careful with automatic tests. For example when a vessel is stopped, measurements can be BAD simply because there is no more water pressure 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



Online help is not yet implemented

C. 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 ¹ 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) |

¹ Varillon D., Shipboard Oceanographic Data Acquisition - S.O.D.A Version 1.00 - Manuel d'utilisateur, 2009

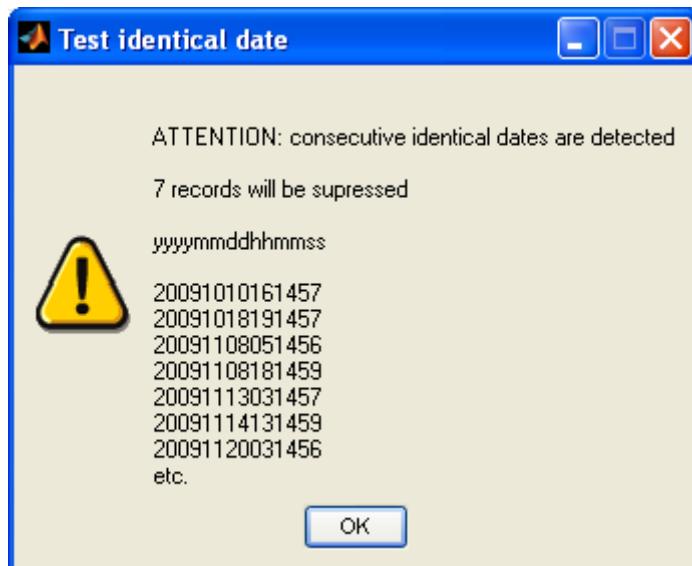
Format description can be found page:

| | |
|------------|-------|
| *.arg | p. 42 |
| *.ast | p. 43 |
| *.btl | p. 44 |
| *.lbv | p. 45 |
| *.nc | p. 44 |
| *.ora | p. ?? |
| *.sdf | p. ?? |
| *.spl | p. 44 |
| *.transmit | p. 45 |
| *.tsgqc | p. 44 |

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.



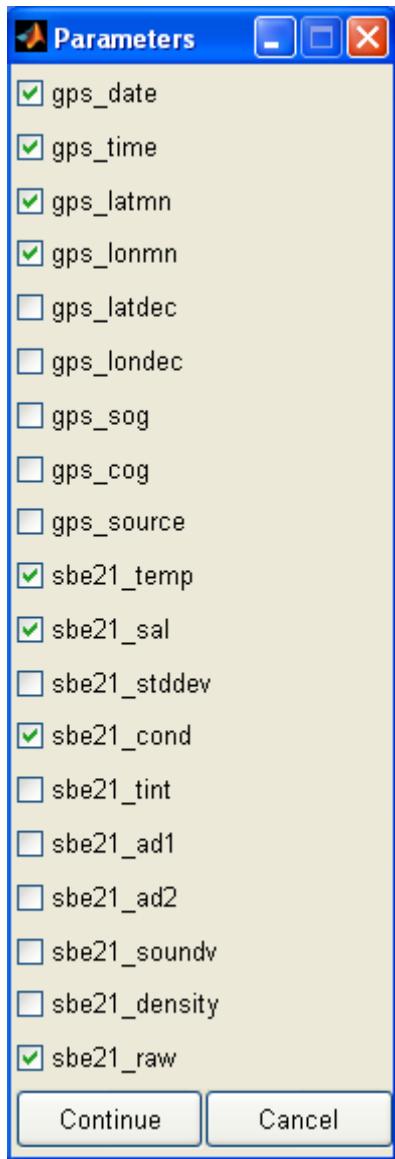
2. **Sample** measurements: Double measurements are detected based on date and hour comparison. No message box is displayed. Double records are deleted.

Sample file (*.btl, *.spl, *.arg) cannot be read if no **TSG** file was read. The following message box is displayed:



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

 When opening a Merchant Vessel file in the **SODA**² format, the following window is displayed:



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 copied in the netCDF FLOW variable.

² Varillon D., Shipboard Oceanographic Data Acquisition - S.O.D.A Version 1.00 - Manuel d'utilisateur, 2009

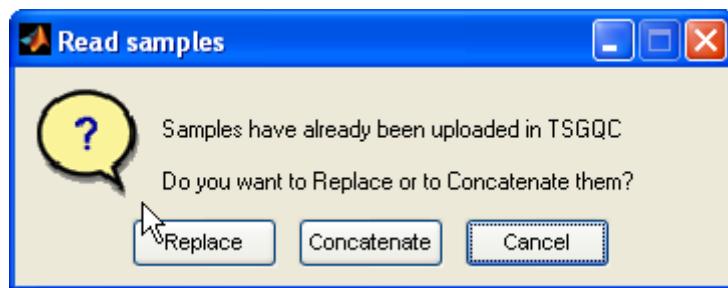
Remark

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.

2. Opening Sample Files (*.btl, *.spl, *argo)

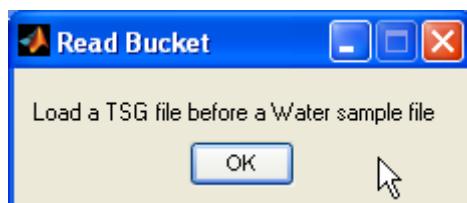
Samples (variable with extension _EXT in the netCDF format) can be used to correct the TSG measurements.

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.



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:



D. Saving your work

1. netCDF format



The default recording format is **netCDF** (see p. 44). 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 

TSG GLOBAL ATTRIBUTES AND VARIABLES

| | | | |
|------------------|---------|--------------------|-----|
| CYCLE MESURE: | N/A | DATE CREATION: | |
| PLATFORM NAME: | N/A | DATE UPDATE: | |
| PROJECT NAME: | ORE-SSS | DATA RESTRICTIONS: | |
| SHIP CALL SIGN: | N/A | CITATION: | |
| SHIP MMSI: | N/A | COMMENT: | |
| TSG INSTALL DATE | N/A | PI NAME: | Det |
| TYPE TSG: | RRF21 | DATA CENTRE: | |

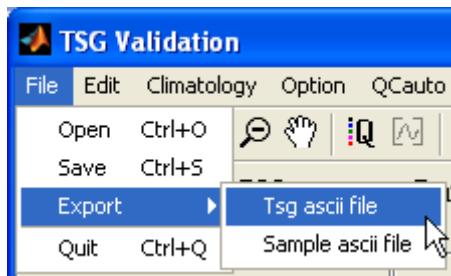
PLATFORM_NAME is the only information necessary to save a file. In general use the ship name in upper-case letters.

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.

2. ASCII format

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



The user can export :

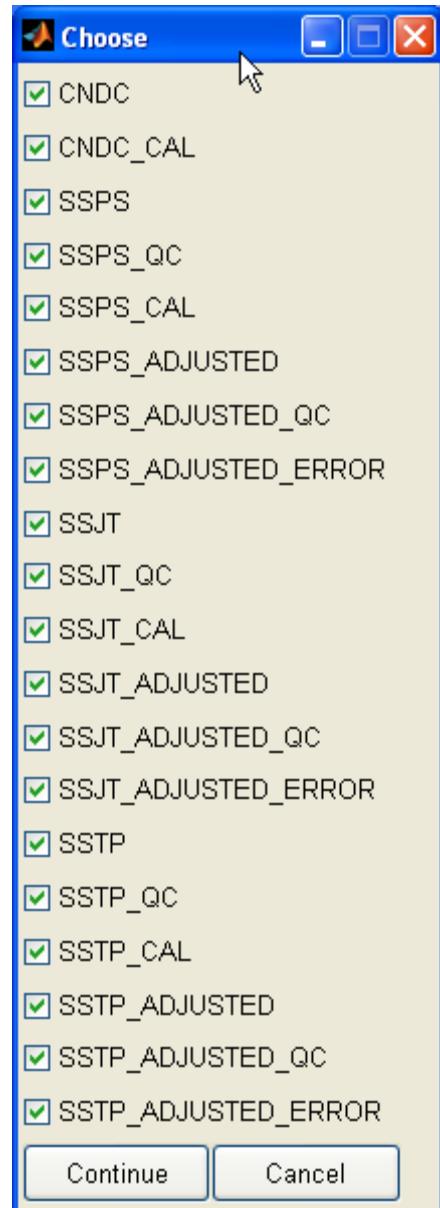
- ✓ Data **samples** (extension name: **.spl**): A **.spl** file contains all data **samples** loaded in **TSGQC**. **TSGQC** proposes to export the following variables:



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:



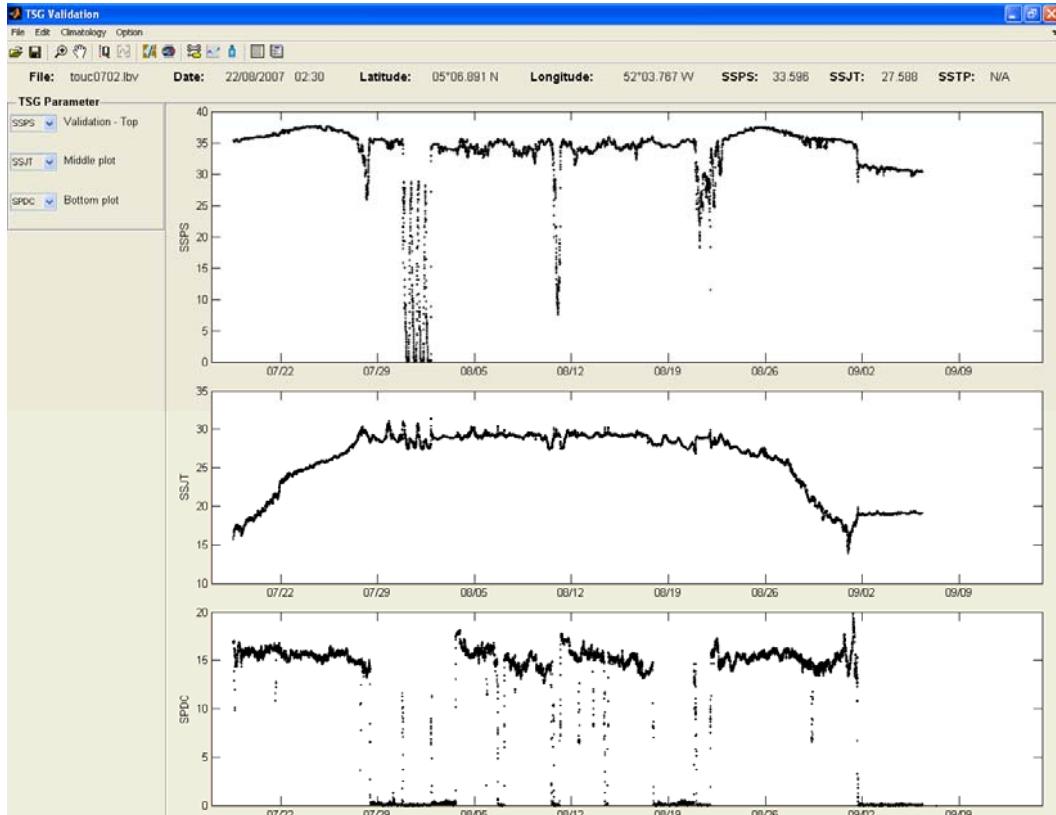
A description of the ASCII format is given p. 44.

E. Using TSGQC

1. 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.

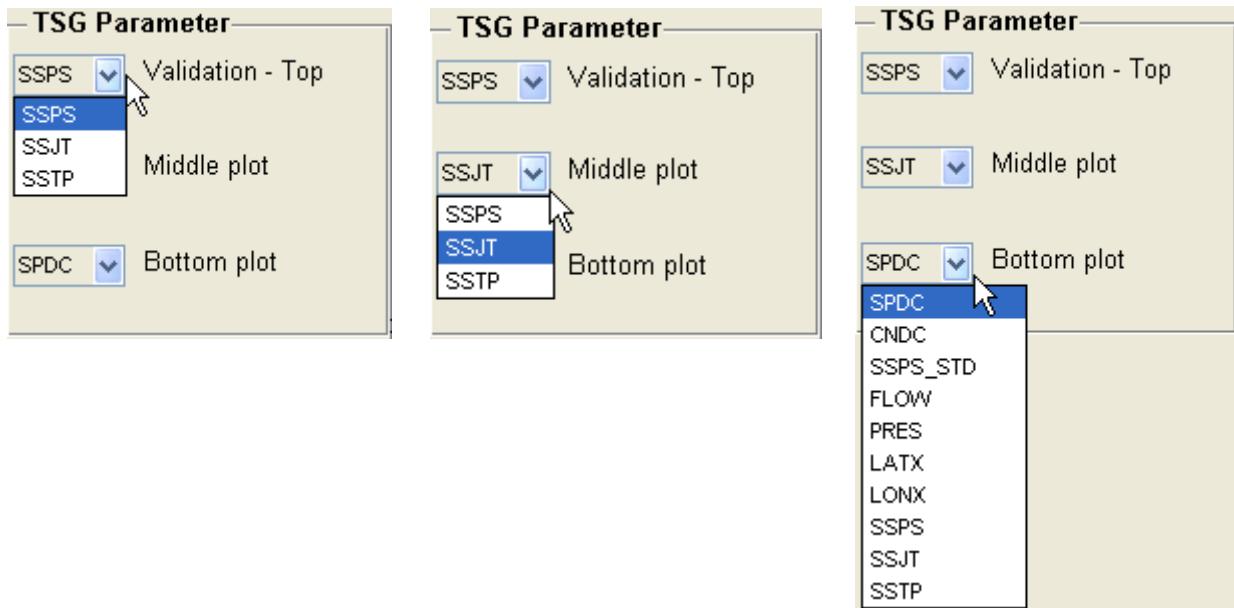


Y-axis labels correspond to the parameter names in the netCDF file.

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

File: touc0702.nc Date: 25/07/2007 14:15 Latitude: 19°03.355 N Longitude: 41°35.439 W SSPS: 37.552 SSJT: 25.901

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.



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.

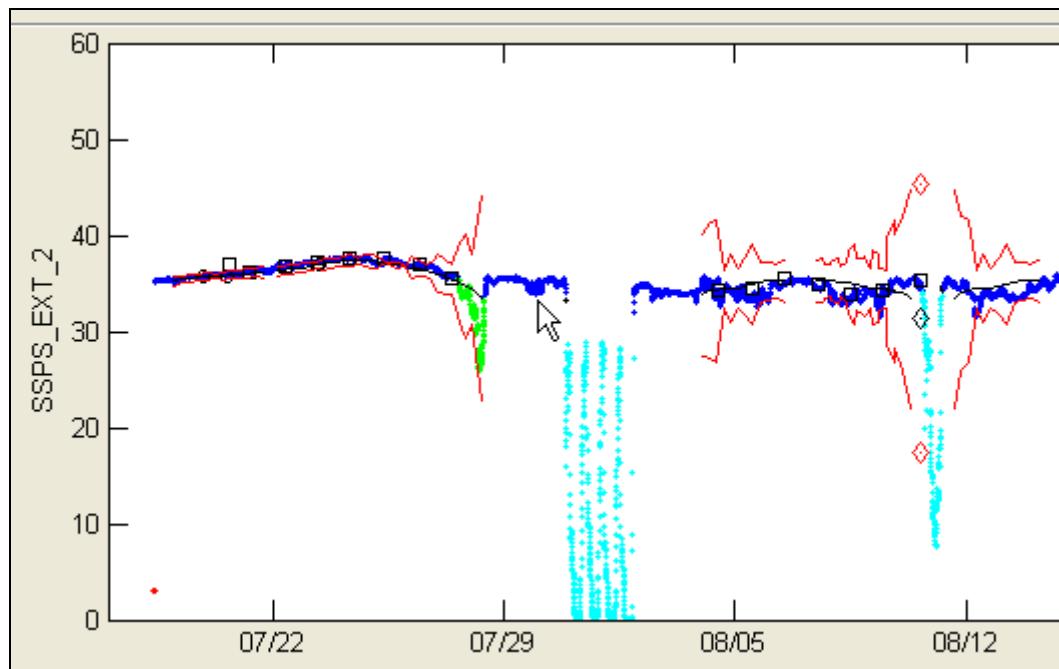
2. Plotting a climatology

The user can choose a climatology file in the **Option - Preferences** menu. The only available climatology are Levitus WOA01 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



3. 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.

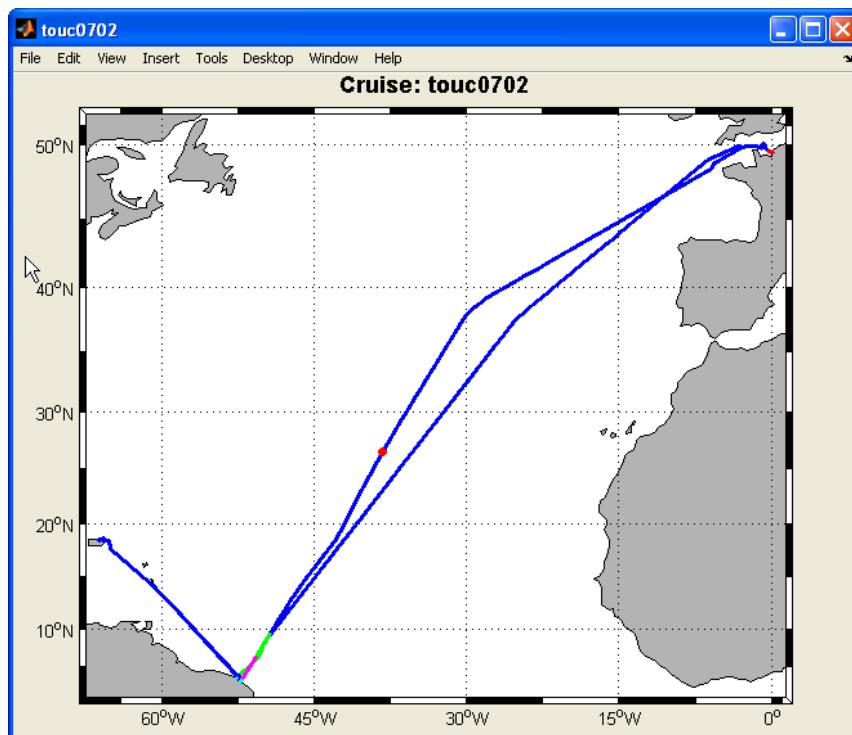
The plot is made taking into account the temporal limits of the upper plot: if the user zooms in the **TSG** time series, the map is also zoomed in. The map limits are updated automatically.

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

Several map resolutions are available. Use the menu « **Option - Preferences** ».

The map is plotted in a MATLAB figure window. The figure menus can be used to print or export the map in a graphic file.

The map can be displayed in several TSGQC modules..



4. Zoom and Pan functions



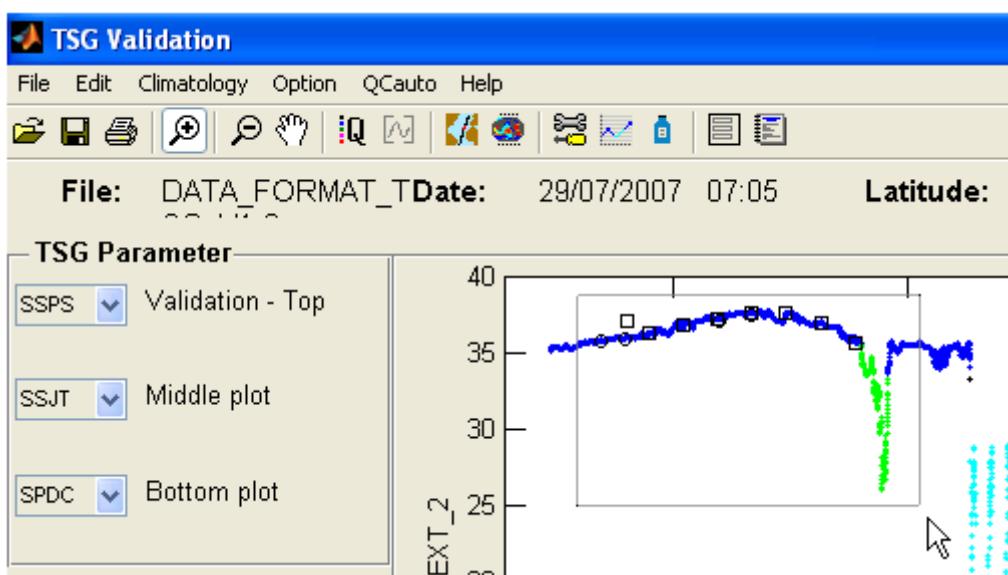
Zoom tools : The user can increase or decrease part of the time series. Zooming is useful to see greater detail in a small area. When in zoom in mode, the user can draw a rectangle with the pointer around the time series to magnify.

The 3 plots undergo the same change.

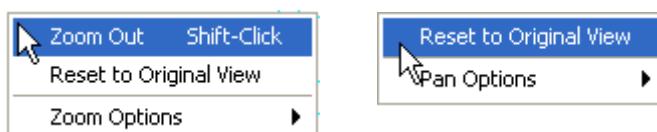


You can move your view of a graph up and down as well as left and right with the **Pan** tool. Panning is useful when you have zoomed in on a graph and want to translate the plot to view different portions.

The 3 plots undergo the same displacement.



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 :

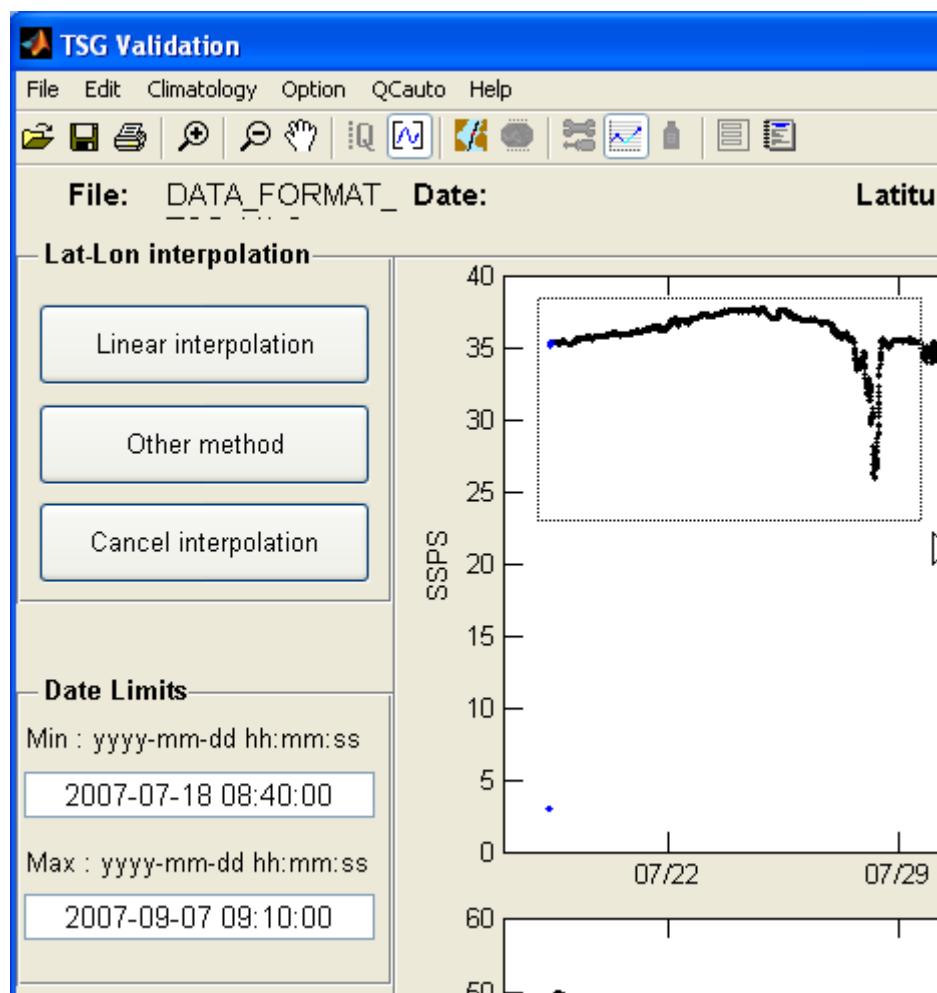
When the validation module is active, (see p.26), the '**Pan**' function is directly available when moving the mouse pointer at the bottom of the upper plot.

5. 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.

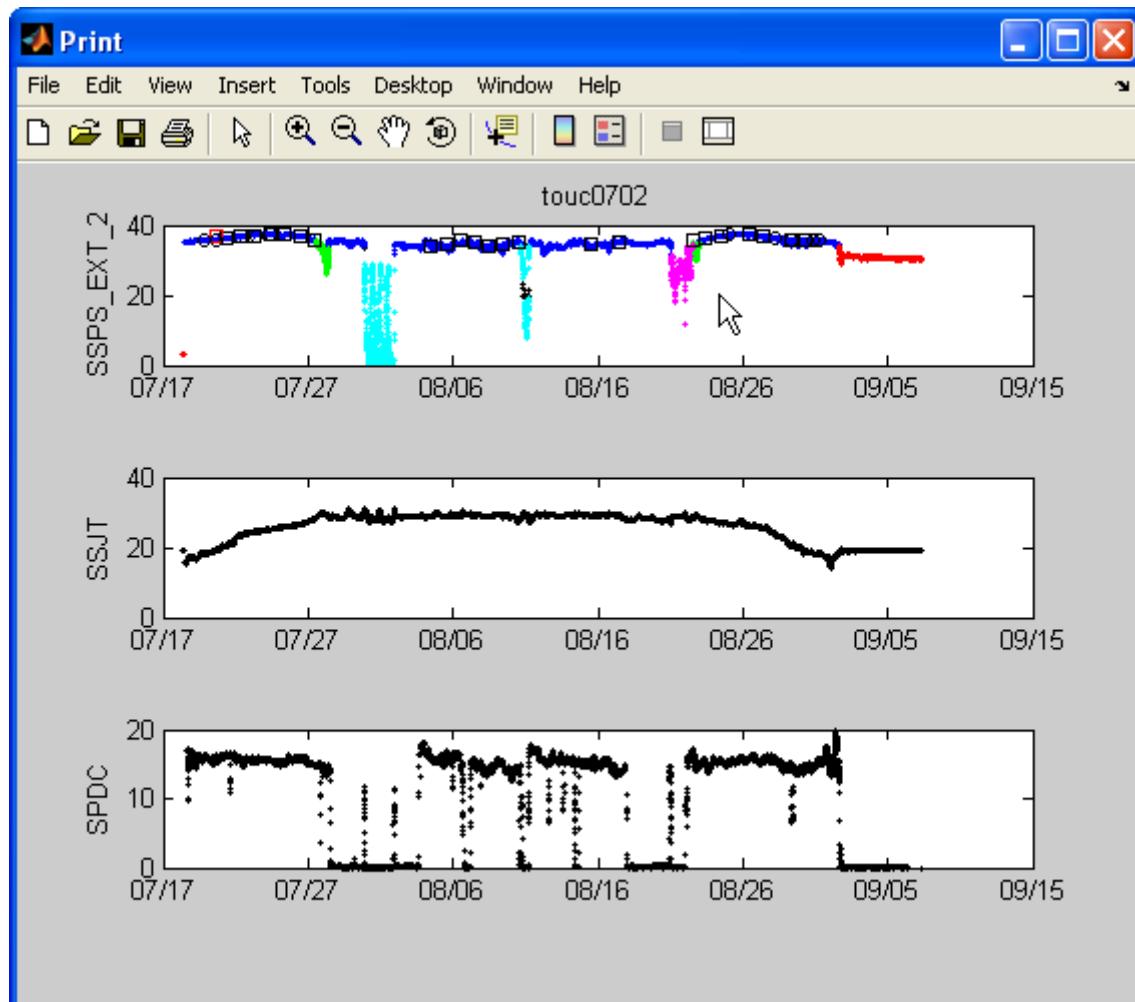


6. Printing figures

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.

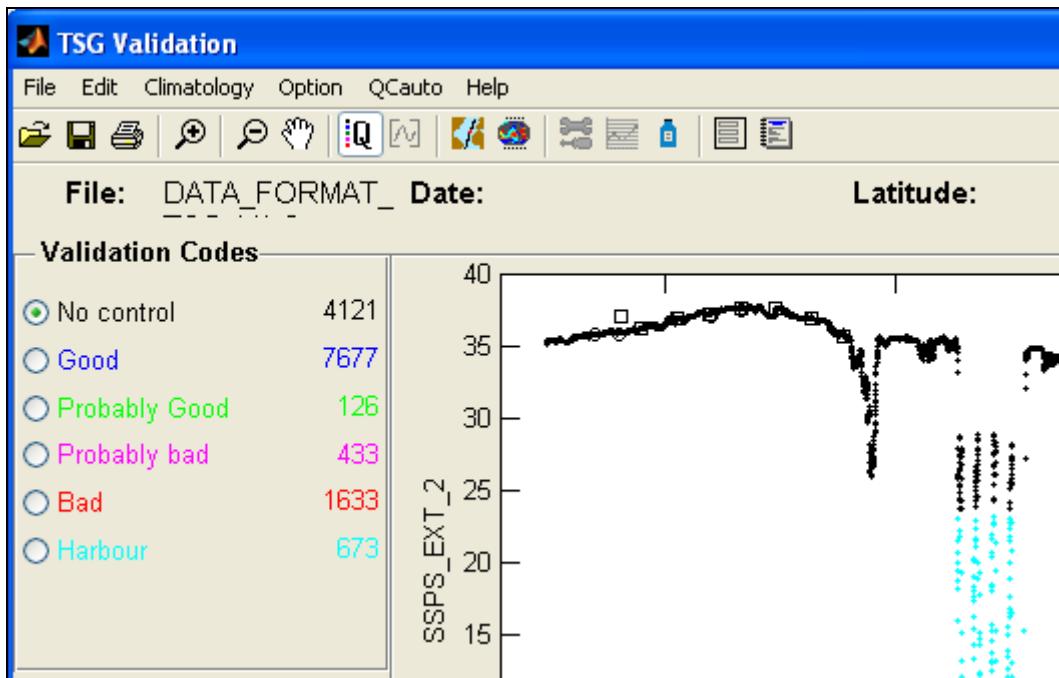
Note that the cruise track is plotted directly in MATLAB FIGURE WINDOW.



F. 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 particular code (7677 have a quality code GOOD in the example below).



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:

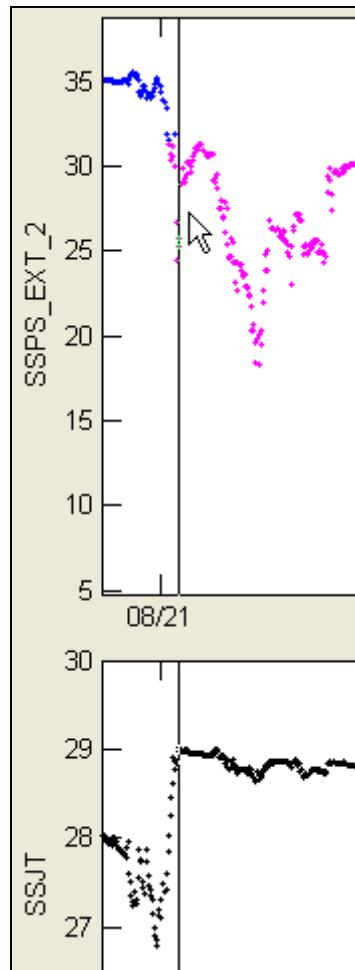


Selected data get the colour of the chosen code. The HARBOUR code is designed to mark good data taken when the ship is in a port. If the data are not of a good quality, choose another code.

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.



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.

G. Calibration

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

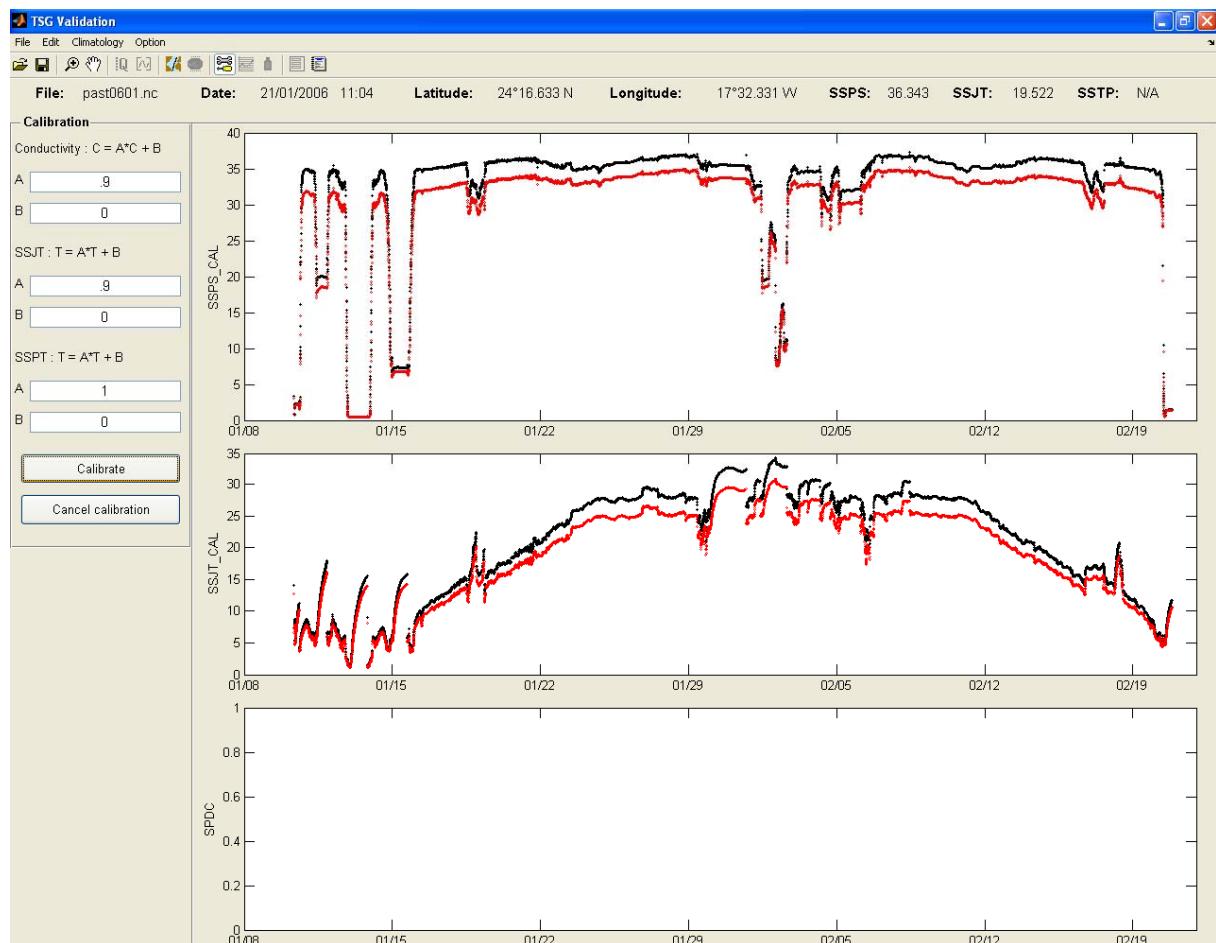
Enter the slope and offset in the input dialog box in the **Calibration** panel for:

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.



Remark

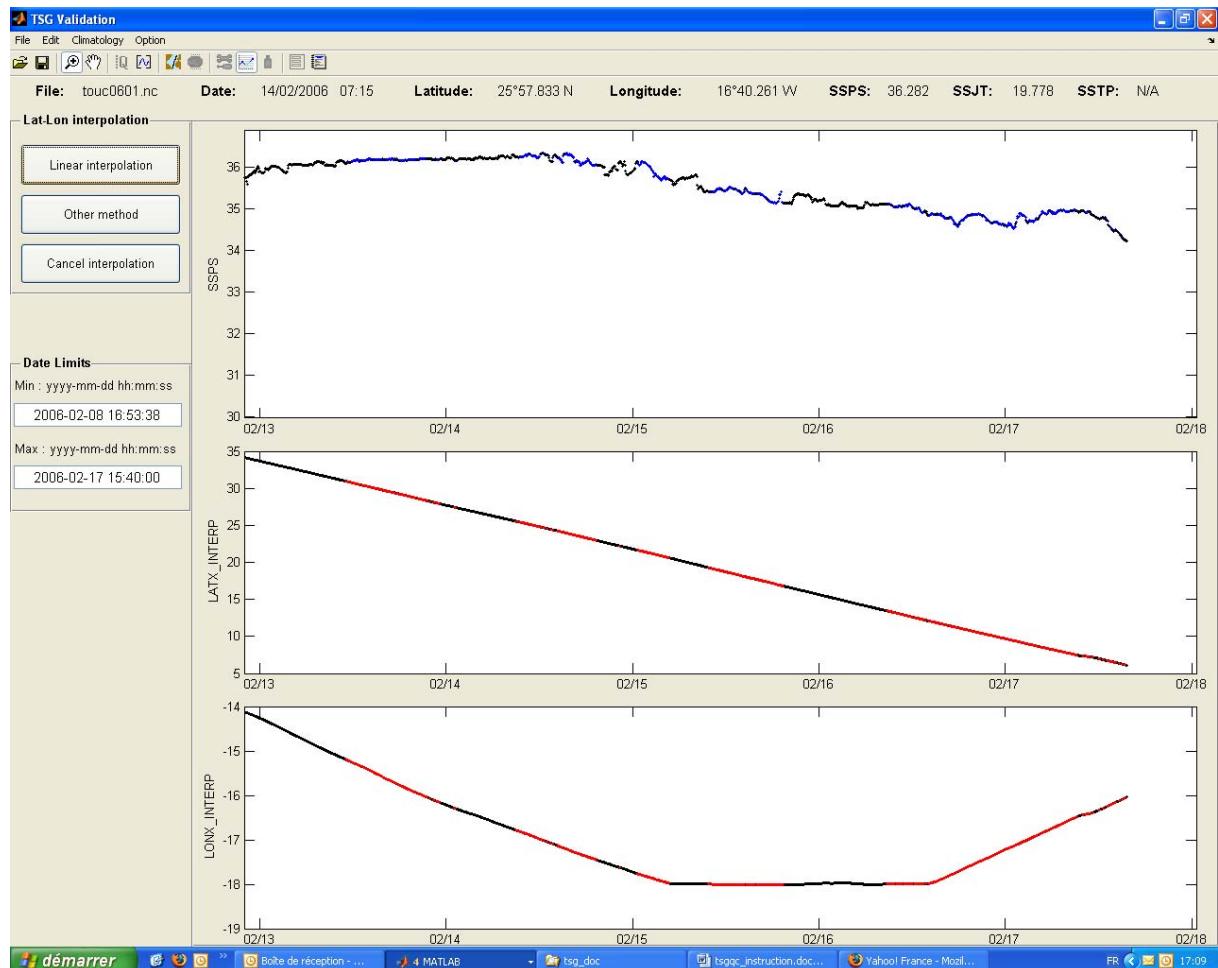
That function is not frequently used. It is better to use Samples to correct/Adjust the data.

H. 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:



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 23).

I. 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).

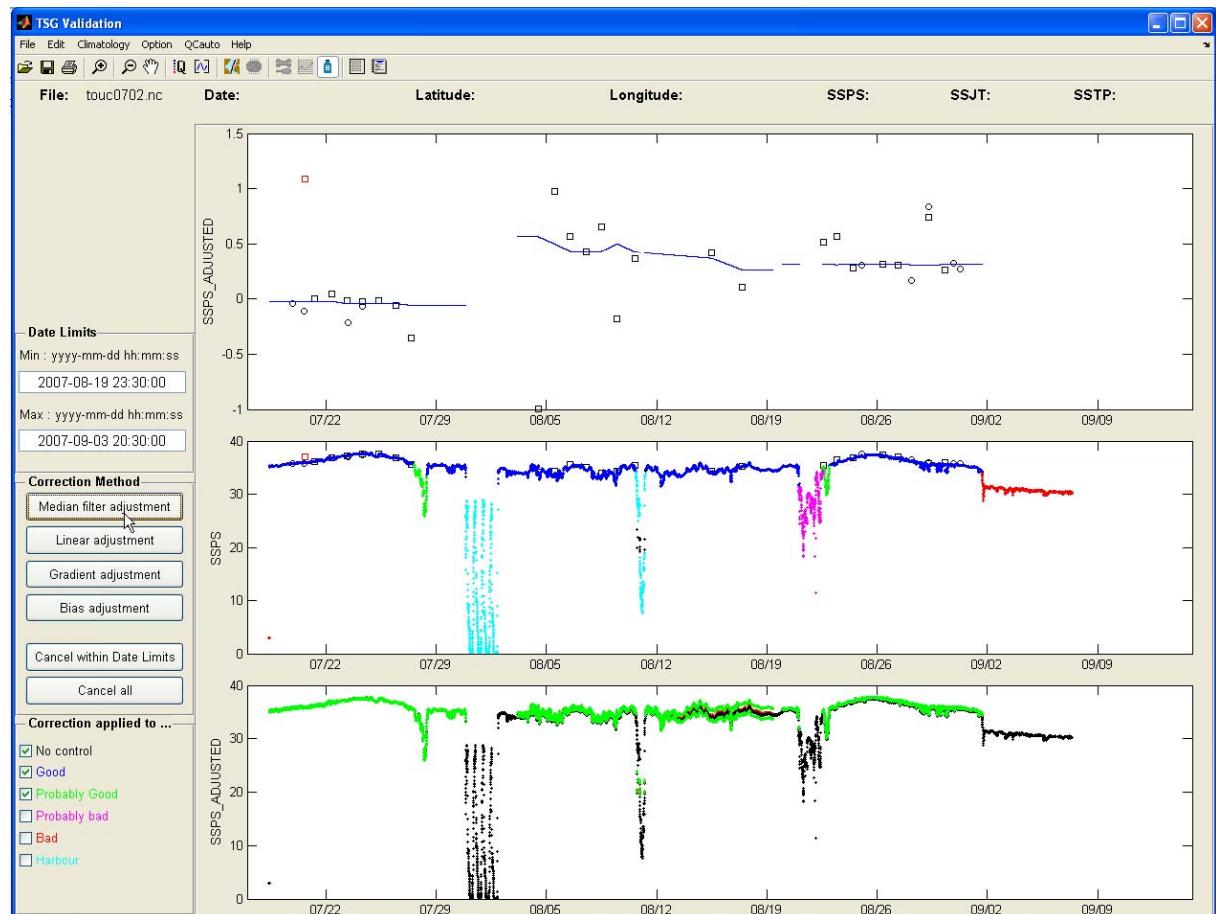
Data corrected are stored in variables with the extension **_ADJUSTED: SSPS_ADJUSTED**, **SSTP_ADJUSTED**, The raw data are not modified.

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 to NaN (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:



1. 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 necessarily 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

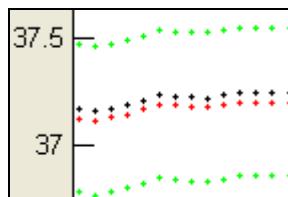
If for some **samples** there is no **TSG** measurements close in time or if the **TSG** measurements have quality code sets to **PROBABLY BAD** or **BAD** the differences are not drawn in the upper plot.

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.
 - a) Either after being calibrated.
 - b) 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.

2. 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

Date Limits

Min : yyyy-mm-dd hh:mm:ss
2007-07-18 08:40:00

Max : yyyy-mm-dd hh:mm:ss
2007-09-07 09:10:00



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 23).

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.

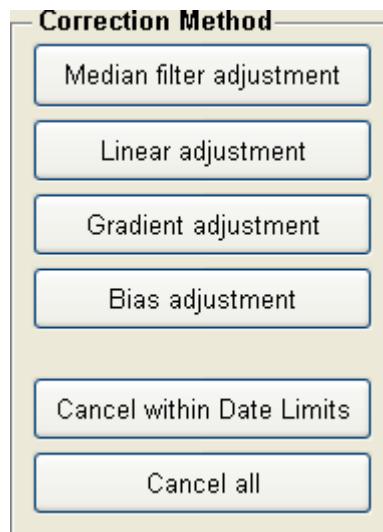
Correction applied to ...

No control
 Good
 Probably Good
 Probably bad
 Bad
 Harbour

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.



Median filter adjustment

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

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

See the algorithm p. 36

Gradient adjustment

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

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:



Cancel within Date Limits

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**').

[W] The time-limits selection is made using the **Date limits** tool (see p 23).

Cancel all

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

3. Algorithms

a) 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`.
 - a) The **TSG** average is computed with measurements with a quality code: **NO_CONTROL**, **GOOD**, and **PROBABLY_GOOD**.
 - b) 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.
 - c) 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.

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 (non 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 $N \geq 4$: error = standard deviation (sample - TSG) / $\sqrt{N-1}$

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

b) 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.

c) 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.

J. 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

K. Quitting 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:



6. Data Format

A. 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.).

1. 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.

2. Remark: The availability of these different quality data can change with time during a single ship journey. 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 (Water Sample) 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) |

B. Input files

TSGQC can read data files with the following format:

| | |
|--|-------|
| 1. ARGO | p. 42 |
| 2. ASCII | p. 44 |
| 3. ASTROLABE | p. 43 |
| 4. Merchant ship (Logiciel SODA - SOERE SSS) | p. 45 |
| 5. NetCDF GOSUD | p. 44 |
| 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. |

C. 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

2. 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. 44

D. 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.

E. 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      -42.8824    147.3407    12.9442    12.8127
            33.1911   -99.0000   -99.0000   -99.0000   -99.0000     1.73
211009      0      1      -42.8824    147.3407    12.9442    12.8133
            33.1935   -99.0000   -99.0000   -99.0000   -99.0000     1.75
211009      0      2      -42.8824    147.3407    12.9442    12.8150
            33.1950   -99.0000   -99.0000   -99.0000   -99.0000     1.75
211009      0      3      -42.8824    147.3407    12.9449    12.8152
            33.1971   -99.0000   -99.0000   -99.0000   -99.0000     1.75
211009      0      4      -42.8824    147.3407    12.9462    12.8171
            33.2006   -99.0000   -99.0000   -99.0000   -99.0000     1.75
211009      0      5      -42.8824    147.3407    12.9471    12.8213
            33.2028   -99.0000   -99.0000   -99.0000   -99.0000     1.75
211009      0      6      -42.8824    147.3408    12.9484    12.8229
            33.2043   -99.0000   -99.0000   -99.0000   -99.0000     1.74
```

F. 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.

G. 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.doc

H. SODA format (*.lby)

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

The acquisition software **SODA**³ is developed under LabView by David Varillon (IRD - US191 'IMAGO' - Nouméa). The software documentation: **SODA_User_manual.pdf** is available on demand..

I. 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 |

J. Format des fichiers ORACLE (*.ora)

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

K. Format des fichiers SDF (*.sdf)

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

L. Climatology file format

TSGQC uses the climatology WOA01 and WOA05 (WORLD OCEAN ATLAS 2001 and 2005). The documentation is available at this address:

<ftp://ftp.nodc.noaa.gov/pub/WOA01/readme.pdf>

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

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

³ Varillon D., Shipboard Oceanographic Data Acquisition - S.O.D.A Version 1.00 - Manuel d'utilisateur, 2009

The available variables are :

WOA01_MEAN_SSTP: temperature
WOA01_MEAN_SSPPS: salinity
WOA01_MEAN_DOX: oxygen

And the standard deviation (WOA01_STD_SSTP) and the number of observations used to build the climatology (WOA01_OBS_SSTP).

In the netCDF files, the WOA01_TIME dimension will take the following values:

WOA01_TIME = 1 for the annual file
WOA01_TIME = 4 for the seasonal file
WOA01_TIME = 12 for the monthly file

Seasonal file (command ncdump):

```
$ ncdump -h woa01_seasonal_surf.nc
```

NetCDF woa01_seasonal_surf {

dimensions:

```
    WOA01_TIME = 4 ;  
    WOA01_DEPTH = 1 ;  
    WOA01_LATX = 180 ;  
    WOA01_LONX = 360 ;
```

variables:

```
    float WOA01_TIME(WOA01_TIME) ;  
    float WOA01_DEPTH(WOA01_DEPTH) ;  
        WOA01_DEPTH:long_name = "Depth" ;  
        WOA01_DEPTH:units = "meters" ;  
        WOA01_DEPTH:_FillValue = -100.f ;  
    float WOA01_LATX(WOA01_LATX) ;  
        WOA01_LATX:long_name = "Latitude" ;  
        WOA01_LATX:units = "degree_north" ;  
        WOA01_LATX:_FillValue = -100.f ;  
    float WOA01_LONX(WOA01_LONX) ;  
        WOA01_LONX:long_name = "Longitude" ;  
        WOA01_LONX:units = "degree_east" ;  
        WOA01_LONX:_FillValue = -100.f ;  
    float WOA01_MEAN_SSTP(WOA01_TIME, WOA01_DEPTH, WOA01_LATX, WOA01_LONX) ;  
        WOA01_MEAN_SSTP:long_name = "Sea Surface Temperature mean" ;  
        WOA01_MEAN_SSTP:units = "degre Celcius" ;  
        WOA01_MEAN_SSTP:_FillValue = -100.f ;  
    float WOA01_MEAN_SSPPS(WOA01_TIME, WOA01_DEPTH, WOA01_LATX, WOA01_LONX) ;  
        WOA01_MEAN_SSPPS:long_name = "Sea Surface Salinity mean" ;  
        WOA01_MEAN_SSPPS:units = "PSU" ;  
        WOA01_MEAN_SSPPS:_FillValue = -100.f ;  
    float WOA01_MEAN_DOX1(WOA01_TIME, WOA01_DEPTH, WOA01_LATX, WOA01_LONX) ;  
        WOA01_MEAN_DOX1:long_name = "Sea Surface Dissolved oxygen mean" ;  
        WOA01_MEAN_DOX1:units = "ml/l" ;  
        WOA01_MEAN_DOX1:_FillValue = -100.f ;  
    float WOA01_STD_SSTP(WOA01_TIME, WOA01_DEPTH, WOA01_LATX, WOA01_LONX) ;  
        WOA01_STD_SSTP:long_name = "Sea Surface Temperature standard deviation" ;  
        WOA01_STD_SSTP:units = "degre Celcius" ;  
        WOA01_STD_SSTP:_FillValue = -100.f ;  
    float WOA01_STD_SSPPS(WOA01_TIME, WOA01_DEPTH, WOA01_LATX, WOA01_LONX) ;  
        WOA01_STD_SSPPS:long_name = "Sea Surface Salinity standard deviation" ;  
        WOA01_STD_SSPPS:units = "PSU" ;  
        WOA01_STD_SSPPS:_FillValue = -100.f ;
```

```

float WOA01_STD_DOX1(WOA01_TIME, WOA01_DEPTH, WOA01_LATX, WOA01_LONX) ;
  WOA01_STD_DOX1:long_name = "Sea Surface Dissolved oxygen standard deviation" ;
  WOA01_STD_DOX1:units = "ml/l" ;
  WOA01_STD_DOX1:_FillValue = -100.f ;
short WOA01_OBS_SSTP(WOA01_TIME, WOA01_DEPTH, WOA01_LATX, WOA01_LONX) ;
  WOA01_OBS_SSTP:long_name = "Sea Surface Temperature number observation" ;
  WOA01_OBS_SSTP:units = "none" ;
  WOA01_OBS_SSTP:_FillValue = -100s ;
short WOA01_OBS_SSPPS(WOA01_TIME, WOA01_DEPTH, WOA01_LATX, WOA01_LONX) ;
  WOA01_OBS_SSPPS:long_name = "Sea Surface Salinity number observation" ;
  WOA01_OBS_SSPPS:units = "none" ;
  WOA01_OBS_SSPPS:_FillValue = -100s ;
short WOA01_OBS_DOX1(WOA01_TIME, WOA01_DEPTH, WOA01_LATX, WOA01_LONX) ;
  WOA01_OBS_DOX1:long_name = "Sea Surface Dissolved oxygen number observation" ;
  WOA01_OBS_DOX1:units = "none" ;
  WOA01_OBS_DOX1:_FillValue = -100s ;

// global attributes:
:description = "WOA01 CLIMATOLOGY Surface Levitus seasonal" ;
:author = "J Grelet IRD US191 Brest" ;
:date = "29 Jan 2008" ;

```

M. Glossary

- GOSUD **Global Ocean Surface Underway Data**
www.ifremer.fr/gosud/
- SOERE SSS **Systèmes d'Observation et d'Expérimentation pour la Recherche en Environnement Sea Surface Salinity**
<http://www.legos.obs-mip.fr/fr/observations/sss/>
- ROSCOP **Report of Observations/Samples Collected by Oceanographic Programmes**
<http://www.ices.dk/Ocean/roscop/index.asp>