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OOI Data QA/QC: Overview and examples with pCO2, pH, Oxygen, CTD, and Acoustic Data

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NE Pacific Workshop
June 2022

NSF

The Challenge

"With great power comes great responsibility…."

- Infrastructure
- Instruments
- Metadata

- Data Flags
- Discrete Validation
- Sensor Deep Dives

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Quality Assurance

- Infrastructure
  - Deployment turn cycles (annual and bi-annual)
  - Biofouling mitigation
  - Sparing
- Instruments
  - Quality conformance testing (QCT) of incoming sensors
  - Integration and burn-in testing before deployments
  - Biweekly cross-MIO instrument meetings and annual meetings with vendors
- Metadata
  - Data about the data, used to answer questions about the who (serial number), what (sensor model), where (deployment location, assembly), how (algorithms, calibration coefficients), when (deployment dates), and why (project priorities)
  - “Critical” metadata, specifically instrument serial numbers, calibration coefficients and instrument assignments, etc. (data impacting)

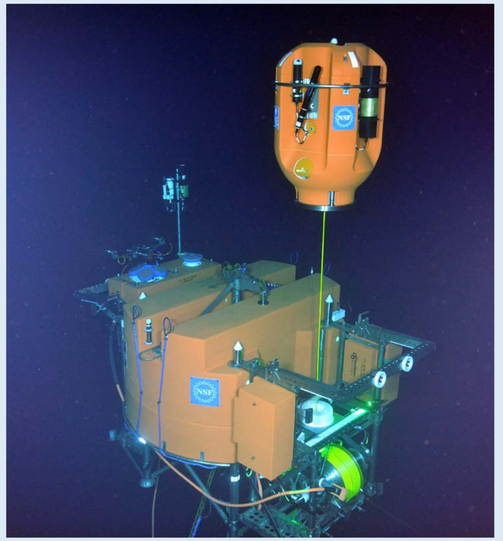
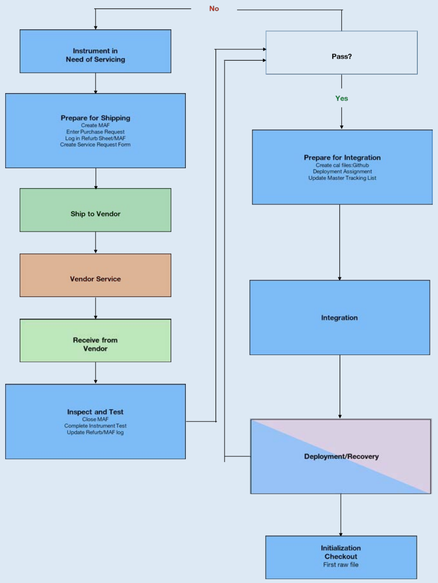
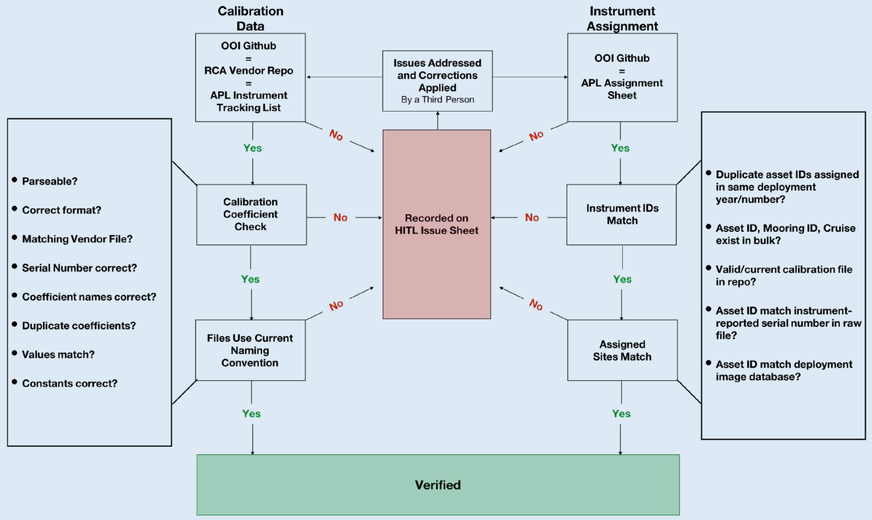


Photo Credit UW/NSF-OOI/CSSF





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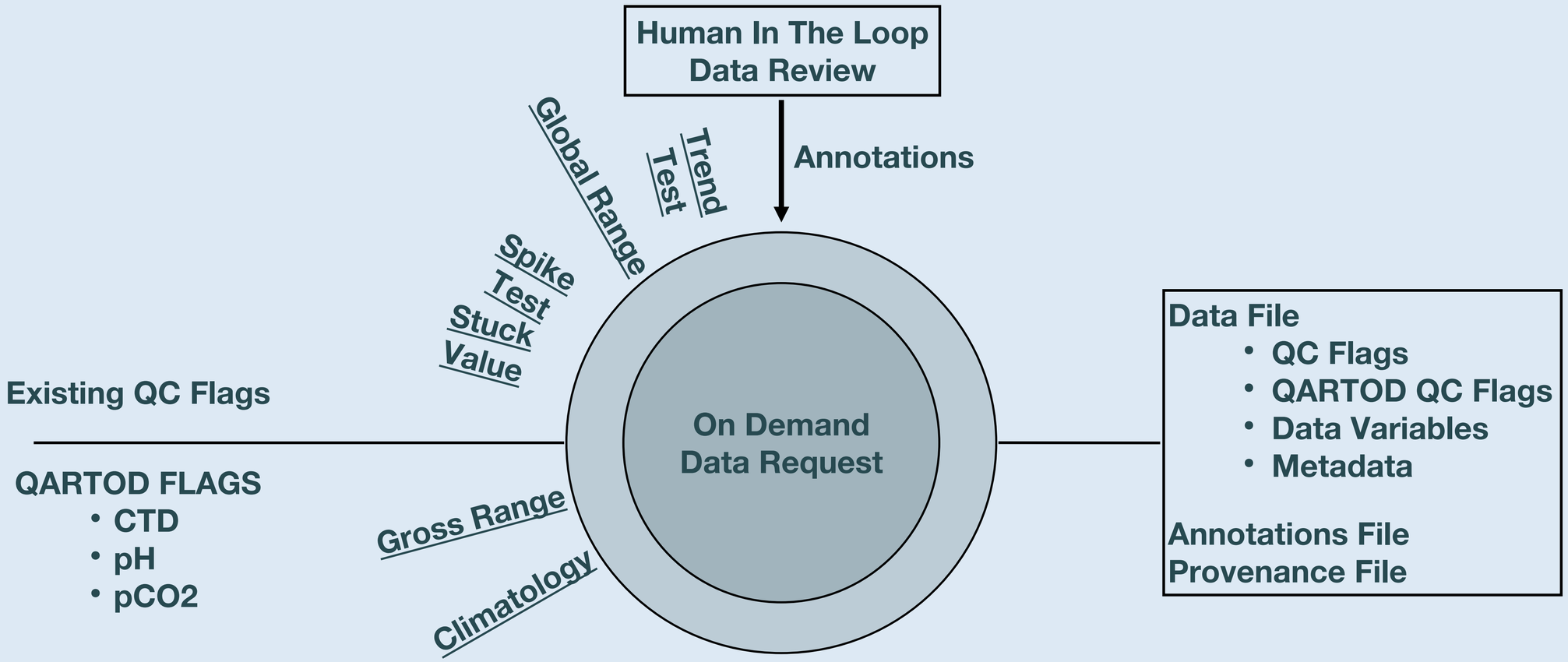
Quality Control



Quality Control: Existing QC Flags

Bit Order	OOI Test	Description
0	Global Range Test	**Data are flagged unless they fall within valid world ocean ranges or instrument limits (whichever is more restrictive)**
1	*Local Range Test*	*Data are flagged unless they fall within locally valid site-specific or depth ranges. Interpolates thresholds between depth and season intervals (not implemented)*
2	Spike Test	**Deviation from mean compared to neighboring points (subject to numerous false positives and false negatives!)**
3	Trend Test	**Data are flagged as having a trend if the standard deviation of the residuals to a polynomial curve < original data, multiplied by some factor. Designed to test for sensor drift**
4	Stuck Value Test	**If 2 neighboring values differ by less than the resolution of the sensor for more than N repetitions, data are flagged**
5	*Gradient Test*	*Will detect if multiple successive points are remote from a baseline of presumably good data points (not implemented)*
7	*Propagate Flags*	*Combines results of all tests based on "logical" or to set a single quality flag for pass or fail (not implemented)*

- Current QC tests applied to select parameters within most datasets
- QC tests results indicated by two variables named with '_qc_results' and '_qc_executed' appended to the variable name, e.g.:
  - practical_salinity
  - practical_salinity_qc_results
  - practical_salinity_qc_executed
- Integer values represent binary bit mask for each test executed and the corresponding result (e.g., _qc_executed = 29 = 00011101)
- pass/applied = 1, fail/not applied = 0
- Need to combine both the _qc_exected and the _qc_result to create a final QC flag
- https://github.com/oceanobservatories/qc-lookup

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Quality Control: QARTOD

- Quality Assurance/Quality Control of Real Time Oceanographic Data
- Developed by the NOAA-led Integrated Ocean Observing System (IOOS) program
- Pros
  - Well-documented, and actively maintained set of QA/QC standards and procedures with broad community engagement
  - Standardized code and flag definitions
  - Simplified, easy to interpret result value
- Cons
  - Not all instrument classes have tests defined (e.g., pCO_2 sensors)
  - Designed for real-time data, while OOI includes both real-time and recovered data

- Results will be added to data sets comparably to existing QC tests with key differences:
  - Results and the tests executed will be named _qartod_results and _qartod_executed, e.g.,
    - practical_salinity
    - practical_salinity_qartod_results
    - practical_salinity_qartod_executed
  - Utilize the QARTOD style flags
    - _qartod_results: summary result of all tests applied (max value of all tests applied), where 1 = pass, 2 = not tested, 3 = suspect/high interest, 4 = fail, 9 = missing
    - _qartod_executed: string with a list of the individual results of each test applied (order and tests applied in the variable metadata)

Quality Control: QARTOD Timeline

QARTOD Planning

Feb 2021

- **Test Prioritization** ✓
  1. GRT/CT
  2. Gap & Timing
- **Instrument Prioritization** ✓
  1. CTD/PHSEN/PCO2/PRESF
  2. FLORT/DOSTA/PAR
  3. METBK/NUTNR/SPIKR/PREST /ADCP/WAVSS/VEL

Gross Range & Climatology Test Production

Mar-Dec 2021

- Develop Test Processes & Data Tools
- Code & Data Generation **GRT/CT**
- Code Testing ✓

Jan 2022

- Deploy GRT/CT for **CTD, PHSEN, PCO2, PRESF**
- (15% of OOI data volume) ✓

July 2022

- Generate & Deploy GRT/CT data tables for **FLORT/DOSTA/PAR**
- (22% of data volume) 🔄

Jan 2023

- Generate & Deploy GRT/CT data tables for **METBK, NUTNR, SPIKR, PREST, ADCP, WAVSS, VEL**
- (52% of data volume)

Gap & Timing Test Production

Jan 2023

- Develop process for Gap & Timing tests

July 2023

- Code & Data Generation Gap & Timing
- Code Testing

Dec 2023

- Deploy Gap & Timing to OOI site

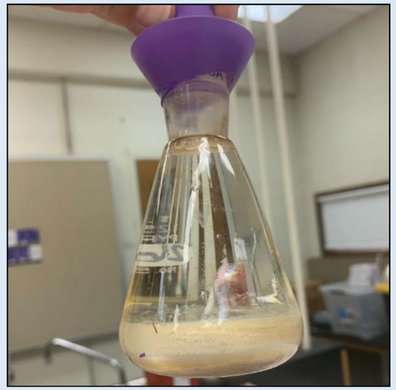
Jan 2024

- QARTOD O&M
- Review QARTOD for further potential tests deployed on an instrument-by-instrument basis

Quality Control: Discrete Validation

Shipboard CTD Profiles and Sample Collection

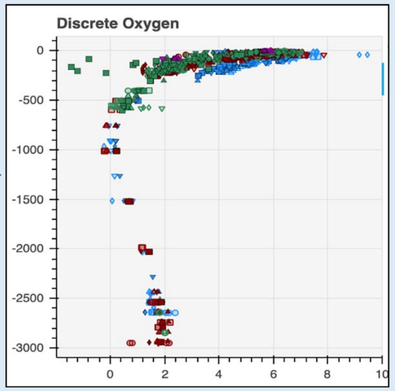
Sample Analysis



Nutrients
Carbon (DIC)
Chlorophyll

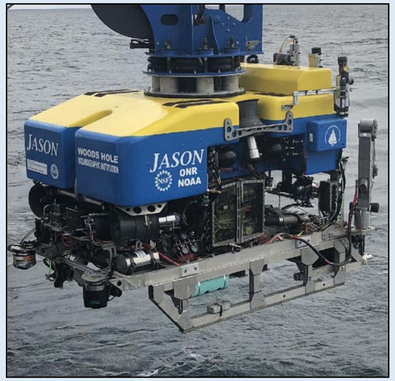
Salinity
Oxygen

Verify Assets

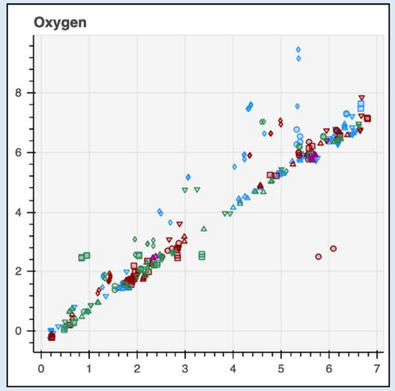


Communication of Results to Users

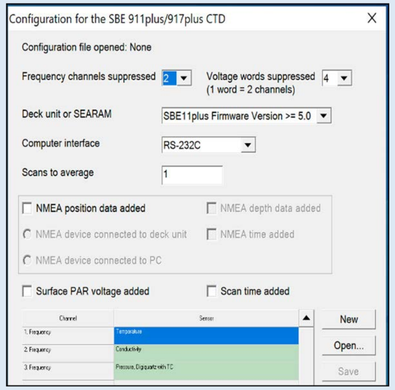
Verification Summary



ROV CTD and Sample Collection



Compare Bottle Samples To Shipboard Profile



Recalculate Profile Sensor Coefficients

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Quality Control: Discrete Validation

OOI collects discrete water samples during CTD casts at each mooring recovery and deployment at each instrument depth. Analysis is performed by outside labs. Analysis include:

- Oxygen
- Salinity
- Nutrients (Nitrate, Nitrite, Ammonium, Phosphate, Silicate)
- Chlorophyll
- Carbon System

Data are publicly available at OOI Alfresco Web Document Server (alfresco.oceanobservatories.org)

OOI > Array > Cruise Data > Cruise > Ship Data > Water Sampling

Currently creating master summary spreadsheets which merged all datasets into a single file.

Cruises with CTD and Bottle Data:

- **Coastal Pioneer** - 18 cruises spaced ~6 months apart dating from 2014
- **Coastal Endurance** - 16 cruises spaced ~6 months apart dating from 2013
- **Irminger** - 8 cruises spaced ~12 months apart dating from 2014
- **Ocean Station Papa** - 9 cruises spaced ~12 months apart dating from 2013
- **Argentine Basin** - 4 cruises spaced ~12 months apart from 2015-2018
- **Southern Ocean -** 6 cruises spaced ~12 months apart from 2015-2020
- **Cabled Array -** 12 cruises spaced ~12 months apart dating to 2013

Quality Control: Discrete Validation: QC Flags

- Quality Flags are provided for each CTD parameter and Discrete Water parameter measured
- Flags are encoded as a 16-bit array, read from right to left
- Definitions for each bit in an array for a particular parameter can be found in a definition table included in the cruise water sampling README.txt file
  - E.g. a flag of *0000000000000010 for the **CTD File Flag** indicates a data cast only
  - E.g. a flag of *0000000000001001 for the **Niskin Flag** indicates that the bottle was leaking and to check for notes about that sample
- Flags also indicate whether a sample is a replicate

Bit Position	Cast Flag	CTD File Flag	CTD Parameter Flag	Niskin Flag	Discrete Sample Flag	Discrete Replicate Flag
0	Notes/Other	Notes/Other	Notes/Other	Notes/Other	Notes/Other	Notes/Other
1	Delayed start to data collection	Data cast only	Not Calibrated	Bottle information unavailable	Sample for this measurement was drawn but analysis not yet received	Duplicate analysis on same Sample
2	Acceptable; normal cast according to SOP	Acceptable; file processed according to SOP	Acceptable measurement	No problems noted	Acceptable; sample processed according to SOP	Single Sample
3	Non-standard winch speed	File processed using modified parameters	Questionable measurement	Leaking	Questionable measurement	Duplicate analysis from same Niskin
4	Non-standard surface soak time	File processed using alternate XMLCON	Bad measurement	Ran out of water during sampling	Bad measurement	Triplicate analysis from same Niskin

Quality Control: Discrete Validation QC Flags

Niskin/Bottle Position	Niskin Flag	CTD Pressure [db]	CTD Pressure Flag	Discrete pH [Total scale]	pH Analysis Temp [deg C]	Discrete pH Flag	Discrete pH Replicate Flag
12	*0000000000000100	131.784	*0000000000000100	-9999999	-9999999	-9999999	-9999999
13	*0000000000000100	101.681	*0000000000000100	7.717	25	*0000000000000100	*0000000000000100
13	*0000000000000100	101.681	*0000000000000100	7.712	25	*0000000000000100	*0000000000001000
15	*0000000000000100	81.656	*0000000000000100	-9999999	-9999999	-9999999	-9999999
17	*0000000000000100	41.487	*0000000000000100	-9999999	-9999999	-9999999	-9999999
19	*0000000000000100	21.261	*0000000000000100	7.7632	25	*0000000000001000	*0000000000000100
20	*0000000000000100	12.965	*0000000000000100	7.7873	25	*0000000000000100	*0000000000000100
21	*0000000000000100	3.017	*0000000000000100	7.789	25	*0000000000000100	*0000000000000100
16	*0000000000000100	30.496	*0000000000000100	7.7455	25	*0000000000000100	*0000000000000100

If you want to simplify, I suggest interpreting the data into the simplified WOCE/QARTOD flagging scheme as:

* 1 = good
* 2 = not run
* 3 = suspect
* 4 = bad
* 9 = missing

The "Replicate Flags" are reduced into a boolean value indicating that either there is a replicate sample or not.

Quality Control: Discrete Validation: QC Flags

Niskin/Bottle Position	Niskin Flag	CTD Pressure [db]	CTD Pressure Flag	Discrete pH [Total scale]	pH Analysis Temp [deg C]	Discrete pH Flag	Discrete pH Replicate Flag
12	1	131.784	1	-9999999	-9999999	-9999999	-9999999
13	1	101.681	1	7.717	25	1	False
13	1	101.681	1	7.712	25	1	True
15	1	81.656	1	-9999999	-9999999	-9999999	-9999999
17	1	41.487	1	-9999999	-9999999	-9999999	-9999999
19	1	21.261	1	7.7632	25	3	False
20	1	12.965	1	7.7873	25	1	False
21	1	3.017	1	7.789	25	1	False
16	1	30.496	1	7.7455	25	1	False

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* 1 = good
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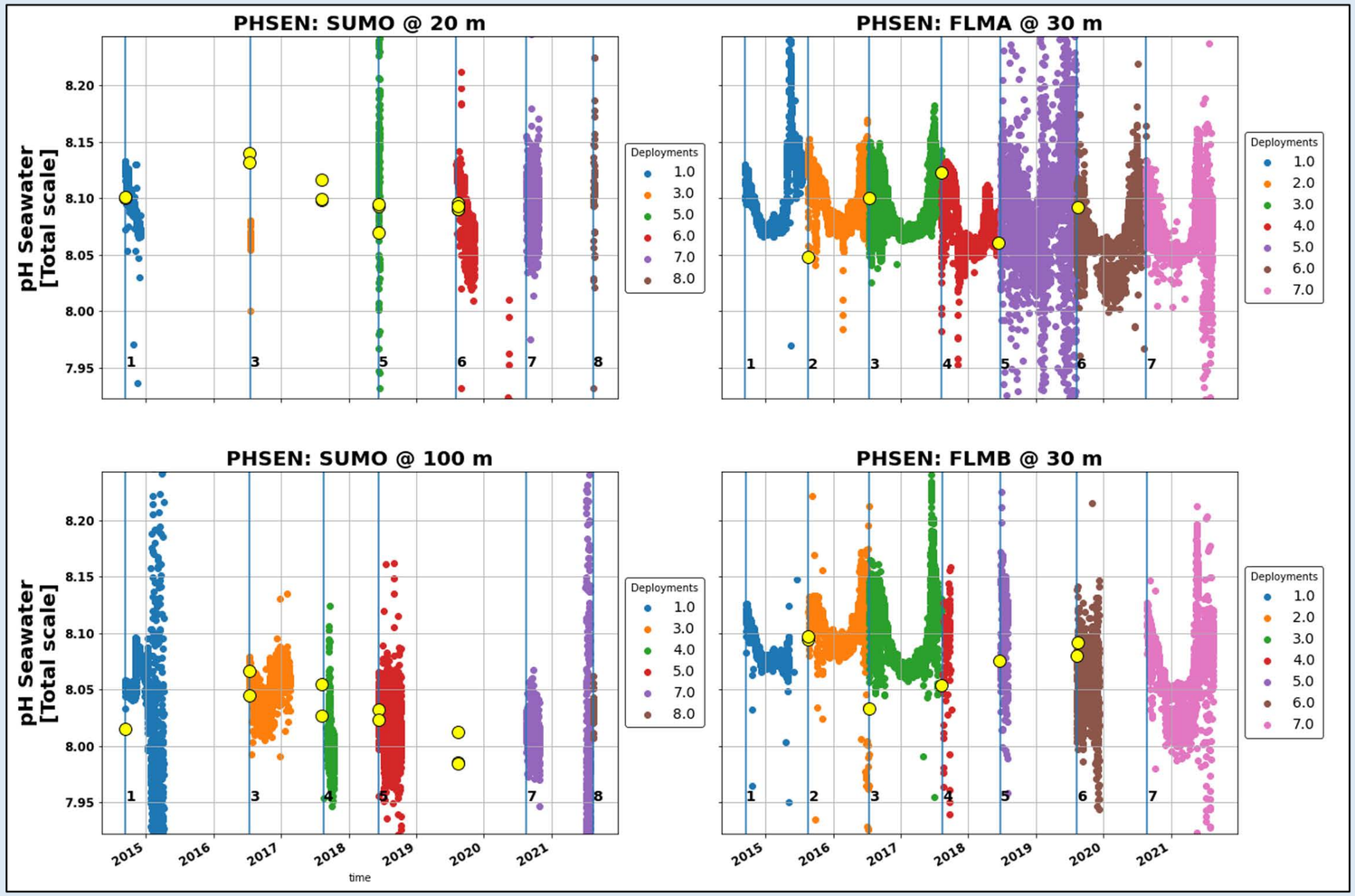
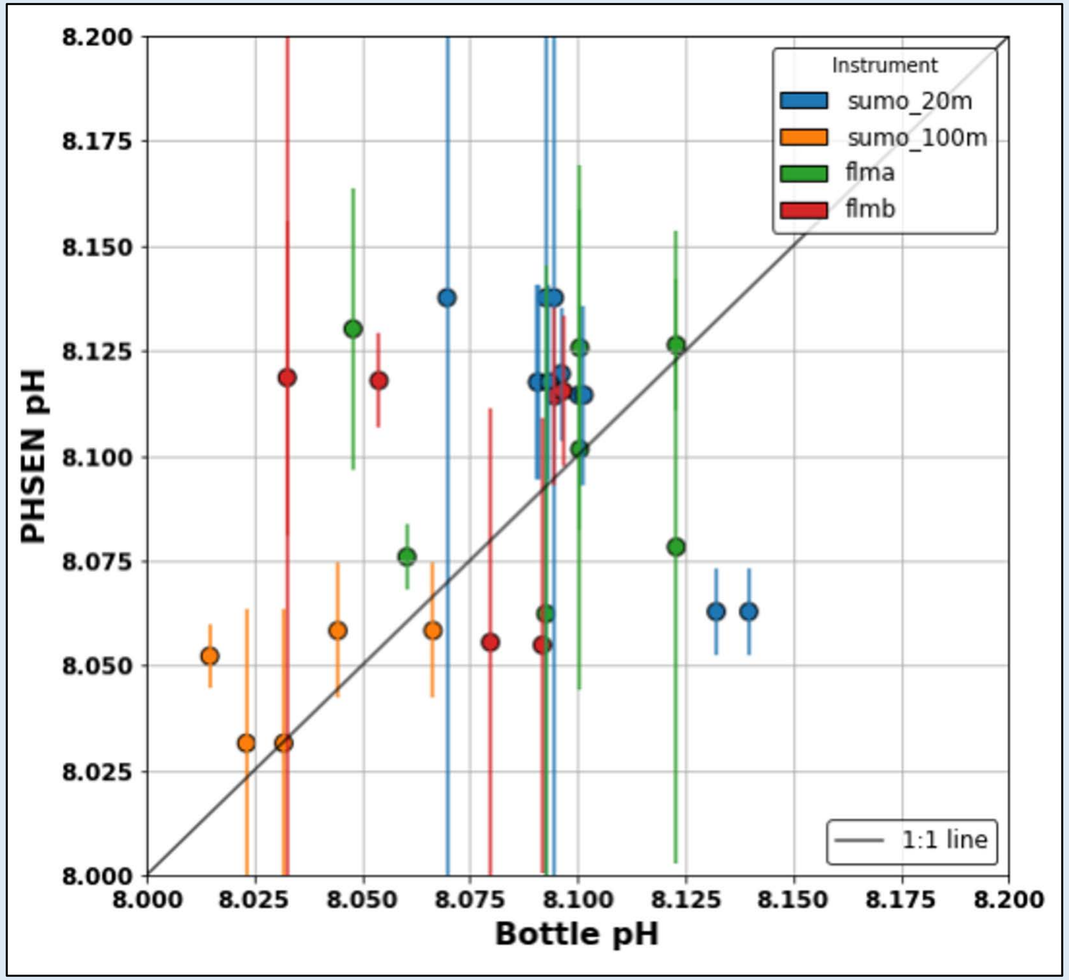
Quality Control: Discrete Validation Example



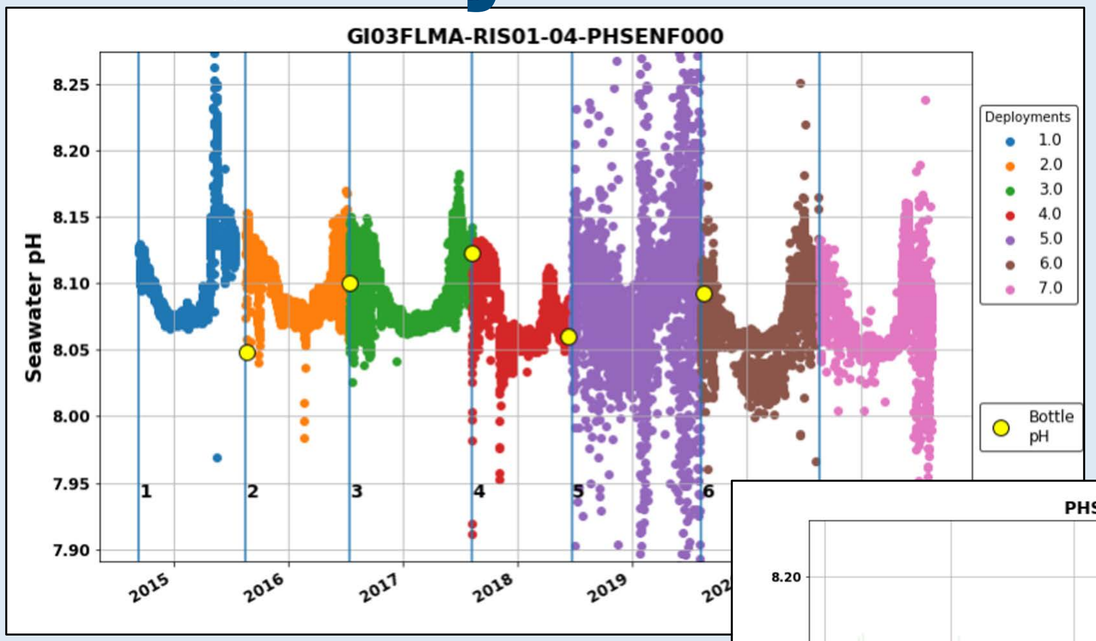
Time series of the Irminger Array's Sunburst SAMI-pH seawater pH, color coded by deployment, with nearest discrete carbon samples overlaid. The instruments on the Flanking Moorings are protected by the buoy and thus have more consistent data returns than the instruments on the Apex Surface Mooring wire.

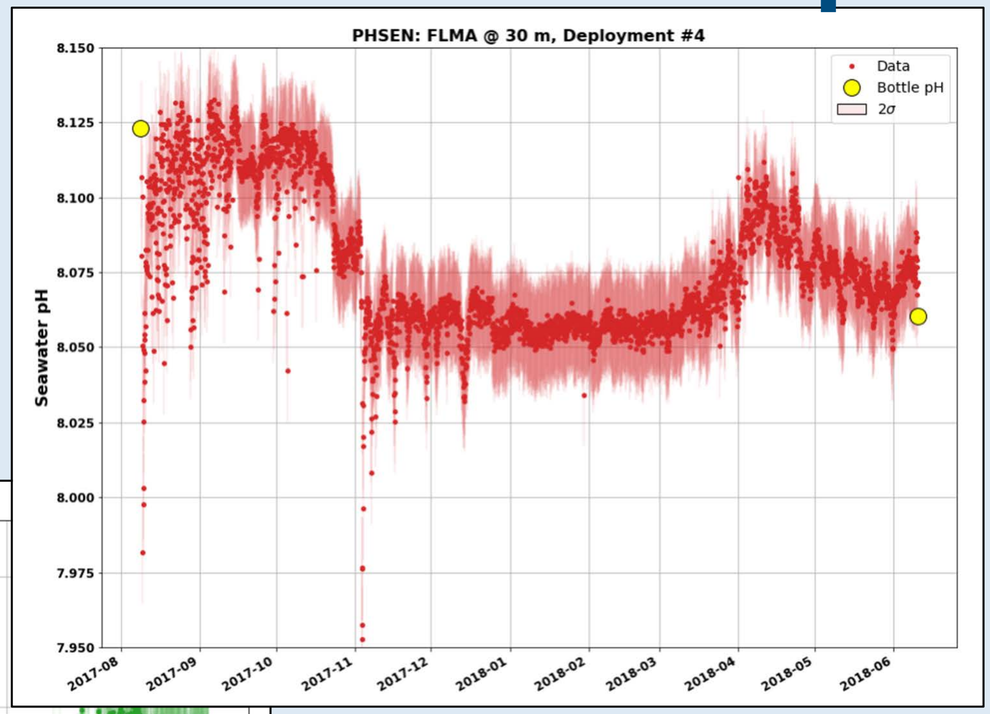
Quality Control: Discrete Validation Example

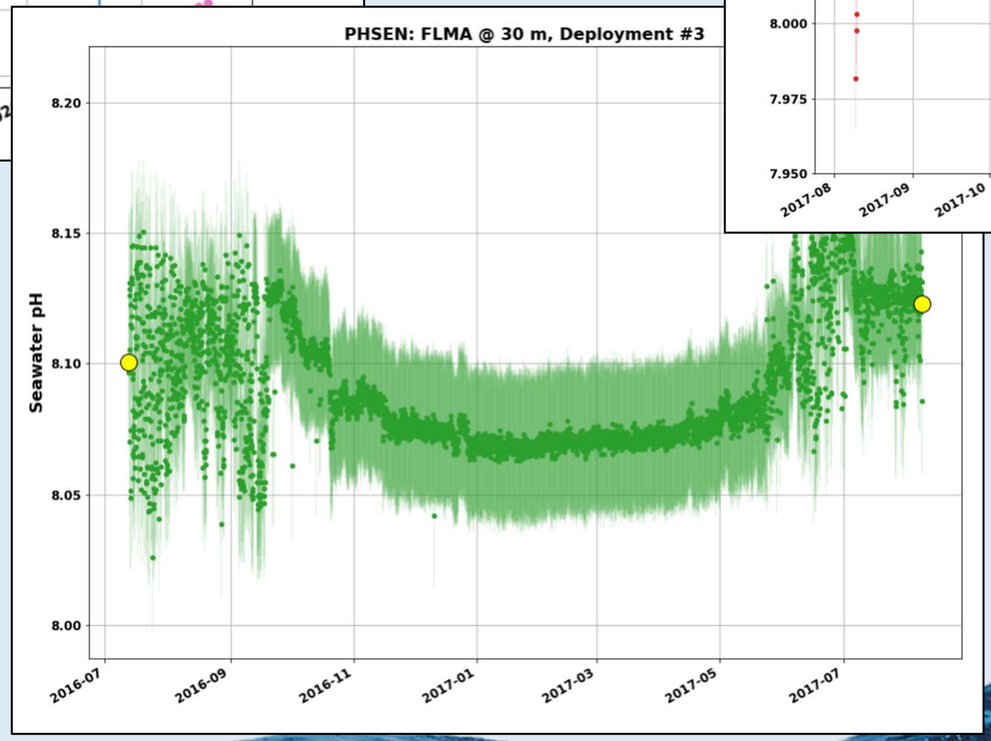


Comparison of the PHSEN measured pH with matched bottle pH, with 1:1 line drawn for comparison. Vertical lines are two standard deviations.

Quality Control: Discrete Validation Example







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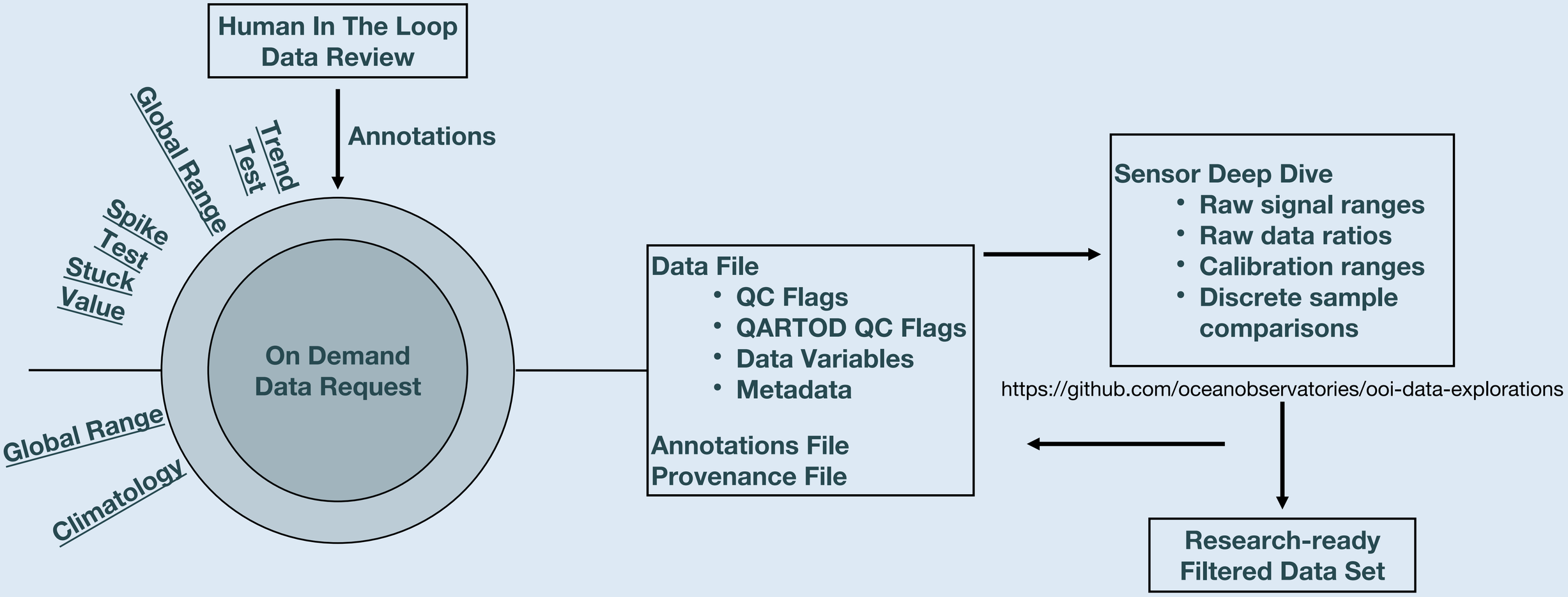
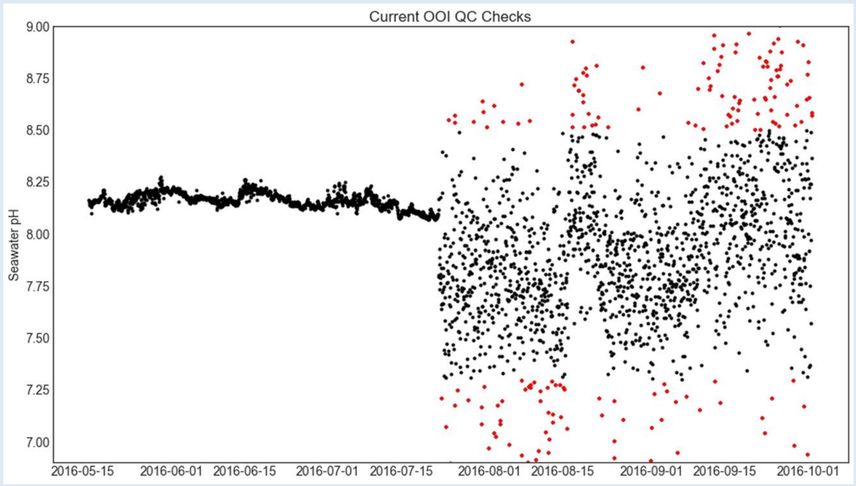
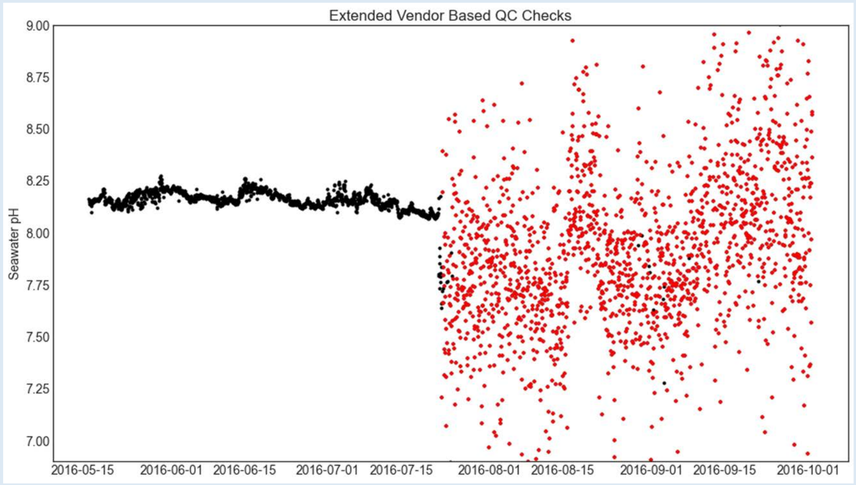
Quality Control: Sensor Deep Dives (HITL)



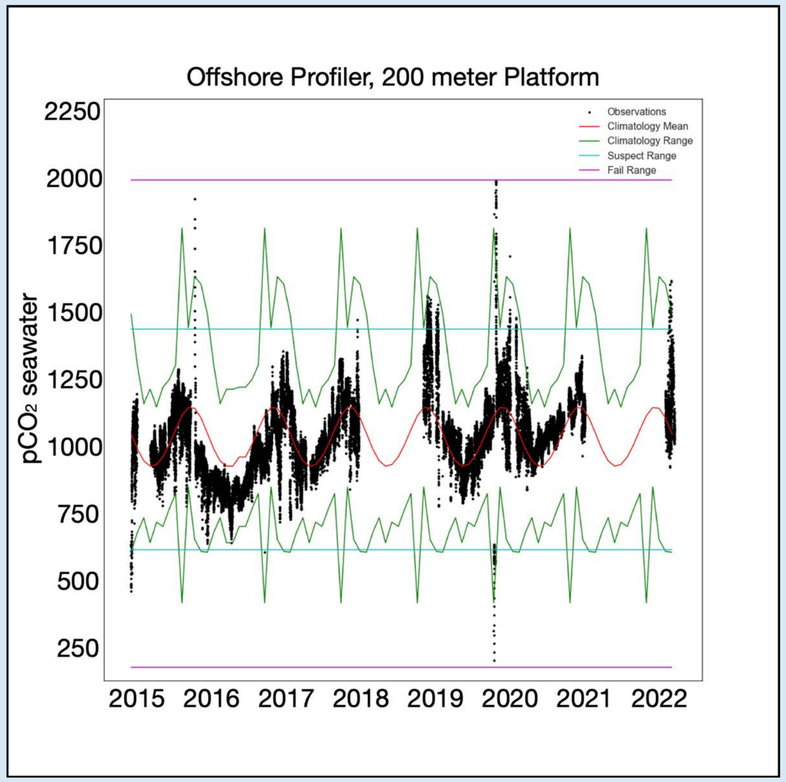
Quality Control: pH

- Automated QC checks of the pH data
  - OOI Gross Range, Spike and Stuck Value tests (https://oceanobservatories.org/quality-control/).
  - QARTOD Gross Range and Climatology tests added 2022-02-23 (https://ioos.noaa.gov/ioos-in-action/ph/).
  - Tests based on limits applied to the calculated seawater pH; most of the bad data is missed.
- Source of Additional QC Checks
  - Vendor provided Matlab code performs a series of QC checks on different variables in the raw data prior to calculating pH.
  - Building these checks into a processing workflow is essential to ensure we are working with the best quality data possible.
- Combination of the extended quality flags and the HITL annotations will flag majority of the bad data.
  - Example notebook showing how to load, flag, and process data through to the creation of QARTOD style Gross Range and Climatology test limits.
  - https://nbviewer.org/github/oceanobservatories/ooi-data-explorations/blob/master/python/examples/notebooks/phsen/creating_annotations.ipynb

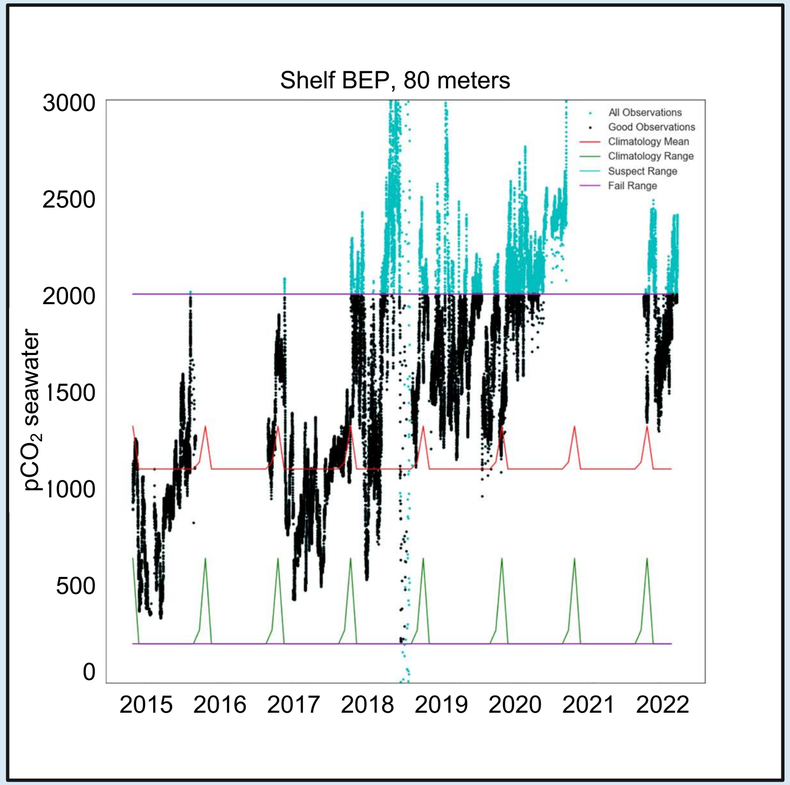


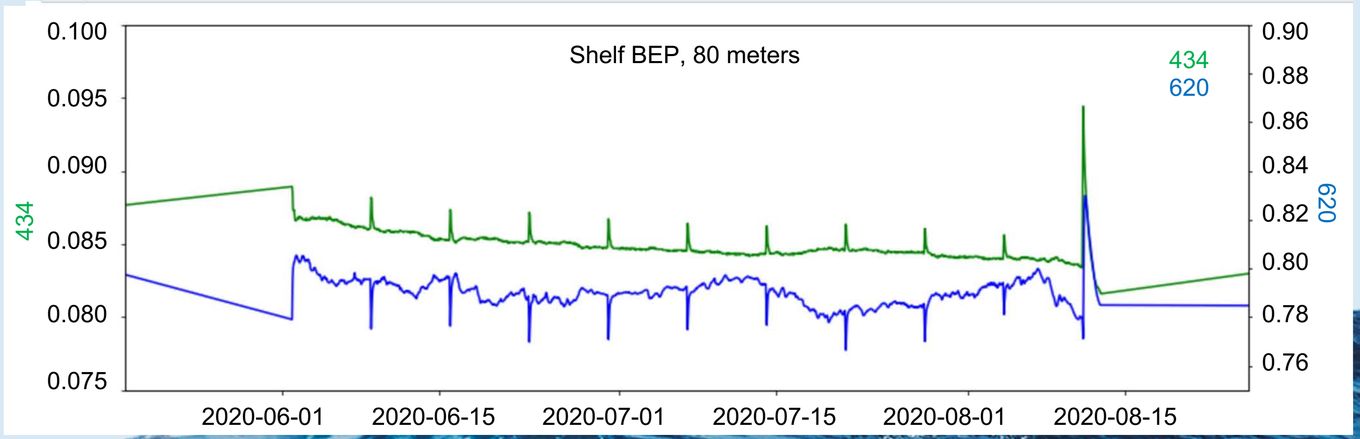


Quality Control: pCO2



- Automated QC flags
  - Global, Gross, Local Ranges
  - Stuck value, spikes
  - Climatology
- HITL annotations and exclusion flags
- Sensor-specific filters
  - Raw signal ratios and ranges
  - Vendor calibration ranges
  - Data spikes





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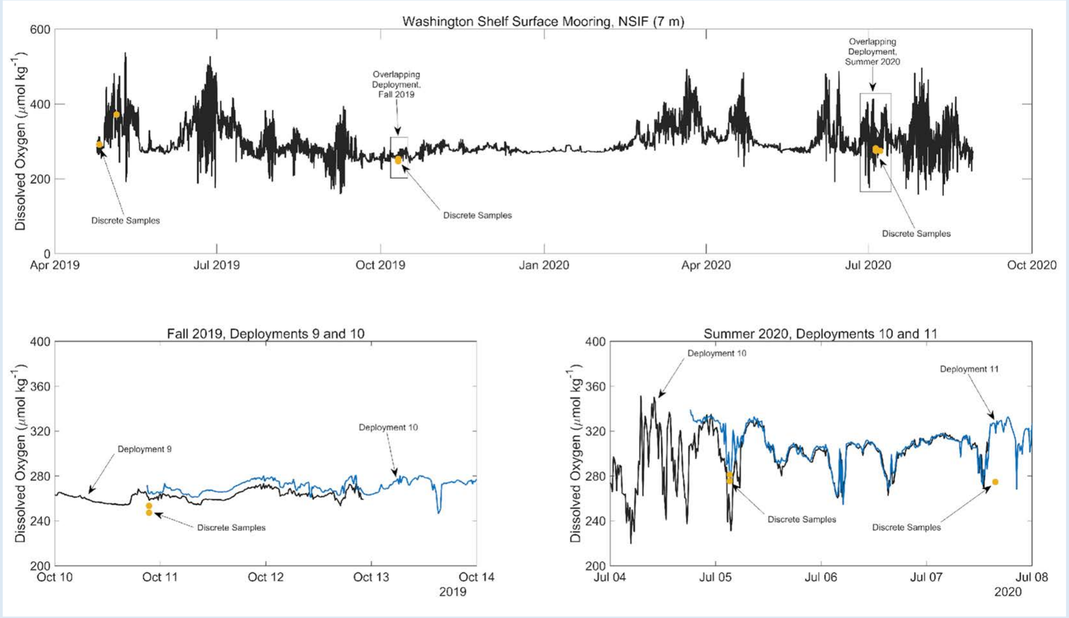
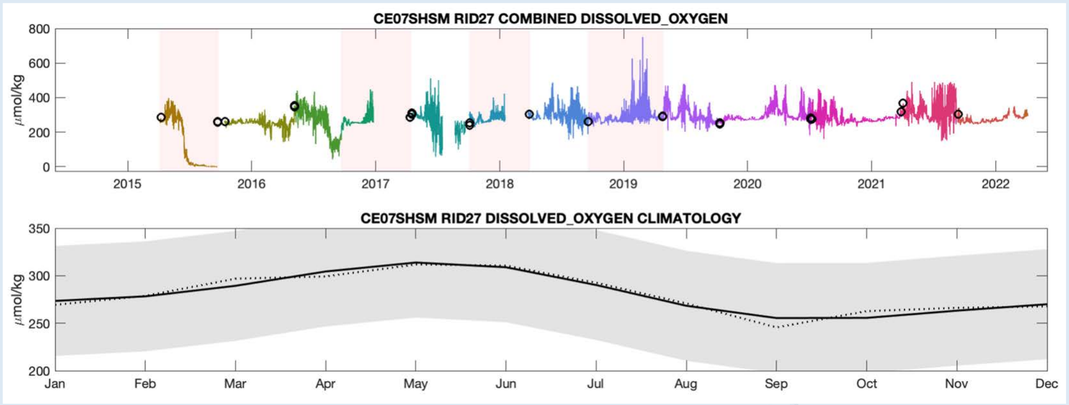
Quality Control: Oxygen

- HITL process with heavy reliance on discrete samples and adjacent (overlapping or close-in-time) deployments
- Some obvious instrument failures, but usually QC is impacted by biofouling
- Implemented UV biofouling control measures in Spring 2018 to great success, but still have some issues (UV lamp and power failures)
- Determining onset of biofouling can be subjective
- Iterative process to review/create HITL annotations, develop QARTOD gross range and climatology limits, and review again





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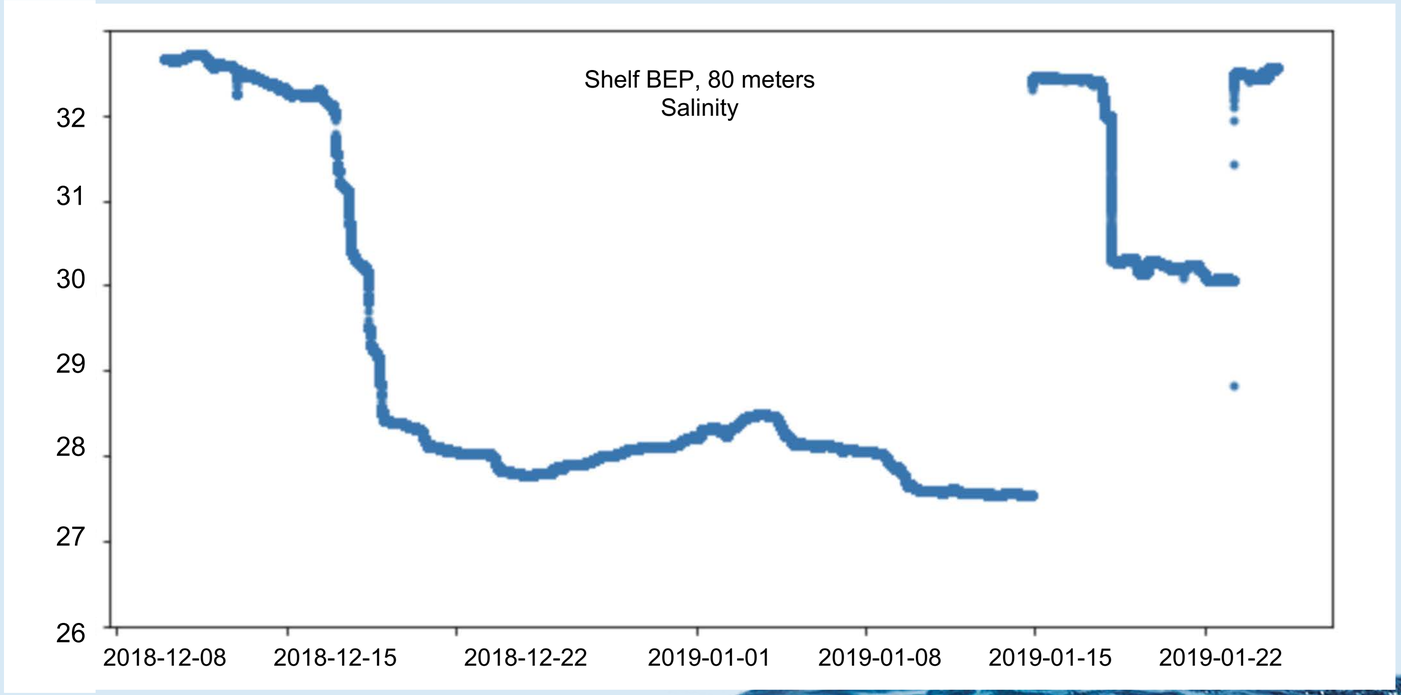
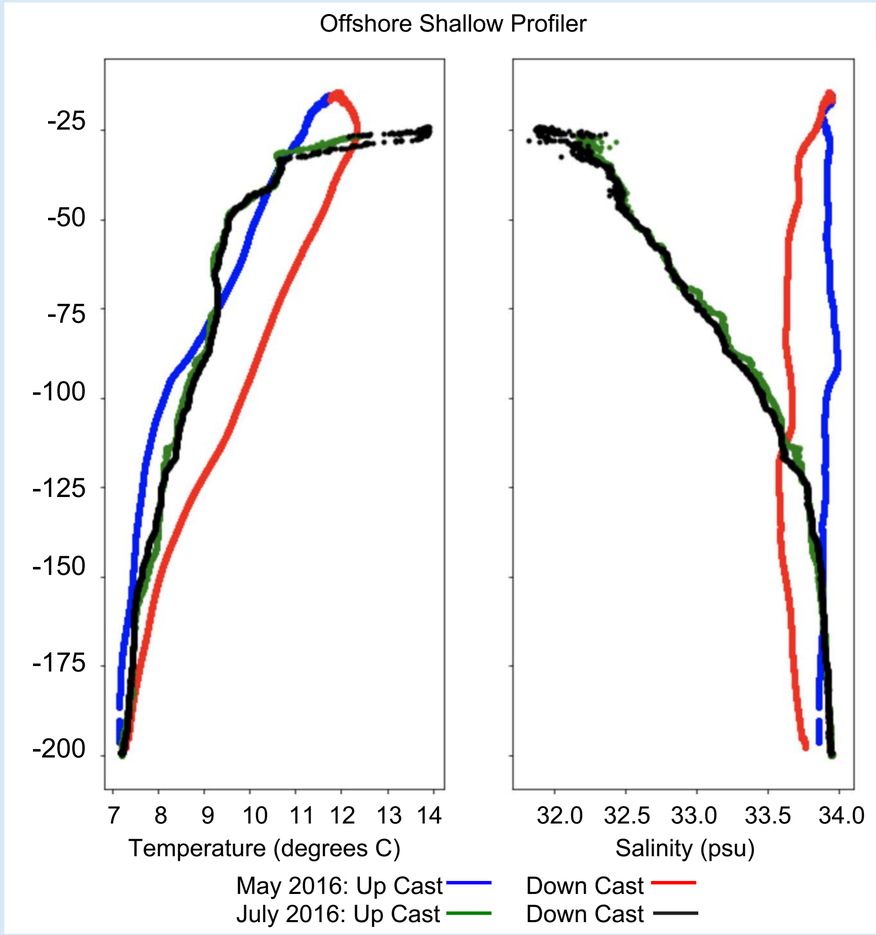
Quality Control: CTD

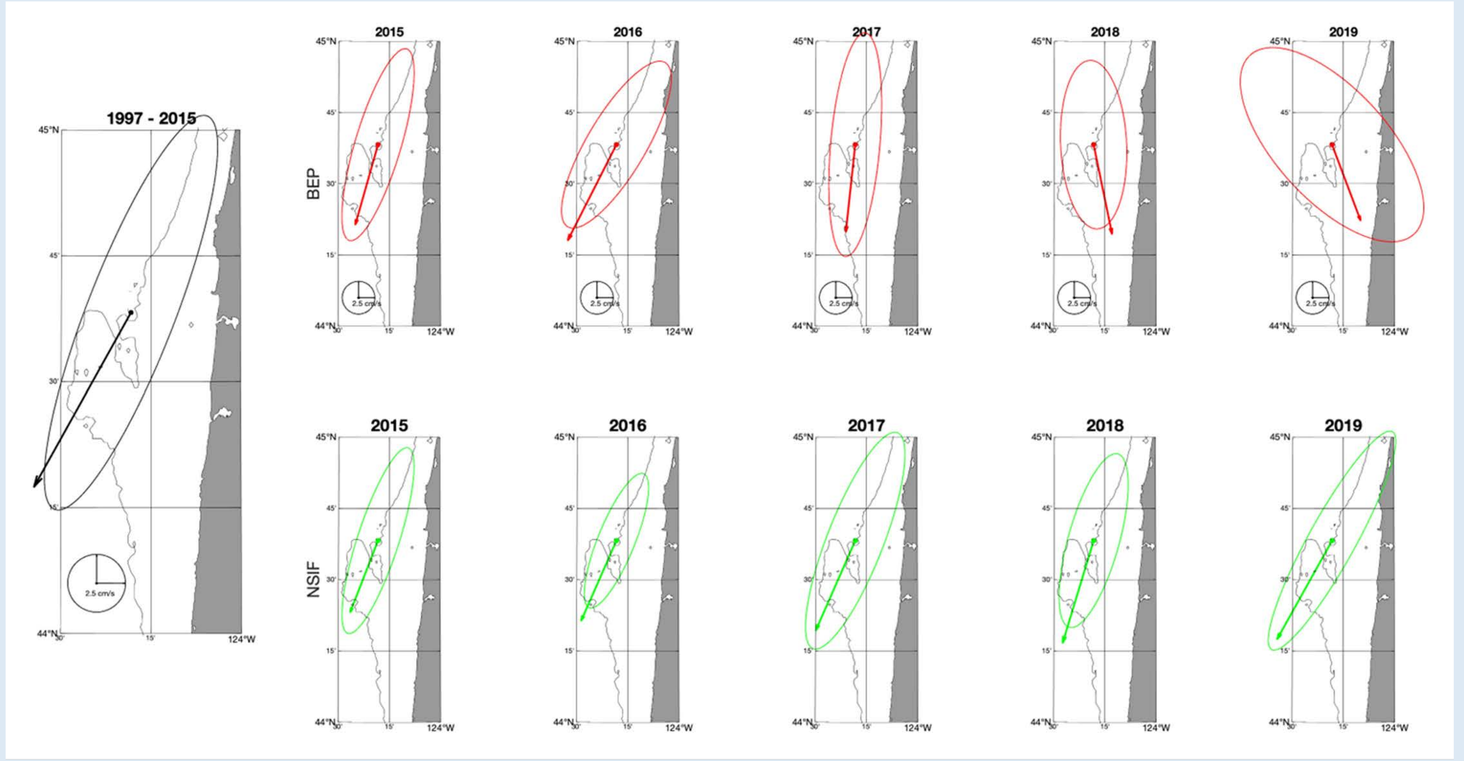
- Overall data quality is good due to robust sensors
- HITL process
  - Nearest neighbor comparisons
  - Pre-recovery / post-deployment
- Biggest issues related to biofouling, clogged cells, pump failures





Quality Control: ADCP

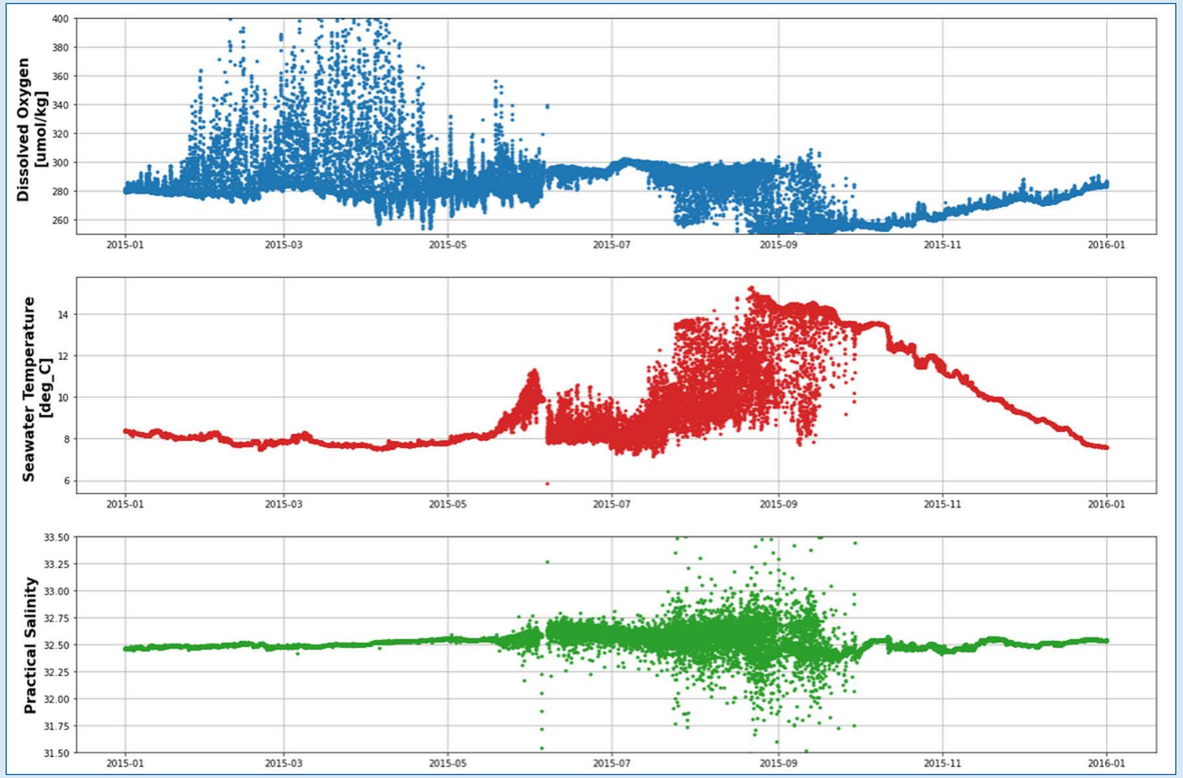
- Largely HITL process, with some automated QC test limits (e.g., pitch or roll > 15°)
- Co-location of multiple velocity sensors (downward looking ADCP and VELPT on the NSIF, and upward looking ADCP on the seafloor) allowing for cross-comparison and validation of the data
- Overall data quality is good with some issues (ADCP orientation) still to address
- Issues during early deployments with configuration control, since automated



Variance ellipses and mean vectors of the depth-averaged, 36-hr low-pass filtered velocity from the composite of ADCP data available at the historic NH-10 mooring (co-located with CE02) for 1997-2015 (left, black) and for 2015-2019 at the BEP (top, red) and NSIF (bottom, green) showing the depth-averaged mean flow from the BEP does not follow the bathymetry in 2018/2019 as it does in other years.

Quality Control: Annotations

- Added to datasets by operators for specified time periods, instrument streams
- Provide metadata on QC, performance, issues, configurations
- Available through M2M, OOI Data Portal



	@class	id	subsite	node	sensor	method	stream	beginDT	endDT	annotation	exclusionFlag	source	qcFlag	parameters
0	.AnnotationRecord	152	GP03FLMA	None	None	None	None	2015-06-06 22:40:00	2016-06-28 19:10:00	Deployment 3: Mooring was deployed 10-15m deep...	False	lgarzio@marine.rutgers.edu	0	[]
1	.AnnotationRecord	151	GP03FLMA	None	None	None	None	2014-06-17 06:00:00	2015-06-05 00:00:00	Deployment 2: Mooring was deployed 15-20m shal...	False	lgarzio@marine.rutgers.edu	0	[]
2	.AnnotationRecord	775	GP03FLMA	RIS01	03-DOSTAD000	None	None	2015-01-01 00:00:00	2015-06-05 00:00:00	Deployment 2: Dissolved oxygen noise increased...	False	lgarzio@marine.rutgers.edu	3	[]

```
2015-06-06 22:40:00 to 2016-06-28 19:10:00: Deployment 3: Mooring was deployed 10-15m deeper than planned.
2014-06-17 06:00:00 to 2015-06-05 00:00:00: Deployment 2: Mooring was deployed 15-20m shallower than planned. Upon recovery of platform, biofouling was apparent on shallow CTDs.
2015-01-01 00:00:00 to 2015-06-05 00:00:00: Deployment 2: Dissolved oxygen noise increased, possibly from biofouling.
```

Data Quality User Tools

Metadata

- Sensor calibration sheets, vendor documentation
- Cruise plans and SOPs
- Discrete samples, shipboard data, discrete summary sheets
- Metadata change GUI, data-affecting changes list

Raw Data

- Public raw data archive
- Public GitHub repositories with raw data parsers, data product algorithms

User Community

- OOI Discourse
- Helpdesk
- Community tools and data repositories on GitHub
- Workshops

Next Steps

- Continue development and implementation of QARTOD tests
  - GRT/CT data tables for FLORT/DOSTA/PAR
  - GRT/CT data tables for METBK, NUTNR, SPIKR, PREST, ADCP, WAVSS, VEL
  - Gap and Timing Tests

- Continue Human-In-The-Loop Data Review and Sensor Deep Dives
  - Communicate results to community through annotations, data flags, github code and notebooks

- Start work to integrate sensor-specific filters developed through deep dives into enhanced data products

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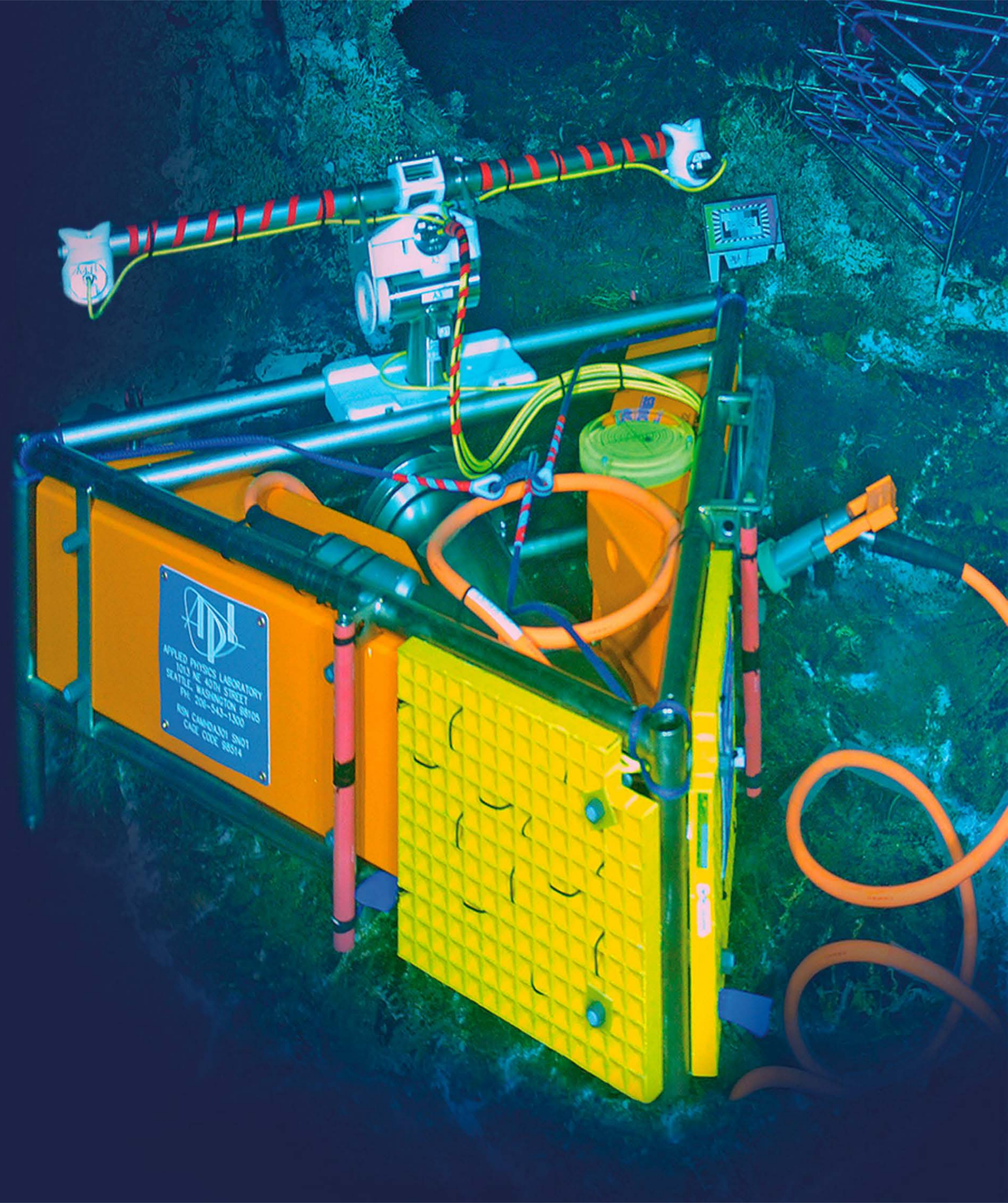
Questions?

OOI Discourse

https://discourse.oceanobservatories.org/

OOI HelpDesk

helpdesk@oceanobservatories.org



Quality Assurance: Infrastructure

- Deployment turn cycles
  - Regional Cabled and Global Scale Arrays: once per year
  - Coastal Pioneer and Endurance Arrays: twice per year
  - Coastal sliders and surface profilers: nominal three month cycle
  - Pioneer AUV's: deployed on an expeditionary basis
- Biofouling mitigation
  - Manufacturer-provided mitigation, copper tape, zinc ointment
  - UV light mitigation being implemented (O_2 optodes, spectral irradiance, digital still cameras)
- Sparing
  - Two sets of instruments and platforms to allow for efficient refurbishment

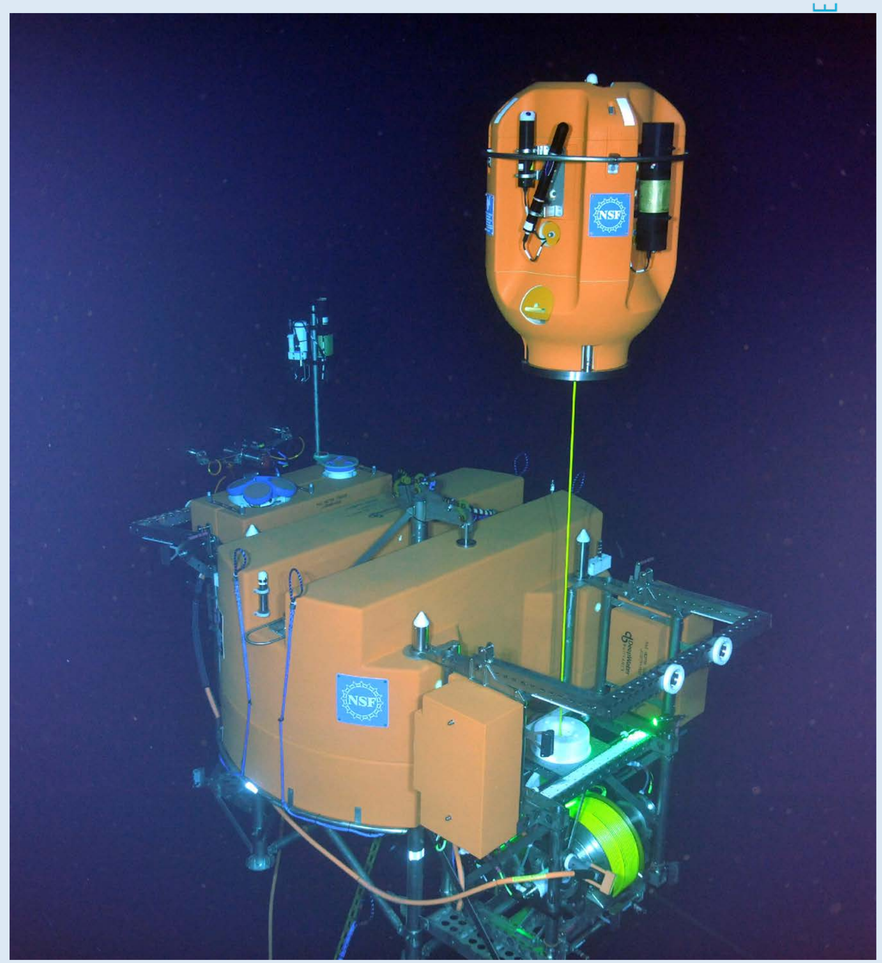
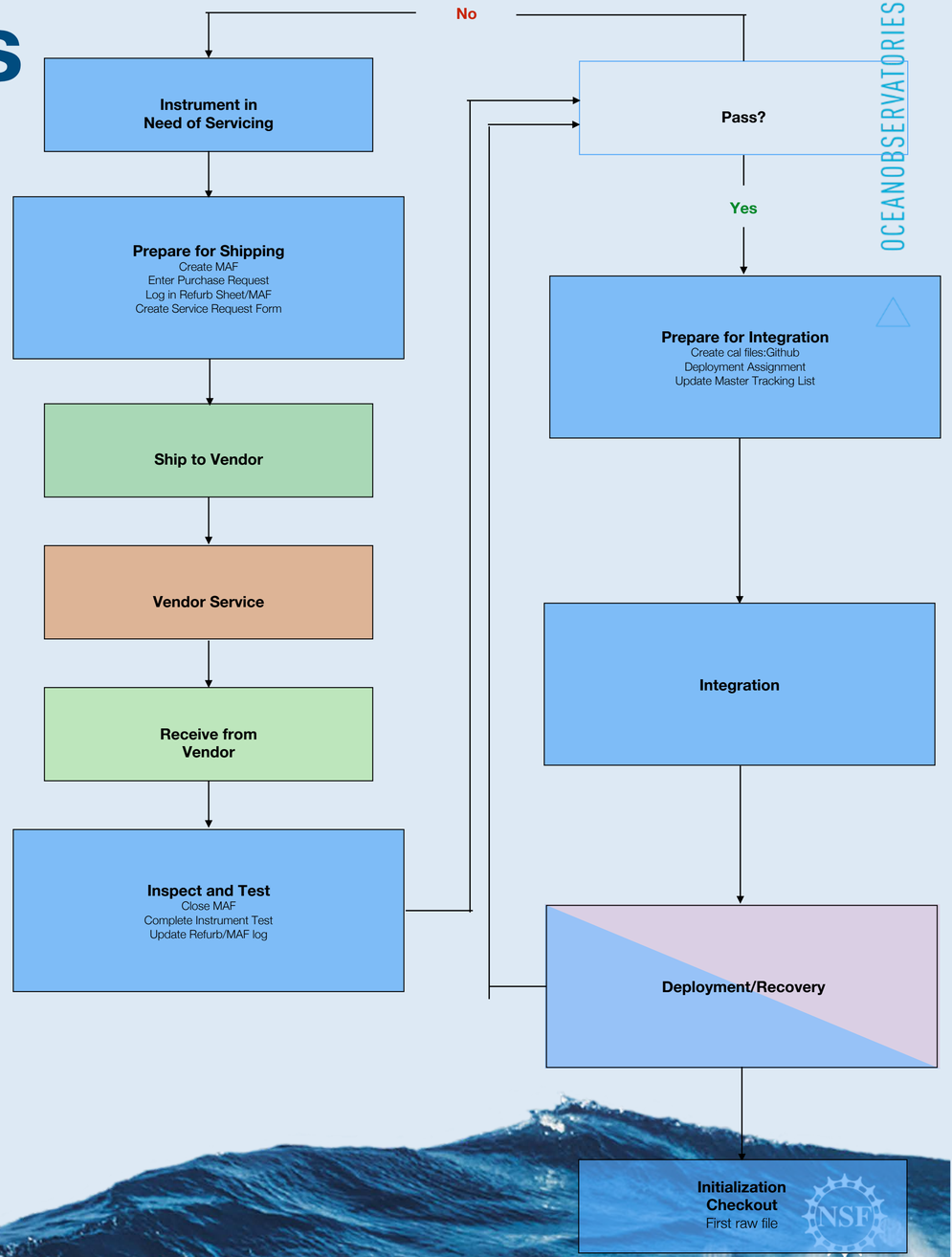


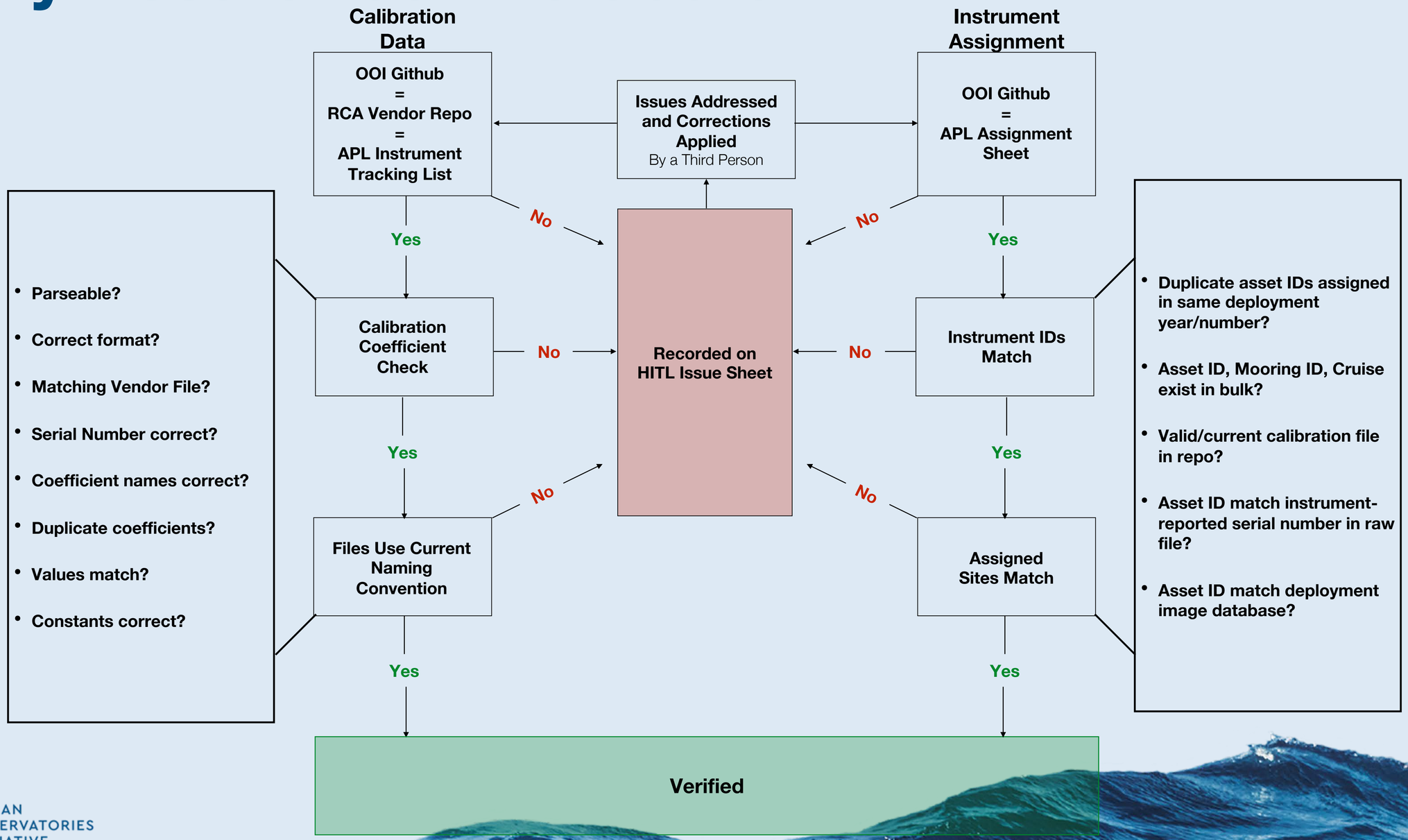
Photo Credit UW/NSF-OOI/CSSF

Quality Assurance: Instruments

- Quality conformance testing of incoming sensors
- Additional validation procedures in house
- Integration and burn in before deployment
- Biweekly cross-MIO instrument meetings



Quality Assurance: Metadata



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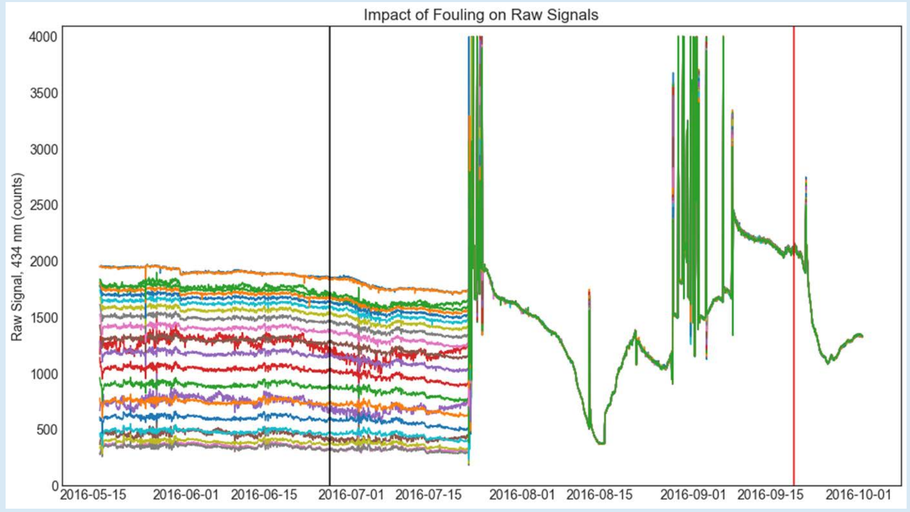
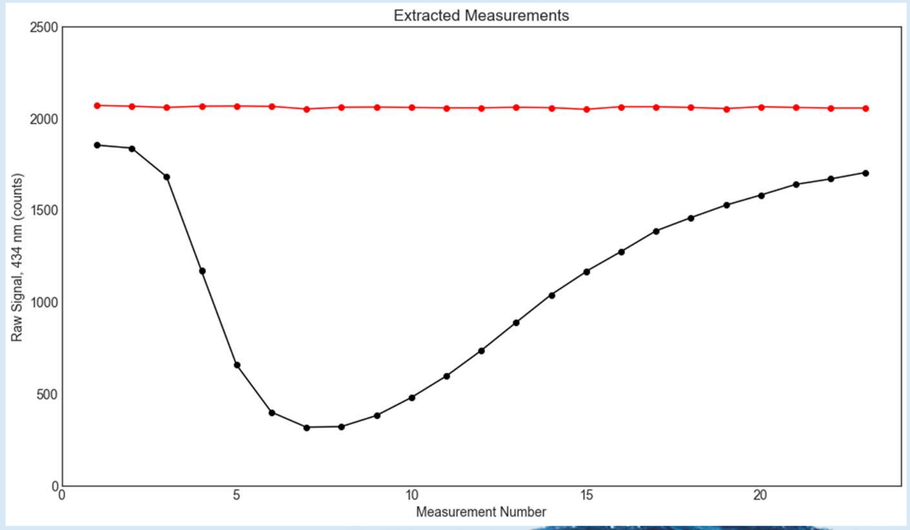
Quality Control: pH

- Reorganize blanks (seawater only)
  - Pull from `reference_light_measurements` (array of 16 points)
  - 4 variables, 4 measurements each
    - 434 nm raw signal and reference (counts)
    - 578 nm raw signal and reference (counts)
  - Test signal and reference levels are within acceptable range (*1st test*).
- Reorganize pH measurements (seawater + indicator)
  - Pull from `light_measurements` (uncabled) or `ph_light_measurements` (cabled) (array of 92 points)
  - 4 variables, 23 measurements each
    - 434 nm raw signal and reference (counts)
    - 578 nm raw signal and reference (counts)
  - Test signal and reference levels are within acceptable range (*2nd test*).
  - Test signal levels span an acceptable range (standard deviation, *3rd test*).
- Calculate seawater pH
  - Test derived value falls between 6.9 and 9.0 (*4th test*).





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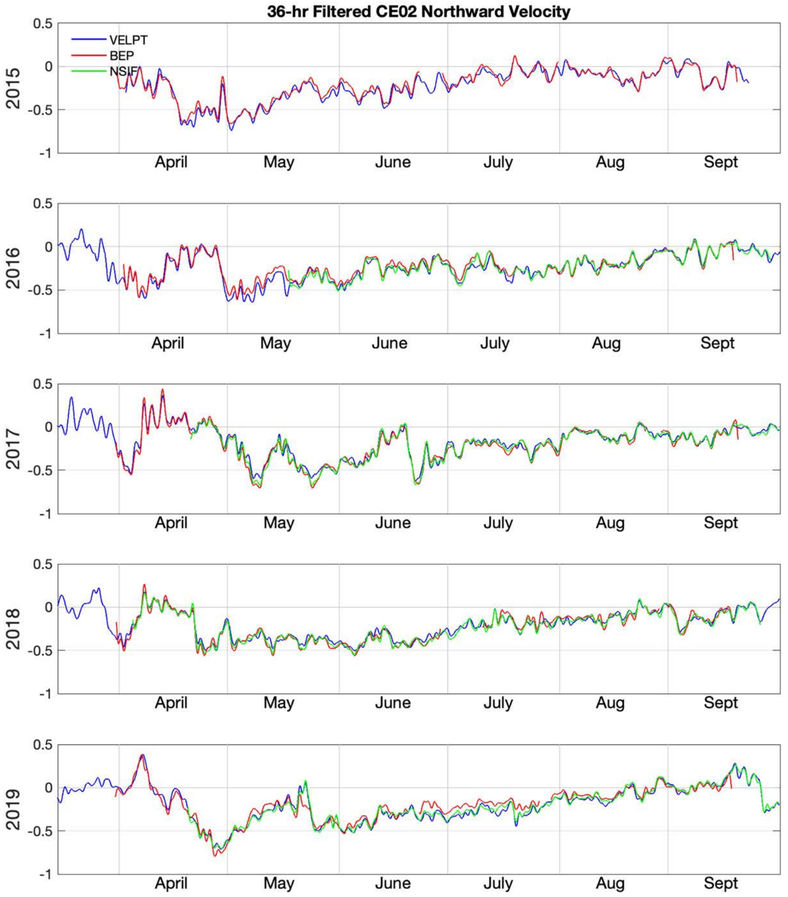
Quality Control: ADCP



BEP Eastward Velocity appears to be the wrong sign