Beta 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
- Beta 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 Provisional maturity stage
- Summary

Maturity Review - Exit Criteria

- Beta 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
  - Beta Maturity Performance
  - Risks, Actions, Mitigations
  - Path forward (to the next maturity stage)

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

BETA 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

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. Results 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 VIIRS SST Algorithms

Day:

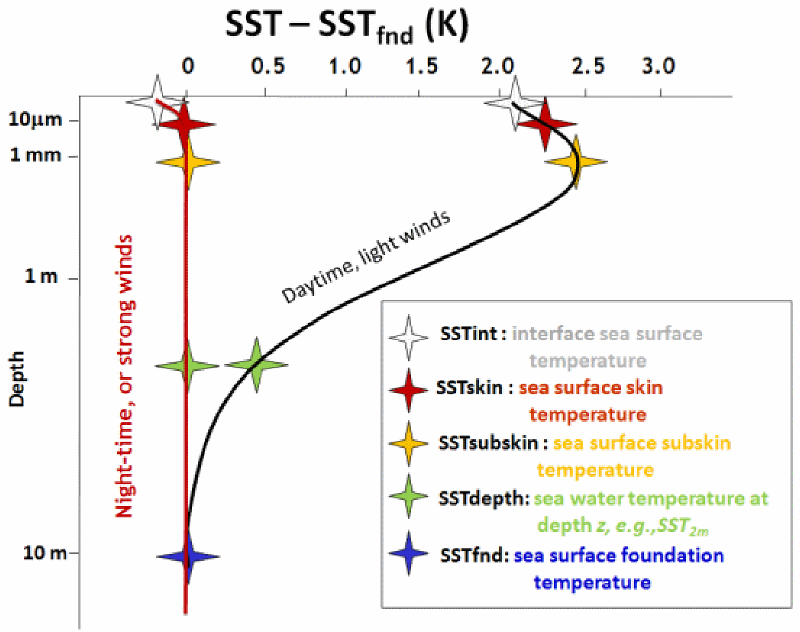
$$T_S = a_0 + a_1 S_\theta + a_2 T_{11} + a_3(T_{11}-T_{8.6}) + a_4(T_{11}-T_{12}) + [a_5 T_{11} + a_6(T_{11}-T_{8.6}) + a_7(T_{11}-T_{12})]S_\theta + [a_8(T_{11}-T_{8.6}) + a_9(T_{11}-T_{12})]T_0$$

Night:

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

$T_{3.7}, T_{8.6}, T_{11}, T_{12}$	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

- ACSPO files report 'subskin' SST (depth of ~1mm) calculated using the Non-Linear SST (NLSST) equation 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 beta maturity review will focus on the 'subskin' SST product.



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].

[1]JPSS GSegDPS (https://www.nesdis.noaa.gov/s3/2022-03/474-01543_JPSS-GSegDPS_A.pdf)
[2]Standard deviation of bias against drifting buoys (day &night, full VIIRS swath, globally)
[3]Mean of bias against drifting buoys (day &night, full VIIRS swath, globally)
[4]The clear-sky ratio (percent of clear-sky SST pixels to the total ice-free ocean pixels) must be at least 18%

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 available for evaluation/testing purposes following this beta maturity review
- **Three products from both 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)

- **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 warmup-cooldown (WUCD) exercises. The SDR team has successfully mitigated the issue for NPP and N20. We assume that they will 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). This suggests that we do use prior SST/Atmosphere, but we do not force retrieved SST into it

Quality Control Analysis/Validation

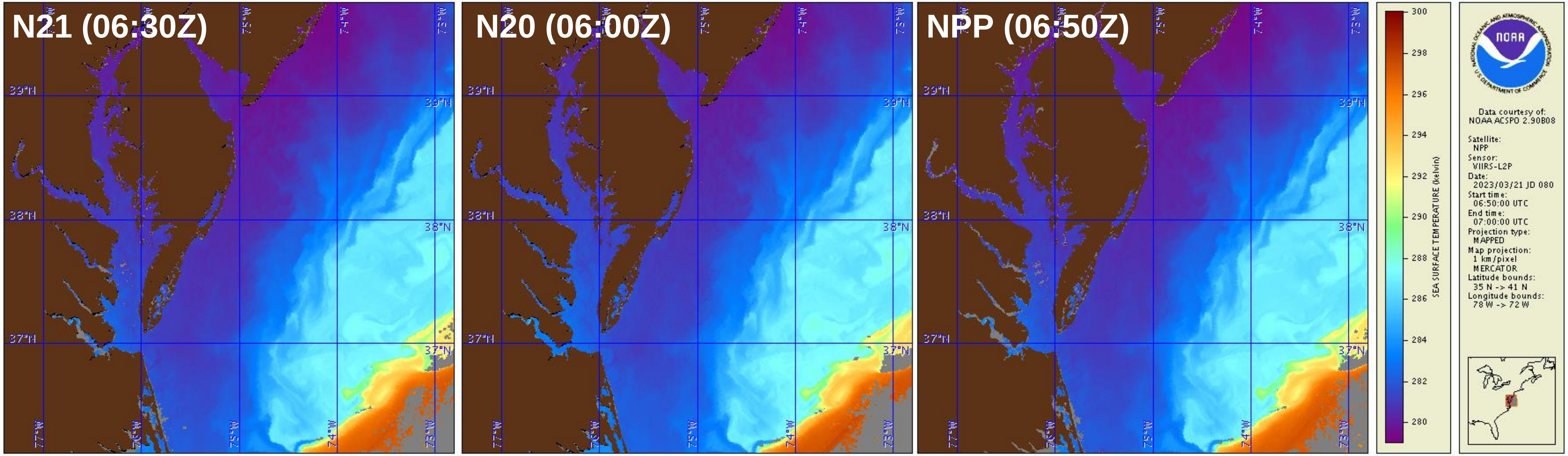
- **Defined Quality Flags**
  - ACSPO has quality levels (QLs). QL=5: Recommended to users; QL=0: Missing data; QL=1: Non-SST (cloudy, probably cloudy, land, etc.); QL=2,3,4 – not used
- **ACSPO Follows GHRSST Data Specifications version 2 (GDS2) and provides error characterization of SST in each pixel**
  - SST bias estimation and uncertainty (vs *in-situ* SST) in each QL=5 pixel is defined by the two extra layers in data files: Singe Sensor Error Statistics (SSES) Bias and SSES Standard Deviation (SD)
  - ‘depth’ SST = ‘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 (sufficient statistics are currently unavailable at the time of beta review)
  - Validation of ‘depth’ SST will be presented during provisional maturity review

Evaluation of SST Performance

- **Product performance evaluation**
  - Global and Regional, using N21 L1B/SDR from Feb 11 2023 – present
  - 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

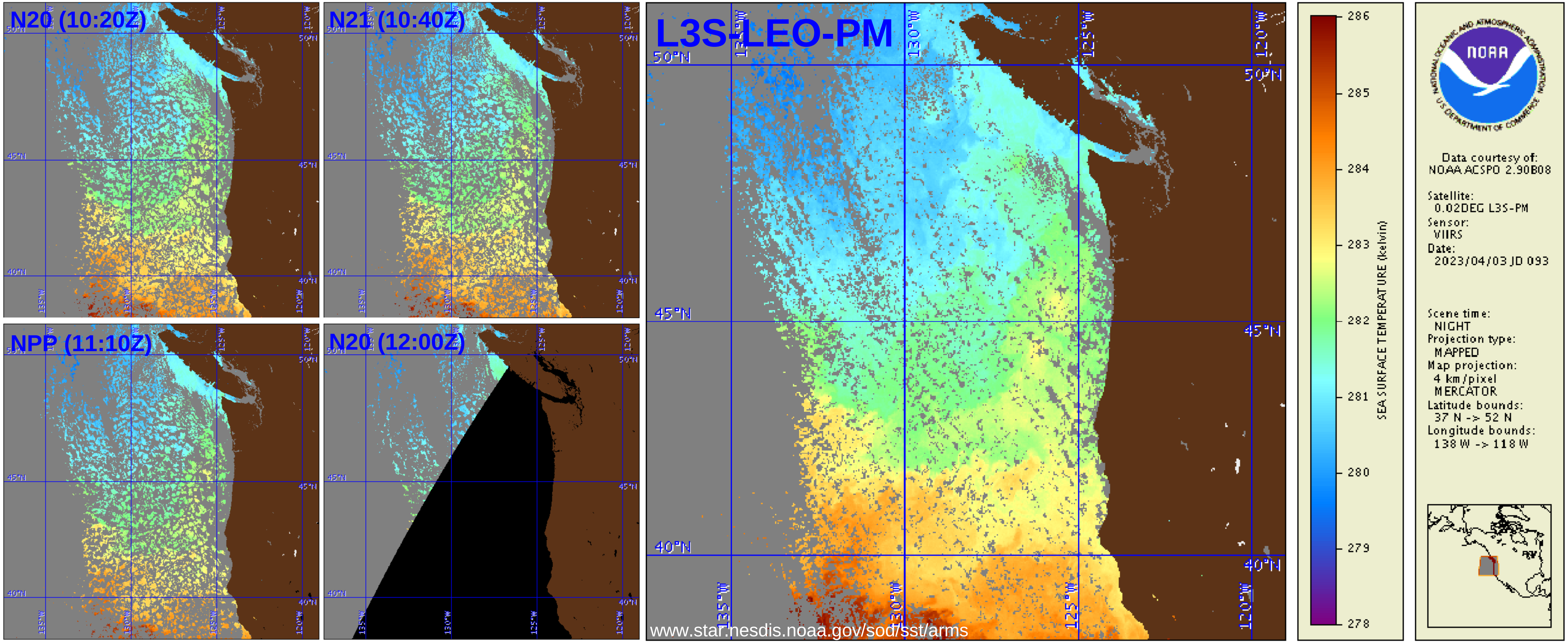
Chesapeake Bay 3 March 2023



- 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

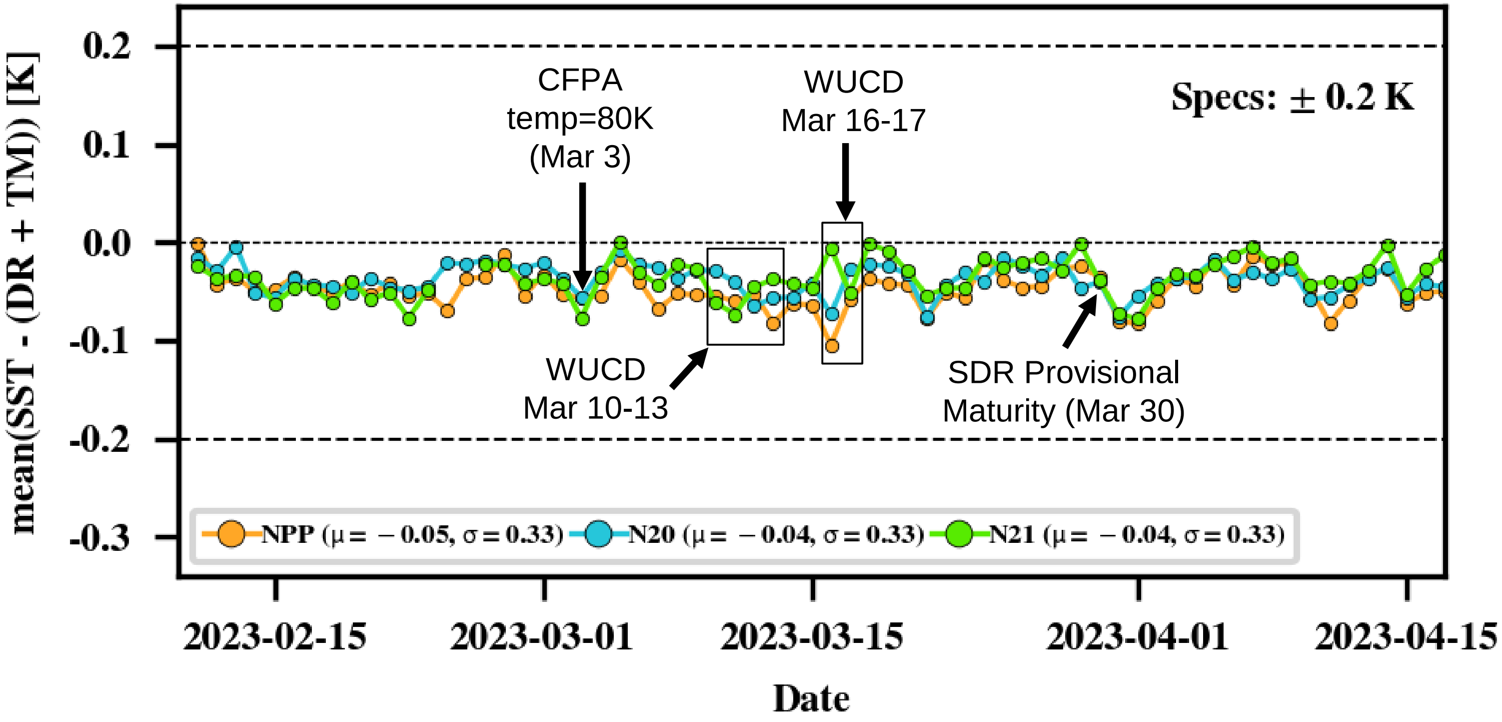
- North-West US Coast (3 Apr 2023; nighttime ‘subskin’ SST)
- Clouds move between satellite overpasses
- Improved coverage in ACSPO L3S-LEO-PM by collating SST from multiple VIIRS overpasses (7 total; 4 shown)



Global 'subskin' SST Bias wrt. *iQuam in situ* SST (night)

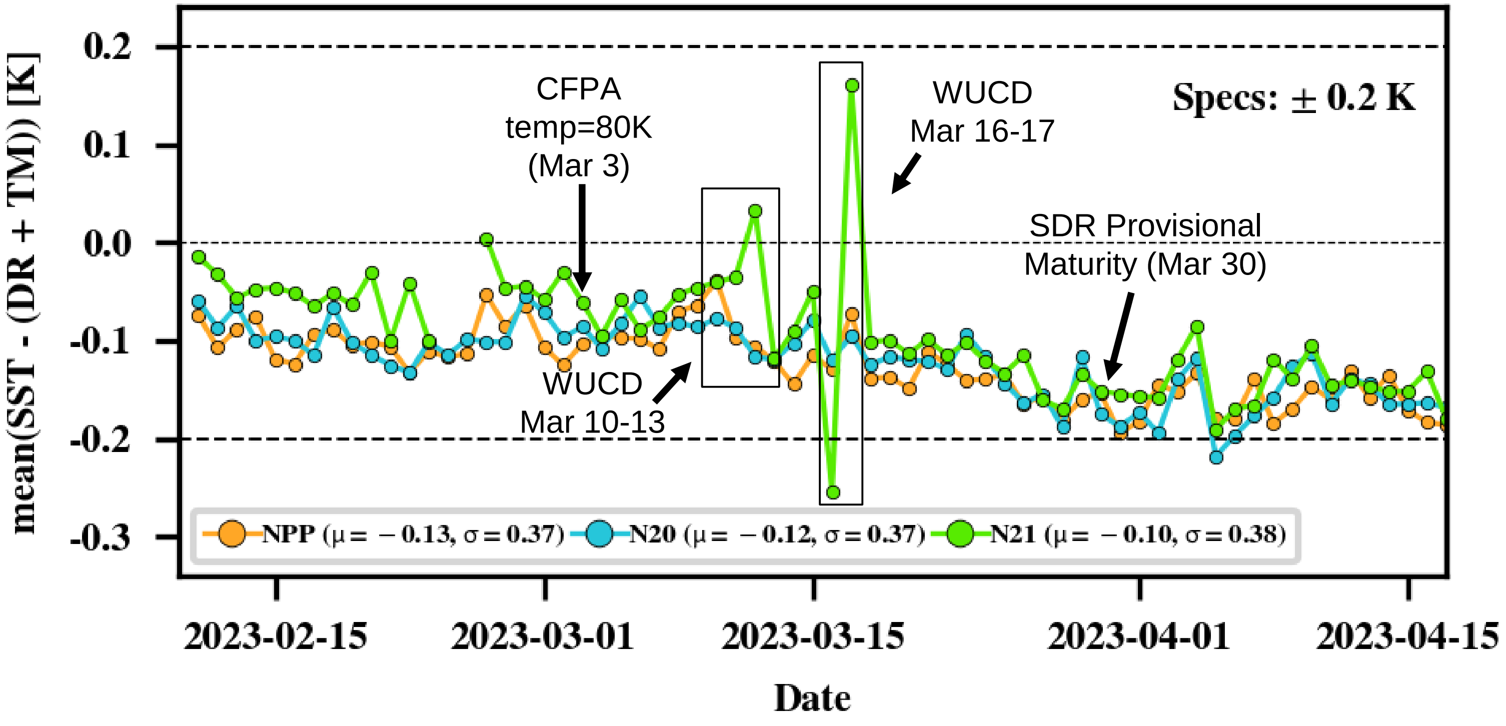
- Nighttime biases are close to ~0K, typically within ±0.05K
- N21, N20, and NPP statistics are very consistent
- CFPA setpoint temperatures was changed from 82 to 80 K on Mar 3 (no visible effect on nighttime SST bias)
- Two warmup cooldown events March 10-13 and March 16-17. Effects of WUCD on nighttime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

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



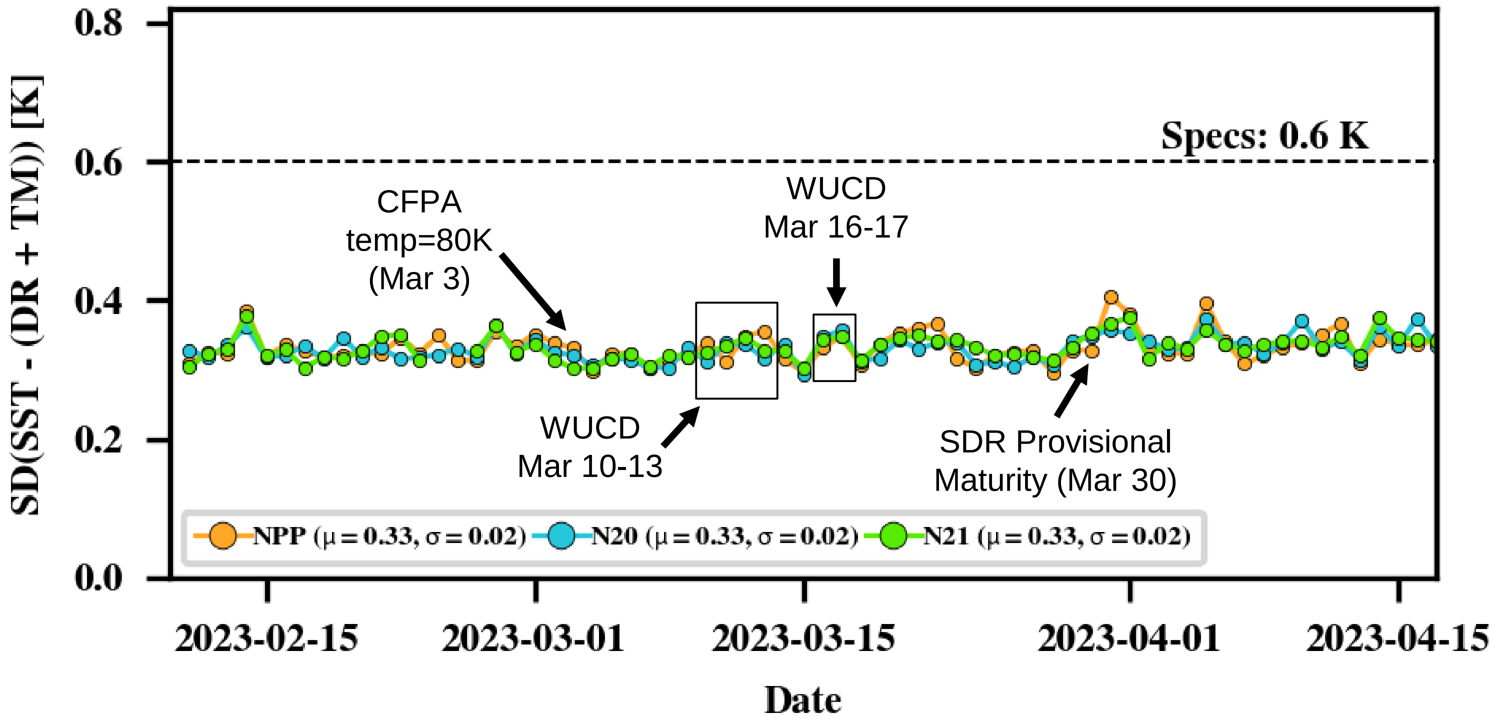
Global 'subskin' SST Bias wrt. *iQuam in situ* SST (day)

- Daytime biases are larger than at night but still within JPSS specs: ±0.2K
- Bias has seasonal cycle (likely due to skin-bulk SST difference) with ~0.2K amplitude (April is near the bottom)
- N21 shows signs of warm ~0.05K bias prior to CFPA temperature switch
- Could also be due to the short N21 time period available for N21 SST coefficient training
- Effects of WUCDs on daytime SST is substantial (up to ~0.25K)
- Excluding WUCD events, N21, N20, and NPP mean bias is very consistent after Mar 3



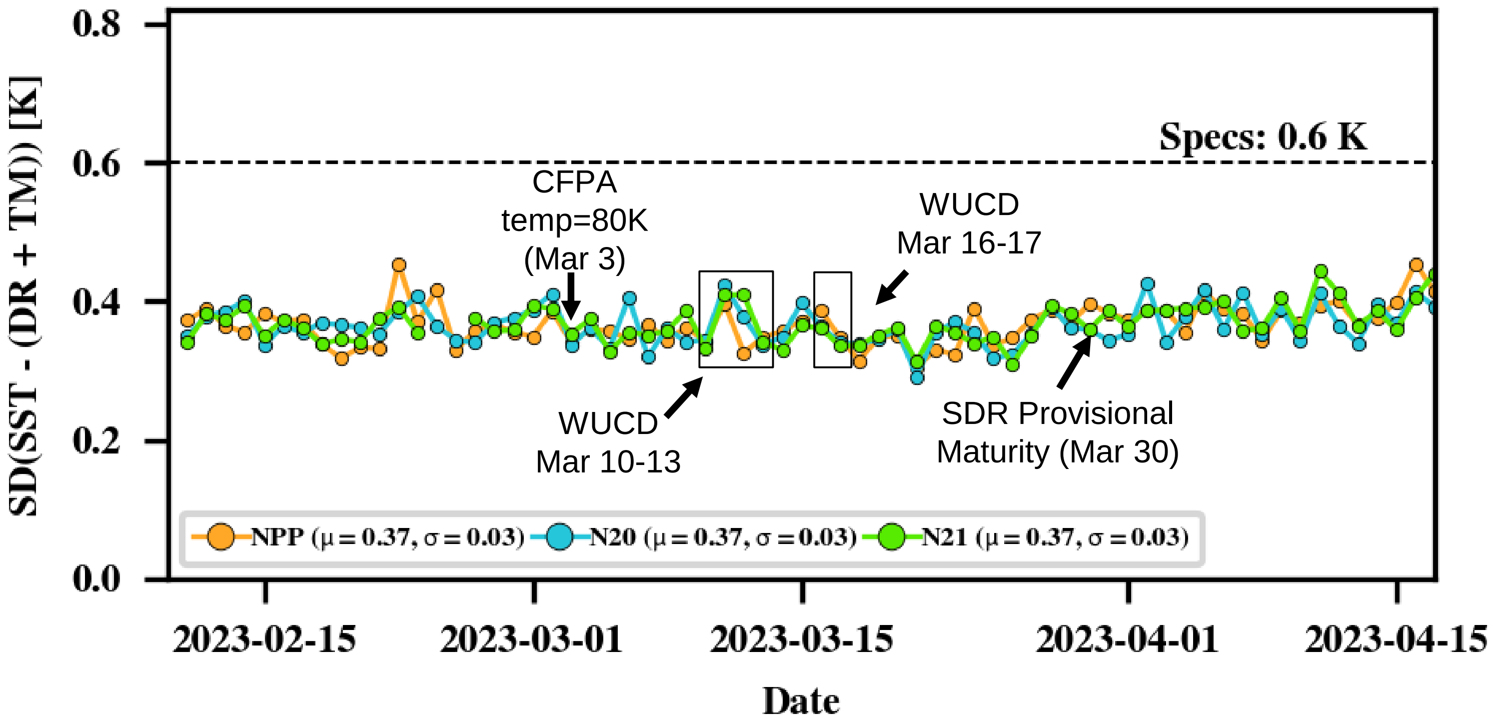
Global 'subskin' SST SD wrt. *i*Quam *in situ* SST (night)

- Nighttime SDs are ~0.33 K
- JPSS specs (0.6 K) are met by a wide margin
- N21 is very consistent with N20 and NPP
- CFPA temperatures change and WUCDs have no visible effect on nighttime SST SD



Global 'subskin' SST SD wrt. iQuam *in situ* SST (day)

- Daytime SDs are ~0.37 K
- Higher than nighttime SDs by ~0.04 K but still meet JPSS specs, and beat by a wide margin
- N21, N20, and NPP statistics are very consistent
- CFPA temperatures change and WUCDs have no visible effect on daytime SST SD



SST Error Budget

- March 4-present (after CFPA change to 80 K), excludes days with WUCD exercises
- Red (daytime); Blue (nighttime)
- All three satellites are consistent
- Less than 0.025 K difference in accuracy (global mean bias)
- Less than 0.01 K 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		
'subskin' SST Accuracy	±0.2 K	DPS-134* L1RDS-139# JERD-2151†	N/A	-0.03 K -0.13 K	-0.04 K -0.14 K	-0.05 K -0.15 K	Yes	Meets/Exceeds Specs/User's Expectations
'subskin' SST Precision	0.6 K	DPS-135* L1RDS-139# JERD-2152†	N/A	0.33 K 0.37 K	0.33 K 0.37 K	0.33 K 0.37 K	Yes	Meets/Exceeds Specs/User's Expectations
Clear-Sky fraction	18%	DPS-134* DPS-135*	N/A	19.8% 20.4%	19.8% 20.6%	19.7% 20.4%	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 available to users for evaluation/testing purposes following this beta 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 - Beta Maturity

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

Cal/Val Summary & Conclusion

- SST Team recommends SST algorithm beta maturity as of March 20 (00:00 UTC)
- N21, N20 & NPP ‘subskin’ SST products are highly consistent, and meet/exceed JPSS specs & users' expectations
- Longer training period needed for validation of N21 VIIRS ‘depth’ SST algorithm
- 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

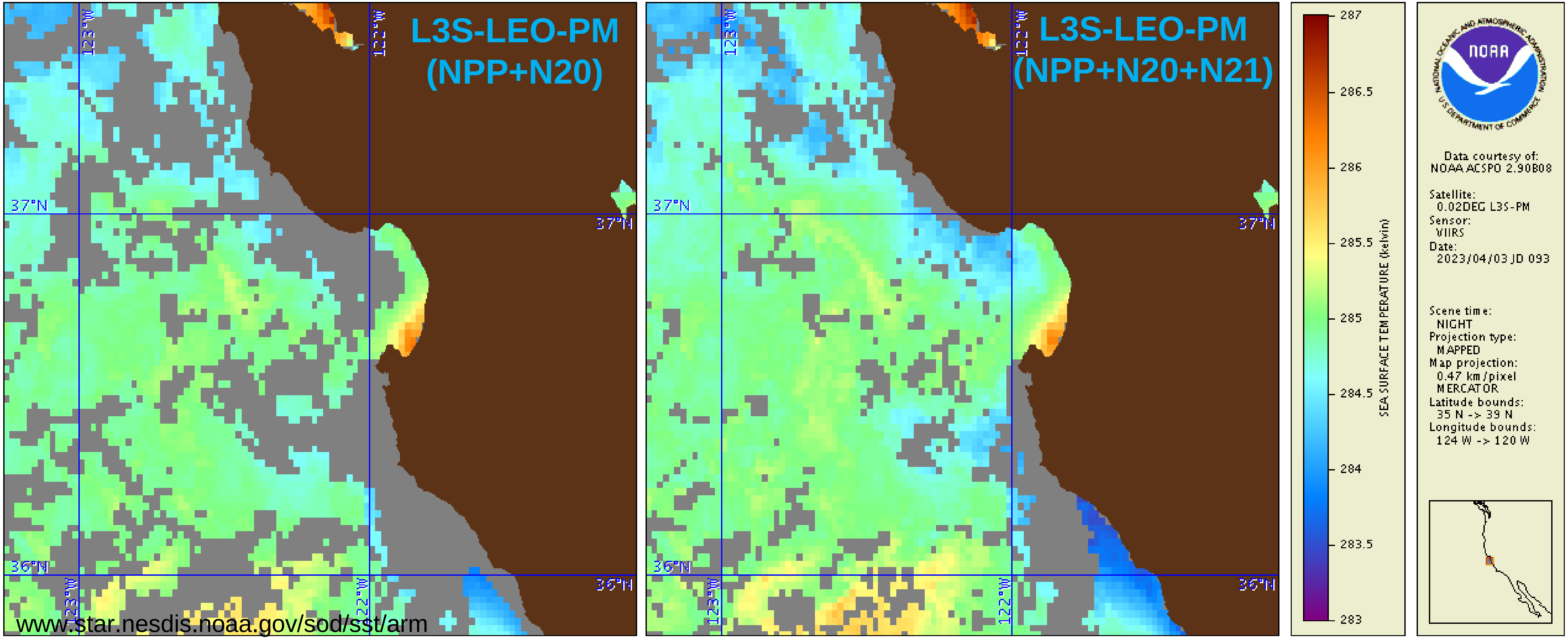
- **Lessons learned from N21 Cal Val**
  - NPP, N20 and N21 VIIRS SST products fully meet and exceed NOAA requirements and users' expectations. ACSPO VIIRS SST products are accurate and consistent
- **Planned improvements**
  - Minimize residual cloud leakages in each individual product. Potentially, revisit clear-sky mask, add new tests
  - Minimize cross-platform, angular, regional SST biases. Potentially, revisit the current NLSST algorithms
  - Include N21 in super-collated ACSPO products (L3S-LEO-PM)
- **Future Cal/Val Activities/Milestones**
  - Train piecewise regression (PWR) algorithm coefficients used to generate ACSPO ‘depth’ SST. Retrain ‘subskin’ SST algorithm coefficients/LUTs using longer timeseries of matchups that covers multiple seasons
  - Make N21 SST data available to users for evaluation/testing purposes
  - Work towards integrating into 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/arm
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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)