great lakes observing system

# QARTOD 101: An Introduction to GLOS Real-Time Quality Control Procedures

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# Agenda

- What is QARTOD?
- QARTOD implementation at GLOS
- QARTOD application and implications
- GLOS and QARTOD: next steps

# What is QARTOD?

- Quality Assurance/Quality Control for Real-Time Oceanographic Data
- Standardized tests
- Ensures available data is of known quality
- IOOS Certification requirement for Regional Information Coordination Entities (RICE)

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# Being a certified RICE means…

- Local observing data are leveraged to expand the pool of federal-quality data available nationwide.
- GLOS data are as reliable as the data you get from federal sources like NOAA.
- Federal sources are able to use this data without spending time and resources on additional QC.
- Data are archived at a national center which facilitates long-term data research.

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# Seven Data Management Laws of QARTOD

1. Every real-time observation distributed to the ocean community must be accompanied by a quality descriptor.
2. All observations should be subject to some level of automated real-time quality test.
3. Quality flags and quality test descriptions must be sufficiently described in the accompanying metadata.
4. Observers should independently verify or calibrate a sensor before deployment.
5. Observers should describe their method/calibration accuracy in the real-time metadata.
6. Observers should quantify the level of calibration accuracy and the associated expected error bounds.
7. Manual checks on the automated procedures, the real-time data collected and the status of the observing system must be provided by the observer on a time scale appropriate to ensure the integrity of the observing system.

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# QARTOD Tests and Parameters

| 26 IOOS CORE VARIABLES | | | |
|---|---|---|---|
| ACIDITY | FISH ABUNDANCE | PATHOGENS | TEMPERATURE* |
| BATHYMETRY | FISH SPECIES | PHYTOPLANKTON SPECIES* | TOTAL SUSPENDED MATTER |
| BOTTOM CHARACTER | HEAT FLUX | SALINITY* | WIND SPEED AND DIRECTION* |
| COLORED DISSOLVED ORGANIC MATTER* | ICE DISTRIBUTION | SEA LEVEL* | ZOOPLANKTON ABUNDANCE |
| CONTAMINANTS | Ocean Color | STREAM FLOW | ZOOPLANKTON SPECIES |
| DISSOLVED NUTRIENTS* | OPTICAL PROPERTIES* | SURFACE CURRENTS* | |
| DISSOLVED OXYGEN* | PARTIAL PRESSURE OF $CO_2$ | SURFACE WAVES* | |

# QARTOD Tests and Parameters

- QARTOD Manuals
  - Real-Time Quality Control of Passive Acoustics Data
  - Real-Time Quality Control of Phytoplankton Data
  - Real-Time Quality Control of HF Radar Observations
  - Real-Time Quality Control of Dissolved Nutrients Observations
  - Real-Time Quality Control of Wind Data
  - Real-Time Quality Control of Water Level Data
  - Real-Time Quality Control of In-Situ Surface Wave Data
  - Real-Time Quality Control of Ocean Optics Data
  - Real-Time Quality Control of In-Situ Temperature and Salinity Data
  - Real-Time Quality Control of In-Situ Current Observations
  - Real-Time Quality Control of Dissolved Oxygen Observations in Coastal Oceans

# QARTOD Tests and Parameters

- US IOOS 26 Core Variables
  - Nine completed
  - Two non-core completed
  - Three supporting docs

| Core Variable Manuals Completed | Core Variable (s) Covered | Other Variables Covered |
|---|---|---|
| Dissolved Oxygen | Dissolved Oxygen | |
| In-Situ Currents | Current Speed and Direction | |
| In-Situ Waves | Surface Waves | |
| Temperature and Salinity | Temperature<br>Salinity | |
| Water Level | Sea Level | |
| Wind Speed and Direction | Wind Speed and Direction | |
| Ocean Optics | CDOM<br>Ocean Color<br>Optical Properties | In-water & above-water radiance/irradiance, Beam attenuation, Turbidity, PAR, Cholorophyll, FDOM, Backscattering/volume scattering |
| Dissolved Nutrients | Dissolved Nutrients | Nitrogen (NO3, NO2, and NH4)<br>Phosphate<br>Silicate |
| Phytoplankton Species | Phytoplankton Species | |
| **Other Manuals (not core variables)** | | |
| Five Year Plan Update | | |
| Data Flags Manual | | |
| HFR Surface Currents | | |
| Glider DAC | | |
| Passive Acoustics | | |

# QARTOD Tests and Parameters

- Required, recommended and suggested QC tests

| | | |
|---|---|---|
| **Group 1** *Required* | Test 1) | Gap Test |
| | Test 2) | Syntax Test |
| | Test 3) | Location Test |
| | Test 4) | Gross Range Test |
| | Test 5) | Climatological Test |
| **Group 2** *Strongly Recommended* | Test 6) | Spike Test |
| | Test 7) | Rate of Change Test |
| | Test 8) | Flat Line Test |
| **Group 3** *Suggested* | Test 9) | Multi-Variate Test |
| | Test 10) | Attenuated Signal Test |
| | Test 11) | Neighbor Test |
| | Test 12) | TS Curve/Space Test |
| | Test 13) | Density Inversion Test |

Example from IOOS *"Manual for Real-Time Quality Control of In-situ Temperature and Salinity Data"*

# QARTOD Tests and Parameters

| Flag | Primary-Level Flag Short Name | Definition |
|---|---|---|
| 1 | Pass / Good | Data have passed critical real-time quality control tests and are deemed adequate for use as preliminary data |
| 2 | Not evaluated, not available or unknown | Data have not been QC-tested or the information on quality is not available |
| 3 | Questionable / suspect | Data are considered to be either suspect or of high interest to data providers and users. They are flagged suspect to draw further attention to them by operators |
| 4 | Fail / Bad | Data are considered to have failed one or more critical real-time QC checks. If they are disseminated at all, it should be readily apparent that they are not of acceptable quality |
| 9 | Missing Data | Used as a placeholder when data are missing |

# GLOS QARTOD Tests and Parameters

| variable | units | gross range | | | | spike | | rate of change | flat_line | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | sensor_min | sensor_max | user_min | user_max | low_threshold | high_threshold | high_threshold | low_reps | high_reps | epsilon |
| Air_Pressure | hPa | 500 | 1110 | 950 | 1030 | 1 | 2 | 1.5 | 6 | 12 | 0.1 |
| Air_Temperature | degree_Celsius | -45.6 | 65.6 | -17.7 | 37.8 | 2.2 | 3.3 | 3.3 | 2 | 6 | 0.1 |
| Dew_Point | degree_Celsius | -45.6 | 65.6 | -28.9 | 37.8 | 2.2222 | 3.3333 | 3.3333 | 2 | 6 | 0.1 |
| **dissolved_oxygen** | mg/L | 0 | 50 | 0 | 20 | 0.5 | 1 | 0.5 | 10 | 100 | 0.1 |
| dissolved_oxygen_saturation | | 0 | 500 | 0 | 110 | 10 | 20 | 2 | 10 | 100 | 0.01 |
| ph | | 0 | 14 | 7 | 10 | 0.25 | 5 | 0.2 | 10 | 20 | 0.01 |
| Relative_Humidity | % | 0 | 100 | 0 | 100 | 15 | 20 | 20 | 6 | 12 | 0.1 |
| **Significant_Wave_Height** | m | 0 | 15.24 | 0.06096 | 9.144 | 0.9144 | 1.524 | 1.2192 | 2 | 6 | 0.1 |
| **Significant_Wave_Period** | sec | 0 | 100 | 0.5 | 10 | 0.2 | 0.4 | 0.5 | 2 | 6 | 0.1 |
| **significant_wave_to_direction** | degrees | 0 | 360 | 0 | 360 | 360 | 360 | 360 | 2 | 6 | 0.1 |
| Solar_Radiation | W/m^2 | 0 | 3000.0 | 0 | 1400 | 400 | 800 | 700 | 100 | 200 | 0.1 |
| **Thermistor_String** | degree_Celsius | -5 | 50 | 0 | 35 | 1 | 2 | 1.5 | 2 | 4 | 0.01 |
| **water_conductivity** | µS/cm | 0 | 600 | | | 25 | 40 | 40 | 2 | 4 | 0.01 |
| **Water_Temperature_at_Surfac** | degree_Celsius | -5 | 50 | 0 | 35 | 1 | 2 | 1.5 | 2 | 4 | 0.01 |
| **Wind_from_Direction** | degrees | 0 | 360 | 0 | 360 | 360 | 360 | 360 | 2 | 6 | 0.1 |
| **Wind_Gust** | m/s | 0 | 100 | 0 | 44.7 | 11.2 | 17.9 | 17.9 | 2 | 6 | 0.1 |
| **Wind_Speed** | m/s | 0 | 100 | 0 | 44.704 | 6.7056 | 8.9408 | 8.9408 | 2 | 6 | 0.1 |
| ysi_blue_green_algae | | -2 | 100 | -2 | 75 | 10 | 25 | 2 | 2 | 4 | 0.01 |
| **ysi_chlorophyll** | | -2 | 100 | -2 | 50 | 10 | 25 | 2 | 2 | 4 | 0.01 |
| **ysi_turbidity** | | 0 | 4000 | 2 | 1000 | 10 | 20 | 1 | 2 | 4 | 0.01 |

# QARTOD Tests and Parameters

**Test 4) Gross Range Test (Required)**

Data point exceeds sensor or operator-selected min/max. Applies to T, SP, C and P.

All sensors have a limited output range, and this can form the most rudimentary gross range check. No values less than a minimum value or greater than the maximum value the sensor can output (T_SENSOR_MIN, T_SENSOR_MAX) are acceptable. Additionally, the operator can select a smaller span (T_USER_MIN, T_USER_MAX) based upon local knowledge or a desire to draw attention to extreme values.

**NOTE:** Operators may choose to flag as suspect values that exceed the calibration span but not the hardware limits (e.g., a value that sensor is not capable of producing or negative conductivity).

| Flags | Condition | Codable Instructions |
|---|---|---|
| Fail=4 | Reported value is outside of sensor span. | If $T_n$ < T_SENSOR_MIN, or $T_n$ > T_SENSOR_MAX, flag = 4 |
| Suspect=3 | Reported value is outside of operator-selected span. | If $T_n$ < T_USER_MIN, or $T_n$ > T_USER_MAX, flag = 3 |
| Pass=1 | Applies for test pass condition. | |

**Test Exception:** None.

**Test specifications to be established locally by the operator.**

**Examples:** The following global range min/max are applied on some climate and forecast standard-names in the IMOS toolbox: depth: -5/12,000 m
sea_water_pressure: -5/12,000 decibars (dbar)
sea_water_pressure_due_to_sea_water: -15/12,000 dbar
sea_water_salinity: 2/41
sea_water_temperature: -2.5/40 °C

Example from IOOS *"Manual for Real-Time Quality Control of In-situ Temperature and Salinity Data"*

# QARTOD Tests and Parameters

**Test 6) Spike Test (Strongly Recommended)**

Data point *n*-1 exceeds a selected threshold relative to adjacent data points. Applies to T, SP, C, and P.

This check is for single value spikes, specifically the value at point *n*-1. Spikes consisting of more than one data point are difficult to capture, but their onset may be flagged by the rate of change test. The spike test consists of two operator-selected thresholds, THRSHLD_LOW and THRSHLD_HIGH. Adjacent data points ($n_{-2}$ and $n_0$) are averaged to form a spike reference (SPK_REF). The absolute value of the spike is tested to capture positive and negative spikes. Large spikes are easier to identify as outliers and flag as failures. Smaller spikes may be real and are only flagged suspect. The thresholds may be fixed values or dynamically established (for example, a multiple of the standard deviation over an operator-selected period).

| Flags | Condition | Codable Instructions |
|---|---|---|
| Fail=4 | High spike threshold exceeded. | If $\lvert T_{n-1} - SPK\_REF \rvert >$ THRSHLD_HIGH, flag = 4 |
| Suspect=3 | Low spike threshold exceeded. | If $\lvert T_{n-1} - SPK\_REF \rvert >$ THRSHLD_LOW and $\lvert T_{n-1} - SPK\_REF \rvert \leq$ THRSHLD_HIGH, flag = 3 |
| Pass=1 | Applies for test pass condition. | N/A |

**Test Exception:** None.

**Test specifications to be established locally by the operator.**
**Examples:** THRSHLD_LOW = 3 °C, THRSHLD_HIGH = 8 °C

Example from IOOS *"Manual for Real-Time Quality Control of In-situ Temperature and Salinity Data"*

# QARTOD Tests and Parameters

**Test 7) Rate of Change Test (Strongly Recommended)**

Excessive rise/fall test. Applies to T, SP, C, and P.

This test inspects the time series for a time rate of change that exceeds a threshold value identified by the operator. T, SP, C, P values can change substantially over short periods in some locations, hindering the value of this test. A balance must be found between a threshold set too low, which triggers too many false alarms, and one set too high, making the test ineffective. Determining the excessive rate of change is left to the local operator. The following show three different examples of ways to select the thresholds provided by QARTOD VI participants. Implementation of this test can be challenging. Upon failure, it is unknown which of the points is bad. Further, upon failing a data point, it remains to be determined how the next iteration can be handled.

The rate of change between temperature $T_{n-1}$ and $T_n$ must be less than three standard deviations (3*SD). The SD of the T time series is computed over the previous 25-hour period (operator-selected value) to accommodate cyclical diurnal and tidal fluctuations. Both the number of SDs (N_DEV) and the period over which the SDs (TIM_DEV) are calculated and determined by the local operator.

The rate of change between temperature $T_{n-1}$ and $T_n$ must be less than 2 °C +2SD.

$|T_{n-1} - T_{n-2}| + |T_{n-1} - T_n| <= 2*N\_DEV*SD$ (example provided by EuroGOOS).

| Flags | Condition | Codable Instructions |
|---|---|---|
| Fail=4 | No fail flag is identified for this test. | N/A |
| Suspect=3 | The rate of change exceeds the selected threshold. | If $\|T_n - T_{n-1}\| > N\_DEV*SD$, flag = 3 |
| Pass=1 | Applies for test pass condition. | N/A |

**Test Exception:** None.

**Test specifications to be established locally by operator.**
**Example:** N_DEV = 3, TIM_DEV = 25

Example from IOOS *"Manual for Real-Time Quality Control of In-situ Temperature and Salinity Data"*

# QARTOD Tests and Parameters

**Test 8) Flat Line Test (Strongly Recommended)**

Invariant value. Applies to T, SP, C, and P.

When some sensors and/or data collection platforms fail, the result can be a continuously repeated observation of the same value. This test compares the present observation *n* to a number (REP_CNT_FAIL or REP_CNT_SUSPECT) of previous observations. Observation *n* is flagged if it has the same value as previous observations within a tolerance value, EPS, to allow for numerical round-off error. Note that historical flags are not changed.

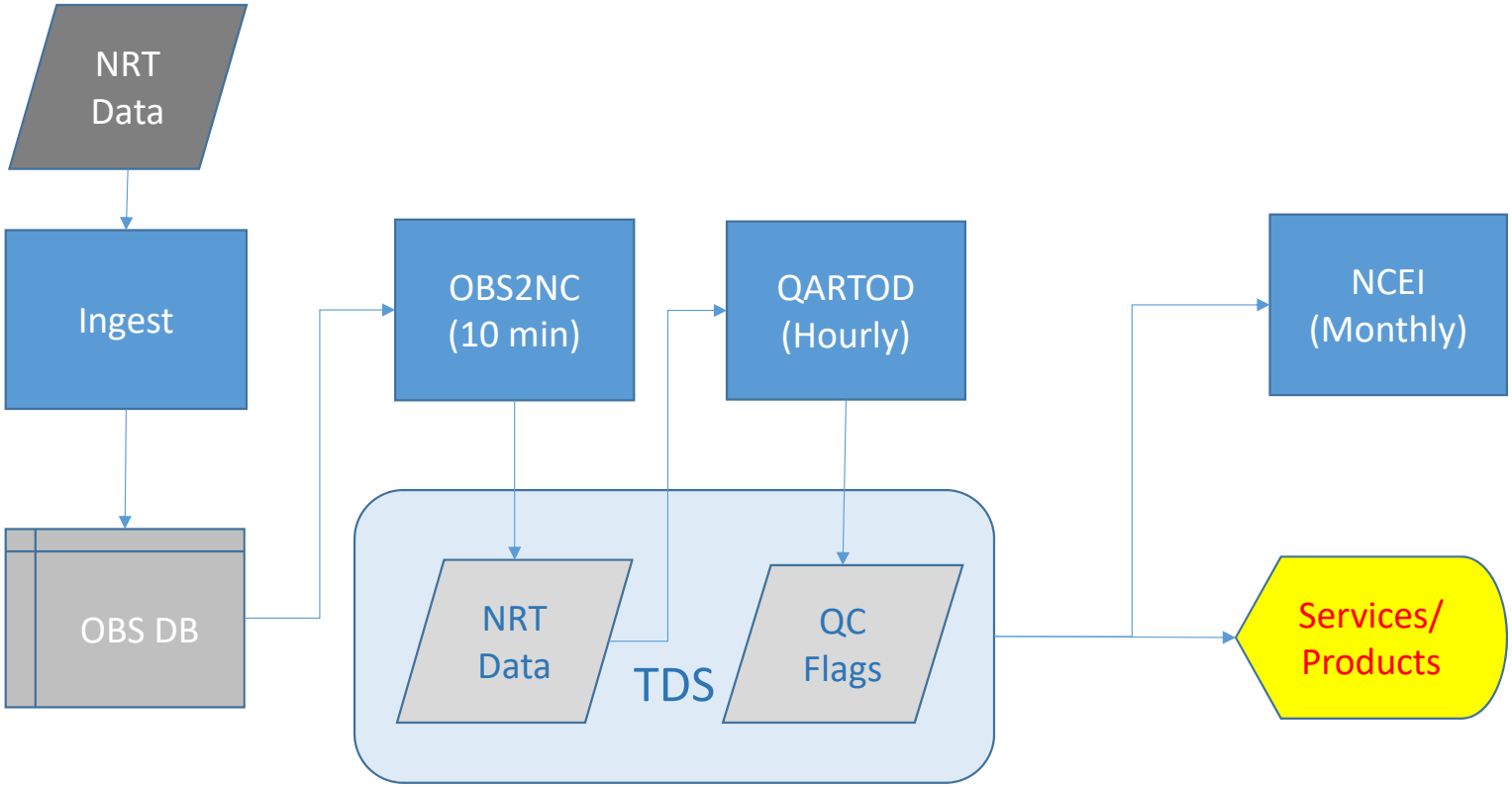
| Flags | Condition | Codable Instructions |
|---|---|---|
| Fail=4 | When the five most recent observations are equal, $T_n$ is flagged fail. | For $i$=1,REP_CNT_FAIL $T_n - T_{n-i}$ <EPS , flag = 4 |
| Suspect=3 | It is possible but unlikely that the present observation and the two previous observations would be equal. When the three most recent observations are equal, $T_n$ is flagged suspect. | For $i$=1,REP_CNT_SUSPECT $T_n - T_{n-i}$ <EPS, flag = 3 |
| Pass=1 | Applies for test pass condition. | N/A |

**Test Exception**: None.

**Test specifications to be established locally by the operator.**
**Examples:** REP_CNT_FAIL = 5, REP_CNT_SUSPECT= 3, EPS = 0.05°

Example from IOOS *"Manual for Real-Time Quality Control of In-situ Temperature and Salinity Data"*

# GLOS QARTOD Implementation: Data Flow



# GLOS QARTOD Implementation: Details

- Default flag values to ‘2’ for ‘Not Evaluated’ on initialization
- Individual flags for each test + primary flag
- Run tests on observations in near real-time (hourly)
- Run QC on-demand for delayed data if necessary
- Standardized spreadsheet for configuration of QC parameters
- NetCDF solution
  - stores flags as values
  - adds many variables to every dataset, but...
  - clear, self-describing

# GLOS QARTOD Implementation: Packages

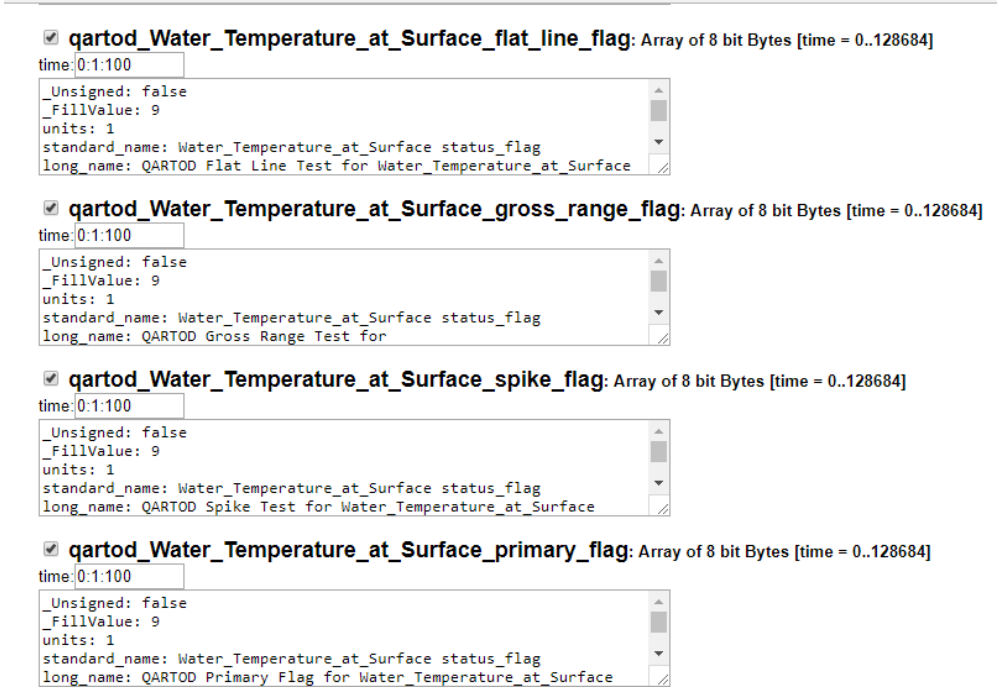
1. IOOS QARTOD: utilities, scripts and tests to assist in automated QARTOD application
   - Implementation agnostic - requires array of data and returns array of flags
   - Includes location, gross range, climatology, spike, rate of change, flat line, attenuated signal
   - Includes tests for the tests
2. GLOS netCDF Wrapper: python utility for applying IOOS QARTOD to netCDF time-series datasets.
   - Reads netCDF files
   - Reads QARTOD config file
   - Initializes/applies the tests
   - Writes the results to netCDF

# QARTOD Examples

- TDS access demo
- RPS tool demo (non-GLOS)

# TDS Access

http://tds.glos.us/thredds/dodsC/buoy_agg_standard_qc/leelyria/leelyria.ncml?Water_Temperature_at_Surface[0:1:100],qartod_Water_Temperature_at_Surface_flat_line_flag[0:1:100],qartod_Water_Temperature_at_Surface_gross_range_flag[0:1:100],qartod_Water_Temperature_at_Surface_spike_flag[0:1:100],qartod_Water_Temperature_at_Surface_primary_flag[0:1:100],qartod_Water_Temperature_at_Surface_rate_of_change_flag[0:1:100]



**qartod_Water_Temperature_at_Surface_flat_line_flag**: Array of 8 bit Bytes [time = 0..128684]

time: 0:1:100

```
_Unsigned: false
_FillValue: 9
units: 1
standard_name: Water_Temperature_at_Surface status_flag
long_name: QARTOD Flat Line Test for Water_Temperature_at_Surface
```

**qartod_Water_Temperature_at_Surface_gross_range_flag**: Array of 8 bit Bytes [time = 0..128684]

time: 0:1:100

```
_Unsigned: false
_FillValue: 9
units: 1
standard_name: Water_Temperature_at_Surface status_flag
long_name: QARTOD Gross Range Test for
```

**qartod_Water_Temperature_at_Surface_spike_flag**: Array of 8 bit Bytes [time = 0..128684]

time: 0:1:100

```
_Unsigned: false
_FillValue: 9
units: 1
standard_name: Water_Temperature_at_Surface status_flag
long_name: QARTOD Spike Test for Water_Temperature_at_Surface
```

**qartod_Water_Temperature_at_Surface_primary_flag**: Array of 8 bit Bytes [time = 0..128684]

time: 0:1:100

```
_Unsigned: false
_FillValue: 9
units: 1
standard_name: Water_Temperature_at_Surface status_flag
long_name: QARTOD Primary Flag for Water_Temperature_at_Surface
```

# TDS Access

```
Dataset {
    Float64 Water_Temperature_at_Surface[time = 101];
    Byte qartod_Water_Temperature_at_Surface_flat_line_flag[time = 101];
    Byte qartod_Water_Temperature_at_Surface_gross_range_flag[time = 101];
    Byte qartod_Water_Temperature_at_Surface_spike_flag[time = 101];
    Byte qartod_Water_Temperature_at_Surface_primary_flag[time = 101];
    Byte qartod_Water_Temperature_at_Surface_rate_of_change_flag[time = 101];
} buoy_agg_standard_qc/leelyria/leelyria.ncml;
---------------------------------------------
Water_Temperature_at_Surface[101]
23.53, 23.41, 23.47, 23.49, 23.45, 23.5, 23.51, 23.51, 23.46, 23.46, 23.45, 23.57, 23.51, 23.48, 23.48, 23.47, 23.46, 23.61, 23.48, 23.46, 23.46, 23.45, 23.52, 23.47, 23.54,
23.47, 23.49, 23.56, 23.48, 23.47, 23.49, 23.44, 23.52, 23.53, 23.46, 23.43, 23.52, 23.44, 23.5, 23.48, 23.52, 23.44, 23.39, 23.47, 23.43, 23.44, 23.44, 23.58, 23.65, 23.43,
23.51, 23.43, 23.44, 23.46, 23.47, 23.44, 23.54, 23.51, 23.44, 23.47, 23.52, 23.49, 23.65, 23.5, 23.46, 23.5, 23.45, 23.46, 23.46, 23.45, 23.51, 23.46, 23.45, 23.43, 23.43,
23.44, 23.43, 23.46, 23.46, 23.45, 23.44, 23.45, 23.41, 23.41, 23.43, 23.46, 23.45, 23.44, 23.49, 23.44, 23.41, 23.28, 23.34, 23.46, 23.38, 23.43, 23.39, 23.38, 23.36, 23.46,
23.38

qartod_Water_Temperature_at_Surface_flat_line_flag[101]
1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
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qartod_Water_Temperature_at_Surface_gross_range_flag[101]
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1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1

qartod_Water_Temperature_at_Surface_spike_flag[101]
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qartod_Water_Temperature_at_Surface_primary_flag[101]
1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 3, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1

qartod_Water_Temperature_at_Surface_rate_of_change_flag[101]
2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1
```
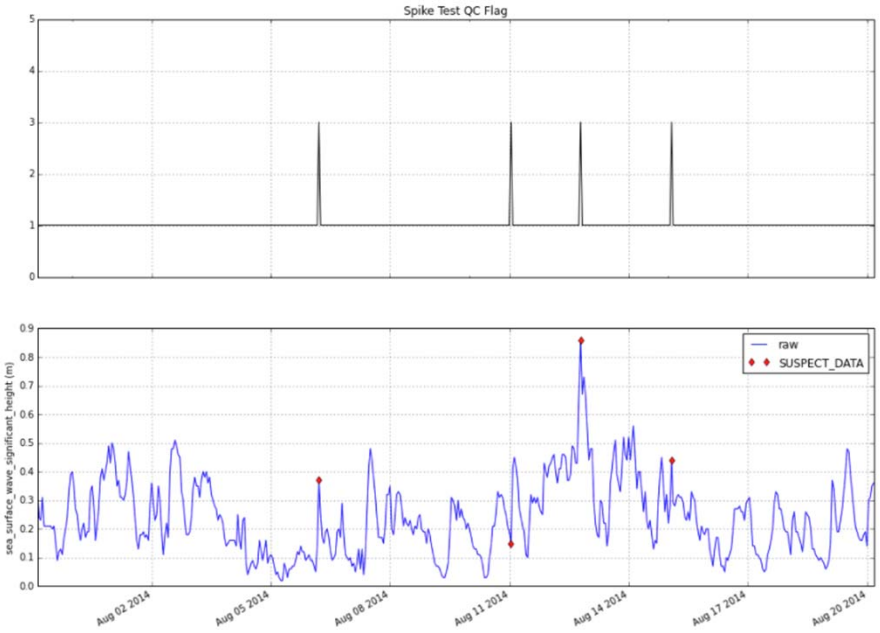
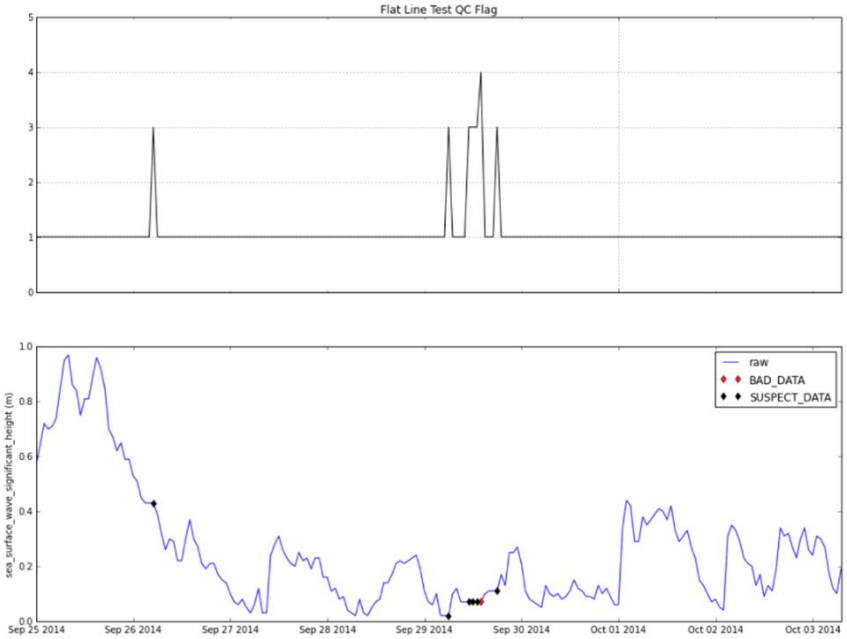

# Jupyter Notebook



# GLOS QARTOD: Next Steps?

- Refine test parameters
- Alerts to data providers
- Add more tests at GLOS or provider level
  - Climatologies?
- Add more parameters
- Integrate flags with retrieval/visualization

# Useful Links

- IOOS QARTOD Project site
  - https://ioos.noaa.gov/project/qartod/
- GitHub QARTOD code
  - https://ioos.github.io/qartod
- GitHub GLOS QARTOD
  - https://github.com/glos/glos-qartod
- RPS Jupyter notebook
  - https://github.com/glos/QARTOD/blob/master/notebooks/plot_QARTOD_results.ipynb
- GLOS TDS
  - http://tds.glos.us/thredds/catalog.html
- Feedback
  - dmac@glos.us

# Wrap-Up

- Questions or comments?
- Thank you …
  - Please fill out our webinar survey!