Beta Maturity Science Review For NOAA-21 V8Pro Ozone Profile EDR

Presented by L. Flynn
Date: 3/30/2023

Disclaimer

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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 (See OMPS SDR presentation.)
- Beta Maturity Performance Validation
  - On-orbit instrument performance assessment
    - Identify all of the instrument and product characteristics you have verified/validated as individual bullets
    - Identify pre-launch concerns/waivers, mitigation and evaluation attempts with on-orbit data
- Users/Downstream-Products feedback (N/A for Beta)
- Risks, Actions, Mitigations
  - Potential issues, concerns
- Path forward (to the next maturity stage)
- Summary

Maturity Review - Exit Criteria

- Beta Maturity Performance is adequately characterized and performance deficits are understood:
  - 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)

BETA MATURITY REVIEW MATERIAL

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

Ozone Cal/Val/Alg Team Membership

EDR	Name	Organization	Task
Lead	Lawrence Flynn	NOAA/NESDIS/STAR	Ozone EDR Team
Sub-Lead	Irina Petropavlovskikh	NOAA/ESRL/CIRES	Ground-based Validation
Sub-Lead	Trevor Beck	NOAA/NESDIS/STAR	Trace Gas Algorithm Development
Member	Jianguo Niu	STAR/IMSG	R&D, trouble shooting, TOAST, V8TOS
Member	Eric Beach	STAR/IMSG	Validation, ICVS/Monitoring, Data Management
Member	Zhihua Zhang	STAR/IMSG	V8 Algorithms implementation & modification
Member	Robert Lindsay	STAR/IMSG	Limb Algorithms implementation
Member	Jeannette Wild	UMD	Applications, CDRs, validation
JAM	Starry Manoharan	JPSS/Aerospace	Coordination
Adjunct	Bigyani Das	STAR/ASSISTT	Deliveries to NDE / NCCF
PAL	Vaishali Kapoor	OSPO	Atmospheric Chemistry Product Area Lead

Product Overview/Requirements:

Attribute	Threshold	Observed/validated
Geographic coverage	60% Global Earth 7 days	SZA < 86°, orbital track
Vertical Coverage	0-60 km	0-60 km
Vertical Cell Size	3-km reporting, 7-10 km	21 layers, averaging kernel
Horizontal Cell Size	250x250 km^2	250x50 km^2
Mapping Uncertainty	25 km	5 km
Measurement Range	0.1-15 ppmv	0.1-15 ppmv
Measurement Accuracy		
h < 25 km, p < 30 hPa	10% or 0.1 ppmv	
25 km < h < 50 km	10%	
h > 50 km, p > 1 hPa	10%	
Measurement Precision		
h < 25 km, p < 30 hPa	20% or 0.1 ppmv	
25 km < h < 50 km	10%	
h > 50 km, p > 1 hPa	10% or 0.1 ppmv	

https://www.jpss.noaa.gov/assets/pdfs/technical_documents/474-01543_JPSS-GSegDPS_A.pdf

Processing Environment and Algorithms

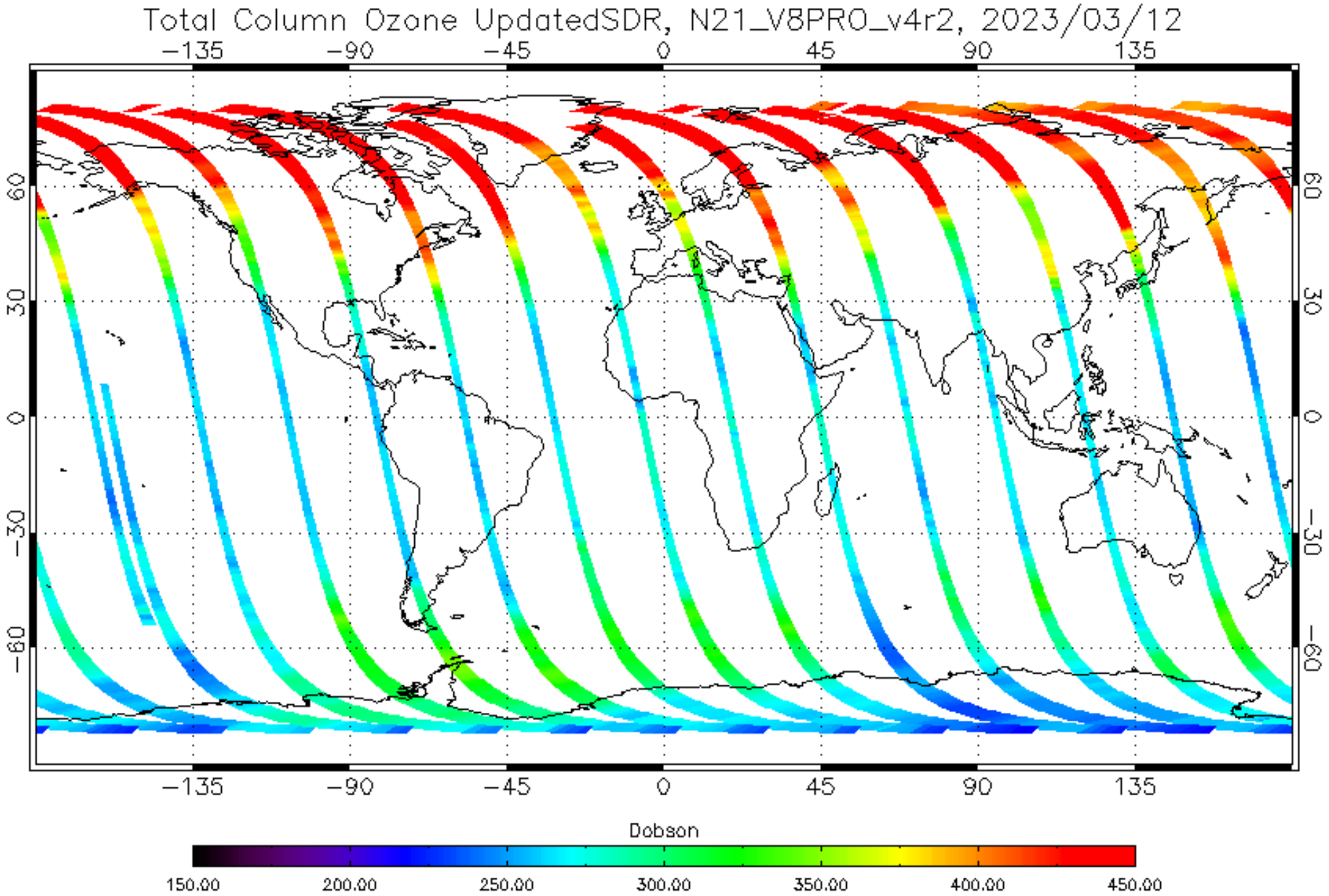
- Description of processing environment and algorithms used to achieve the maturity stage:
  - Algorithm version: NDE I&T V8Pro v4r2
  - Version of LUTs used: Pre-launch
  - Effective date: 3/24/2023

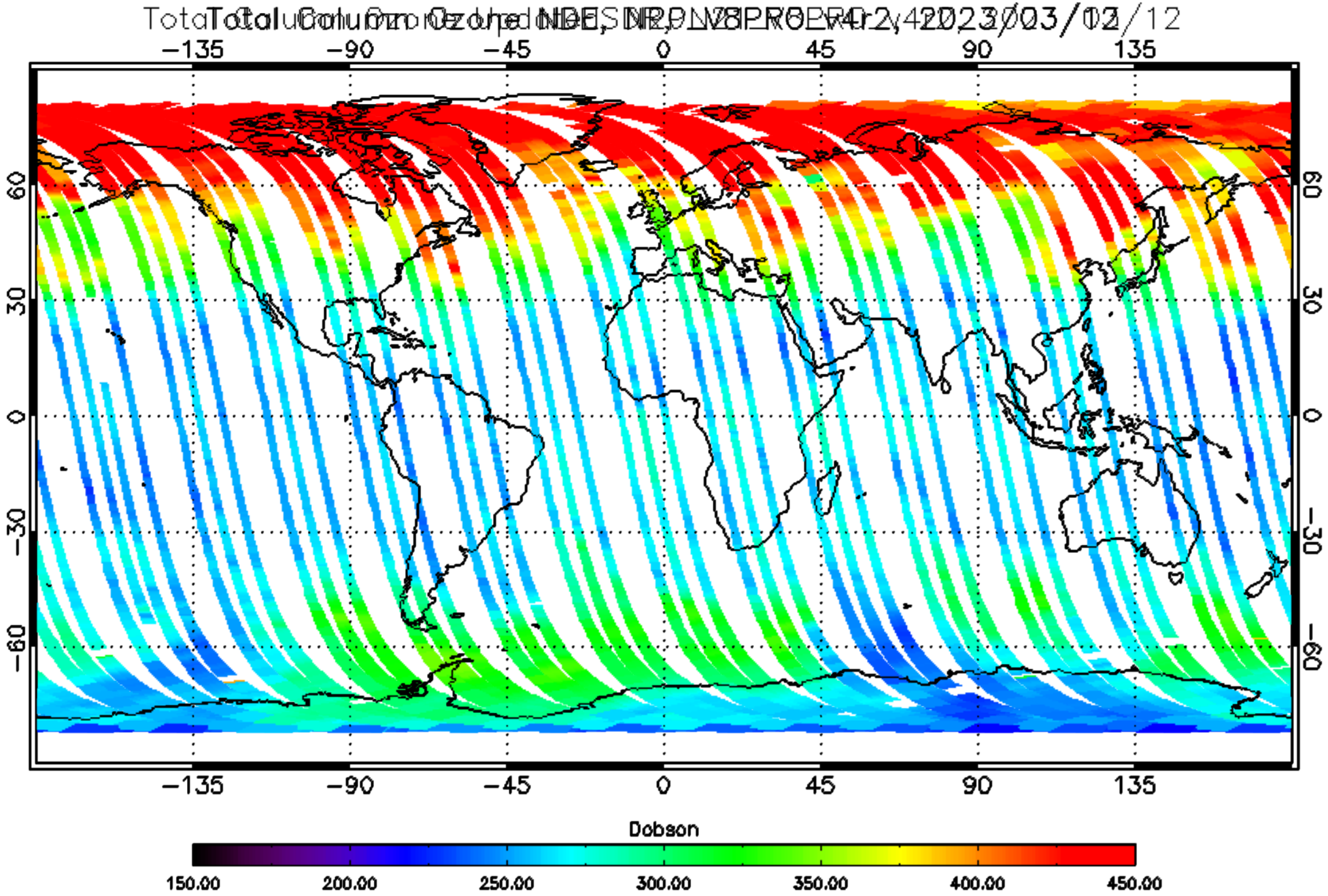
Evaluation of algorithm performance to specification requirements (3-5 slides)

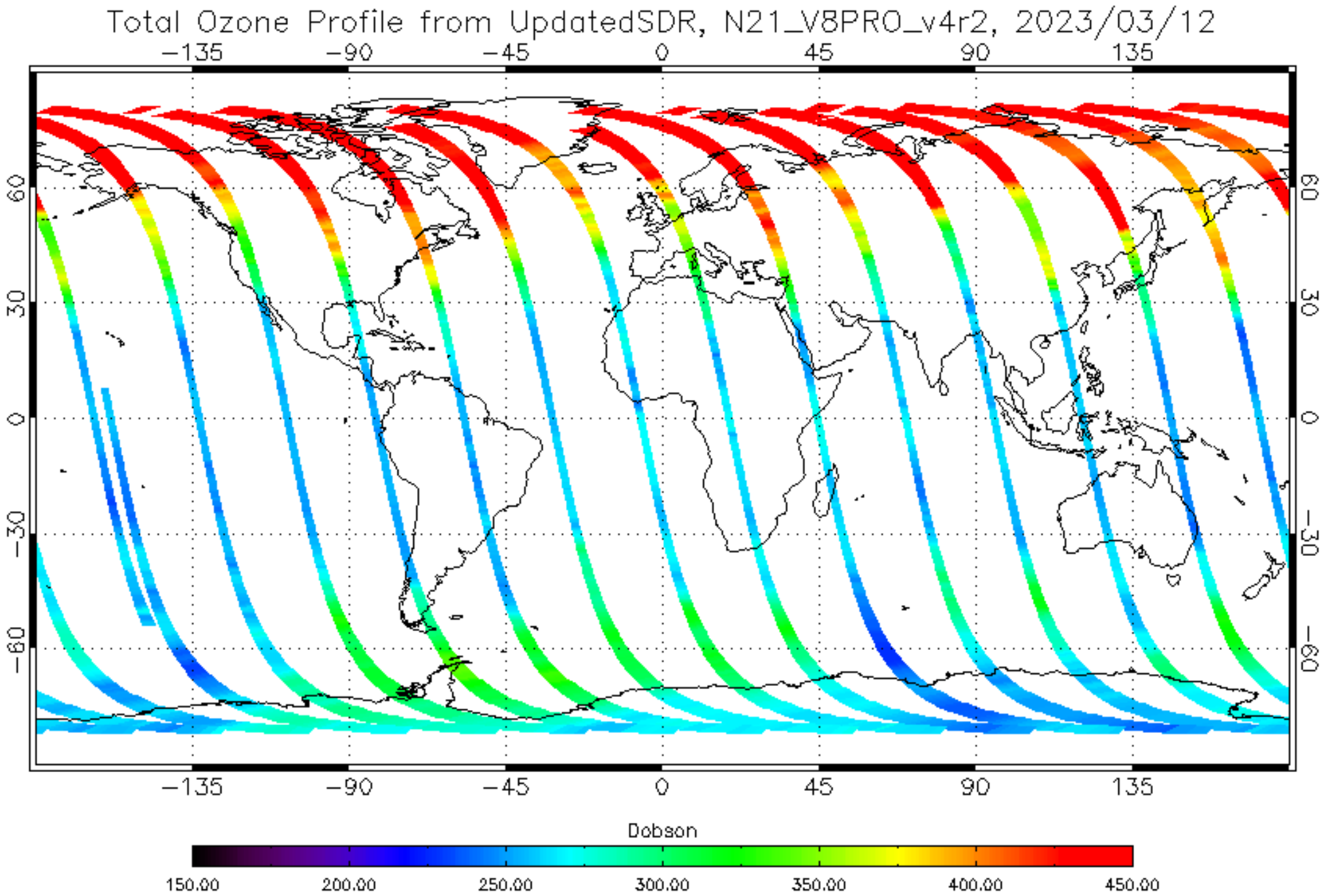
- Findings/Issues from {previous-maturity}/last Review
- Improvements since {previous-maturity}/last Review
  - Algorithm Improvements
  - LUT / PCT updates
- Algorithm performance evaluation
  - Validation data sets (type, periods, coverage)
  - Validation strategies / methods
  - Validation results
  - Long term monitoring readiness
- Inter-sensor comparison
  - Compare with S-NPP and NOAA-20
  - ~~Compare with other satellite product~~

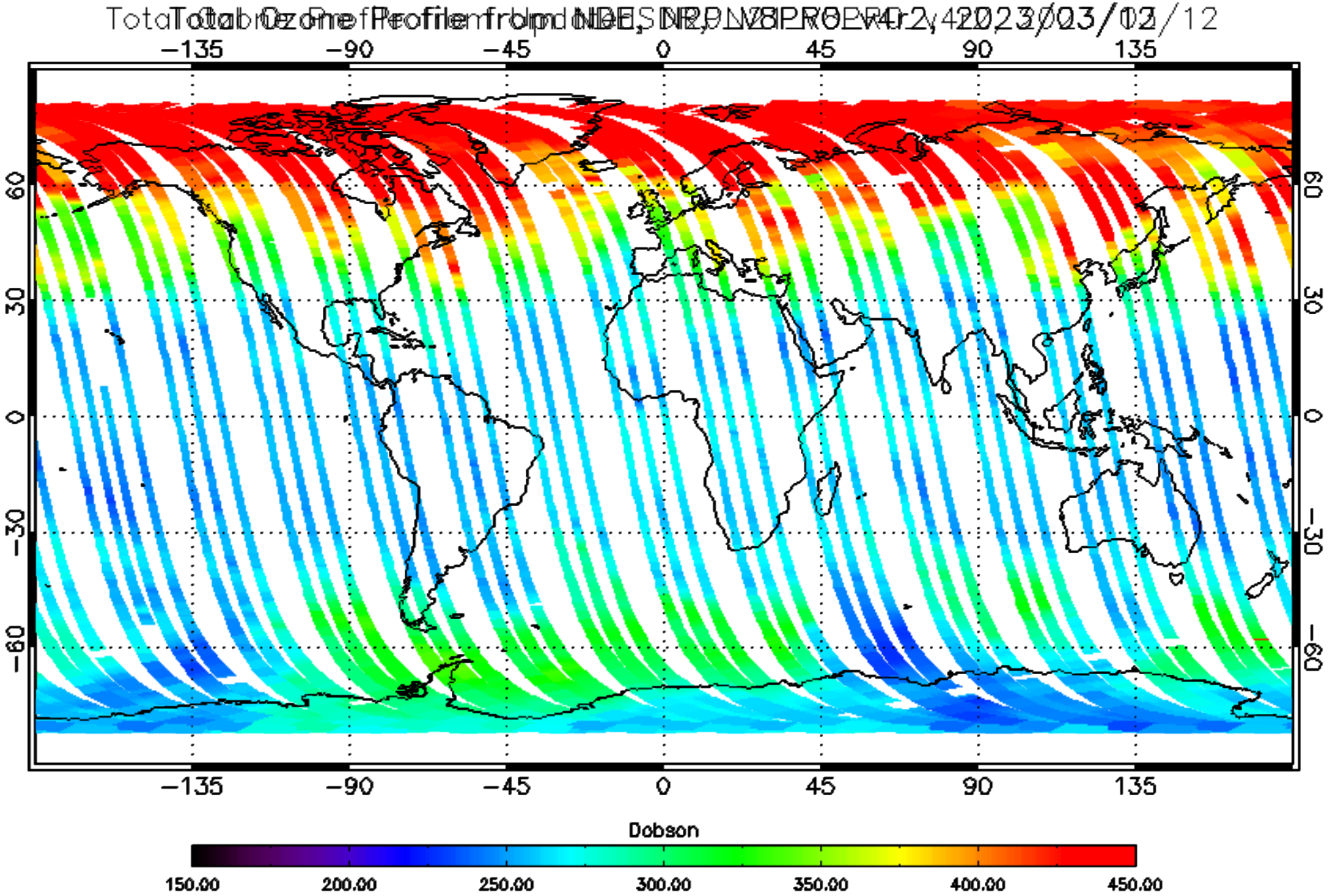
Major changes since Launch

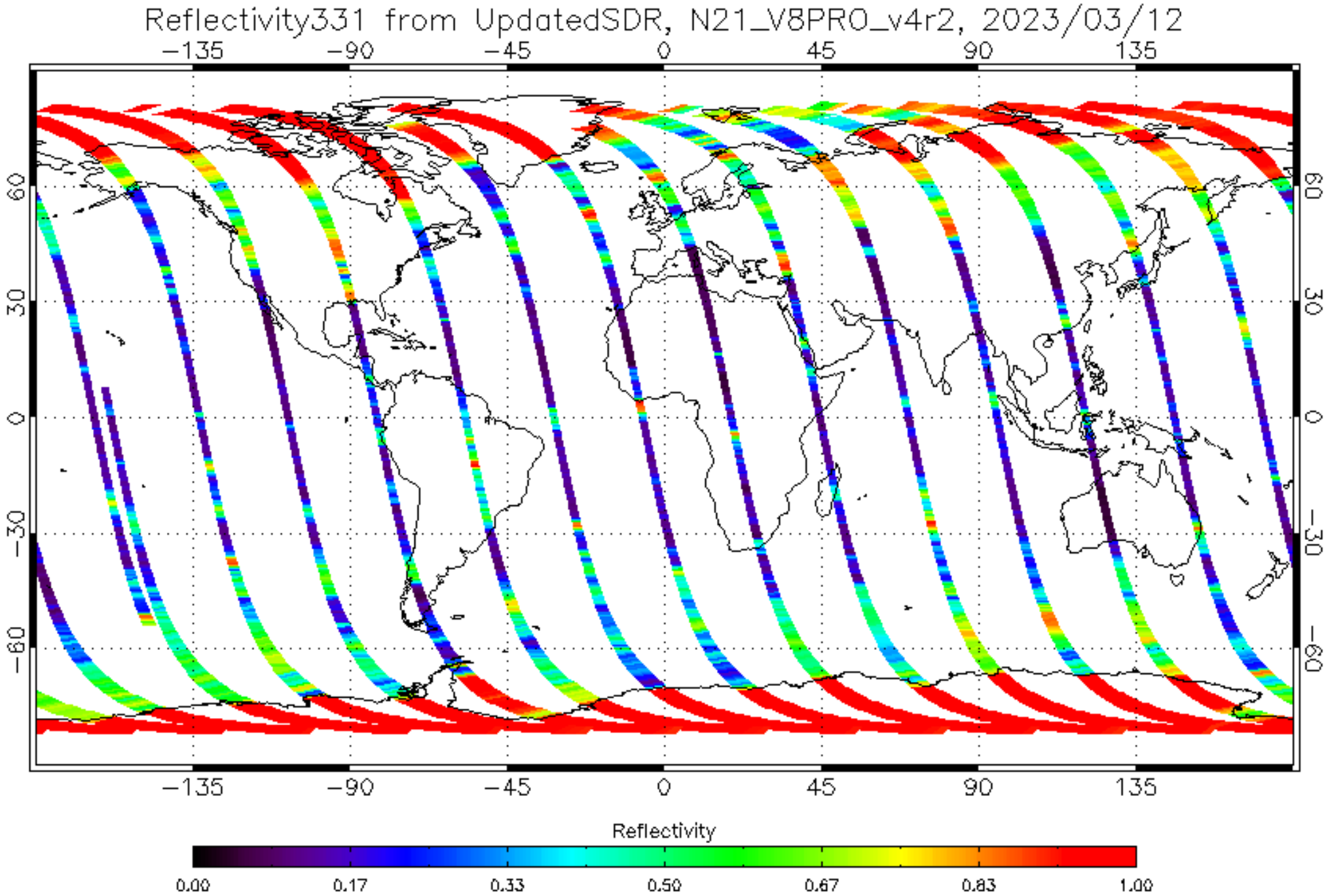
- Regular weekly dark table and biweekly Solar and wavelength table updates for both SDRs.
  - Solar and wavelength updates for ground-to-orbit wavelength shifts based on first solar measurements for both OMPS NM (-0.14 nm) and NP SDRs (-0.09 nm).
  - Solar and wavelength updates for three pixel offset error for OMPS NM SDR.
  - Solar and wavelength updates for twelve pixel offset error for OMPS NP SDR.
- OMPS NM SDR changes and performance are discussed in the OMPS NM SDR and the OMPS V8TOz EDR briefings.
- NOAA-21 OMPS NM & NP SDRs have all major updates neeede for beta maturity as of 3/24/2023.
- No changes to the V8Pro EDR algorithm or tables.

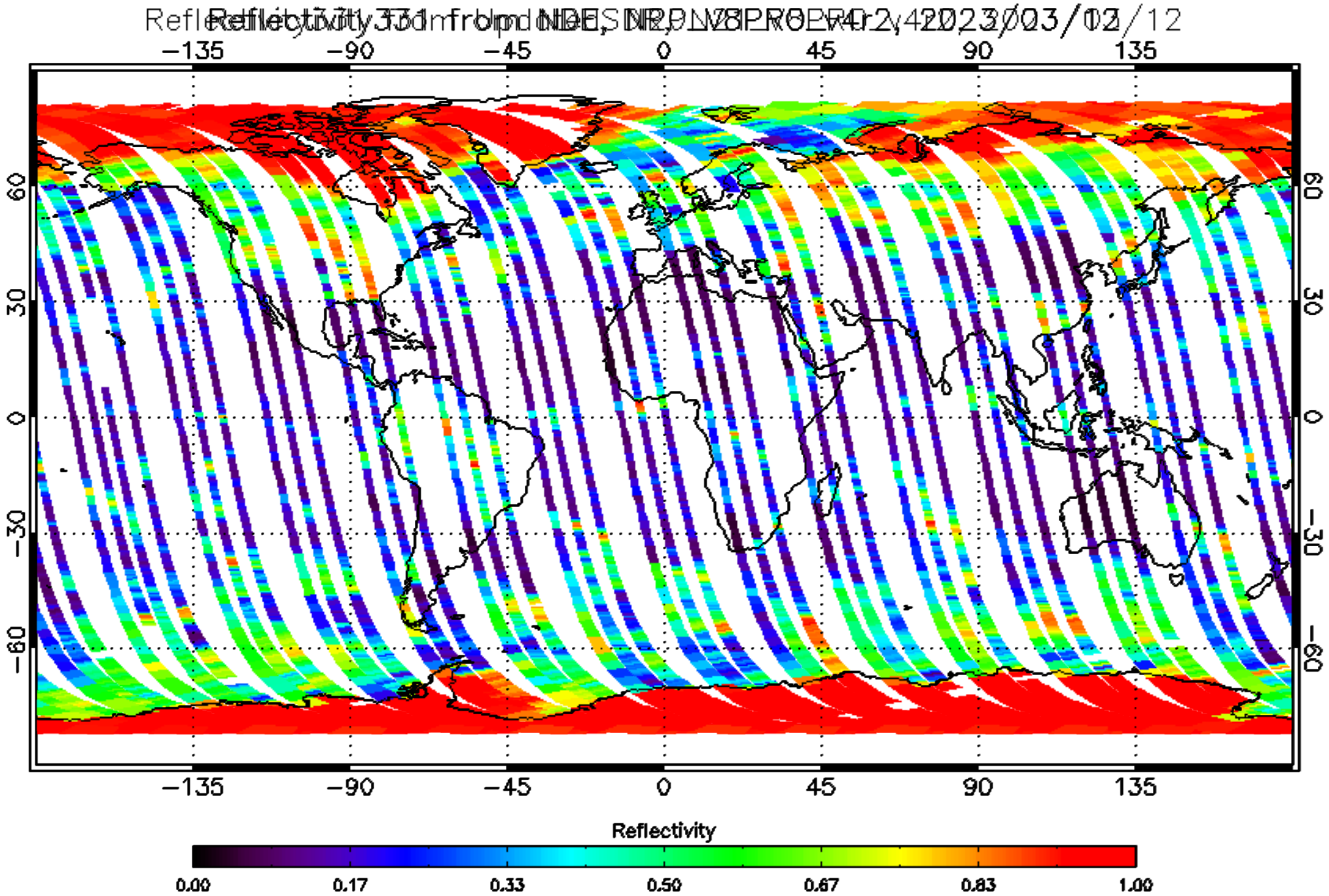

Total Column Ozone UpdatedSDR, N21_V8PRO_v4r2, 2023/03/12
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
Dobson
150.00
200.00
250.00
300.00
350.00
400.00
450.00

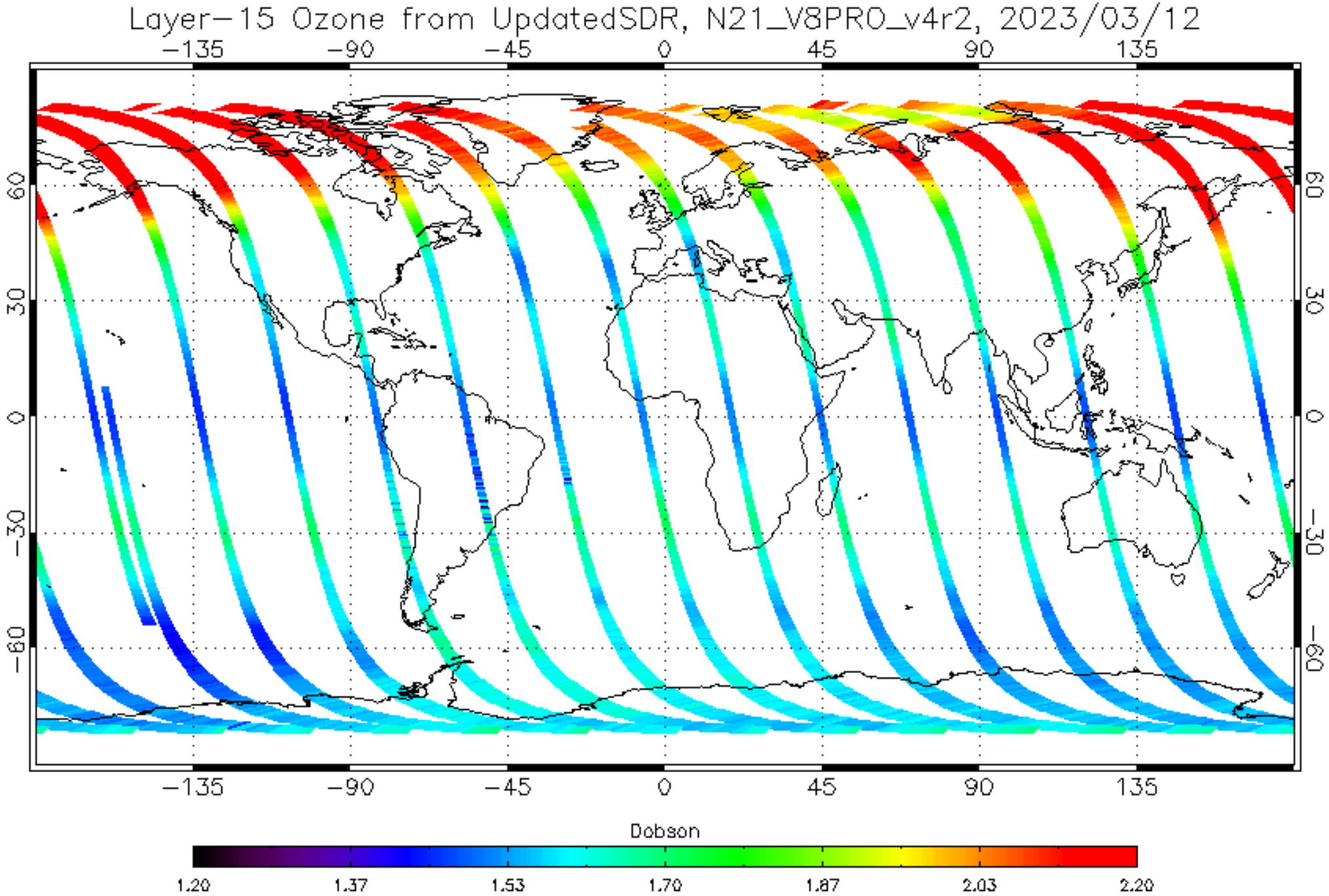

Total Column Ozone NOAA-20 OMPS NPP V8PROEV2 2023/03/12
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
Dobson
150.00
200.00
250.00
300.00
350.00
400.00
450.00

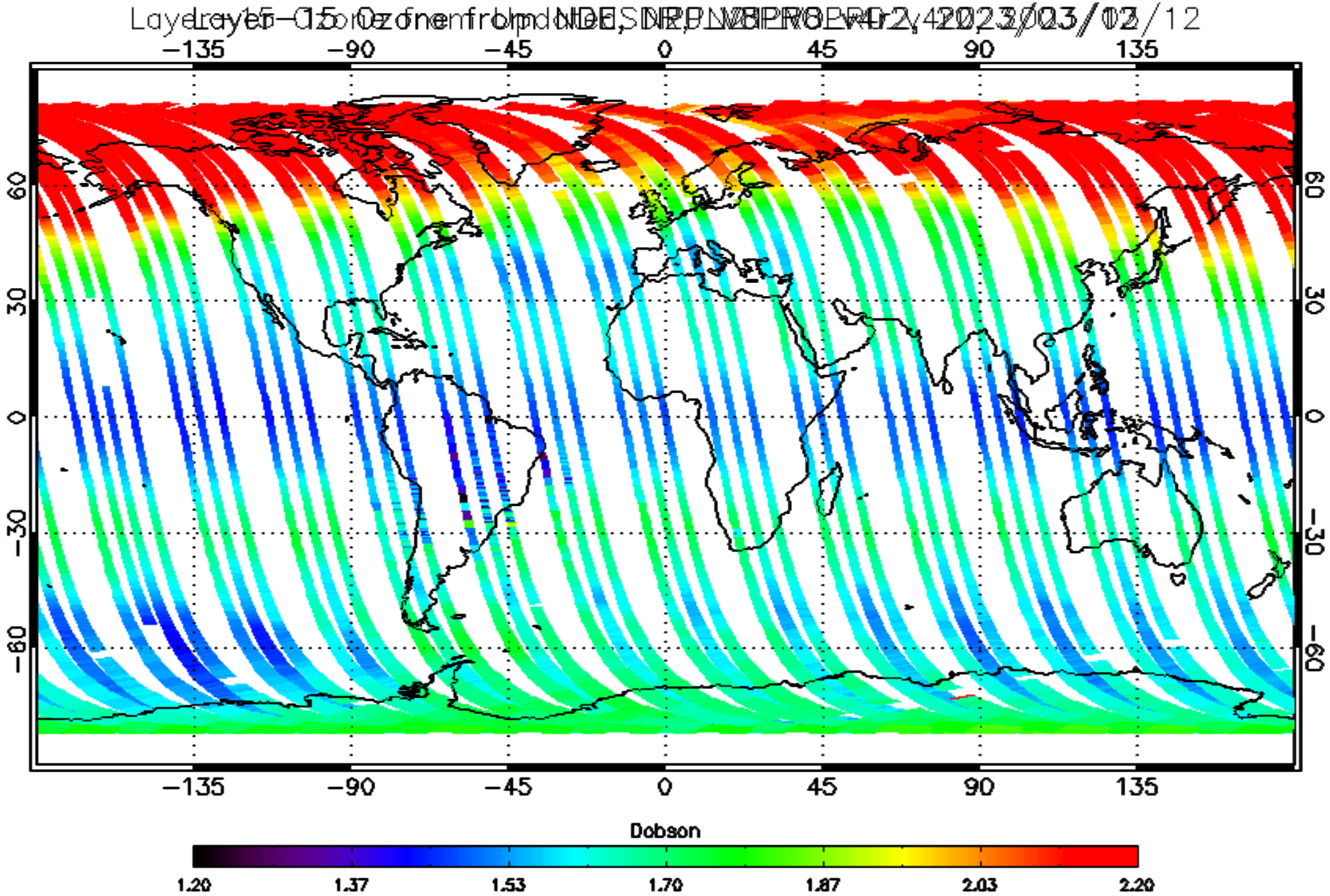

Total Ozone Profile from UpdatedSDR, N21_V8PRO_v4r2, 2023/03/12
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
Dobson
150.00
200.00
250.00
300.00
350.00
400.00
450.00


Total Ozone Profile from NOAA-20 OMPS NM SDR V8PROEV 2023/03/12
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
Dobson
150.00
200.00
250.00
300.00
350.00
400.00
450.00


Reflectivity331 from UpdatedSDR, N21_V8PRO_v4r2, 2023/03/12
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
Reflectivity
0.00
0.17
0.33
0.50
0.67
0.83
1.00


Reflectivity from NOAA-20 VIIRS on 2023/03/12
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
Reflectivity
0.00
0.17
0.33
0.50
0.67
0.83
1.00


Layer−15 Ozone from UpdatedSDR, N21_V8PRO_v4r2, 2023/03/12
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
Dobson
1.20
1.37
1.53
1.70
1.87
2.03
2.20

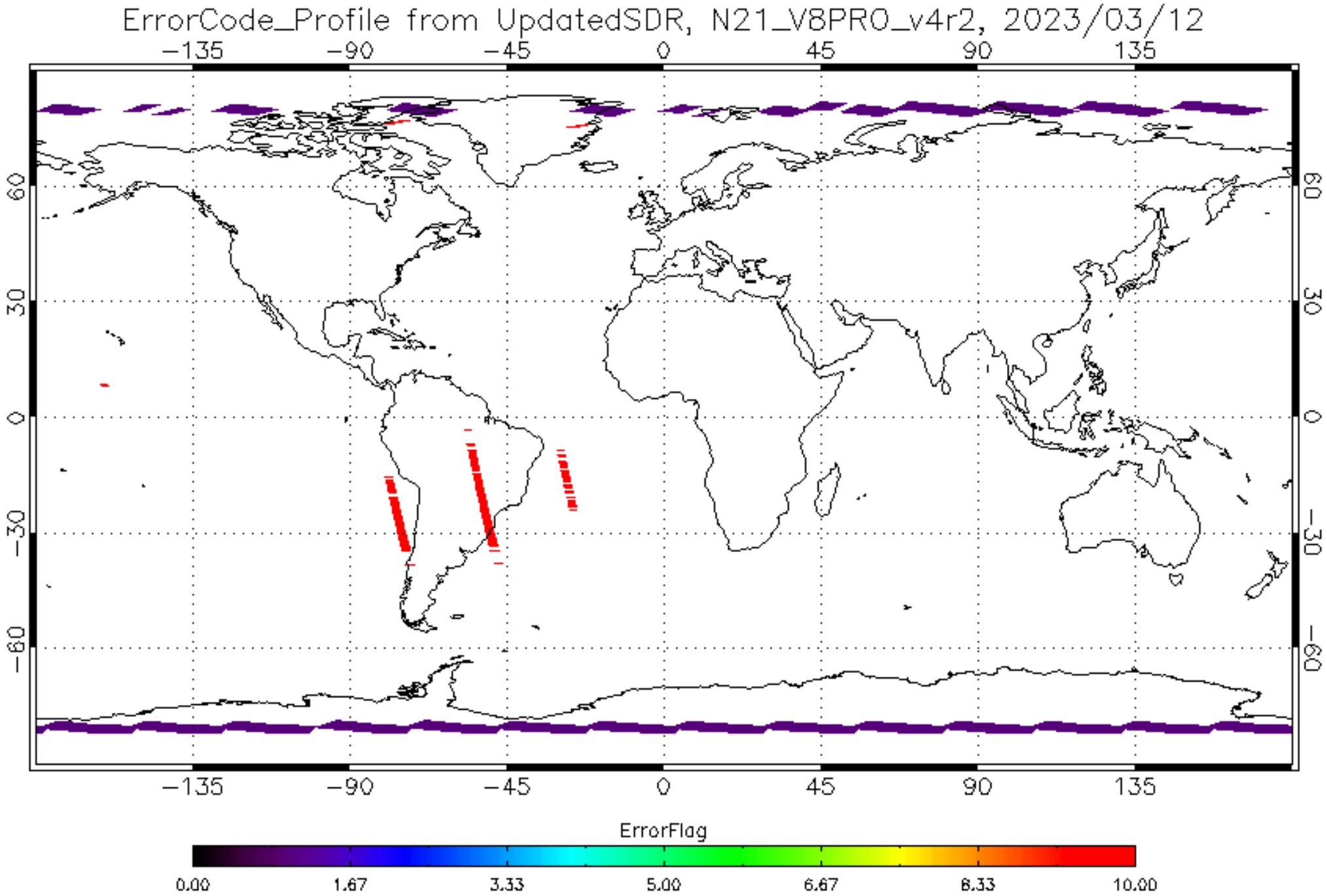

Layer 15 Ozone from NOAA-20 NOAA-21 SNPP 2023/03/12
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
Dobson
1.20
1.37
1.53
1.70
1.87
2.03
2.20

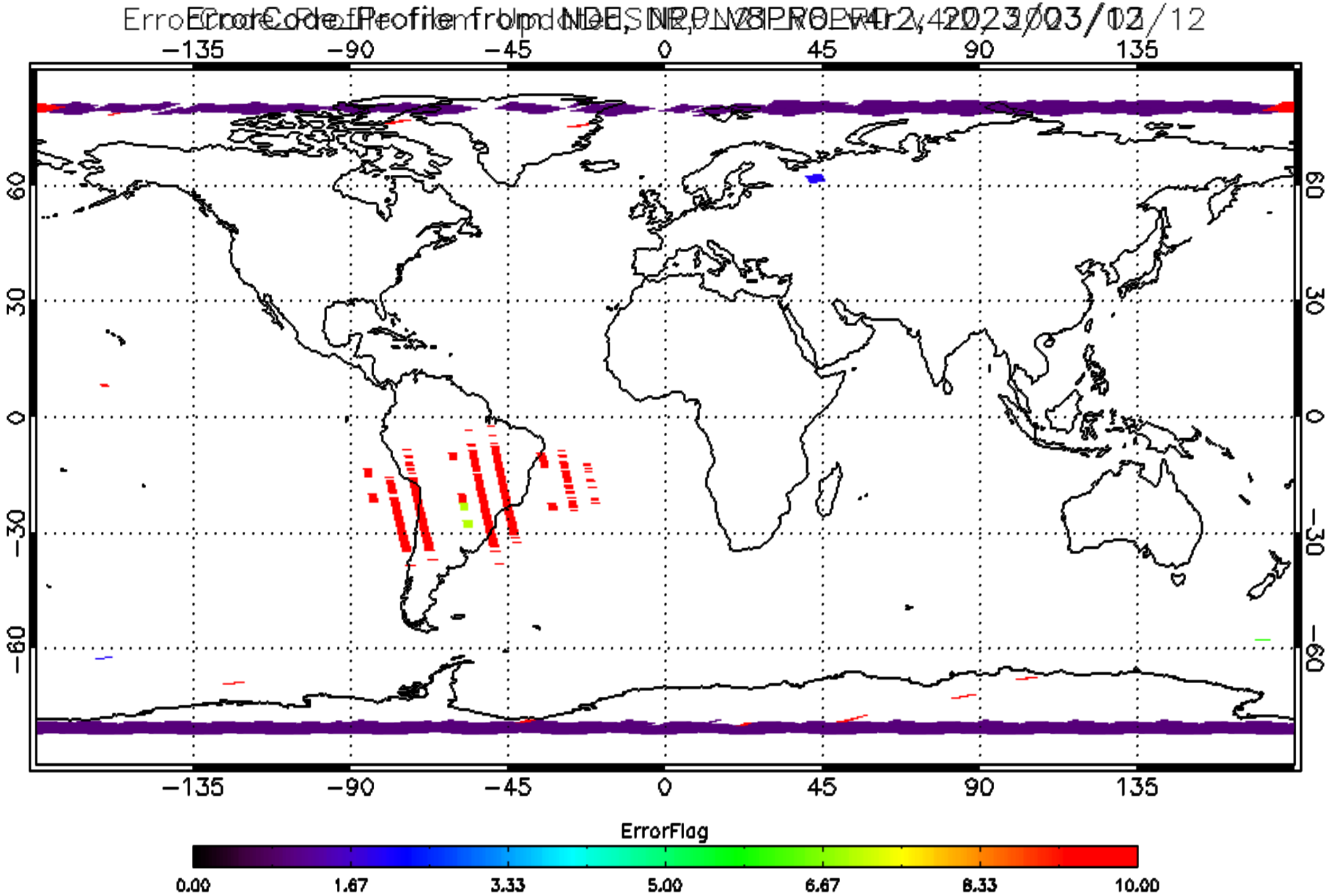
Quality flag analysis/validation

- Defined Quality Flags
  - Variable
  - Description
  - Value
- Quality flag analysis/validation
  - Test / example / ground truth data sets
  - Analysis / validation results
  - Analysis / validation plan

V8Pro Profile Error Code and Descriptions

Profile Error Code	Description
0.0	Good retrieval
1.0	SZA > 84 degrees
2.0	|Step3O3 – Profile Total| > 25 DU
3.0	Average |Final Residual| for retrieval channels > threshold
4.0	|Final residue| greater than 3 times instrument error
5.0	|Retrieved - a priori| greater than 3 times a priori error
6.0	Non-convergent solution
7.0	Stray light anomaly
8.0	Initial residue >18.0 N-value units or upper level profile anomaly
9.0	Total ozone algorithm failure
+10.0	10 is added - to the flag values to designate descending portions of the orbit. The unit's value is unchanged.
+20.0 or +40.0	Thresholds on number of deviations from the polynomial fit. +20 for >30%, +40 for >60%.

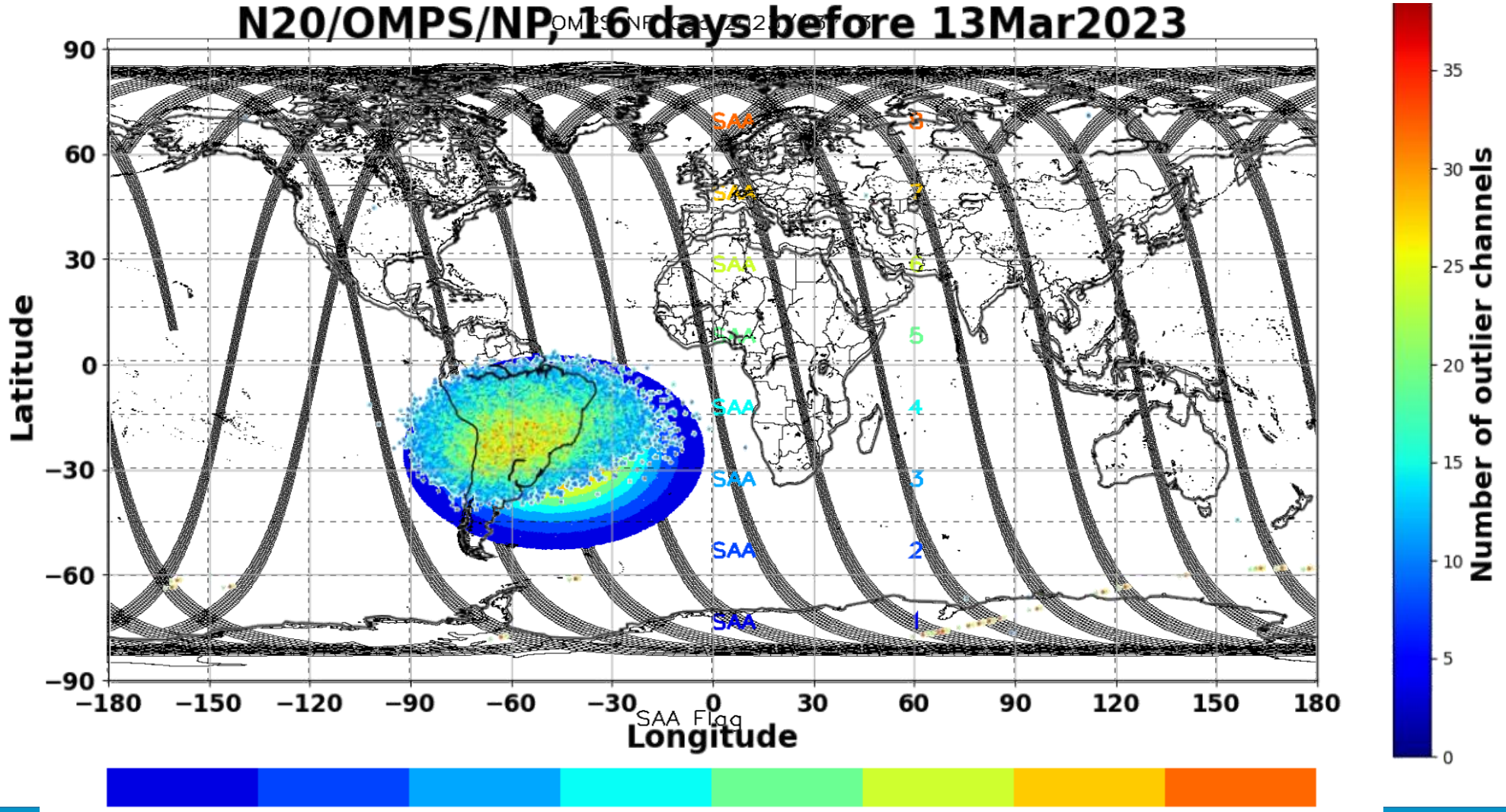

ErrorCode_Profile from UpdatedSDR, N21_V8PRO_v4r2, 2023/03/12
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
ErrorFlag
0.00
1.67
3.33
5.00
6.67
8.33
10.00


Error Code of Profile from NDE, NRT V2.42 2023/03/12
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
ErrorFlag
0.00
1.67
3.33
5.00
6.67
8.33
10.00

Need to update IDPS SAA location. It has moved to the west.

Change the name to South American Anomaly?

Can we create a time series for NPP for March 2012-2023?

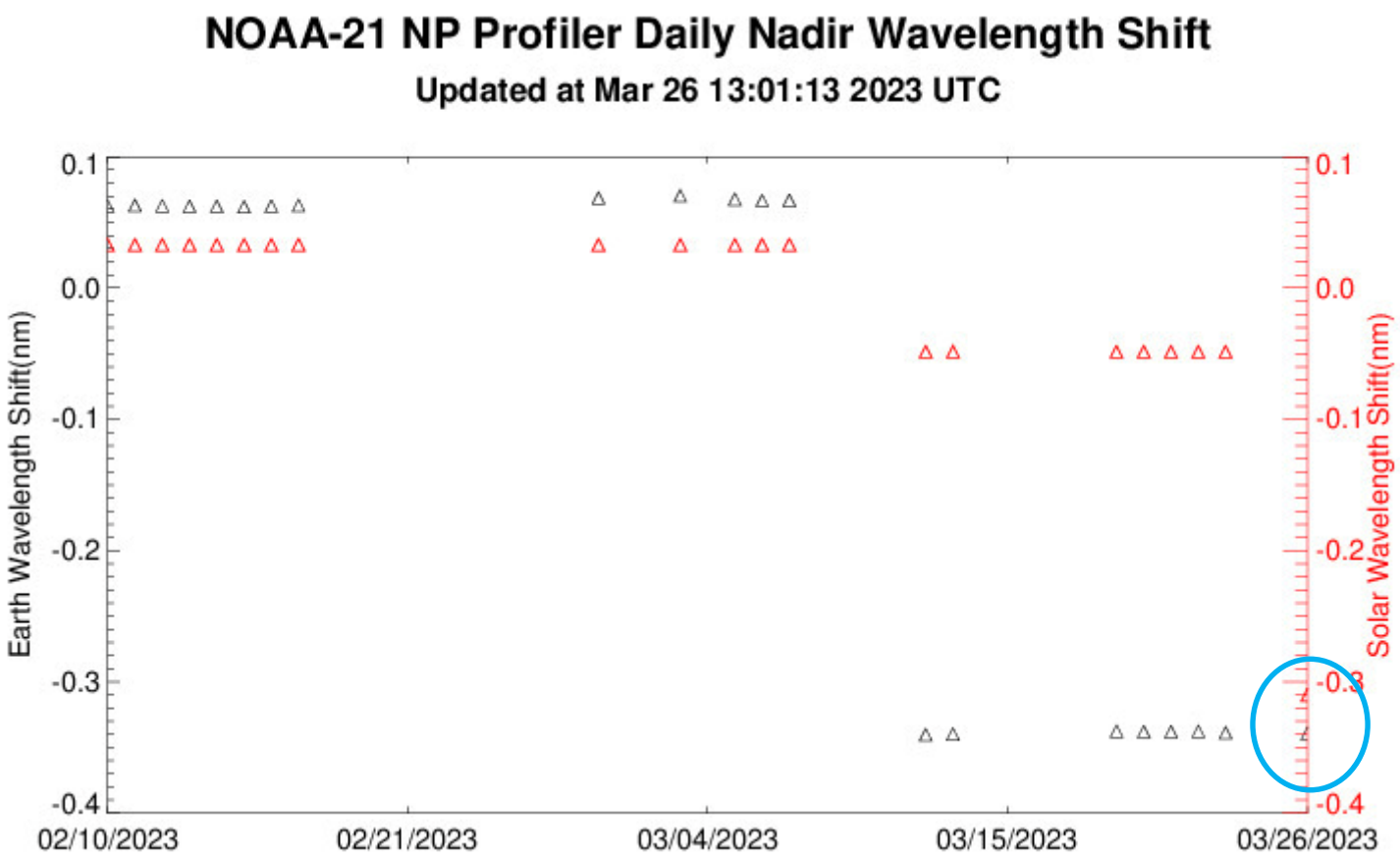


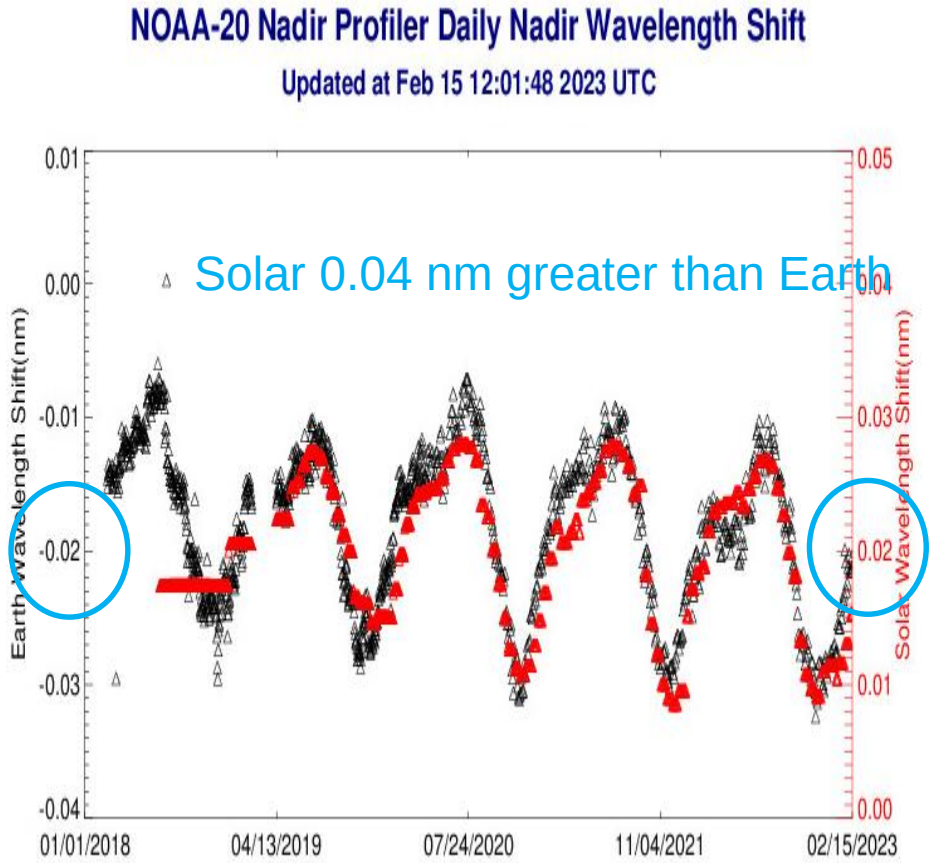
Evaluation of the effect of required algorithm inputs

- Required Algorithm Inputs
  - OMPS Nadir Mapper SDR and GEO
  - OMPS Nadir Profiler SDR and GEO
  - Instrument interpolation tables
  - Soft calibration tables (currently zero adjustments)
- Evaluation of the effect of required algorithm inputs
  - Study / test cases
  - Results

ICVS Mg II wavelength shifts – Earth vs. Solar

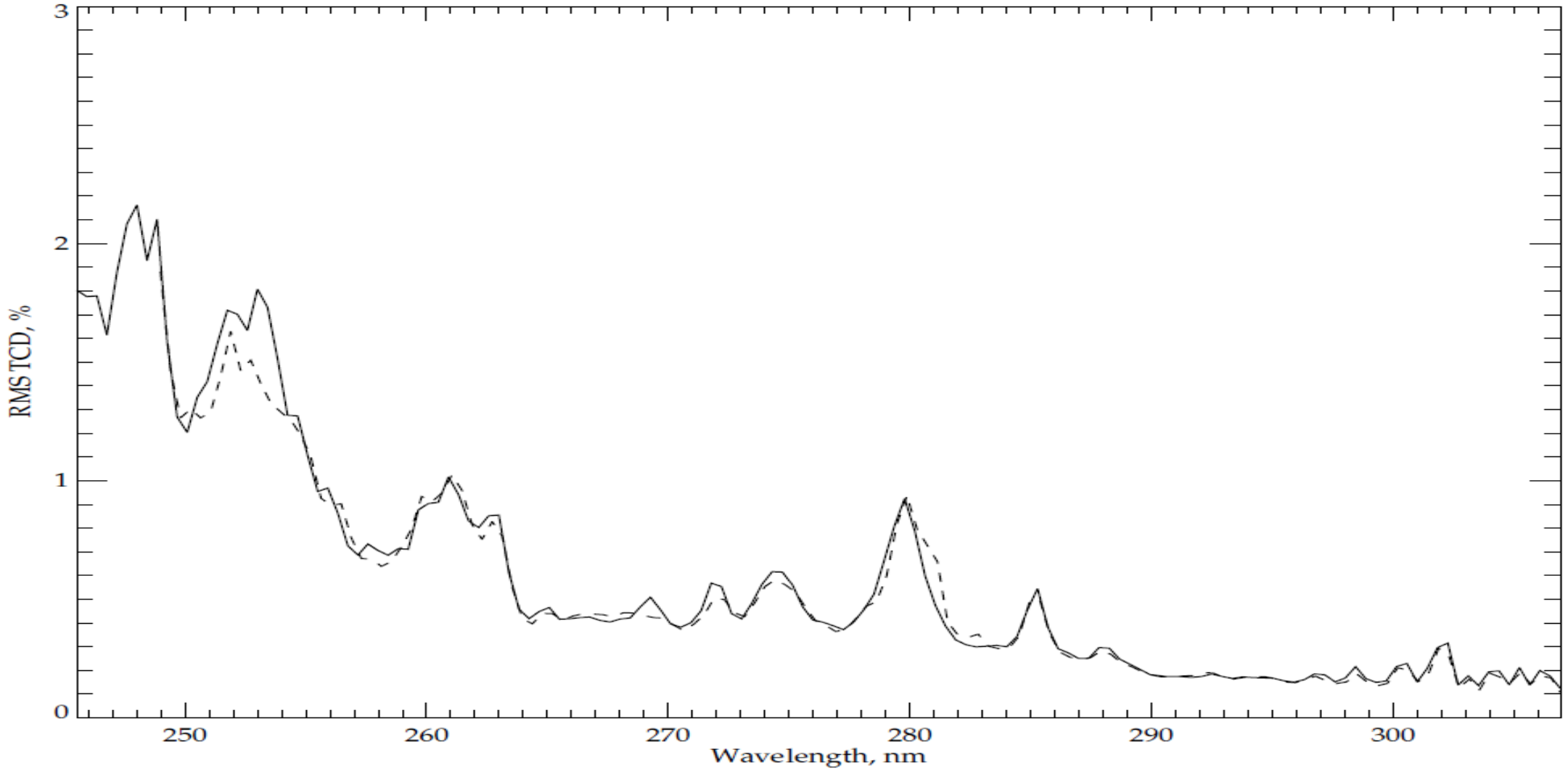
Earth and Solar wavelength scales now show the expected relationship.





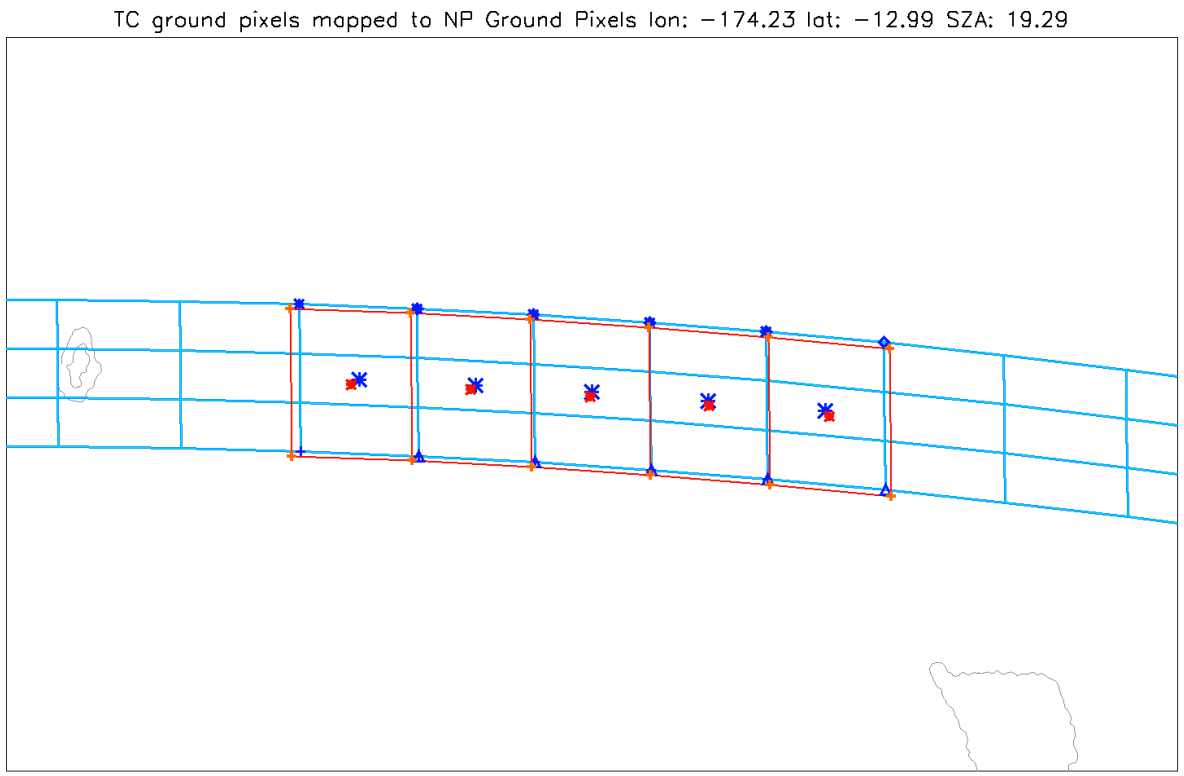
https://www.star.nesdis.noaa.gov/icvs-beta/status_J02_OMPS_NP.php

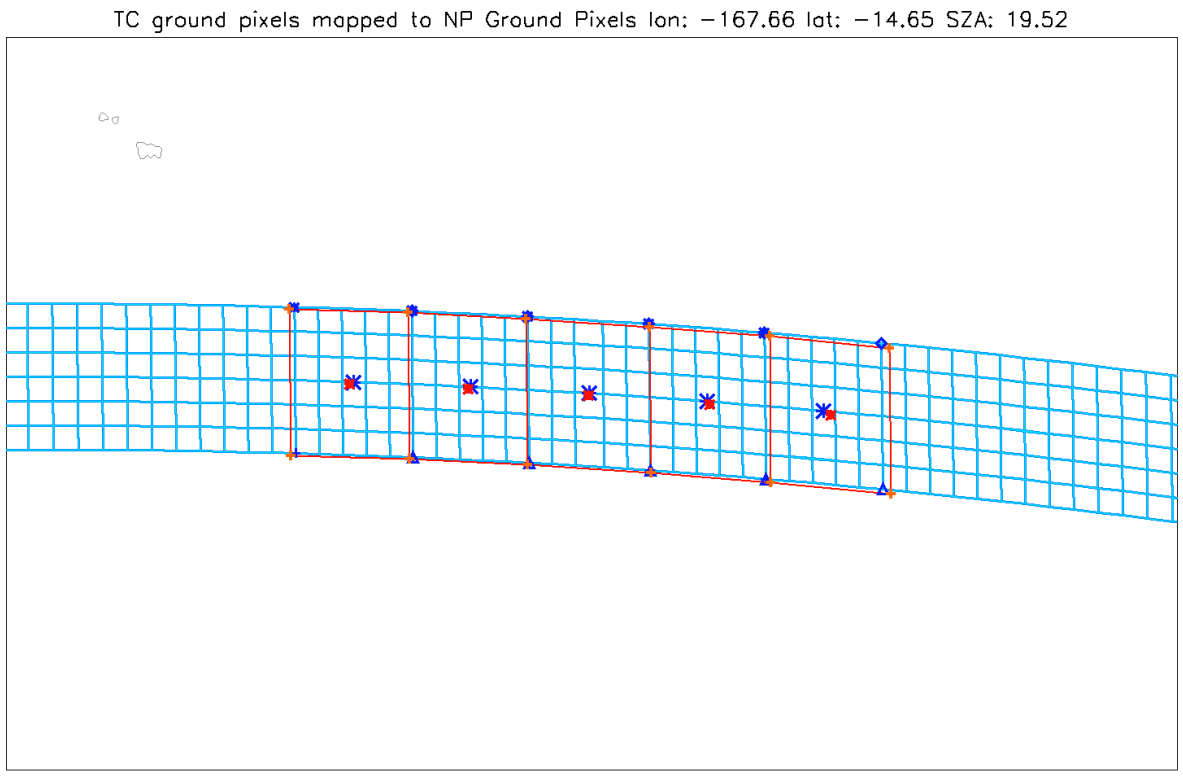
NOAA-21(Solid) & NOAA-20(Dash) OMPS NP SDR Noise estimates for Earth Radiances using triple centered differences for March 22, 2023, using all cross-tracks, no SAA



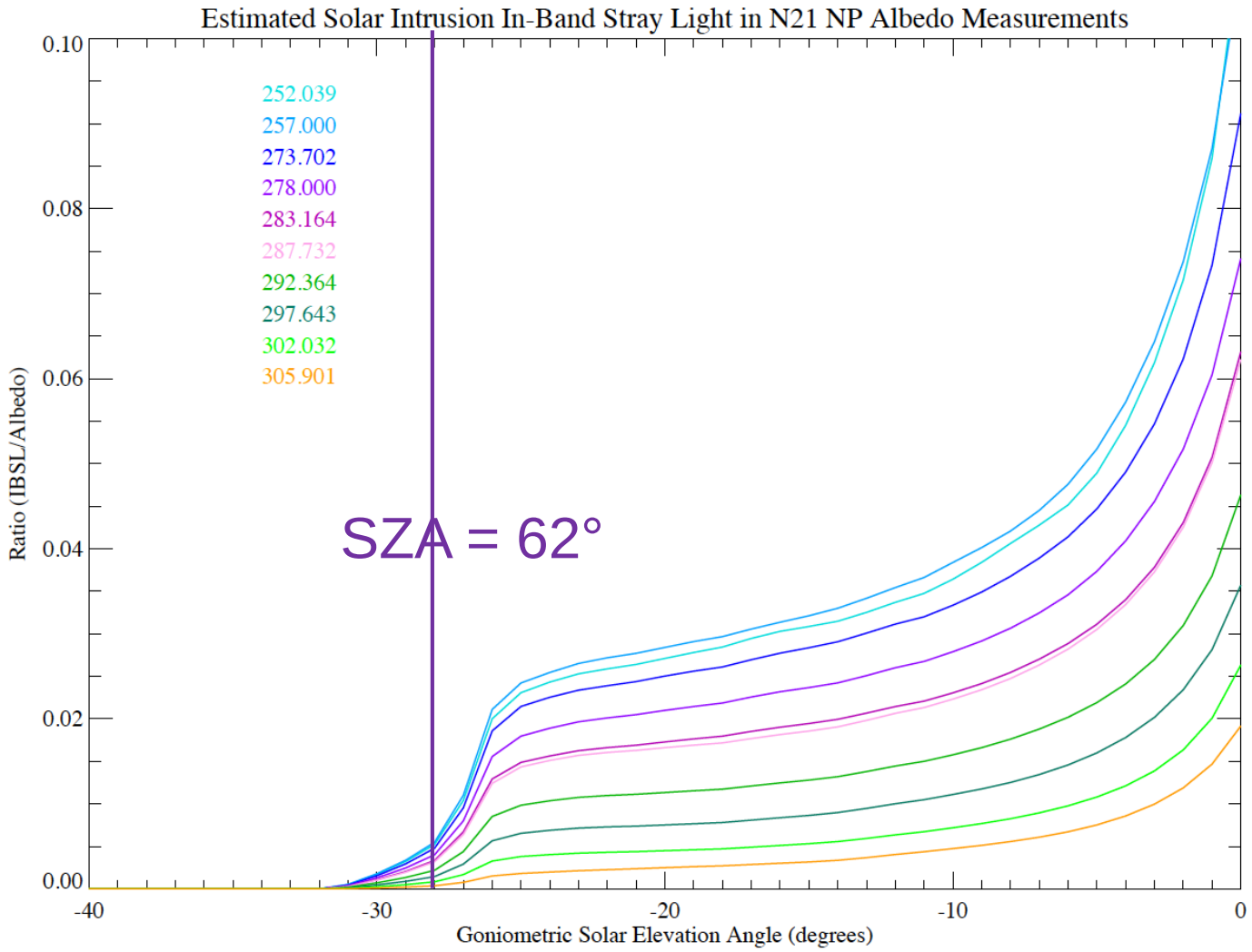
N20/N21 Representative GEO scene

- Red: NP ground pixel corners, centers, and edges. One 7.5 second scan, 5 NP pixels
- Blue: TC ground pixel corners, centers, edges. Three 2.5 second TC scans, lower left.
- Blue: TC ground pixel corners, centers, edges. Six 1.25 second TC scans, lower right.
- Mapped scene is northwest of the island of Samoa.
- There are 1CT and 3AT TC ground pixels per each NP pixel, lower left.
- There are 5CT and 6AT TC ground pixels per each NP pixel, lower right.



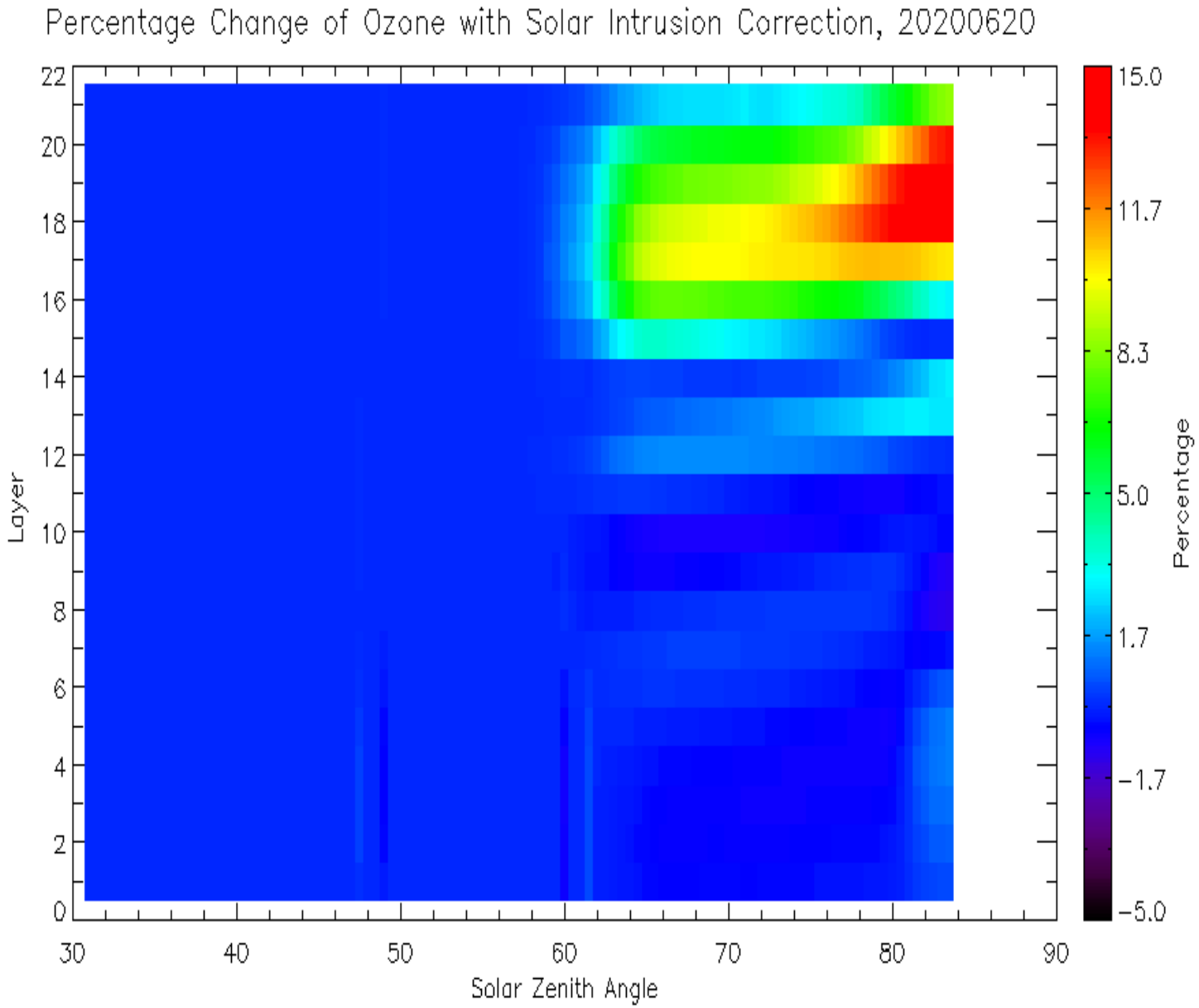


NOAA-21 OMPS NP Solar Intrusion Northern Hemisphere Stray Light Estimates



NOAA-20 V8Pro profile retrieval change with the In-band Stray Light Solar Intrusion correction

NOAA-21 OMPS NP has approximately two-thirds of the IBSL of NOAA-20 OMPS NP. Errors in the upper layers of the V8Pro EDR will be present for the Northern Hemisphere for Solar Zenith Angles greater then 62 degrees until a model of the NOAA-21 stray light is developed and the correction is implemented by the SDR Team.



Documentations (Check List, 1 slide)

Science Maturity Check List	Yes ?
ReadMe for Data Product Users	Yes (after approval)
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	Performance shows good agreement compared to NOAA-20 for a Beta Maturity level.
Information/data from validation efforts can only be used to make initial qualitative or very limited quantitative assessments regarding product fitness-for-purpose	Performance shows good agreement compared to NOAA-20 for a Beta Maturity level.
Documentation of product performance and identified product performance anomalies, including recommended remediation strategies, exists	Improvement is needed in the form of soft calibration adjustments in the EDR processing and solar stray light model development and correction in the SDR processing.

Conclusion & Caveats

- The NOAA-21 OMPS NP & NM GEOs have good, well-aligned Geolocations.
- The NOAA-21 OMPS NP & NM SDRs have good performance.
  - The OMPS NM SDRs have a small error in the wavelength / solar table for three near-nadir FOVs. This will be fixed with the fast-track table updates on 4/7/2023.
  - The OMPS NP SDRs have stray light at high solar zenith angles (SZA) in the Northern Hemisphere. While the contamination is approximately 2/3 of the NOAA-21 stray light, upper layers for ozone profiles in the Northern Hemisphere for SZA > 62° will have large errors until a correction is implemented.
- While the NOAA-21 V8Pro EDR values are reasonable, the total and profile ozone values have not been fully validated. Soft calibration adjustments to force agreement with S-NPP and NOAA-20 V8Pro EDRs are under development. This has to be done in concert with possible SDR changes to the calibration coefficients and out-of-band stray light corrections as they progress from provisional to fully validated.
- We recommend NOAA-21 V8Pro v4r2 EDRs from NDE I&T be released at Beta Maturity as of 3/24/2023. The instruments are still making extensive calibration and diagnostic measurements, so the Earth Science coverage is less than for regular operations. Regular operations will begin next month.