NOAA in situ SST Quality Monitor Version 2 (*i*Quam2)

Current url: www.star.nesdis.noaa.gov/sod/sst/iquam/v2

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Motivation and Objective

- NOAA is responsible for wide range of polar and geostationary satellite SST products (including swath – L2, gridded – L3) and blended/analysis L4 SSTs.
- High-quality, unified *in situ* standard is needed for consistent Cal/Val
  - Covers full satellite era 1981 – pr
  - Includes all available normal-quality and high-quality *in situ* SSTs suitable for satellite Cal/Val (drifters, moorings, ARGO floats, ships)
  - Uniformly processes all *in situ* data using state-of-the-art QC, consistent with wider oceanographic, meteorological, and climate communities such as Met Office, NOAA NCEP, ICOADS. Preserve all heritage QFs for user's option.
  - Provides data in community consensus, user friendly format, via web interface with minimal latency, to support NRT Cal/Val applications
  - Reprocesses data periodically, to support long-term satellite consistent/climate data records (CDRs)

Motivation and Objective

- **In 2008, conducted inventory of available *in situ* SSTs for the use in Cal/Val**
  - ICOADS r2.40 (Sep 1981 – Jul 2007; not available in NRT; suboptimal QC for satellite Cal/Val)
  - FNMOC (Sep 1998 – pr; available in NRT; suboptimal QC for satellite Cal/Val)
  - NCEP GTS (Jan 1991 – pr; available in NRT; no QC)
  - Documented in: *Xu, Ignatov, 2010: Evaluation of in situ SSTs for use in Cal/Val, JGR, 115, C09022.*

- **In 2009, launched *in situ* SST Quality Monitor version 1 (*i*Quam1)**
  www.star.nesdis.noaa.gov/sod/sst/iquam/ (google "iquam")
  - Uses NCEP GTS data as feed (1991-pr)
  - Included drifters, tropical and coastal moorings, ships
  - State of the art UK MO Bayesian QC
  - Documented in: *Xu, Ignatov, 2014: In situ SST Quality Monitor (iQuam), JTECH, 31, 164.*

Today, *i*Quam has become a GHRSST community resource which is widely used nationally and internationally, to support Cal/Val and data assimilation for various blended and satellite SST products

*i*Quam users (we are aware of)

- NOAA STAR/OSPO – JPSS, GOES-R, Himawari, AVHRR (SQUAM, USA)
- JPL MUR (US) – M. Chin
- U. Miami MODIS, VIIRS Teams (US) – K. Kilpatrick, L. Williams
- Felyx (France/UK) – J.-F. Piolle
- CMS (France) – A. Marsouin
- JAXA (Japan) – Y. Kurihara, M. Kachi
- Ocean University (China) – L. Guan
- CMA (China) – S. Wang
- SOA (China) – Q. Tu
- NOAA geo-polar blended team (USA) – P. Koner, J. Mittaz, A. Harris, E. Maturi
- NOAA NCEI/Silver Spring (USA) – K. Saha
- NOAA NCEI/Asheville (USA) – V. Banzon
- EUMETSAT (Germany) – P. Dash, A. O'Carroll
- NASA GMAO (USA) – Ricardo Todling, Santha Akella, Guillaume Vernieres
- ABoM (Australia) – Irina Sakova, Helen Beggs

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Enhancements in *i*Quam2

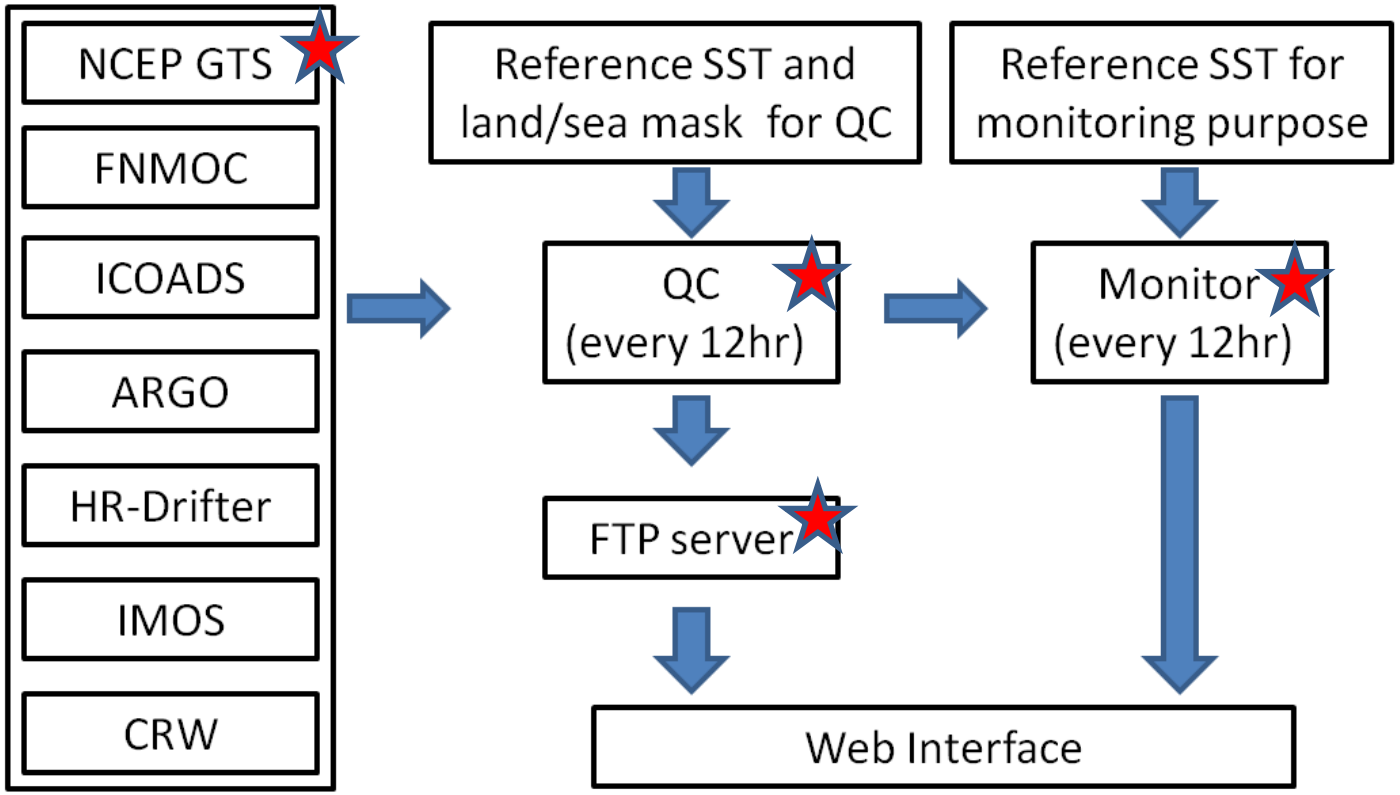
As *i*Quam user community grows, it requested several enhancements

- Extend time series to full satellite era (Sep 1981 – on)
- Improve QC, by adding
  - the 2nd reference SST (CMC)
  - performance history check (*i*Quam check similar to the UKMO/CMS "black lists")
  - CMS black list; and individual QFs from data producers (ICOADS, ARGO, IMOS)
- Improve web interface
  - Redesign web engine (from flash player to High Charts)
  - Add daily (hourly) statistics
  - Enhance graphics (interactive display, and print/save functions)
- Add new *in situ* data
  - ARGO Floats (in NRT and post-processing modes)
  - High-Resolution Drifters
  - IMOS Ships
  - Coral Reef Watch buoys
- Change output data files to NetCDF4. (Maximally reconcile with GHRSST GDS2 satellite L2/L3 format).

Functionality and Data Flow

The *i*Quam is a web-based near-real time system. It performs 4 major functions

- Ingests various *in situ* SSTs
- Performs a uniform Quality Control (QC)
- Monitors QCed *in situ* SSTs online
- Serves reformatted *in situ* SST data with quality flags appended



Quality Control in *i*Quam

Category	Check	Type of error handled	Physical basis
Preprocessing	Duplicate Removal	Duplicates arise from multiple transmission or data set merging	Identical space/time/ID
Plausibility	Geo-location checks	Unreasonable Geolocation	Range of single fields & Relationships among them
Internal consistency	Tracking	Points falling out of track	Travel speed exceeds limit
	Spike check	Discontinuities in SST time series along track	SST gradient exceeds limit
External consistency	Reference Check	Measurements deviating far away from reference	Bayesian approach (Ref. SST: daily OI SST v2 and CMC 0.2)
Mutual consistency	Cross-platform Check	Mutual verification with nearby measurements ("buddies check")	Bayesian approach based on space/time correlation of SST field
Performance consistency	Performance history check	Bad performance of single platform ID	Outlier rate exceeds limit (50%) in single platform
Heritage quality flags	All the heritage QFs are preserved in iQuam2 output files, including ICOADS, ARGO Floats, HR-Drifters, IMOS Ship and CMS blacklist.		

Quality level

iQuam2 quality level definition:

string quality_level:flag_meanings = "invalid not_used not_used low_quality acceptable_quality best_quality" ;

string quality_level:flag_values = "0b, 1b, 2b, 3b, 4b, 5b" ;

quality_level = 5 :

- ✓ Geo-location check pass
- ✓ Duplicate check pass
- ✓ Platform ID check pass
- ✓ Tracking check pass
- ✓ Spike check pass
- ✓ Performance history check pass
- ✓ Reference check probability < 0.5
- ✓ Cross-platform check probability < 0.1

quality_level = 4 :

- ✓ Geo-location check pass
- ✓ Duplicate check pass
- ✓ Platform ID check pass
- ✓ Tracking check pass
- ✓ Spike check pass
- ✓ Performance history check pass
- ✓ Cross-platform check probability < 0.5

Or

- ✓ Geo-location check pass
- ✓ Duplicate check pass
- \- Platform ID check fail
- \- Tracking check fail
- ✓ Spike check pass
- ✓ Performance history check pass
- ✓ Reference check probability < 0.5
- ✓ Cross-platform check probability < 0.1

quality_level = 3 :

- ✓ Fails to meet the criteria of ql = 5 or ql = 4

quality_level = 0 :

- ✓ Both references are unavailable

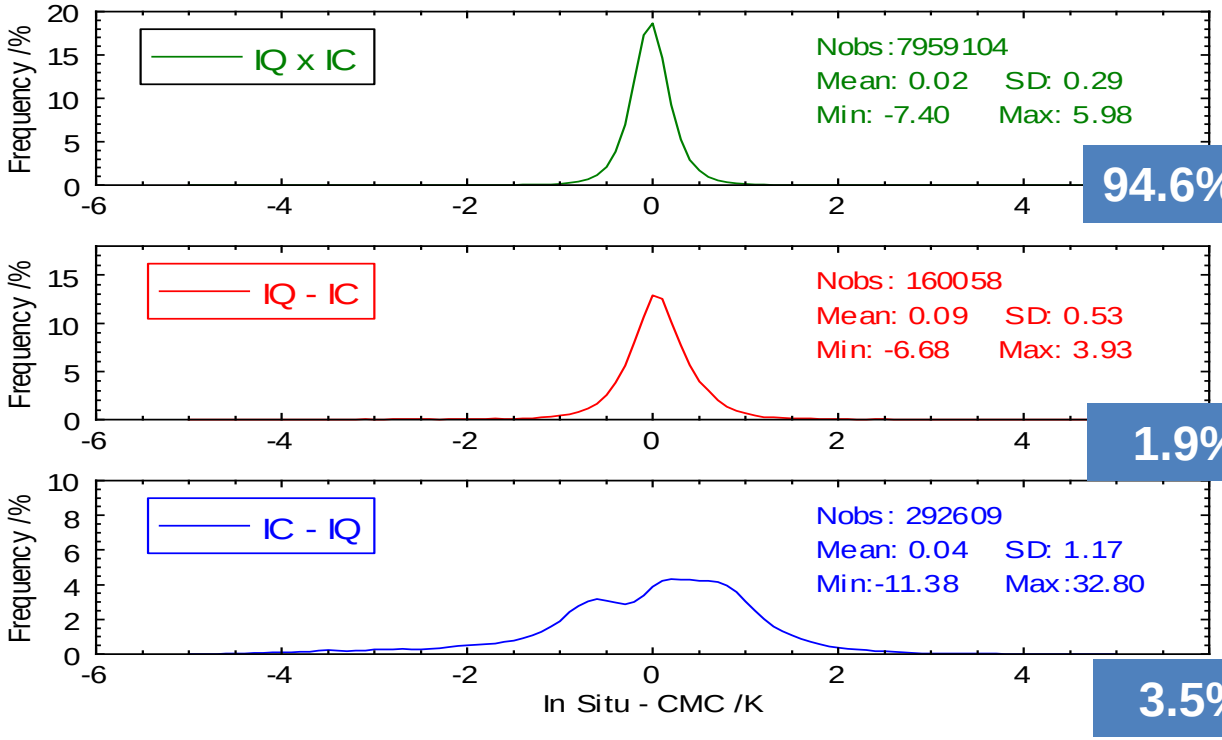
% of Data by Quality Levels Example for Feb 2017

	Total Num	% of QL = 5	% of QL = 4	% of QL = 3
Argo floats	12,469	92.8	2.1	5.1
Drifters	607,840	91.6	2.4	6.0
HR-Drifters	156,951	74.7	1.8	23.5
Tropical Moorings	25,942	95.7	2.1	2.2
Coastal Moorings	235,223	79.3	2.7	18.0
CRW Moorings	15,340	95.1	2.0	2.9
Ships	80,745	66.9	4.3	28.8
IMOS Ships	63,849	65.8	0.6	33.6

Based on our observation, QL = 0 is not exist

Drifters QC
*i*Quam vs. ICOADS

Jan 2006 – Dec 2006



94.6%

1.9%

3.5%

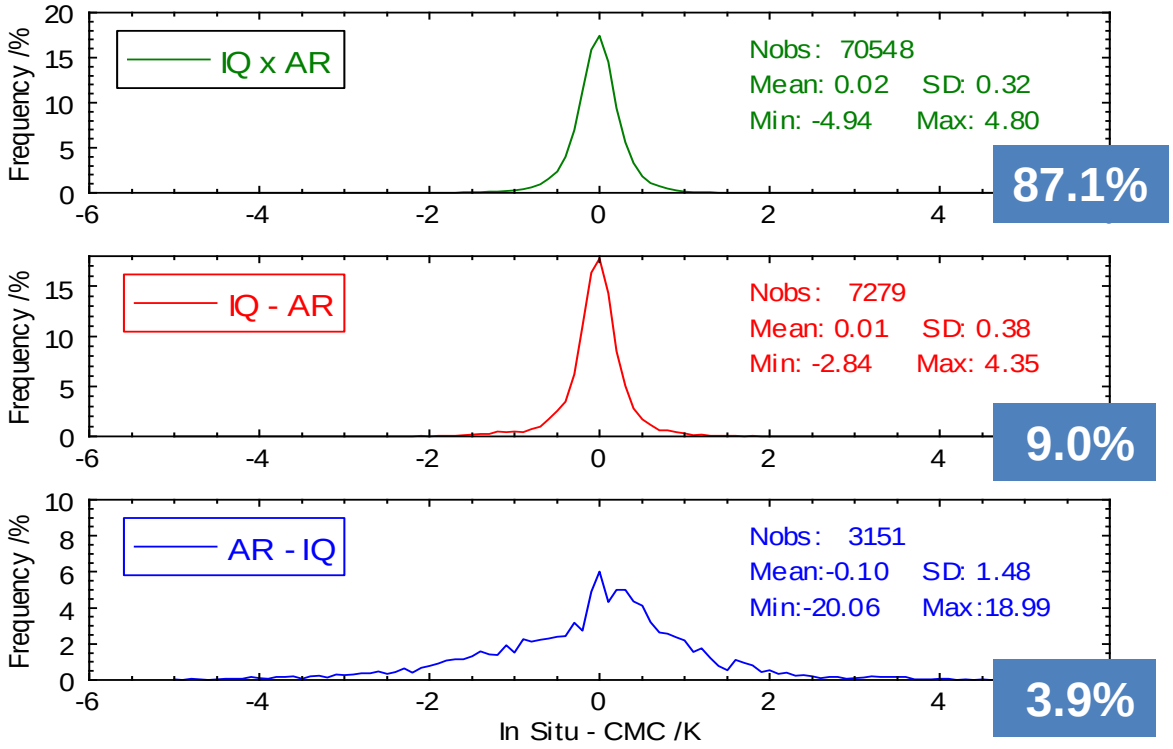
Data passing both QCs show a Gaussian distribution with Bias~0.02K and SD~0.29K

"iQuam leakages" (data pass iQuam QC but fail IC) are close to Gaussian shape but with degraded statistics. Suggests that this portion of data is noisier but still normal.

"IC leakages" (data pass IC QC but fail iQuam QC) significantly deviate from normal distribution with SD exceeding 1K.

ARGO floats QC
*i*Quam vs. Heritage

Jan 2006 – Dec 2006



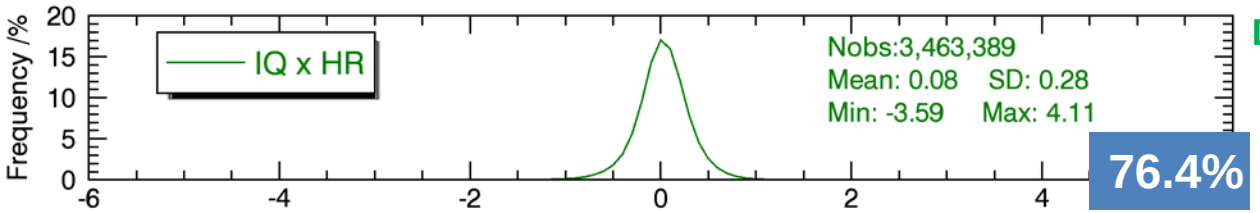
Data passing both QCs show a Gaussian distribution with Bias~0.02K and SD~0.32K

"iQuam leakages" (data pass iQuam QC but fail AG) are comparable with IQ x AG. This suggests that these data are normal but with little bit higher noise.

"AG leakages" (data pass AG QC but fail iQuam QC) deviate from normal distribution and SD over 1.4K.

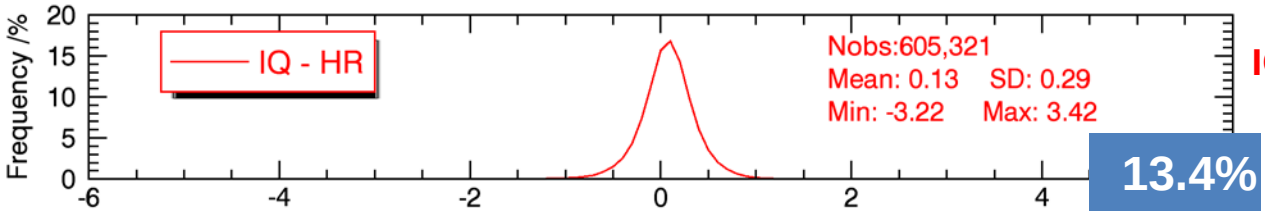
HR-Drifter QC
*i*Quam vs. Heritage

Jan 2012 – Mar 2015



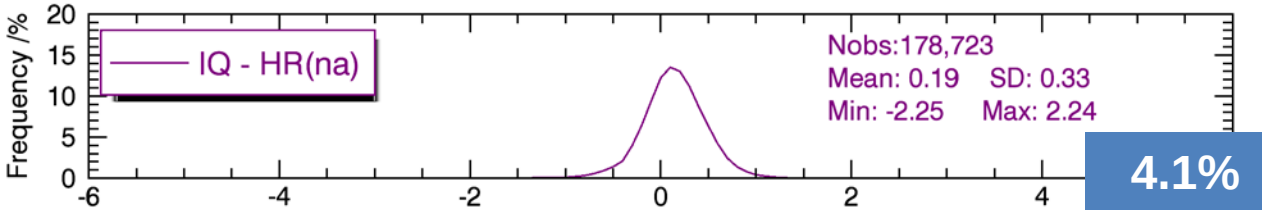
76.4%

Data passing both QCs show a narrow Gaussian distribution with Bias~0.08K and SD~0.28K



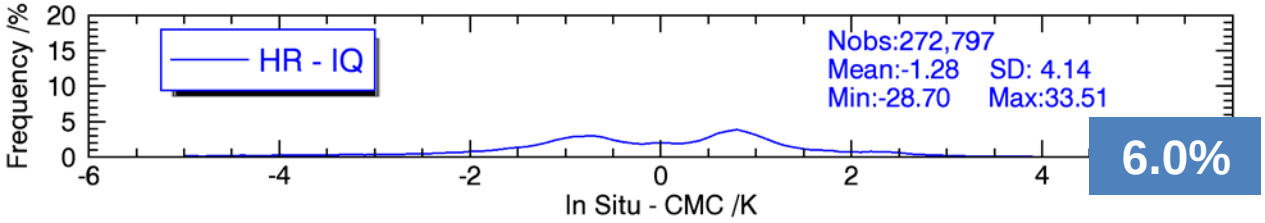
13.4%

IQ 'leakage' has comparable stats with IQxHR, suggesting that HR QC is overly conservative



4.1%

HR(na) stats are slightly degraded, likely due to regional biases

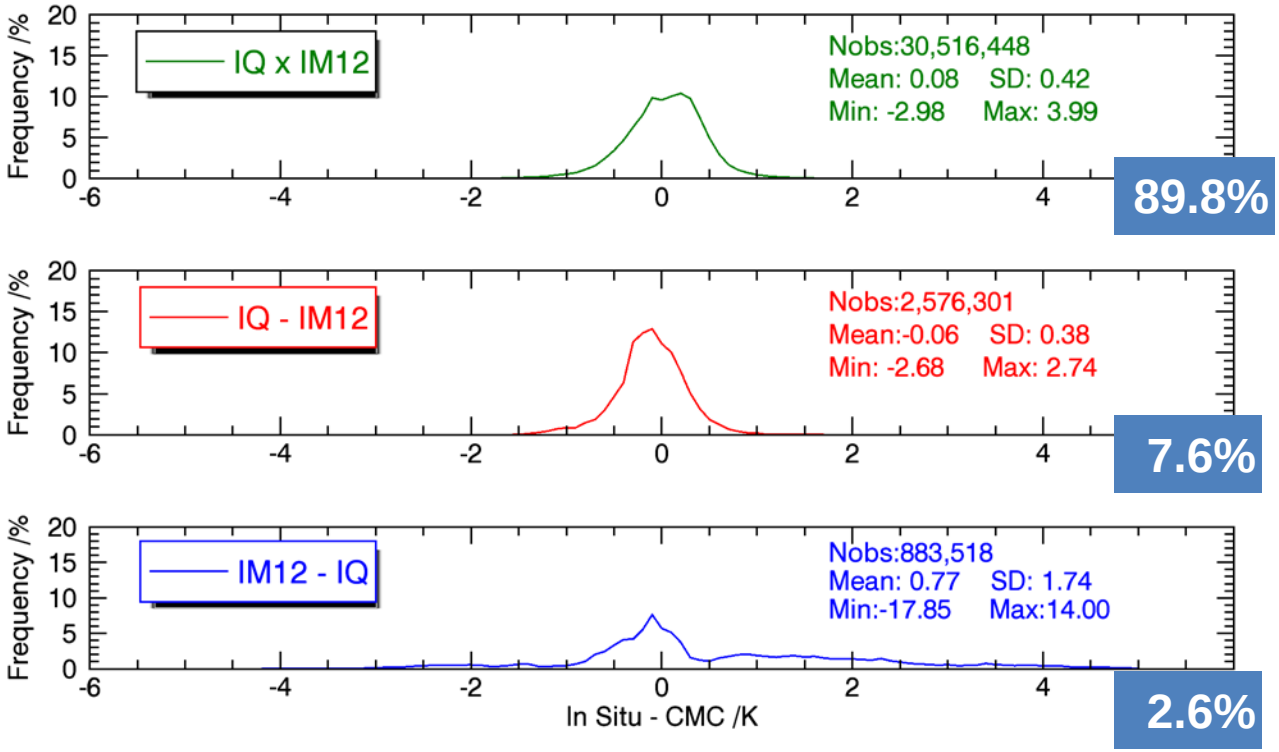


6.0%

HR 'leakages' (data pass HR QC but fail iQuam) are significantly degraded

IMOS IM12 Ships QC
*i*Quam vs. Heritage

Aug 2012 – Dec 2014



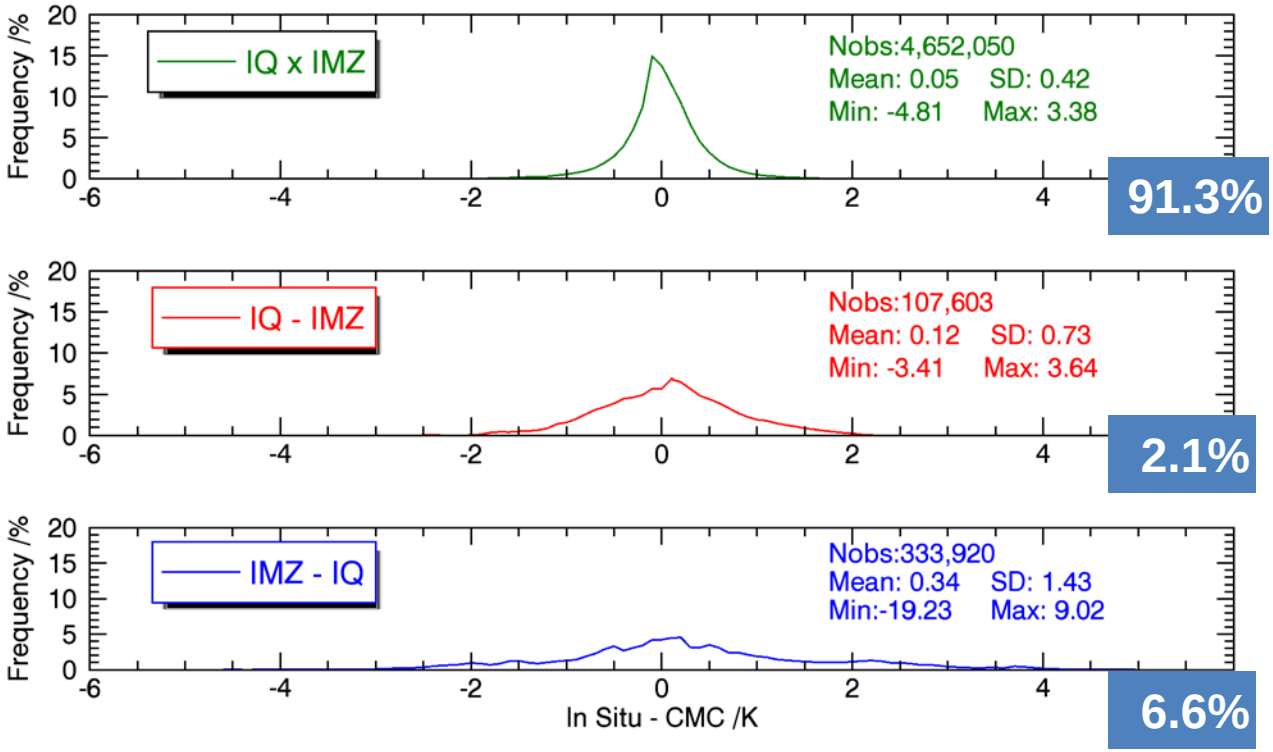
Data passing both QCs show a Gaussian distribution with Bias~0.08K and SD~0.42K

"iQuam leakages" (data pass iQuam QC but fail IM12) are comparable with IQ x IM12. This suggests that the IM12 QC is overly conservative. It removes 7.6% of data.

"IM12 leakages" (data pass IM12 QC but fail iQuam QC) are significantly degraded. This suggests that iQuam QC is instrumental, for ~2.6% of data

IMOS IMZ Ships QC
*i*Quam vs. Heritage

Aug 2012 – Dec 2014



Data passing both QCs show a narrow Gaussian distribution with Bias~0.05K and SD~0.41K

Stats for "iQuam leakages" (data pass iQuam QC but fail IMZ) are degraded. Suggests that IMZ QC contain valid and independent info that iQuam2 doesn't have. (~2% of the data)

"IMZ leakages" (data pass IMZ QC but fail iQuam QC) are significantly degraded. Suggests that iQuam QC is instrumental to improve the quality of IMOS data (~6% of the data)

What *i*Quam QFs/QLs should I use?

1. Using iQuam QL=5 is recommended. This is what we monitor in the *i*Quam web page and use for NOAA Cal/Val
2. All heritage QFs are also reported in iQuam. Our “confusion matrix” analyses suggest that they do not add much to the iQuam QFs. (The only heritage QF which was found unique, the IMOS IMZ, is included in the iQuam2 QL=5)
3. All individual iQuam QFs are also reported in data files. Advanced users are welcome to build their own QLs

Monitor Interface (1)

NOAA NESDIS STAR

iQUAM

in situ SST quality monitor v2.0

NOAA / NESDIS / STAR

Monitor Data About

www.star.nesdis.noaa.gov/sod/sst/iquam/v2

Maps
Statistics
Time Series
Platforms

2017 03 26

Show hour 0

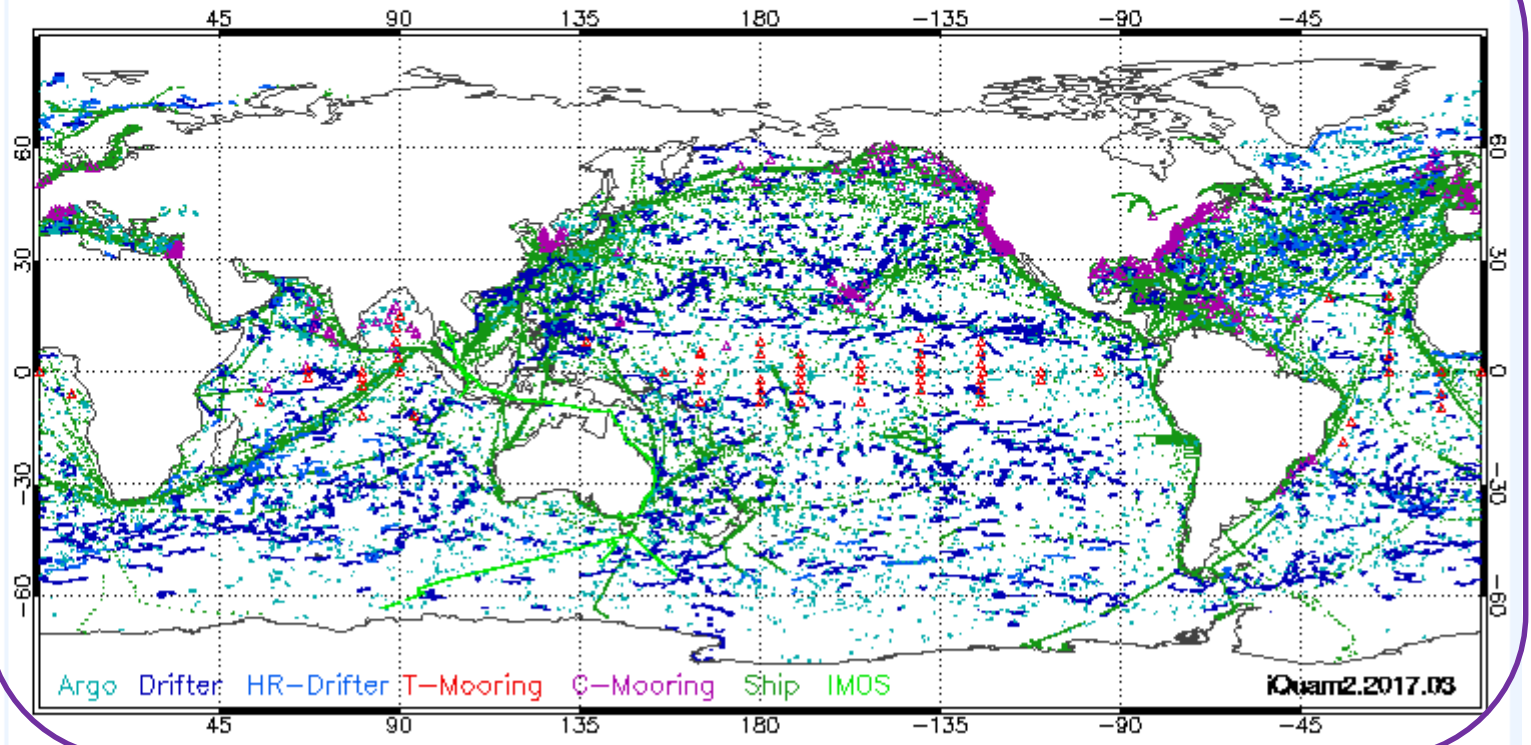
Month Day

Ref SST used in QC

Reyn CMC

QCed Outlier

All Platforms | Argo | Drifter | HR-Drifter | T-Mooring | C-Mooring | CRW | Ship | IMOS



- Argo - Argo Floats
- Drifter - Conventional drifters
- HR-Drifter - High-Resolution Drifters
- T-Mooring - Tropical Moorings
- C-Mooring - Coastal Moorings
- CRW - Coral Reef Watch Buoys
- Ship - Conventional ships
- IMOS - IMOS Ships

Symbol = one observation.

Monitor Interface (2)

iQUAM

Maps | Statistics | Time Series | Platforms

2017 ▼ 03 ▼ 26 ▼

◉ Month ○ Day

Ref SST used in QC
☑ Reyn ☐ CMC

Ref SST used in Monitoring
○ Reyn ◉ CMC

N_Obs - number of obs;
N_QC - number of obs passed QC;
DR,GL,TS,SG,RS,XP,PH,XQ - nobs detected by each check:

- AL - All checks combined.
- DR - Duplicate Removal
- GL - Geo-Location
- TS - Travel-Speed (aka. Tracking)
- SG - SST-Gradient (aka. Spike)
- RS - Ref SST (aka. background); 1 - Reynolds, 2 - CMC
- XP - Cross-Platform (aka. buddy). Performed on top of RS. 1- Reynolds, 2 - CMC
- PH - Performance History (aka. iQuam blacklist)
- XQ - External QC (from input data)

Statistics are calculated over (In situ - Ref SST).
In situ: obs that passed iQuam QC
Ref1 = Reynolds; Ref2 = CMC

Note: N_Mtchp - number of (in situ - Ref) match ups. (Smaller than N_QC due to missing Ref SST in some points.)

For more information, see About.

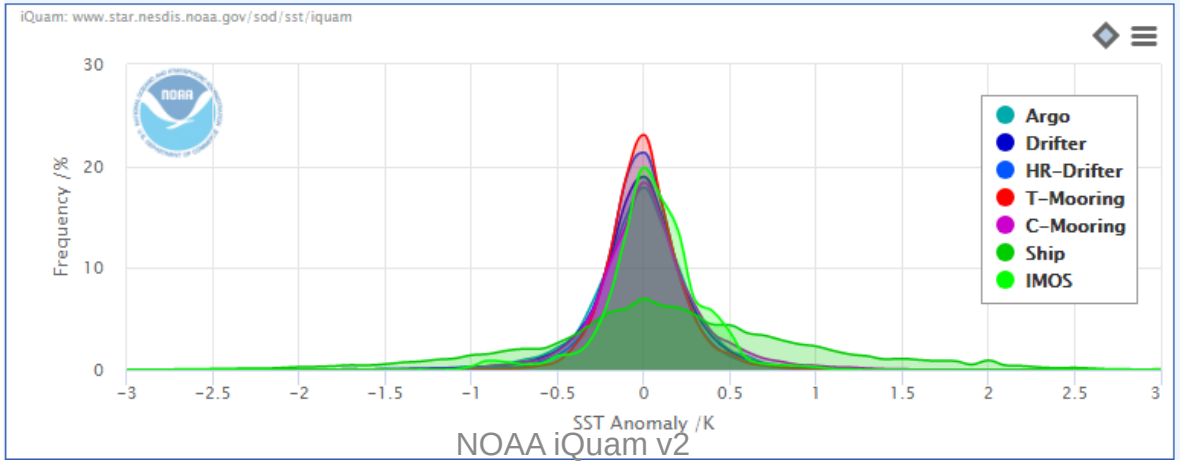
QC Statistics - NOBS | QC Statistics - Percent

Platform	N_ID	N_Obs	N_QC	AL	DR	GL	TS	SG	RS	XP	PH	XQ
Argo	3,771	9,495	8,914	581	0	0	0	0	392	373	0	208
Drifter	1,578	602,147	555,279	46,868	1,377	8,817	119	787	32,155	32,155	3,613	0
HR-Drifter	266	125,642	96,410	29,232	0	18,949	41	87	9,934	9,934	221	96,410
T-Mooring	62	23,132	22,016	1,116	89	1	2	4	902	853	167	0
C-Mooring	294	215,950	201,111	14,839	0	1	7,123	321	7,101	7,056	338	0
Ship	1,658	101,912	80,212	21,700	23	352	358	232	18,837	18,951	1,784	0
IMOS	4	40,988	40,638	350	0	0	0	0	63	79	0	271

In situ - Ref SST Statistics

Platform	N_Mtchp	MEAN	MED	SD	RSD	MIN	MAX	SKEW	KURT
Argo	8,914	0.04	0.04	0.33	0.24	-6.77	2.79	-1.16	25.42
Drifter	543,534	0.03	0.04	0.33	0.21	-5.22	3.89	-2.27	23.31
HR-Drifter	96,410	0.04	0.04	0.26	0.19	-3.87	3.80	-0.86	14.28
T-Mooring	21,566	0.05	0.04	0.22	0.18	-1.35	1.71	0.39	3.02
C-Mooring	196,685	0.07	0.06	0.34	0.24	-3.27	2.72	-0.11	7.03
Ship	78,187	0.21	0.17	0.85	0.67	-4.78	6.20	0.07	1.25
IMOS	40,638	0.10	0.10	0.29	0.21	-2.70	1.54	-0.43	2.85

Histograms (Normalized at NOBS) | Histograms (Normalized at MAX)



Monitor Interface (3)

iQUAM

Maps
Statistics
Time Series
Platforms

Monthly Daily

Ref SST Used in QC
Reyn CMC Both

Ref SST Used in Monitoring
Reyn CMC

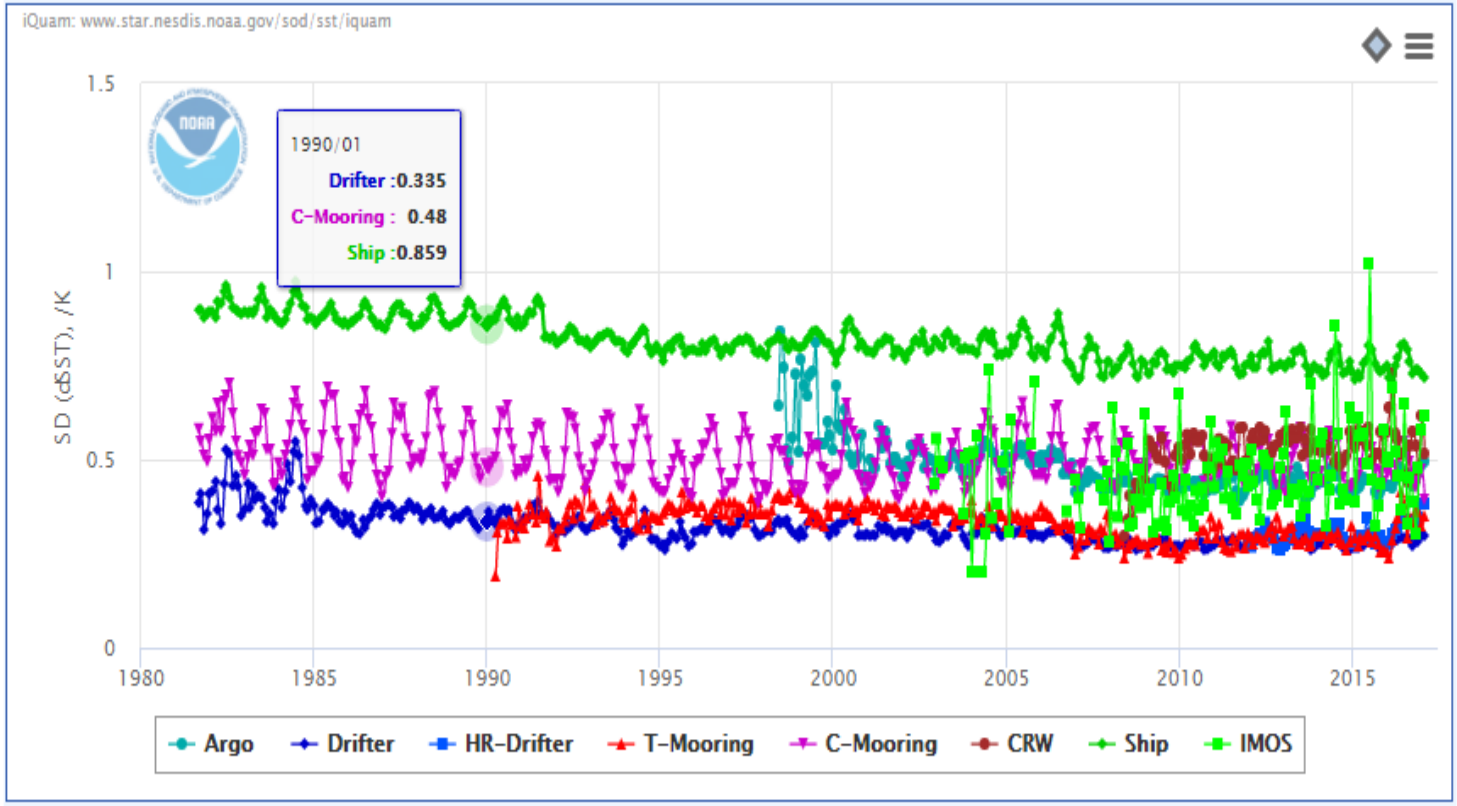
N_ID - number of platforms/IDs; N_Obs - number of obs passed QC; Mean, Median, SD, RSD, Max, Min - statistics of dSST (In situ - Ref).

QC statistics by check:

- *DR - Duplicate Removal*
- *GL - Geo-Location Check*
- *TS - Travel-Speed (aka. Tracking)*
- *SG - SST-Gradient (aka. Spike)*
- *RS - Reference SST (aka. background); 1-Reynolds, 2-CMC*
- *XP - Cross-Platform (aka. buddy). Performed on top of RS. 1-Reynolds, 2-CMC*
- *PH - Performance History (aka. iQuam blacklist)*
- *XQ - External QC (from input data)*
- *AL - All checks combined.*

N_ID | N_ID_norm | N_Obs | N_Obs_norm | Mean | Median | SD | RSD | Min | Max

Argo QC | Drifter QC | HR-Drifter QC | T-Mooring QC | C-Mooring QC | CRW QC | Ship QC | IMOS QC



Monitor Interface (4)

Monitor | Data | About

Maps
Statistics
Time Series
Platforms

2017 ▾ 03 ▾
<< < > >>

◉ Monthly ○ Daily

Ref SST Used in QC
○ Reyn ○ CMC ◉ Both

Ref SST Used in Monitoring
◉ Reyn ○ CMC

NOBS - number of obs;
N_QC - nobs of passed QC;
Err% - rate of obs denied by QC;
N_Mp - nobs of passed QC match-ups;
Mean,SD,Max,Min - statistics calculated over (In situ - Reference) SST.
In situ: obs that passed iQuam QC
Ref: Reynolds or CMC

DR,GL,TS,SG,RS,XP,PH,XQ - nobs detected by each check

- *AL - All checks combined.*
- *DR - Duplicate Removal*
- *GL - Geo-Location*
- *TS - Travel-Speed (aka. Tracking)*
- *SG - SST-Gradient (aka. Spike)*
- *RS - Reference SST (aka. background); 1-Reynolds, 2-CMC*
- *XP - Cross-Platform (aka. buddy). Performed on top of RS. 1-Reynolds, 2-CMC*
- *PH - Performance History (aka. iQuam blacklist)*
- *XQ - External QC (from input data)*

Lat,Lon - starting location of in-situ

Tips:
Click column header to sort.
Click ID to show individual ID monitor window.

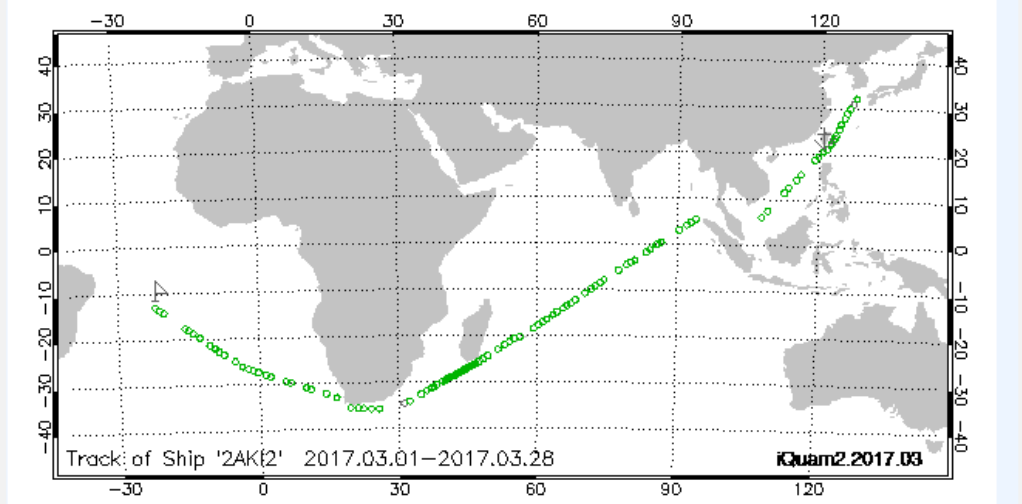
Argo | Drifter | HR-Drifter | T-Mooring | C-Mooring | **Ship** | IMOS

Showing 1 to 29 of 1,403 entries Search:

ID	NOBS	N_QC	Err%	N_Mp	Mean	SD	Min	Max	AL	DR	GL	TS	SG	RS	XP	PH	XQ	Lat	Lon
2AJU5	7	4	42.9	4	-0.20	0.63	-0.69	0.73	3	0	0	0	0	2	3	0	0	-18.6	153.4
2AKI2	120	117	2.5	115	0.59	0.51	-2.14	1.76	3	0	0	0	0	3	3	0	0	-12.9	-22.1
2AKI3	17	17	0.0	15	0.50	0.31	-0.17	0.81	0	0	0	0	0	0	0	0	0	4.4	80.0
2AKI4	6	6	0.0	6	0.67	0.43	0.35	1.46	0	0	0	0	0	0	0	0	0	3.2	122.6
2ARS4	13	13	0.0	13	0.38	0.46	-0.10	1.13	0	0	0	0	0	0	0	0	0	57.1	2.2
2BOK5	7	1	85.7	1	1.58		1.58	1.58	6	0	0	0	0	6	6	0	0	52.9	-166.3
2BUH7	2	2	0.0	2	-0.47	0.91	-1.12	0.17	0	0	0	0	0	0	0	0	0	50.8	-133.0
2CWB2	84	68	19.1	51	-0.25	0.80	-2.10	1.51	16	0	1	0	2	13	13	0	0	29.1	-93.7
2DTQ2	6	4	33.3	4	-0.04	0.68	-0.59	0.92	2	0	0	1	0	1	1	0	0	49.2	178.6
2FGX5	56	46	17.9	45	0.41	0.66	-1.05	2.15	10	0	0	0	0	8	8	2	0	26.8	-17.2
2FRE8	18	17																	
2GNG3	36	34																	
2GYL6	17	17																	
2HCH5	11	10																	
2HDG2	34	32																	
2HDG3	2	2																	
2HFZ6	32	28																	
2HFZ7	45	44																	
2HHG5	58	56																	
2ICH7	23	0																	
2ICH8	19	5																	
2ICH9	36	36																	
2ICI2	40	40																	
2ICI3	55	46																	
2ICI4	25	16																	
2ICI5	45	43																	
2ICI6	3	3																	
2ICI9	112	111																	

Platform '2AKI2'

Track map for the month | SST anomaly for the month | Performance in history



FTP Interface

Monitor Data About

Download from FTP

Data are in self-documented NetCDF4 format. Refer to attributes for more information.

Suggested usage of quality_level:

- *high-accuracy applications: quality_level == 5*
- *general applications: quality_level == 4*
- *advanced users: refer to definitions of iquam_flags and original_flags.*

All statistics in iQuam page are for "high accuracy" data only, i.e (quality_level == 5).

Quality level and flags are only set for SST. Other measurements in iQuam have not been QCed.

Data are organized in monthly files. Latest file isrefreshed every 12hrs with a 2hr latency.

File Name	Update Time
201703-STAR-L2i_GHRSST-SST-iQuam-V2.00-v01.0-fv00.0.nc	2017-03-28 10:16
201702-STAR-L2i_GHRSST-SST-iQuam-V2.00-v01.0-fv01.0.nc	2017-03-01 10:30
201701-STAR-L2i_GHRSST-SST-iQuam-V2.00-v01.0-fv01.0.nc	2017-02-02 12:32
201612-STAR-L2i_GHRSST-SST-iQuam-V2.00-v01.0-fv01.0.nc	2017-01-06 15:25
201611-STAR-L2i_GHRSST-SST-iQuam-V2.00-v01.0-fv01.0.nc	2016-12-02 01:13
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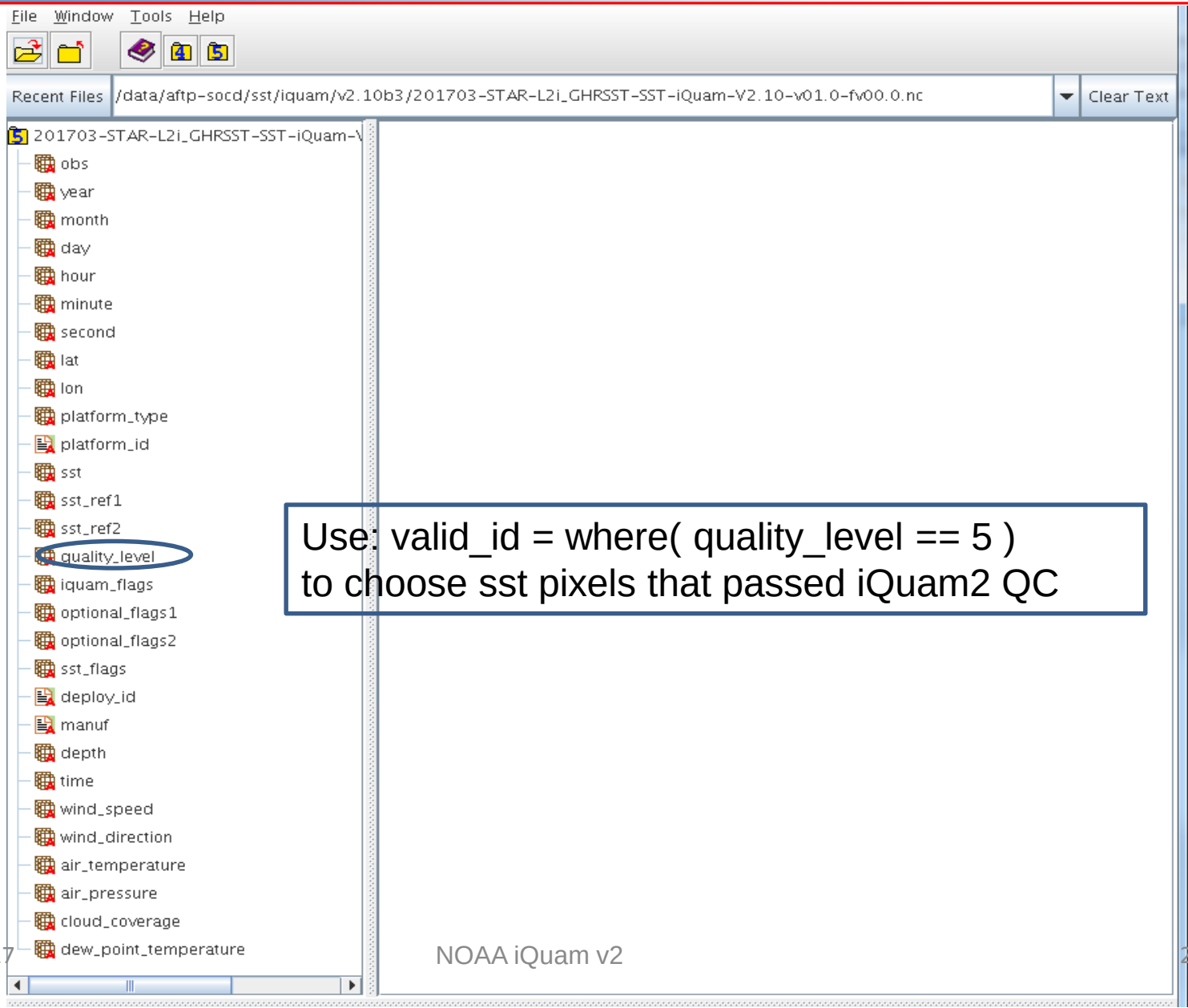
File format (opened in hdfview)



Use: valid_id = where(quality_level == 5)
to choose sst pixels that passed iQuam2 QC

Help Page

iQUAM

Monitor Data About

- System Overview
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- Acknowledgement

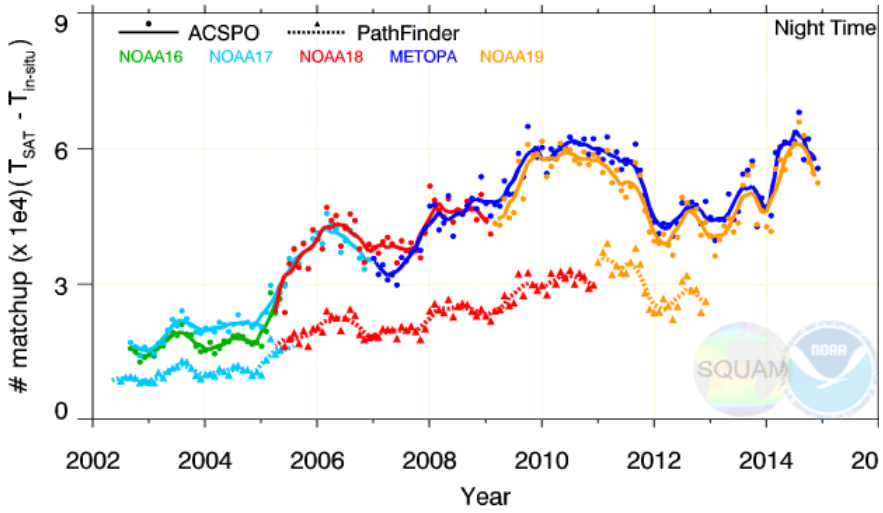
Journal Papers

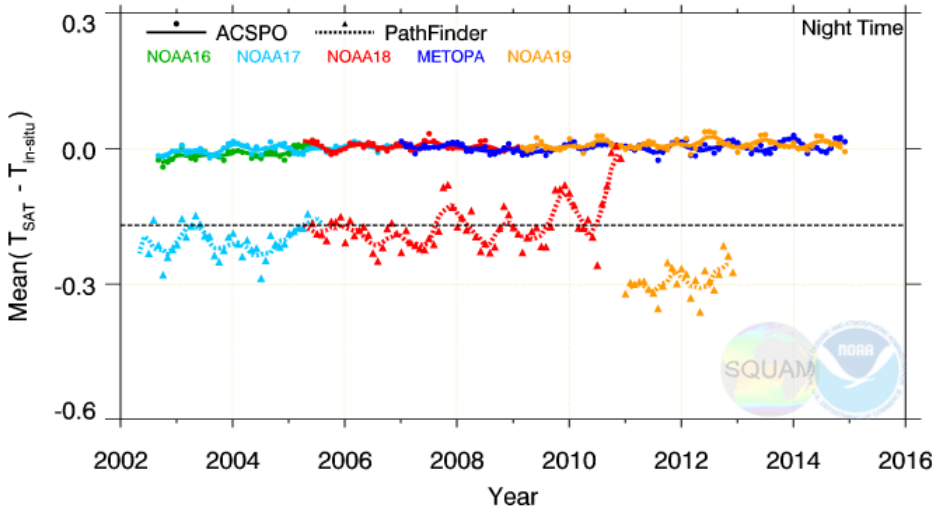
- Xu, F. and A. Ignatov, 2014: *in situ* SST quality monitor (*i*Quam), JTECH. link
- Xu, F. and A. Ignatov, 2010: Evaluation of *in situ* SSTs for use in the calibration and validation of satellite retrievals, JGR. link

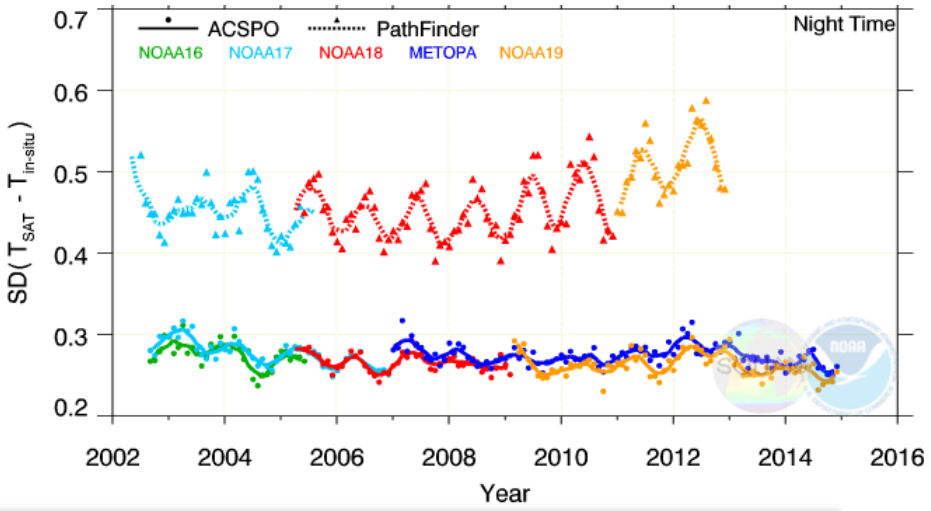
Conference Presentations

- Ignatov, A., F. Xu, and X. Zhou, 2014: In situ SST Quality Monitor (*i*Quam), CLIMAR4 Workshop, Asheville, NC, June 2014.link
- Ignatov, A. and Xu, F., 2013: *in situ* SST quality monitor: from *i*Quam1 to *i*Quam2, 14th GHRSST meeting, Woods Hole, MA, July 2013. download
- Xu, F. and A. Ignatov, 2010: Implementation and evaluation of quality control for *in situ* SST for use in satellite Cal/Val, 2010 AGU Ocean Sciences Meeting, Portland, OR, Feb 2010. download

Val of AVHRR GAC RAN1 Against Drifters + Tropical Moorings



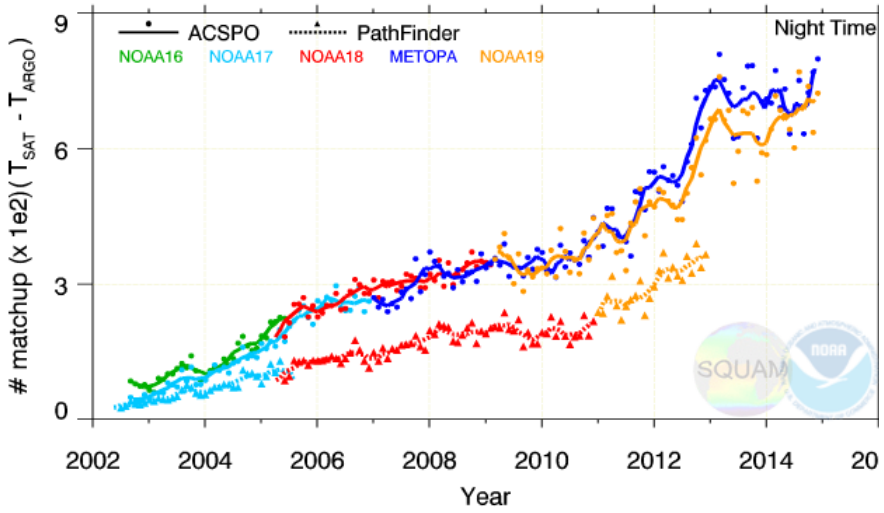


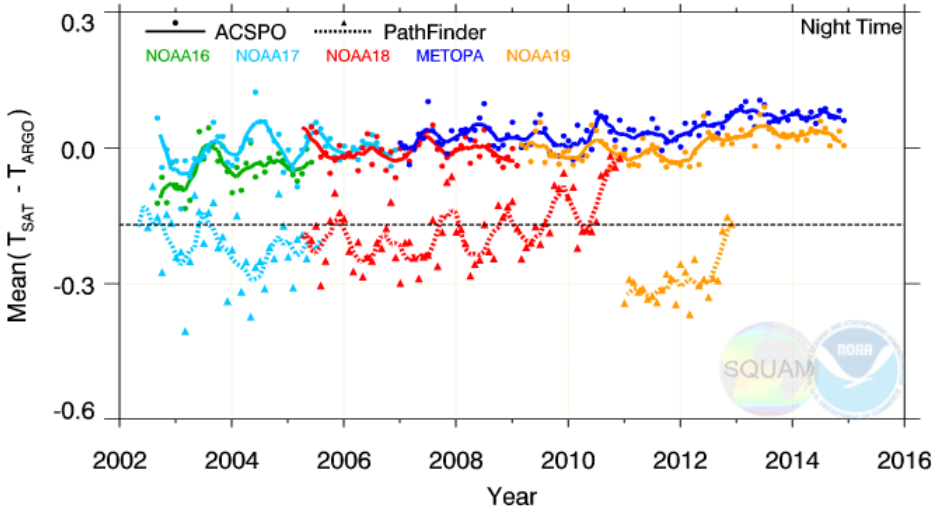


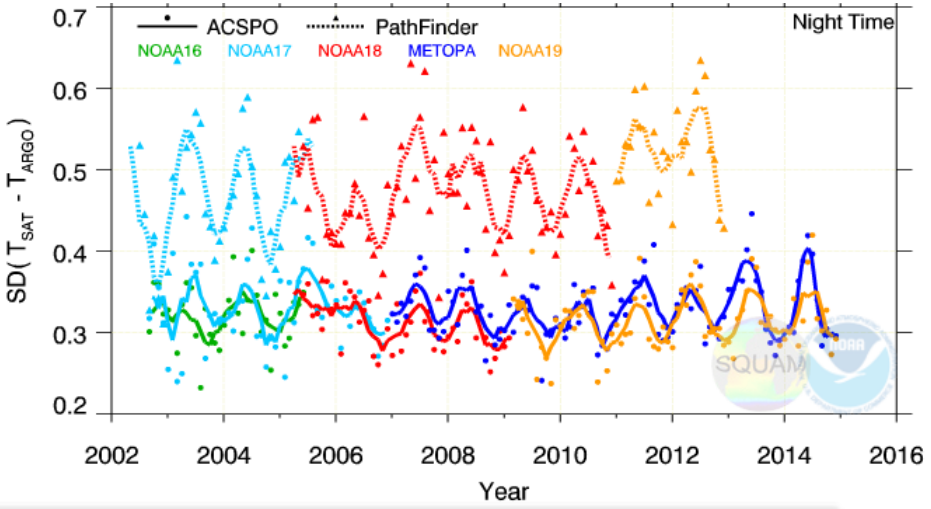
Ignatov, et al., AVHRR GAC SST Reanalysis Version 1 (RAN1), Remote Sensing, 2016

Fig. 1: Drifter and Tropical mooring matchup with Satellite SST, **sample number** (left), **mean bias** (right upper) and **standard deviation** (right lower)

Val of AVHRR GAC RAN1 Against Argo Floats



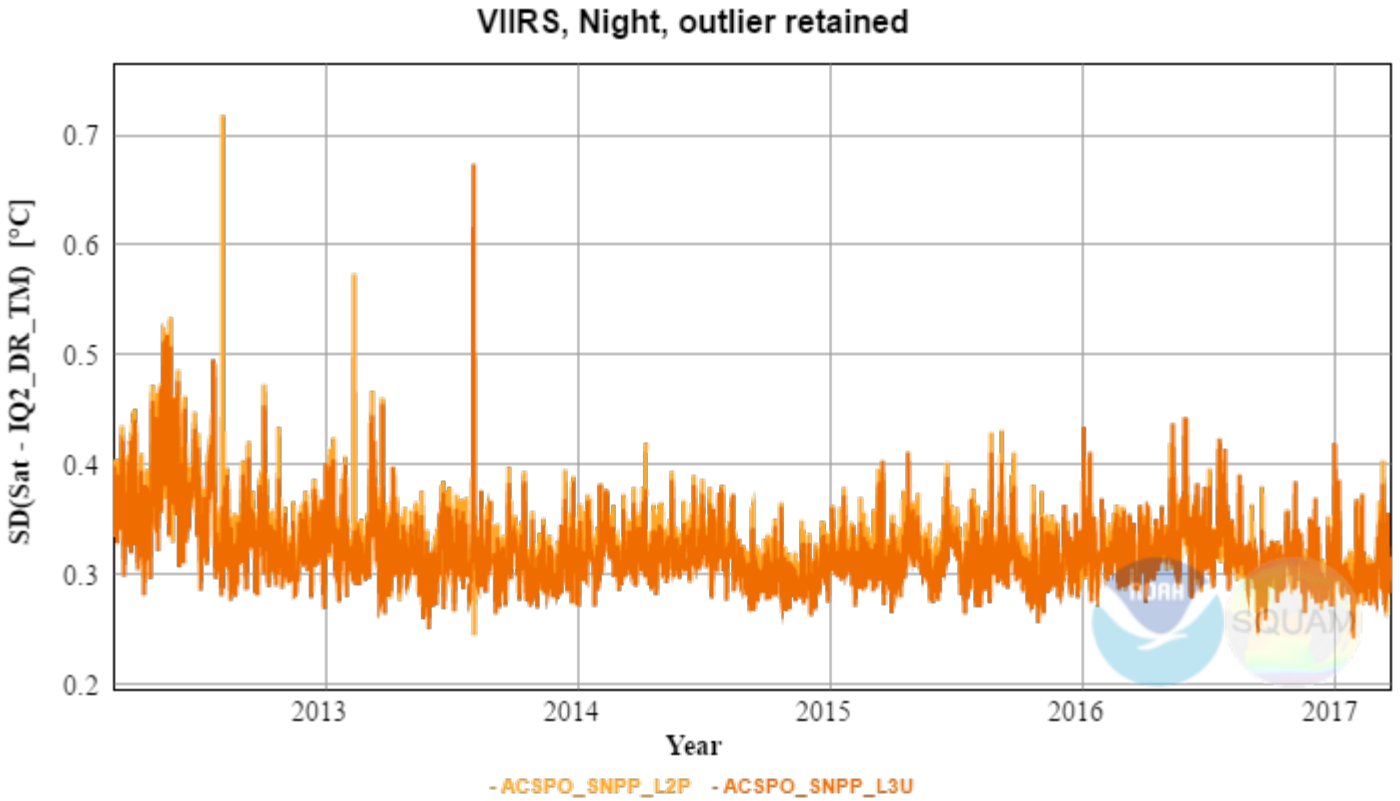




See more plots on squam2/polar at:
www.star.nesdis.noaa.gov/socd/sst/squam2/polar/avhrrgac/

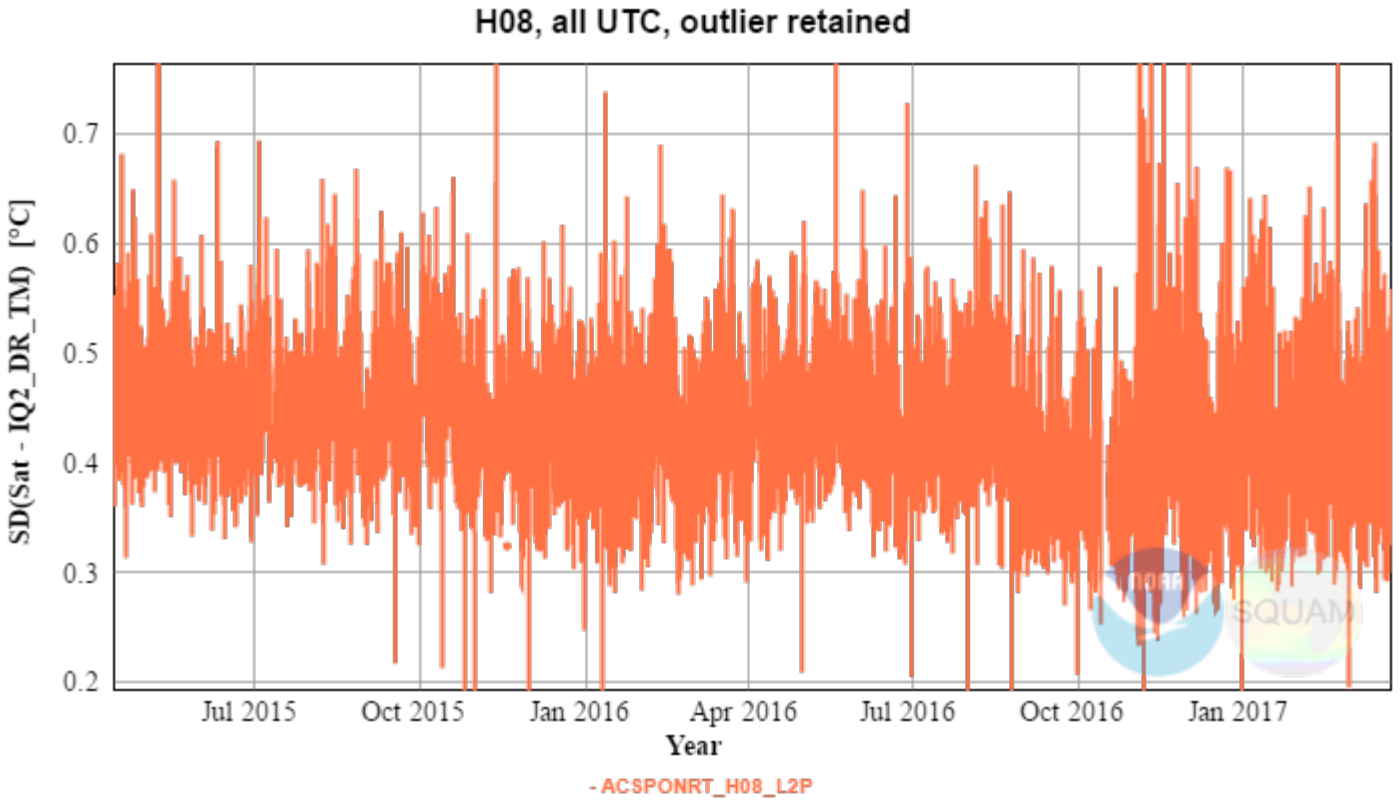
Fig. 2: Argo floats matchup with Satellite SST, **sample number** (left), **mean bias** (right upper) and **standard deviation** (right lower)

Standard Deviation of VIIRS SST Against Drifters + Tropical Moorings



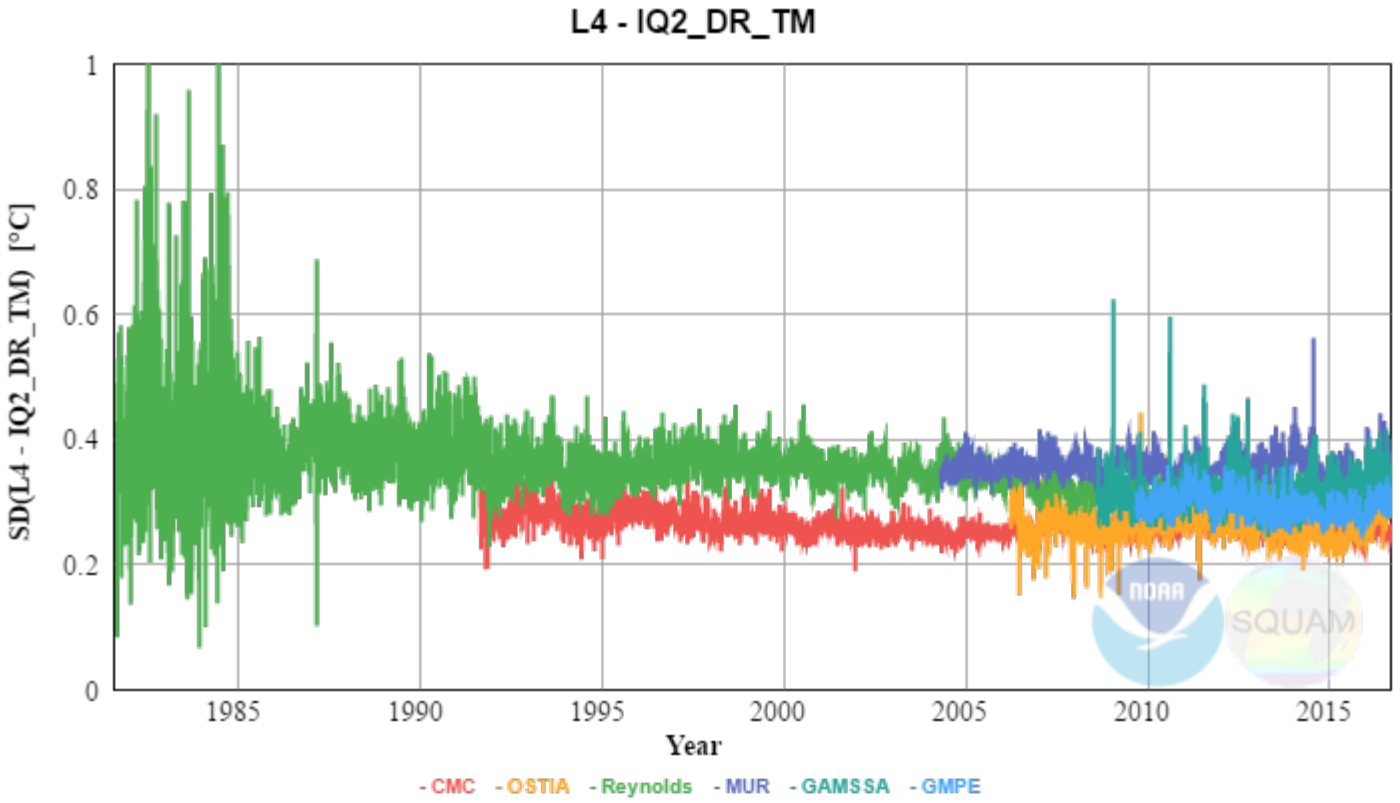
See more plots on squam2/polar at: www.star.nesdis.noaa.gov/socd/sst/squam2/polar/viirs/

Comparison with GEO



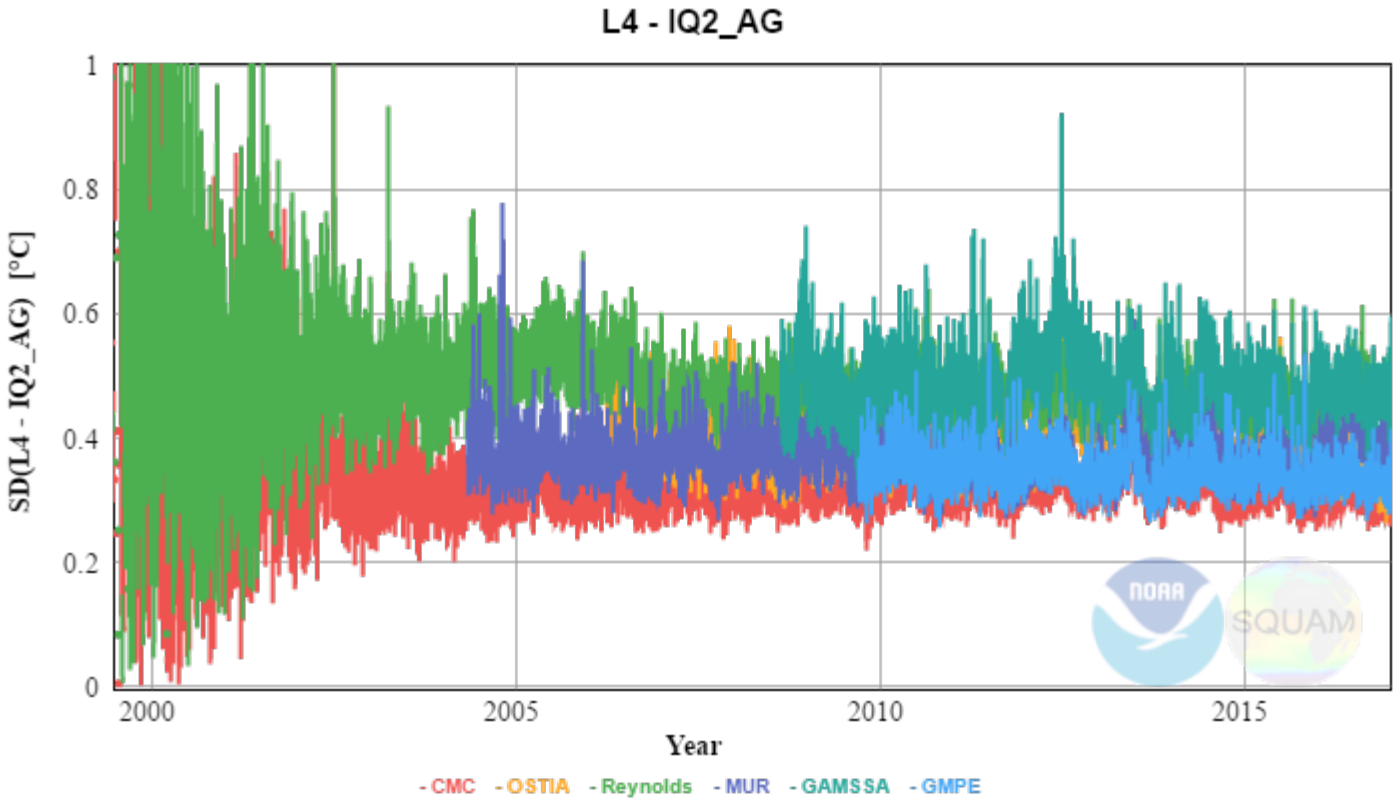
See more plots on squam2/geo at: www.star.nesdis.noaa.gov/socd/sst/squam2/geo/ahi_abi/

Comparison with L4 (1)



See more plots on squam2/analysis at: www.star.nesdis.noaa.gov/socd/sst/squam2/analysis/l4

Comparison with L4 (2)



See more plots on squam2/analysis at: www.star.nesdis.noaa.gov/socd/sst/squam2/analysis/l4

Conclusion and Future Work

Summary of enhancements in iQuam2

- ✓ Longer time series cover full satellite era (Sep 1981 – on)
- ✓ Improved QC
- ✓ Improved web interface
- ✓ Add more *in situ* data
- ✓ Change output data files to NetCDF4

Ongoing work

1. Collect users' feedback and implement iQuam2. Retire iQuam1
2. Archive w/GHRSST (PO.DAAC/NCEI). Document in literature
3. Transition to *i*Quam2 in all NOAA Cal/Val applications including SQUAM
4. Work towards *i*Quam3
   a) Add more *in-situ* data types from SAMOS Ships, Ocean Profilers et al.
   b) Test 3-way error analysis, to determine errors in individual *in situ* data and append sses
   c) Include ship radiometers?

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Thank you!
Questions? Comments?