Provisional Maturity Science Review For NOAA-21 SST

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JPSS/GOES-R Data Product Validation Maturity Stages - COMMON DEFINITIONS (Nominal Mission)

1. Beta

- Product is minimally validated, and may still contain significant identified and unidentified errors.
- Information/data from validation efforts can be used to make initial qualitative or very limited quantitative assessments regarding product fitness-for-purpose.
- Documentation of product performance and identified product performance anomalies, including recommended remediation strategies, exists.

2. Provisional

- Product performance has been demonstrated through analysis of a large, but still limited (i.e., not necessarily globally or seasonally representative) number of independent measurements obtained from selected locations, time periods, or field campaign efforts.
- Product analyses are sufficient for qualitative, and limited quantitative, determination of product fitness-for-purpose.
- Documentation of product performance, testing involving product fixes, identified product performance anomalies, including recommended remediation strategies, exists.
- Product is recommended for potential operational use (user decision) and in scientific publications after consulting product status documents.

3. Validated

- Product performance has been demonstrated over a large and wide range of representative conditions (i.e., global, seasonal).
- Comprehensive documentation of product performance exists that includes all known product anomalies and their recommended remediation strategies for a full range of retrieval conditions and severity level.
- Product analyses are sufficient for full qualitative and quantitative determination of product fitness-for-purpose.
- Product is ready for operational use based on documented validation findings and user feedback.
- Product validation, quality assurance, and algorithm stewardship continue through the lifetime of the instrument.

Maturity Review - Entry Criteria

- Product Requirements
- Pre-launch Performance Matrix/Waivers
- Provisional Maturity Performance Validation
  - On-orbit instrument performance assessment
    - Identify instrument/product characteristics verified/validated
    - Pre-launch concerns/waivers, mitigation and evaluation attempts with on-orbit data
- Users/Downstream-Products feedback
- Risks, Actions, Mitigations
  - Potential issues, concerns
- Path forward to the Validated maturity stage
- Summary

Maturity Review - Exit Criteria

- Provisional Maturity Performance is well characterized and meets/exceeds the requirements:
  - On-orbit instrument performance assessment
    - Provide summary for each identified instrument and product characteristic you have validated/verified as part of the entry criteria
    - Provide summary of pre-launch concerns/waivers mitigations/evaluation and address whether any of them are still a concern that raises any risk.
- Updated Maturity Review Slide Package addressing review committee's comments for:
  - Cal/Val Plan and Schedules
  - Product Requirements
  - Provisional Maturity Performance
  - Risks, Actions, Mitigations
  - Path forward (to the next maturity stage)

NOAA-21 Visible Infrared Imaging Radiometer Suite (VIIRS) Sea Surface Temperature (SST)

PROVISIONAL MATURITY REVIEW

Outline

- Algorithm Cal/Val Team Members
- Product Overview/Requirements
- Evaluation of algorithm performance to specification requirements
  - Algorithm version, processing environment
  - Evaluation of the effect of required algorithm inputs
  - Quality flag analysis/validation
  - Error Budget
- User Feedback
- Downstream Product Feedback
- Risks, Actions, and Mitigations
- Documentation (Science Maturity Check List)
- Conclusion
- Path Forward
- Potential Benefits of 3 JPSS Satellites

NOAA-21 SST Algorithm and Cal/Val Team

Algorithm Cal/Val Team Members

Name	Organization	Major Task
Ignatov, Sasha	STAR	JPSS Algorithm & Cal/Val Lead
Jonasson, Olafur	STAR-GST	SST Algorithm Training; SST Reanalysis (RAN); SST Quality Monitor (SQUAM/MICROS); In situ match-ups; SST data collation (L3S-LEO)
Petrenko, Boris	STAR-GST	ACSPO Clear-Sky Mask; SST Algorithms; Error Characterization
Gladkova, Irina	STAR–CCNY CREST/GST	SST data collation; SST/Clear-Sky Mask and Resampling/Pattern Recognition/Ocean Fronts Algorithms
Kihai, Yury	STAR-GST	SST Hardware; ACSPO L2P Code; ARMS
Johnson, Frank	STAR-GST	SST system administrator; ARMS; Processing software (Airflow)
Pryamitsyn, Victor	STAR-GST	Assisted with analysis of long-term trends in VIIRS SST
Roy, Priyanka	ASSISTT-GAMA-1	ASSISTT liaison with SST team
Sheekela Baker-Yeboah	OSPO	OSPO PAL

ACSPO VIIRS SST Bands

- VIIRS SST is produced using the NOAA enterprise Advanced Clear Sky Processor for Ocean (ACSPO) system
- ACSPO produces SST from low earth orbit (LEO: VIIRS, AVHRR GAC/FRAC & MODIS) and geostationary (GEO: ABI, AHI, FCI) sensors
- Mid and longwave IR window bands are used to retrieve SST in clear-sky conditions
- Atmospherically transparent midwave bands cannot be used during daytime due to contribution from reflected solar insolation, but result in more accurate SST retrievals during nighttime
- ACSPO VIIRS clear-sky mask also employs two reflectance bands centered at 0.67/0.86μm (M5/M7) during daytime (equivalent bands also used for other sensors when available)

Algorithm	Emissive Bands Used
VIIRS (night)	3.7 (M12), 8.6 (M14), 11 (M15), 12 μm (M16)
VIIRS (day)	8.6 (M14), 11 (M15), 12 μm (M16)

Algorithm	Emissive Bands Used
AVHRR/ MODIS (night)	3.7, 11, 12 μm
AVHRR/ MODIS (day)	11, 12 μm

Algorithm	Emissive Bands Used
ABI/AHI/FCI (day & night)	8.5, 10.3, 11.2 & 12.3 μm

ACSPO v2.80 VIIRS SST Algorithms

Day:

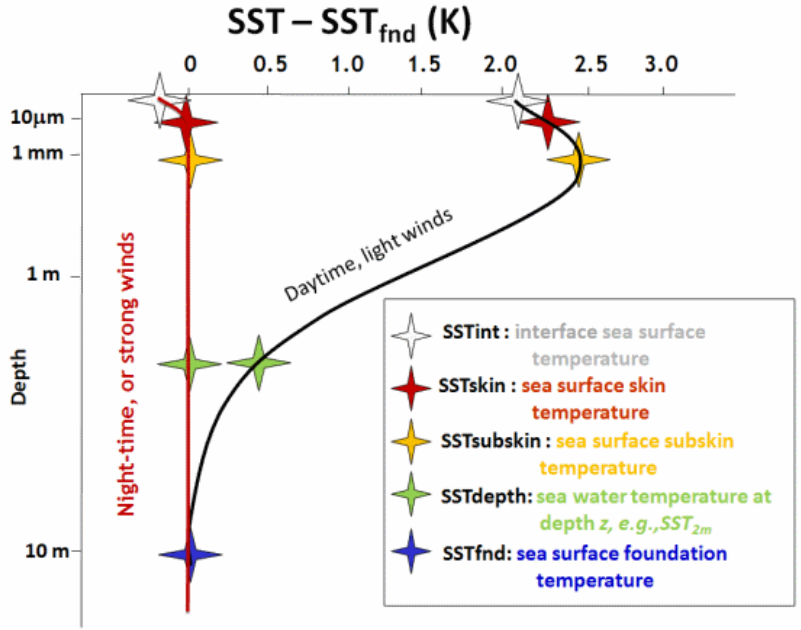
$$T_S = a_0 + a_1 S_\theta + a_2 T_{11} + a_3(T_{11}-T_{8.6}) + a_4(T_{11}-T_{12}) + [a_5 T_{11} + a_6(T_{11}-T_{8.6}) + a_7(T_{11}-T_{12})]S_\theta + [a_8(T_{11}-T_{8.6}) + a_9(T_{11}-T_{12})]T_0$$

Night:

$$T_S = a_0 + a_1 S_\theta + a_2 T_{11} + a_3(T_{11}-T_{3.7}) + a_4(T_{11}-T_{8.6}) + a_5(T_{11}-T_{12}) + [a_6 T_{11} + a_7(T_{11}-T_{3.7}) + a_8(T_{11}-T_{8.6}) + a_9(T_{11}-T_{12})]S_\theta + [a_{10}(T_{11}-T_{3.7}) + a_{11}(T_{11}-T_{8.6}) + a_{12}(T_{11}-T_{12})]T_S^0$$

- ACSPO files report ‘subskin’ SST (depth of ~1mm) calculated using the Non-Linear SST (NLSST) equations listed above for day and night
- ACSPO also reports ‘depth’ SST, which is a proxy of SST at typical drifting buoy depth of ~0.2m
- ‘Depth’ SST is calculated using the NLSST, but with coefficients stratified in the space of regressors (piecewise regression; PWR)
- Regression coefficients trained using matchups with SST from drifting and tropical moored buoys
- 1 month of matchups is often sufficient to train ‘subskin’ SST. 6-12 months of matchups needed to train ‘depth’ SST (PWR) coefficients. This provisional maturity review covers both SST products

$T_{3.7}$, $T_{8.6}$, T_{11}, T_{12}	BTs for channels centered at 3.7, 8.6, 11 and 12 μm
$S_\theta = 1/\cos(\theta) - 1$	θ is view zenith angle
T_S^0	First guess SST in °C
a_i/b_i	Regression coefficients, trained against in-situ SST



SSTfnd: SST at depths below diurnal variations

Product Requirements

DPS[1]	Description	Comment
DPS-133[1]	The Sea Surface Temperature product shall provide sea surface temperature, globally day and night, for clear conditions, for ice-free ocean, excluding lakes and rivers, at the refresh rates of the instrument	Requirement is met and exceeded. ACSPO also reports surface temperature for major lakes and rivers.
DPS-813[1]	The Sea Surface Temperature BUFR product shall provide geolocated sea surface temperature, converted from the Sea Surface Temperature product, in BUFR format.	GDS2 to BUFR file format conversion handled by NDE/OSPO
DPS-134[1]	The Sea Surface Temperature product shall provide sea surface temperatures with a measurement **precision**[2] of 0.6 kelvin over the measurement range of the instrument.	Verified against *in-situ* SST. Verification must include 18% of ocean pixels[4].
DPS-135[1]	The Sea Surface Temperature product shall provide sea surface temperature products with a measurement **accuracy**[3] of 0.2 kelvin over the measurement range of the instrument.	Verified against *in-situ* SST. Verification must include 18% of ocean pixels[4].

Processing Environment, Data Products & Versions

- **Today, both NPP and N20 ACSPO SSTs are operational at NDE and also produced in best effort mode at STAR**
  - ACSPO v2.80 is the current version
  - v2.80 data from NDE distributed via PDA & NCEI
  - v2.80 data from STAR distributed via PO.DAAC & CoastWatch
  - Complete archive of v2.80 data available in PO.DAAC (L2P/L3U) and CoastWatch (L3U only) back to the beginning of both NPP and N20 missions
  - N21 data produced at STAR will be made publicly available following this provisional maturity review
- **Three SST products from NPP/N20/N21**
  - L2P (original swath projection; 10-min granules; 144 granules/day)
  - Equal-grid 0.02° L3U (U=uncollated; 10-min granules; 144 granules/day)
  - Super collated 0.02° L3S (L3S-LEO-PM; S=super-collated; 2 granules/24hr: Day&Night)
- **Majority of ACSPO VIIRS SST users prefer L3U/L3S (OISST, GLSEA, Coast Watch, NCEP, EumetCast, NOS, BoM, JMA, Met Office)**
  - There are only two known L2P users: STAR geo-polar blended group and NCEP
  - Users are encouraged to use super-collated L3S-LEO products

ACSPO Inputs

- **Required Algorithm Inputs**
  - No upstream algorithms (ACSPO is stand-alone)
  - VIIRS SDRs
    - Day: M14/M15/M16 (+M5/M7 for masking)
    - Night: M12/M14/M15/M16
  - SST LUTs: 2 per platform/sensor (1 day, 1 night)
  - Land mask file
  - Ancillary Data: CMC L4 foundation SST; GFS/MERRA forecast/analysis (surface wind speed & atmosphere profiles of temperature and humidity)

- **Evaluation of the effect of required algorithm inputs**
  - Quality and stability of BTs in SST bands is critical for SST
  - N21 VIIRS SST is sensitive to thermal IR anomaly during warm-up/cool-down (WUCD) exercises. The SDR team has successfully mitigated the issue for NPP and N20. Work is underway in SDR Team to mitigate WUCD effects for N21, too.
  - Effect of Missing/Delayed ancillary data is mitigated by using the latest available CMC/GFS/MERRA file. There is no noticeable effect of this “graceful degradation” on the ACSPO SST, if data are missing for not too long (1-2 days). Low sensitivity to small uncertainties in SST/Atmospheric priors is expected and a positive sign

Quality Control Analysis/Validation

- **Defined Quality Flags**
  - ACSPO has quality levels (QLs). Only data with QL=5 are recommended to users. [QL=0: Missing data; QL=1: Non-SST (cloudy, probably cloudy, land, etc.); QL=2,3,4 – not used]

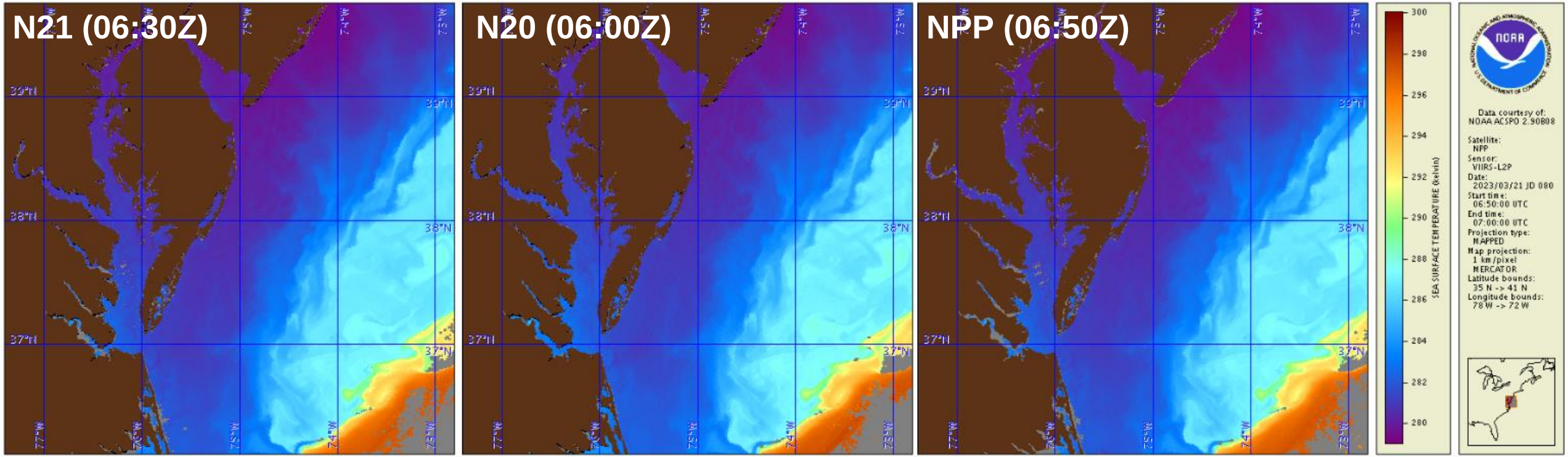
- **ACSPO Follows GHRSST Data Specifications version 2 (GDS2) standard and provides error characterization of SST in each pixel**
  - SST Single Sensor Error Statistics (SSES) in each QL=5 pixel is defined by the two extra layers in data files: Bias and SSES Standard Deviation (SD) wrt. *in-situ* SST
  - 'depth' SST is defined as 'subskin' SST – (SSES bias)
  - SSES algorithm ('depth' SST) is based on piecewise regression (PWR) algorithm and requires a longer time period (more in-situ matchups) for training than 'subskin' SST.
  - At the time of the beta review insufficient training data was available for PWR
  - Sufficient training data is now available for this provisional maturity review
  - Training data for 'depth' SST should include at least 6-12 months
  - We plan to retrain SST LUTs prior to fully validated review, and evaluate the need to replace

Evaluation of SST Performance

- **Product performance evaluation**
  - Global and Regional, using N21 L1B/SDR from 11 Feb 2023 – on
  - Validation strategies:
    1. Validation vs. global QC'ed drifters & tropical moorings, and ARGO Floats from the NOAA *in situ* Quality Monitor (*i*Quam; www.star.nesdis.noaa.gov/sod/sst/iquam/)
    2. Global comparisons with several high-quality L4 SST analyses
    3. Comparisons with NPP/N20, Aqua/Terra MODIS, Metop-B/C AVHRR FRAC
  - Long term monitoring:
    1. SST Quality Monitor (SQUAM; www.star.nesdis.noaa.gov/sod/sst/squam/)
    2. ACSPO Regional Monitor for SST (ARMS; www.star.nesdis.noaa.gov/sod/sst/arms/)
    3. Performance of full-mission VIIRS SSTs from NPP/N20 is documented in the journal paper titled "JPSS VIIRS SST Reanalysis Version 3" (doi.org/10.3390/rs14143476)

N21/N20/NPP SST Imagery Consistency

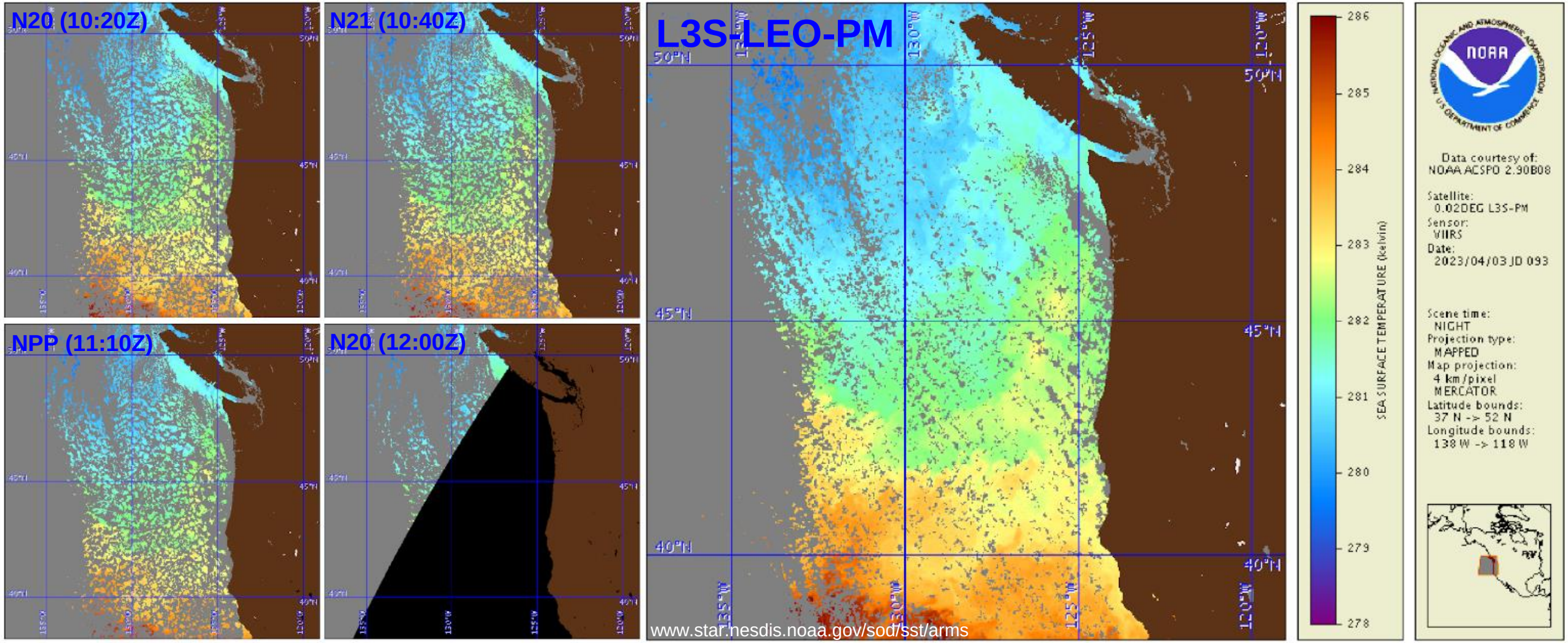
Chesapeake Bay 3 Mar 2023



- Nighttime ACSPO ‘subskin’ L2P SST imagery
- N21 VIIRS SST imagery quality is comparable to N20 and NPP
- Imagery from ACSPO Regional Monitor for SST (ARMS; www.star.nesdis.noaa.gov/sod/sst/arms/)

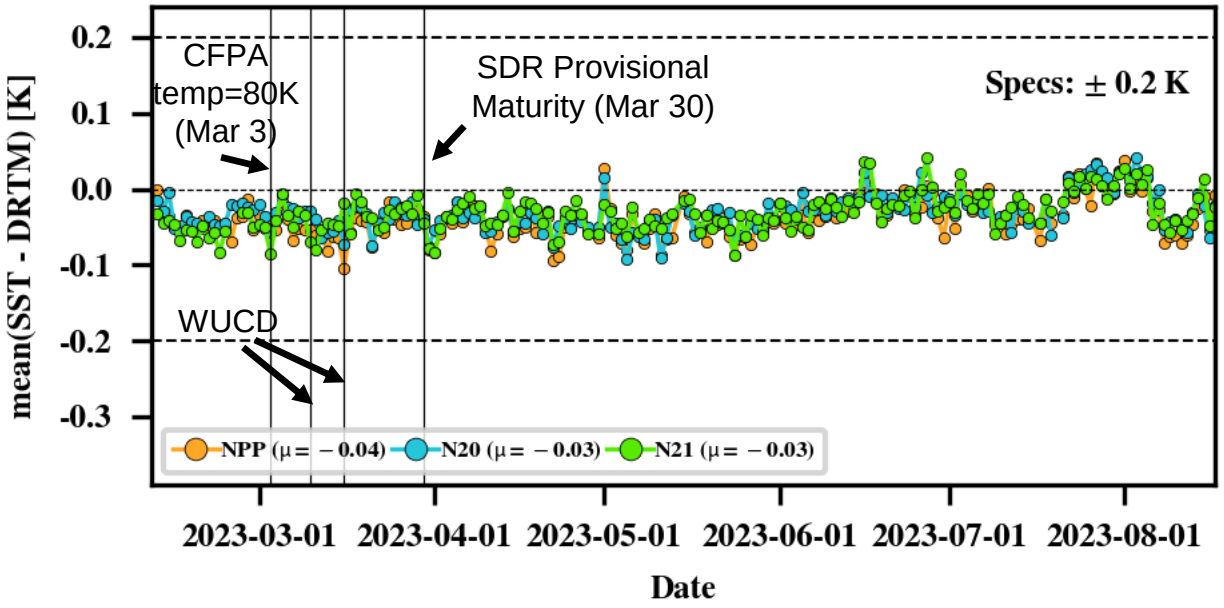
N21/N20/NPP SST Complementarity

- North-West US Coast (3 Apr 2023; nighttime ‘subskin’ SST)
- Clouds move between satellite overpasses
- Improved coverage in ACSPO L3S-LEO-PM by collating SST from multiple VIIRS overpasses (7 total; 4 shown)

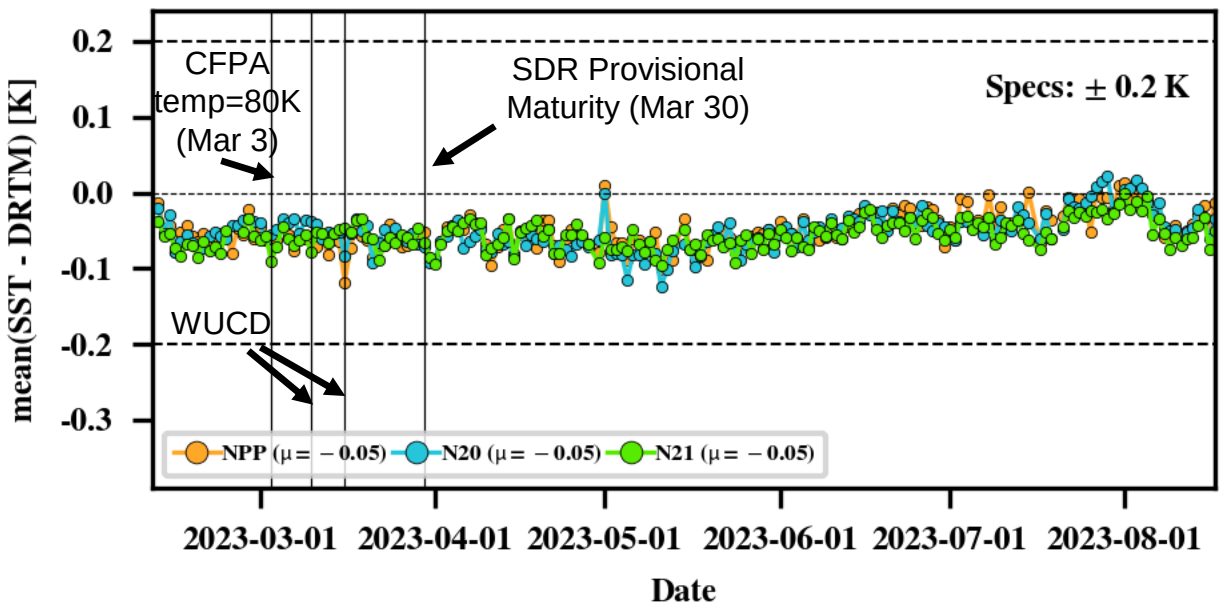


Global SST Bias wrt. *i*Quam *in situ* SST (night)

Nighttime ‘**subskin**’ SST



Nighttime ‘**depth**’ SST

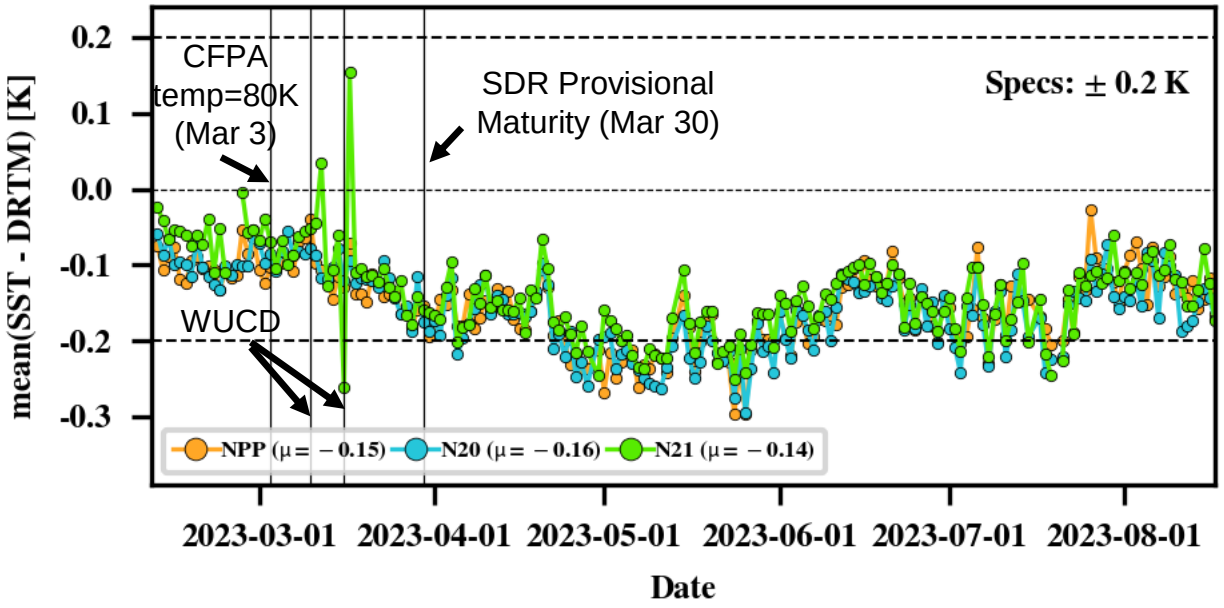


- Nighttime ‘subskin’ and ‘depth’ SST biases are close to ~0K, typically within ±0.05K
- N21, N20, and NPP statistics are very consistent
- CFPA setpoint temperatures was changed from 82 to 80 K on 3 Mar 2023 (no visible effect on nighttime SST bias)
- Two warm-up/cool-down (WUCD) events from 10-13 and 16-17 Mar 2023. Effects of WUCD on nighttime SST is minor (< 0.05 K)

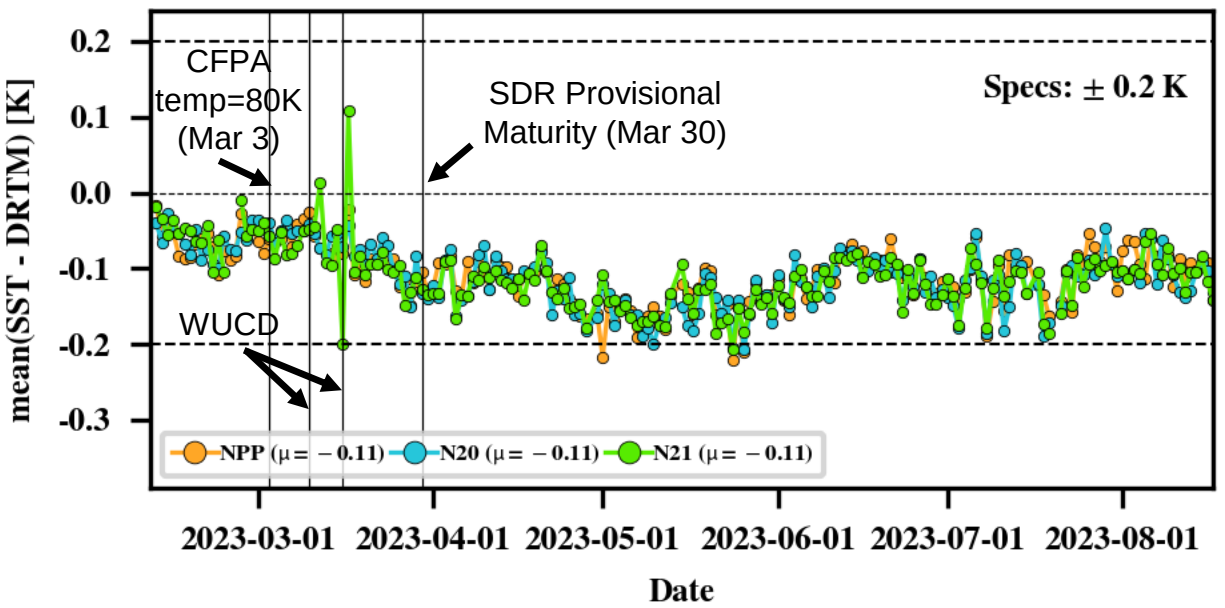
Each Data point: Global 24hr statistic supported by ~130K match-ups with drifters and tropical moorings

Global SST Bias wrt. *i*Quam *in situ* SST (day)

Daytime **'subskin'** SST



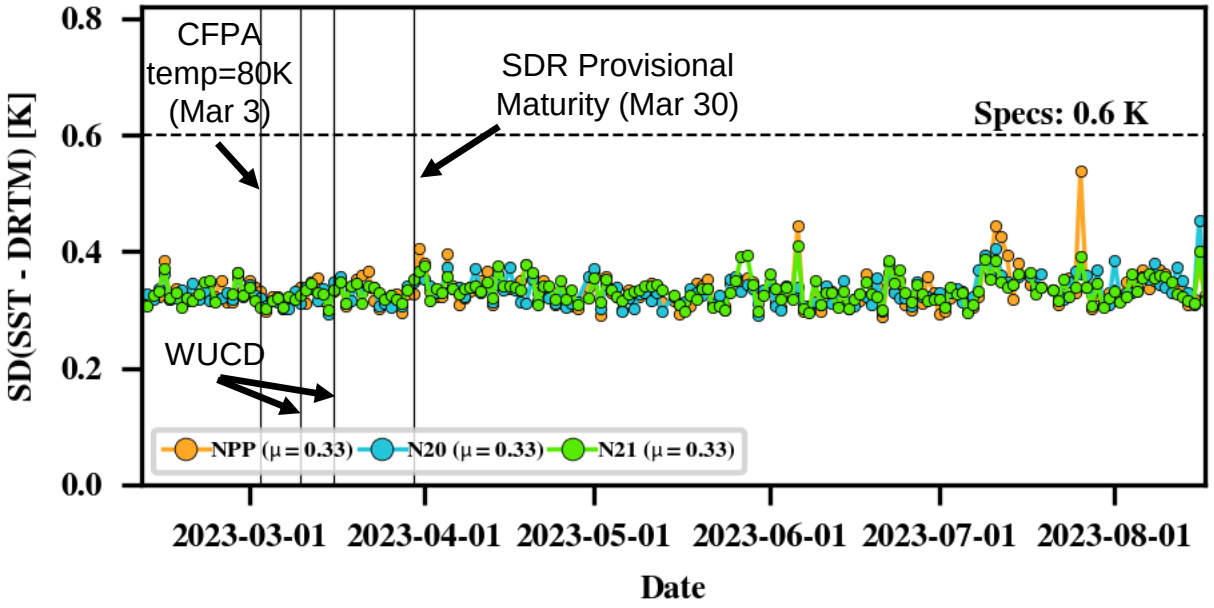
Daytime **'depth'** SST



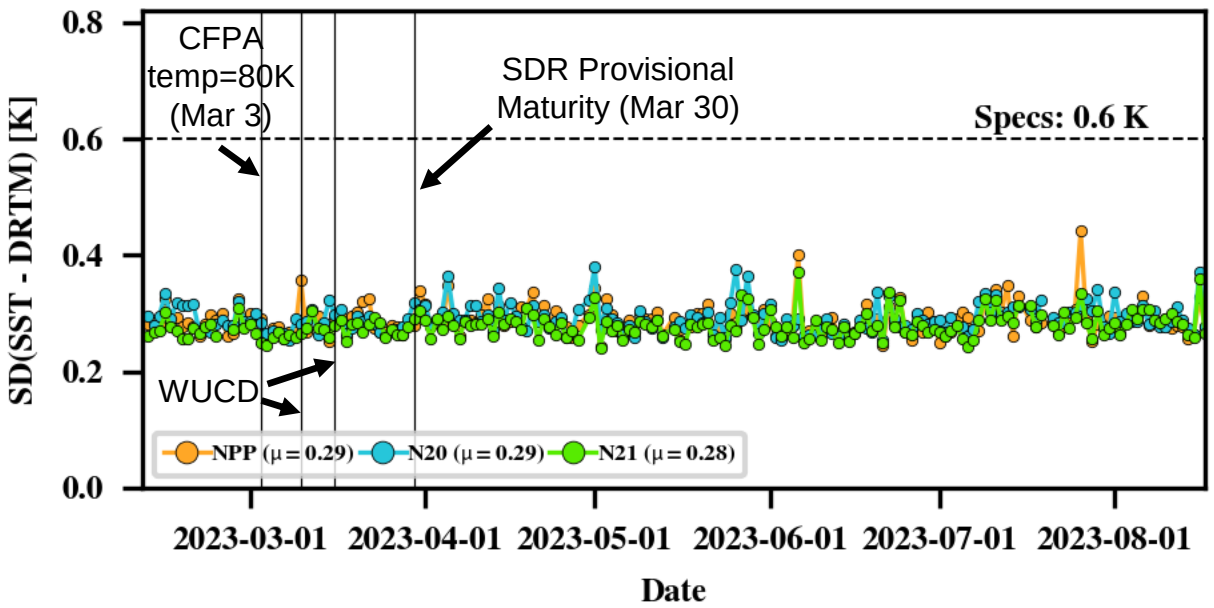
- Daytime biases are close to being within specs of ±0.2K, but larger than at night and more variable in time. They reach -0.25K, due to drift of daytime VIIRS SSTs possibly due to drift of VIIRS longwave BTs (cf. doi.org/10.3390/rs14143476)
- Global mean bias has seasonal cycle (likely due to skin-bulk SST difference) with ~0.2K amplitude (May is near the bottom)
- N21 'depth' SST mean bias is improved over 'subskin', with only 1 day outside ±0.2K
- N21 shows signs of warm ~0.05K bias vs NPP/N20 prior to CFPA temperature switch (3 Mar 2023)
- Effects of WUCDs (10-13 and 16-17 Mar 2023) on daytime SST is substantial (up to ~0.25K)
- Excluding WUCD events, N21, N20, and NPP mean bias is very consistent after 3 Mar 2023

Global SST SD wrt. *i*Quam *in situ* SST (night)

Nighttime ‘**subskin**’ SST



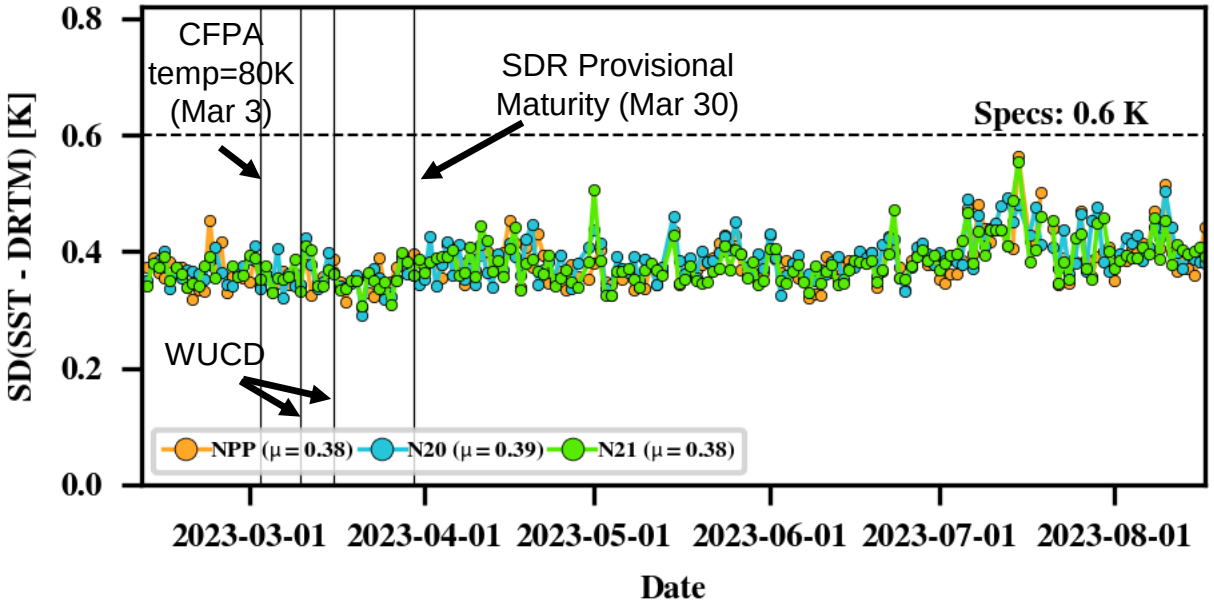
Nighttime ‘**depth**’ SST



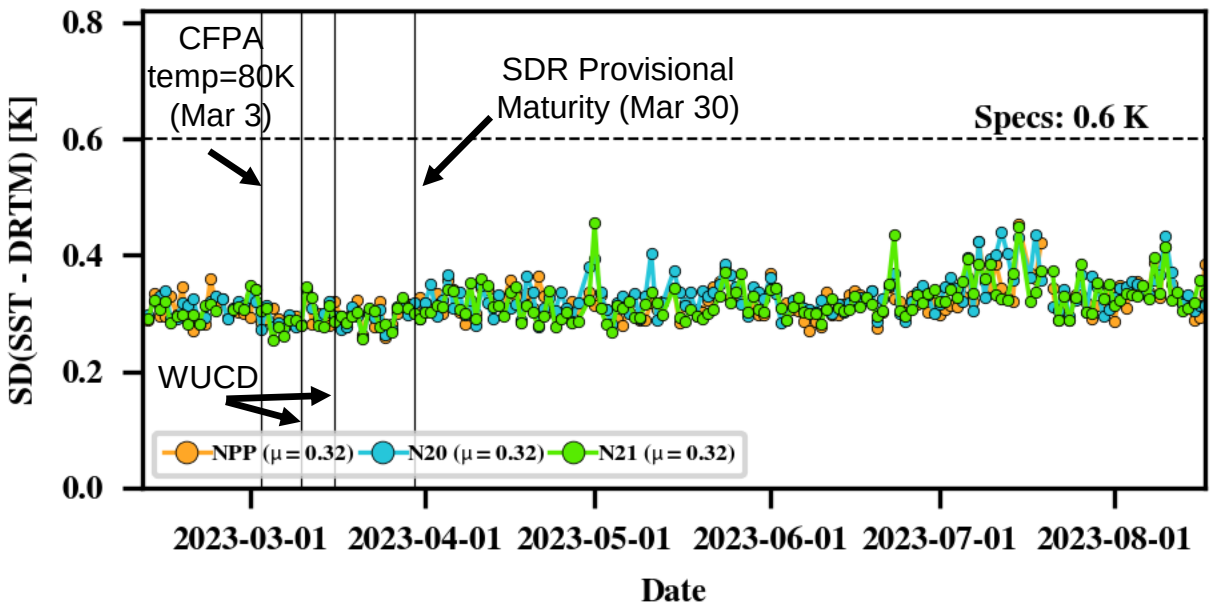
- Nighttime ‘subskin’ SDs are 0.33 K
- As expected, ‘depth’ SDs of 0.28-0.29 K are improved for ‘depth’ SST
- JPSS specs (0.6 K) are met by a wide margin
- N21 is very consistent with N20 and NPP (within 0.01 K)
- CFPA temperatures change and WUCDs have no visible effect on nighttime SST SD

Global SST SD wrt. *i*Quam *in situ* SST (day)

Daytime **'subskin'** SST



Daytime **'depth'** SST



- Daytime 'subskin' SDs are 0.38-0.39K
- SDs are improved for 'depth' SST to ~0.32K, as expected for comparison with in situ depth SST
- Higher than nighttime SDs by 0.03-0.06K but still meet JPSS specs, and exceed by a wide margin
- N21, N20, and NPP statistics are very consistent (within 0.01 K)
- CFPA temperatures change and WUCDs have no visible effect on daytime SST SD

SST Error Budget ('subskin' SST)

- From 4 Mar 2023 – pr (after CFPA change to 80 K), and excluding days with WUCD exercises
- Blue (nighttime) / Red (daytime)
- All three satellites are consistent
- 0.02 K or less difference in accuracy (global mean bias)
- 0.01 K or less difference in precision (global SD)
- 0.2% or less difference in clear-sky fraction

Attribute Analyzed	Req./ Thresh.	DPS	Pre-Launch Performance	On-orbit Performance			Meet Requirement?	Additional Comments
				NOAA-21	NOAA-20	S-NPP		
'subskin' SST Accuracy	±0.2 K	DPS-134* L1RDS-139# JERD-2151†	N/A	-0.03 K -0.15 K	-0.03 K -0.17 K	-0.04 K -0.16 K	Yes	Meets/Exceeds Specs/User's Expectations
'subskin' SST Precision	0.6 K	DPS-135* L1RDS-139# JERD-2152†	N/A	0.34 K 0.38 K	0.33 K 0.38 K	0.34 K 0.38 K	Yes	Meets/Exceeds Specs/User's Expectations
Clear-Sky fraction	18%	DPS-134* DPS-135*	N/A	19.1% 20.0%	19.2% 20.1%	19.0% 19.9%	Yes	Meets/Exceeds Specs/User's Expectations

* JPSS GSegDPS (https://www.nesdis.noaa.gov/s3/2022-03/474-01543_JPSS-GSegDPS_A.pdf)
# L1RDS (https://www.nesdis.noaa.gov/s3/2022-03/L1RDS.pdf)
† JERD (https://www.nesdis.noaa.gov/s3/2022-03/JERDV2_Version_3_Updated_11292019-mcl-FinalDRAFT-mcl.pdf)

SST Error Budget ('depth' SST)

- From 4 Mar – pr (after CFPA change to 80 K), excludes days with WUCD exercises
- Blue (nighttime) / Red (daytime)
- All three satellites are consistent
- 0.01K or less difference in accuracy (global mean bias)
- Less than 0.01K difference in precision (global SD)
- 0.3% or less difference in clear-sky fraction

Attribute Analyzed	Req./ Thresh.	DPS	Pre-Launch Performance	On-orbit Performance			Meet Requirement?	Additional Comments
				NOAA-21	NOAA-20	S-NPP		
'depth' SST Accuracy	±0.2 K	DPS-134* L1RDS-139# JERD-2151†	N/A	-0.05 K -0.12 K	-0.05 K -0.12 K	-0.05 K -0.11 K	Yes	Meets/Exceeds Specs/User's Expectations
'depth' SST Precision	0.6 K	DPS-135* L1RDS-139# JERD-2152†	N/A	0.29 K 0.32 K	0.29 K 0.32 K	0.29 K 0.32 K	Yes	Meets/Exceeds Specs/User's Expectations
Clear-Sky fraction	18%	DPS-134* DPS-135*	N/A	19.1% 20.0%	19.2% 20.1%	19.0% 19.9%	Yes	Meets/Exceeds Specs/User's Expectations

* JPSS GSegDPS (https://www.nesdis.noaa.gov/s3/2022-03/474-01543_JPSS-GSegDPS_A.pdf)
# L1RDS (https://www.nesdis.noaa.gov/s3/2022-03/L1RDS.pdf)
† JERD (https://www.nesdis.noaa.gov/s3/2022-03/JERDV2_Version_3_Updated_11292019-mcl-FinalDRAFT-mcl.pdf)

User Feedback

- ACSPO VIIRS N21 SST data will be made publicly available to users for evaluation/testing purposes following this provisional maturity review

Name	Organization	Application	User Feedback - User readiness dates for ingest of data and bringing data to operations

No External users yet

Downstream Product Feedback

Algorithm	Product	Downstream Product Feedback - Reports from downstream product teams on the dependencies and impacts
ACSPO L3S-LEO	L3S-LEO-PM (super collated SST from afternoon orbit LEO satellites)	Improved coverage by 12-13% (relative). Minor improvement to precision (~0.01 K)

Risks, Actions, and Mitigations

Identified Risk	Description	Impact	Action/Mitigation and Schedule
1	N21 VIIRS Thermal IR anomalies during WUCD exercises	High (during daytime)	SDR team works on mitigating similarly to NPP/N20 (see SDR provisional review)

Documentations

Science Maturity Check List	Yes ?
ReadMe for Data Product Users	Yes
Algorithm Theoretical Basis Document (ATBD)	Yes
Algorithm Calibration/Validation Plan	Yes
(External/Internal) Users Manual	Yes
System Maintenance Manual (for ESPC products)	Yes
Peer Reviewed Publications (Demonstrates algorithm is independently reviewed)	Yes
Regular Validation Reports (at least annually) (Demonstrates long-term performance of the algorithm)	Yes

Check List - Provisional Maturity

Provisional Maturity End State	Assessment
Product performance has been demonstrated through analysis of a large, but still limited (i.e., not necessarily globally or seasonally representative) number of independent measurements obtained from select locations, periods, and associated ground truth or field campaign efforts.	Yes
Product analysis is sufficient to communicate product performance to users relative to expectations (Performance Baseline).	Yes
Documentation of product performance exists that includes recommended remediation strategies for all anomalies and weaknesses. Any algorithm changes associated with severe anomalies have been documented, implemented, tested, and shared with the user community.	Yes
Product is ready for operational use and for use in comprehensive cal/val activities and product optimization.	Yes

Cal/Val Summary & Conclusion

- SST Team recommends SST algorithm provisional maturity as of 20 Mar 2023 @00:00 UTC
- N21, N20 & NPP SST products are highly consistent, and meet/exceed JPSS specs & users' expectations
- N21 SST anomalies during WUCD exercises
  - SDR team is aware and working towards correction (see SDR Provision Review)
  - WUCD correction was successfully implemented for NPP/N20 by SDR team
- No N21-specific caveats or reservations have been observed

Path Forward

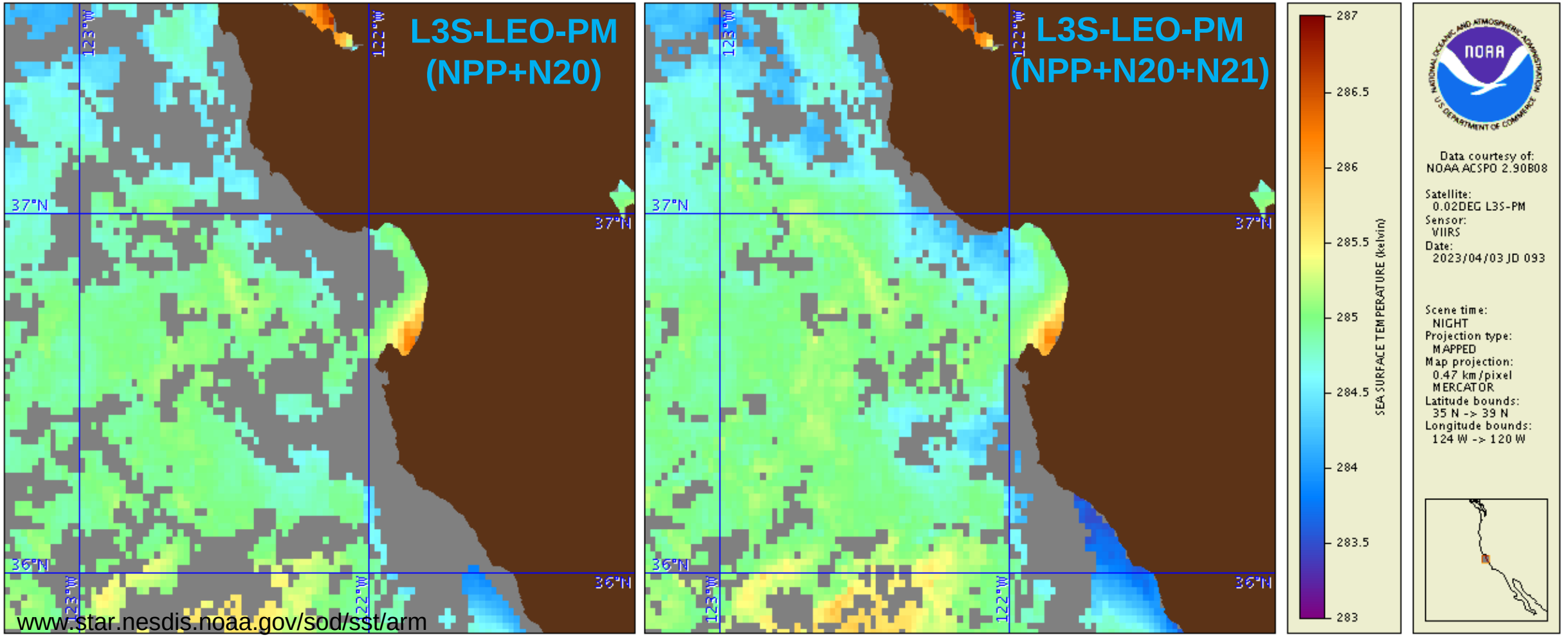
- **Lessons learned from N21 Cal Val**
  - NPP, N20 and N21 VIIRS SST products fully meet and exceed NOAA requirements and users' expectations. ACSPO VIIRS SST products are accurate and consistent
- **Planned improvements**
  - Include N21 in super-collated ACSPO products (L3S-LEO-PM)
  - Minimize residual cloud leakages in each individual product. Potentially, revisit clear-sky mask (ACSPO v3.00; estimated delivery Spring/Summer 2024)
  - Minimize cross-platform, angular, regional SST biases. Potentially, revisit the current NLSST algorithms (ACSPO v3.00; estimated delivery Spring/Summer 2024)
- **Future Cal/Val Activities/Milestones**
  - ACSPO N21 SST quality may benefit from more training data (up to a year)
  - Explore retraining ‘subskin’ and ‘depth’ SST algorithm coefficients/LUTs using longer timeseries of matchups
  - Make N21 SST data publicly available to users on CoastWatch and PO.DAAC
  - Integrate N21 into public ally available L3S-LEO product

Back-up Slides

Potential Benefits of 3 JPSS Satellites

A third JPSS satellite (N21) improves coverage in partially cloudy scenes

- Nighttime L3S-LEO-PM ‘subskin’ SST from Monterey Bay (3 Apr 2023)
- Multiple looks at the same scene at different times provides improved clear-sky coverage



www.star.nesdis.noaa.gov/sod/sst/arms

Potential Benefits of 3 JPSS Satellites

A third JPSS satellite (N21) mitigates data voids caused by clear-sky masking

- L3S-LEO-PM nighttime ‘subskin’ SST from Chesapeake Bay (2 Apr 2023)
- Multiple looks at the same scene at different facilitates improved cloud screening (red rectangle) and improved coverage (green rectangle)