



Ozone Mapping and Profile Suite (OMPS) Nadir Mapper and Nadir Profiler Version 8 Ozone Algorithms

L. Flynn

STAR JPSS Enterprise Algorithms Workshop

March 30, 2016



I. V8TOz Algorithm Status & Approach

- Current status
 - The Version 8 total ozone algorithm (V8TOz) and Linear Fit SO₂ (LFSO₂) algorithm were developed by NASA TOMS and OMI Science Teams.
 - Versions of the total ozone algorithm have been in use at NOAA for operational processing of SBUV/2 and GOME-2 measurements and for offline processing of the OMPS NM measurements.
- The products will provide the operational estimates of daily global total columns of atmospheric ozone from the OMPS Nadir Mapper measurements.



V8TOz: Brief Algorithm Description



The Version 8 total column O₃ algorithm (V8TOz) is the most recent version of a series of BUV (backscattered ultraviolet) total O₃ algorithms and includes better understanding of UV radiation transfer, internal consistency checks, and comparison with ground-based instruments. The algorithm makes two key assumptions about the nature of the BUV radiation.

Firstly, we assume that the BUV radiances at wavelengths greater than 310 nm are primarily a function of total O₃ amount, with only a weak dependence on O₃ profile that can be accounted for using a set of standard profiles.

Secondly, we assume that a relatively simple radiative transfer model that treats clouds, aerosols, and surfaces as Lambertian reflectors can account for most of the spectral dependence of BUV radiation, though corrections are required to handle special situations.

The recent algorithm versions have incorporated procedures for identifying these special situations, and apply semi-empirical corrections, based on accurate radiative transfer models, to minimize the errors that occur in these situations.



Linear Fit Algorithm: Path to SO₂

- The V8 ATBD describes the Linear Fit algorithm to create SO₂ product (LFSO2). The algorithm uses the V8TOz as a starting point as a linearization step to derive an initial estimate of total ozone assuming zero SO₂. The residuals at the twelve wavelengths are then calculated as the difference between the measured and computed N-values ($N = -100 \cdot \log_{10}(I/F)$, I is Earth radiance and F is solar irradiance) using a forward model radiative transfer code.
- In the presence of SO₂, the residuals contain spectral structures that correlate with the SO₂ absorption cross-section. To reduce this interference, a median residual for a sliding group of SO₂-free and cloud-free scenes, radiative cloud fraction < 0.15) covering sixteen consecutive OMPS granules (approximately 30 degrees of latitude along-track).
- For each OMPS scene, the product provides three different estimates of the column density of SO₂ in Dobson Units ($1\text{DU} = 2.69 \cdot 10^{16}$ molecules/cm²) obtained by making different assumptions about the vertical distribution of the SO₂:
 - Lower tropospheric SO₂ column (**ColumnAmountSO2_TRL**, height ~2.5 km)
 - Middle tropospheric SO₂ column, (**ColumnAmountSO2_TRM**, height ~7.5 km),
 - Upper tropospheric and Stratospheric SO₂ column (**ColumnAmountSO2_STL**, height ~17.5 km).



V8TOz Concept of Operations

- Obtain OMPS NM SDR and GEO from IDPS at NDE
- Process SDRs to V8TOz EDRs granule by granule
- Process 16 V8TOz EDR granules at a time to produce the final SO_2/O_3 estimates.
- The algorithms currently read in static sets of climatological data and Radiative Transfer Look-Up Tables.
 - The use of better forecasts of snow/ice cover, surface pressure and temperature profiles will be explored for future improvements.
- The algorithms use a set of soft calibration adjustments that will be updated infrequently.



Integrated Product Team (IPT)



- IPT Lead: L. Flynn (STAR)
- IPT Backup Leads: V. Kapoor (OSPO), C.T. Beck (STAR)
- NESDIS team:
 - STAR: W. Wolf, L. Zhou
 - OSPO: R. Lindsay, Z. Cheng, C. Sisko, D. McNamera
 - OSGS: T. Schott
 - NOAA JPSS: A. Layns, L. Dunlap
 - Data Center: P. Jones (NCEI)
 - Others: Z. Zhang (IMSG), J. Niu (SRG), B. Das (IMSG), E. Beach (IMSG), V. Mikles (IMSG), D. Powell (Lockheed Martin), S. Bunin
- User team
 - C. Long (NCEP/CPC), J. Derber (NCEP/EMC)
 - Others: International NWP users, NWP FOs, Climate Users
- Atmospheric Chemistry POP
- Other POPs involved: ICAPOP



Customers/ Users



- NCEP/CPC
- NCEP/EMC
- International NWP Users
- NRL
- WMO Ozone Assessment



Current Operational Product



- The current OMPS NM total ozone product is made at IDPS with the Multiple Triplet Algorithm.
- We expect to complete a delivery (DAP) of the V8TOz algorithm for use with S-NPP and J-01 OMPS to NDE tomorrow (3/31/2016).
- The NDE implementation will use the OMPS NM SDR and GEO HDF5 files.
- The NOAA operational processing of Metop-A and Metop-B GOME-2 uses this algorithm.
- The NOAA operational processing of SBUV/2 measurements uses this algorithm to create their total ozone estimates.



Enterprise Credentials (1)



- The V8TOz algorithm is currently used to generate products for
 - SBUV/2 (as part of V8Pro to create NOAA operational and CDR products)
 - GOME-2 (to create NOAA operational products)
 - OMI (to create NASA direct broadcast, NRT and CDR products)
 - OMPS (as part of V8Pro to create IDPS Nadir Profile EDRs, at NOAA and NASA to create CDRs, and to create NASA direct broadcast)
 - TOMS (to create historic CDR products)



Enterprise Credentials (2)

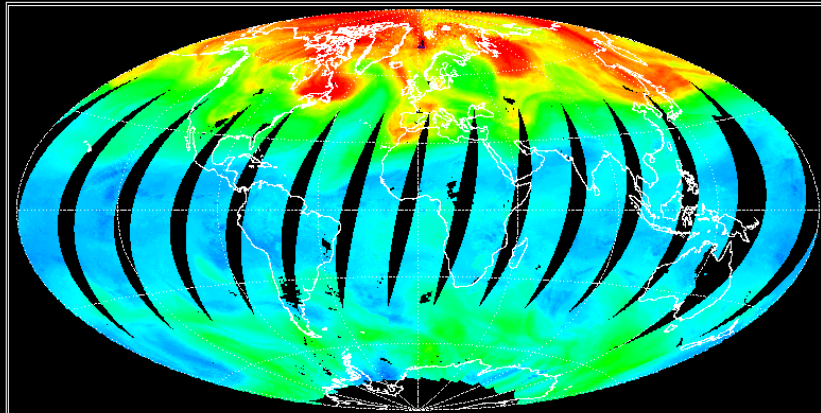
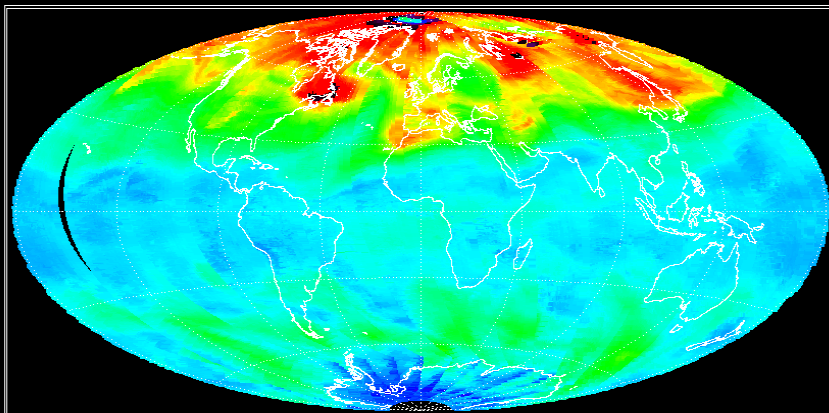


- A Master Radiative Transfer (RT) Table and a reference solar spectrum both at high spectral resolution are combined with bandpass information to produce an instrument-specific set of RT Look-Up Tables.
- For each scene, a set of measurements (Solar irradiance and Earth radiance at twelve Wavelengths) and viewing conditions (Day of Year, Latitude, Longitude, Solar Zenith and Azimuth and Satellite Viewing Zenith and Azimuth Angles) are identified and used to retrieve the total column ozone and other estimates.

Enterprise Credentials (3) Daily maps of total column ozone.

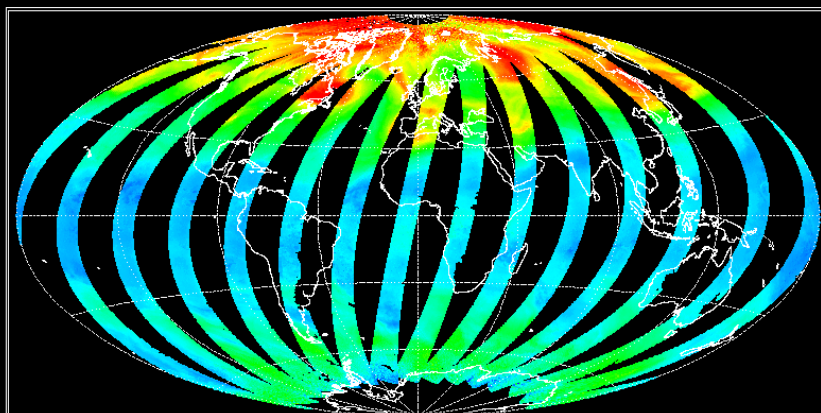
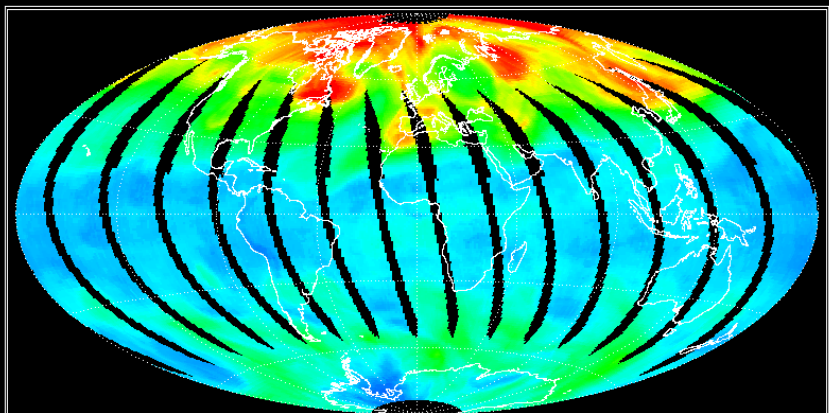
OMPS V8 Total Ozone for 20160323

Metop_B GOME-2 Total Ozone for 20160323



OMI Total Ozone for 20160323

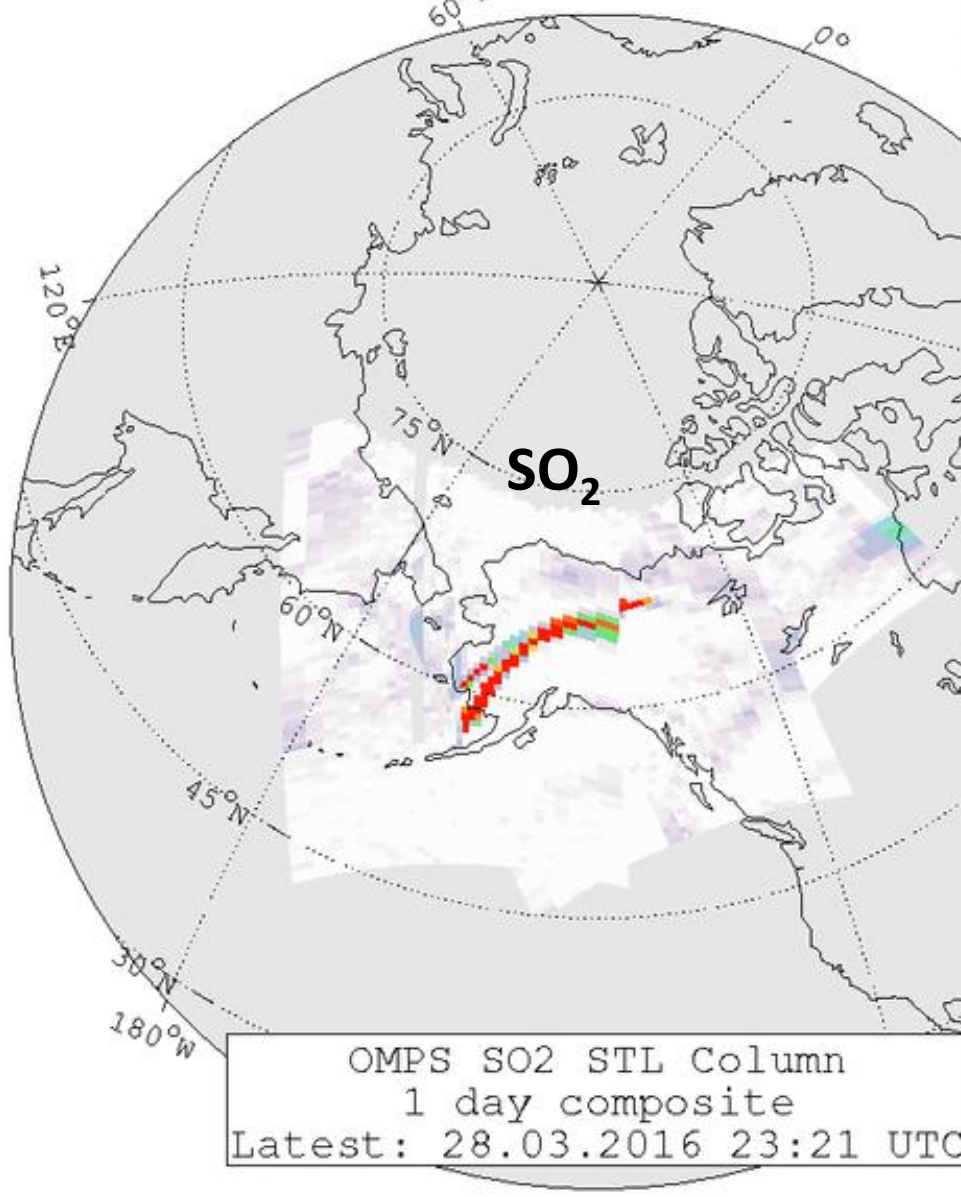
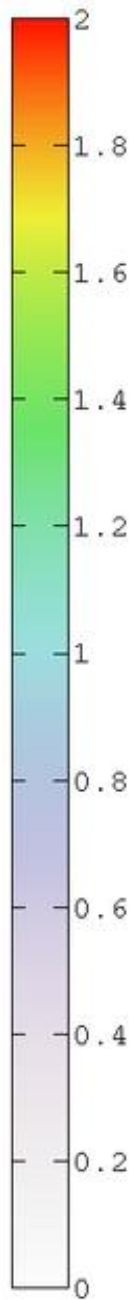
Metop_A GOME-2 Total Ozone for 20160323



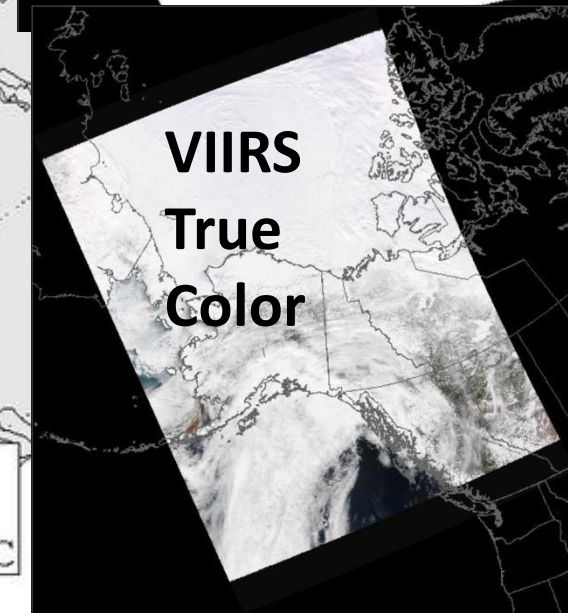
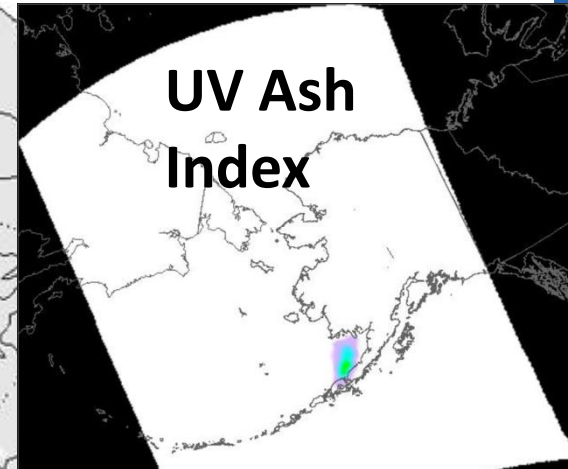
False color maps of total column ozone in Dobson Units for March 23, 2016 for the V8TOz algorithm applied to S-NPP OMPS (Top Left), Metop-B GOME-2 (Top Right), EOS Aura OMI (Bottom Left) and Metop-A GOME-2 (Bottom Right).

SNPP/OMPS Direct readout data

SO₂



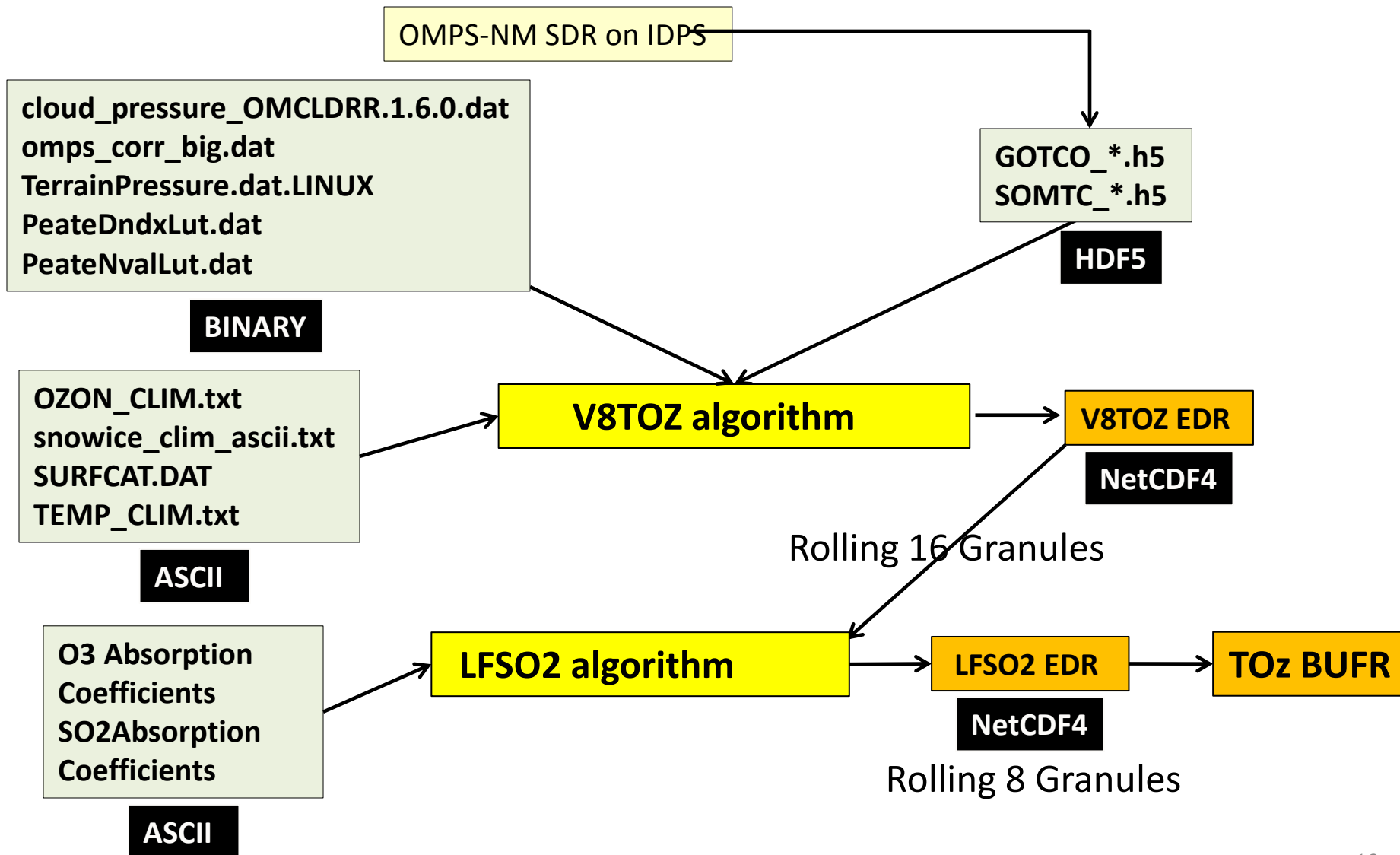
OMPS SO2 STL Column
1 day composite
Latest: 28.03.2016 23:21 UTC



DU

FMI-GINA-NASA







Lessons Learned



- **Implementation of product in NDE system**

The initial implementation will use static climatologies and radiative transfer look up tables. There is one table with soft calibration adjustments that will be updated infrequently.

The LFSO2 algorithm operates on multiple granules of the V8TOz output. We are working with NDE to develop an operational approach.
- **Interdependency with other NDE products**

The baseline implementation does not use other NDE products.

The output will be used to make BUFR product for NWS delivery.



Path Forward



- Anticipated developments
 - Algorithm Readiness Review Completed last week and V8TOz DAP is scheduled for delivery this week.
- Upcoming Deliveries/Reviews
 - Delta ARR and DAP for the LFSO2 expected in April.
- Risks
 - The V8TOz delivered to NDE is designed to accept the full range of S-NPP and J-01 OMPS NM SDRs.
 - The delivery and implementation schedules are tight for implementation before the possible J-01 launch.



Summary



- Current Status
 - The V8TOz transition to NDE has progressed well.
 - The LFSO2 is following close behind.
- Outstanding issues
 - The details of 16-granule processing for the LFSO2 algorithm are yet to be determined.
 - NDE has lots of new algorithms on the way and will have build moratoria or freezes which could impact implementation schedules.



II. Version 8 Ozone Profile (V8Pro)



- The V8Pro algorithm is currently used to generate products with measurements from
 - SBUV/2 (at NOAA to create operational and CDR products)
 - OMPS (at IDPS to create Nadir Profile EDRs, and at NOAA and NASA to create CDRs)
 - SBUV and BUUV (at NASA to create historic CDR products)
- The products will provide the operational estimates of atmospheric ozone profiles from the combined OMPS Nadir Profiler (NP) and Nadir Mapper (NM) measurements.



Version 8 Ozone Profile (V8Pro)



- The V8Pro algorithm uses a maximum likelihood retrieval to generate estimates of the vertical profile distribution of atmospheric ozone from Solar Backscatter Ultraviolet measurements.
- The retrievals uses measurements at twelve wavelength from 252 nm to 380 nm. The eight measurements for wavelengths shorter than 310 nm are from the OMPS NP and the four measurements for longer wavelengths are from the OMPS NM.
- The ozone profile is provided for 21 layers each approximately 3-km in vertical extent. The product contains accompanying parameters including measurement residuals and averaging kernels. The products are used as the input for BUFR products delivered to the NWS.



Concept of Operations



- Obtain OMPS NM and NP SDR and GEO from IDPS
- Matchup a single OMPS NP SDR Granule with one or two OMPS NM SDR Granules.
- Aggregate NP and NM measurements as needed to create input for cross-track FOVs.
- Process each cross-track FOV's set of measurements at twelve wavelengths to create V8Pro ozone profile estimates.
- The algorithms currently reads in static sets of climatological data and Radiative Transfer Look-Up Tables.
 - The use of better forecasts of snow/ice cover, surface pressure and temperature profiles will be explored for future improvements.
- The algorithms use a set of twelve soft calibration adjustments that will be updated infrequently.



Integrated Product Team (IPT)



- IPT Lead: L. Flynn (STAR)
- IPT Backup Leads: C.T. Beck (STAR), V. Kapoor (OSPO)
- NESDIS team:
 - STAR: W. Wolf, L. Zhou
 - OSPO: R. Lindsay, Zhaohui Cheng, C. Sisko, D. McNamera
 - OSGS: T. Schott.
 - NOAA JPSS: A. Layns, L. Dunlap
 - Data Center: P. Jones (NCEI)
 - Others: Z. Zhang (IMSG), J. Niu (SRG), B. Das (IMSG), E. Beach (IMSG), V. Mikles (IMSG), D. Powell (Lockheed Martin), S. Bunin
- User team
 - C. Long (NCEP/CPC), J. Derber (NCEP/EMC)
 - Others: International NWP users, NWP FOs, Climate Users
- Atmospheric Chemistry POP
- Other POPs involved: ICAPOP



Customers/ Users



- NCEP/CPC
- NCEP/EMC
- International NWP Users
- NRL
- WMO Ozone Assessment

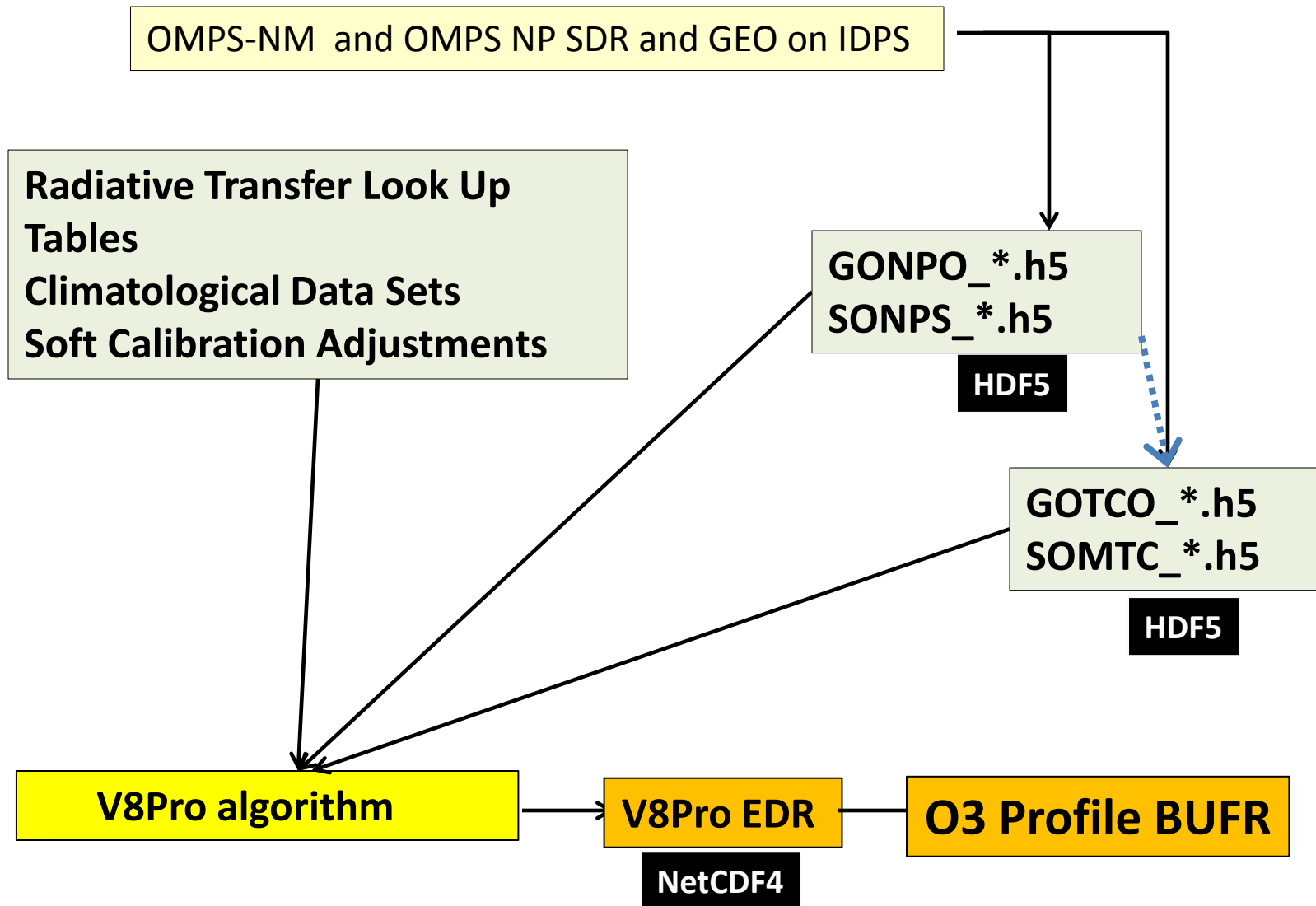


Current Operational Product



- The V8Pro is used to create the operational NOAA POES SBUV/2 Product Master Files (PMFs) and this in turn is used to create the BUFR files delivered to NWS and other users.
- The V8Pro is used at IDPS to make the S-NPP OMPS Nadir Ozone Profile EDR (IMOPO) and this in turn is used to create Ozone Profile BUFR files at NDE for delivery to NWS and other users.
- No OMPS Nadir Ozone Profile EDR is currently produced at NDE.

V8Pro Algorithm High Level Flow





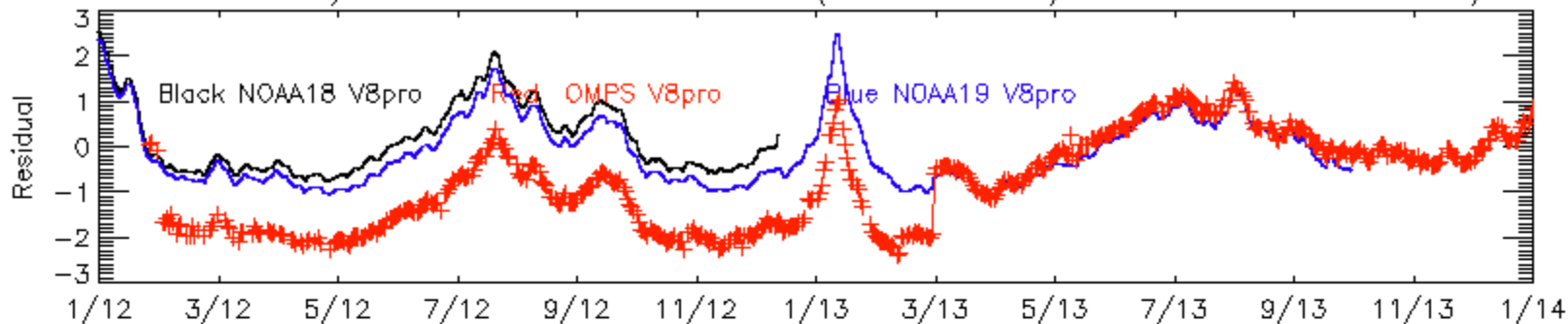
Monitoring and Soft Calibration



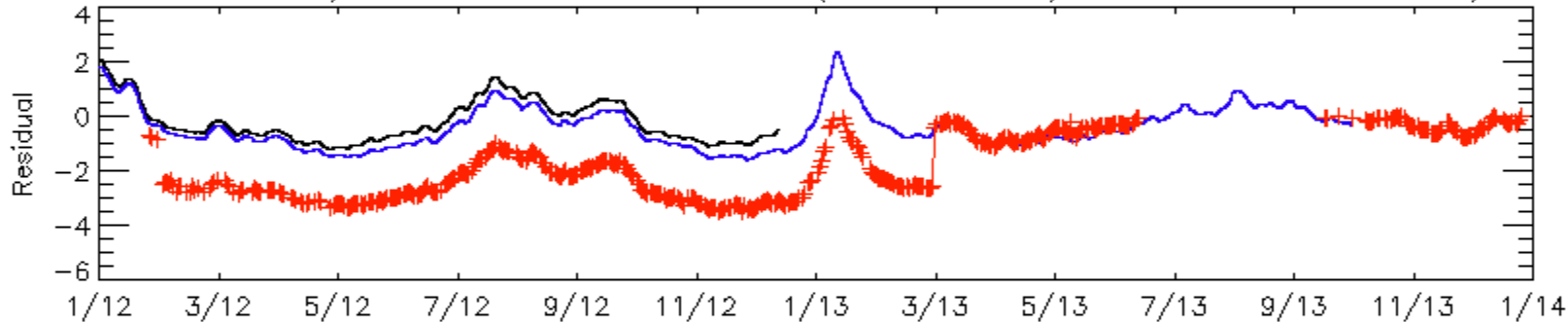
- The figures on the next slide show time series of initial measurement residuals (measured N-values minus those predicted by a radiative transfer forward model using the first guess profile).
- The three figures show how the off-line processing of the OMPS V8Pro was adjusted with a soft calibration in March 2013 and kept good alignment with the NOAA-19 SBUV/2 results until new SDR calibration was implemented.



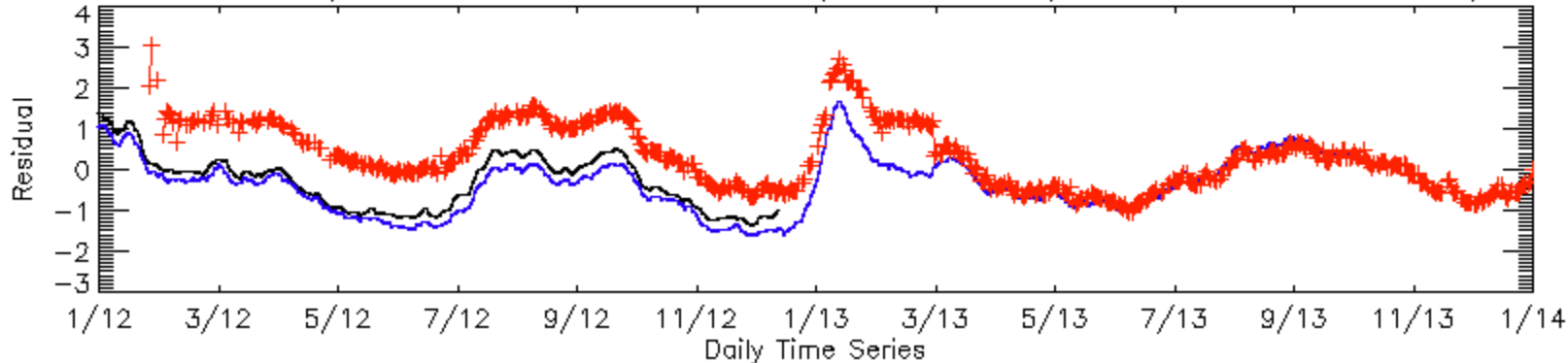
N18N19 OMPS Daily Zonal Mean Initial Residual (Cha4@288nm) 1.2012-2.2014 20S20N/-90W0



N18N19 OMPS Daily Zonal Mean Initial Residual (Cha5@292nm) 1.2012-2.2014 20S20N/-90W0



N18N19 OMPS Daily Zonal Mean Initial Residual (Cha6@298nm) 1.2012-2.2014 20S20N/-90W0





Lessons Learned



- LINUX to LINUX migration is simplifying testing.
- The product currently only depends on static tables and files and the OMPS NM and OMPS NP SDR and GEO for inputs.
- We are rewriting the code that performs the functions of the IDPS Glueware and making it more general for processing the new medium resolution FOV J-01 OMPS SDRs.



Path Forward



- Anticipated developments
 - Output files have been converted to NetCDF4.
 - Soft calibration adjustments are under development.
 - Adaptations to process Medium FOV J-01 OMPS data are in testing.
- Upcoming Deliveries/Reviews
 - The Algorithm Readiness Review will take place next month with a DAP to follow closely.
- Risks
 - Matching NP and NM FOVs and Granules is not yet tested at NDE.
 - The delivery and implementation schedules are tight for implementation before the possible J-01 launch.



Refinements for V8Pro



→ Solar Activity and Wavelength Scales

The daily Mg II Index values from GOME-2 can be used to adjust the Day 1 solar by using scale factors. Earth Radiances can also be used to get daily estimates.

The day of year values can be used to give the expected wavelength scale from intra-annual variations. The can be used to adjust the Day 1 solar and its wavelength scale. (The V8Pro can accommodate small variations in the wavelength scale about some mean values.)

→ Information concentration/Noise reduction for Outlier Detection & Removal

Information concentration can be performed at the same step as the N-value creation. SONPO will maintain spectral coverage for smaller FOVs.

→ Smaller FOVs

NM/NP Matchups modifications are being made to handle new cases of FOVs J01.

→ New ancillary Input

The NDE system can access better data for snow/ice and surface pressure for use in the V8Pro processing.



Summary



- Current Status
 - The V8Pro is already in use operationally at IDPS for S-NPP OMPS with a full set of reviews and documentation.
 - The adaptations to process Medium FOV J-01 OMPS data and to run the code at NDE are progressing well.
- Outstanding issues
 - The code to handle the full range of OMPS NM and OMPS NP FOVs/SDRs is in development.
 - NDE has lots of new algorithms on the way and will have build moratoria or freezes which could impact implementation schedules.



Supporting Content





Version 8 Total Column Ozone (V8TOz)



- Overview of technical approach of the algorithm and its implementation
 - The V8TOz will be implemented on a granule processing to create an EDR. The algorithm combines radiance/irradiance ratios at 12 channels with climatological information and radiative transfer tables for standard ozone profiles to compute estimates of total column ozone, effective reflectivity and aerosols.
 - The LFSO₂ algorithm uses the measurement residuals from the V8TOz retrievals to estimate the SO₂ using three sensitive channels and adjusts the final ozone estimate for the SO₂ absorption effects.
 - The V8TOz algorithm uses the OMPS NM SDR and GEO products, climatological ancillary data, and radiative transfer look-up tables. We expect to refine the ancillary data in the future, e.g., use daily snow/ice tiles in place of climatology.



OMPS Total Ozone Product Requirements



- JPSS Level 1 Requirements Document (L1RD) Supplement for the OMPS Ozone Total Column Environmental Data Records (EDRs)

Table 5.2.11 - Ozone Total Column (O₃)

EDR Attribute	Threshold
Ozone TC Applicable Conditions:	
1. Threshold requirements only apply under daytime conditions with Solar Zenith Angles (SZA) up to 80 degrees.	
2. The EDR shall be delivered for all SZA.	
a. Horizontal Cell Size	50 x 50 km ² @ nadir
b. Vertical Cell Size	0 - 60 km
c. Mapping Uncertainty, 1 Sigma	5 km at Nadir
d. Measurement Range	50 - 650 milli-atm-cm
e. Measurement Precision	
1. $X < 0.25$ atm-cm	6.0 milli-atm-cm
2. $0.25 < X < 0.45$ atm-cm	7.7 milli-atm-cm
3. $X > 0.45$ atm-cm	2.8 milli-atm-cm + 1.1%
f. Measurement Accuracy	
1. $X < 0.25$ atm-cm	9.5 milli-atm-cm
2. $0.25 < X < 0.45$ atm-cm	13.0 milli-atm-cm
3. $X > 0.45$ atm-cm	16.0 milli-atm-cm
g. Refresh	At least 90% coverage of the globe every 24 hours (monthly average)

Verification of Performance:

- 20-Pixel Aggregation and 7-S along track integration.
- 318 nm channel BUV comes from surface to top of atmosphere.
- Confirmed by coastlines and comparison to 750 m VIIRS.
- Confirmed by standard profiles and four years of processing.
- Precision estimates from Nearest Neighbor analysis.
- Accuracy is adjusted by soft calibration as described on Slide 79, confirmed on Slides 84 & 86.
- 105° cross-track swath provides full daily coverage.



V8TOz Validation



- Validation concept
 - Validation is concentrating on comparisons to total ozone retrievals from other total ozone mapping satellite instruments (e.g., SBUV/2, OMI, and GOME-2) and to ground-based records from Dobson and Brewer stations.
 - Products have been validated by the NOAA JPSS Ozone Team and NASA S-NPP Science Team for the first four years of S-NPP data from the V8TOz offline records. SO₂ products are in use at the European VAAC from the FMI Fast Delivery direct broadcast system.



OMPS Ozone Profile Product Requirements

Table 4.2.4 - Ozone Nadir Profile (OMPS-NP)

Attribute	Threshold	Objective
Ozone NP Applicable Conditions: 1. Clear, daytime only (3)		
a. Horizontal Cell Size	250 X 250 km (1)	50 x 50 km ²
b. Vertical Cell Size	5 km reporting	
1. Below 30 hPa (~ < 25 km)	10 -20 km	3 km (0 -Th)
2. 30 -1 hPa (~ 25 -50 km)	7 -10 km	1 km (TH -25 km)
3. Above 1 hPa (~ > 50 km)	10 -20 km	3 km (25 -60 km)
c. Mapping Uncertainty, 1 Sigma	< 25 km	5 km
d. Measurement Range		
Nadir Profile, 0 - 60 km	0.1-15 ppmv	0.01 -3 ppmv (0-TH) 0.1-15 ppmv (TH-60 km)
e. Measurement Precision (2)		
1. Below 30 hPa (~ < 25 km)	Greater of 20 % or 0.1 ppmv	10% (0 -TH)
2. At 30 hPa (~ 25 km)	Greater of 10 % or 0.1 ppmv	3%
3. 30 -1 hPa (~ 25 -50 km)	5% -10%	1%
4. Above 1 hPa (~ > 50 km)	Greater of 10% or 0.1 ppmv	3%
f. Measurement Accuracy (2)		
1. Below 30 hPa (~ < 25 km)	Greater of 10 % or 0.1 ppmv	10% (0 -15 km)
2. 30 -1 hPa (~ 25 -50 km)	5% -10%	5% (15 -60 km)
3. At 1 hPa (~ 50 km)	Greater of 10 % or 0.1 ppmv	5% (15 -60 km)
4. Above 1 hPa (~ > 50 km)	Greater of 10 % or 0.1 ppmv	5% (15 -60 km)
g. Refresh	At least 60% coverage of the globe every 7 days (monthly average) (2,3)	24 hrs. (2,3)
	(16.7° FOV)	v2,0, 9/22/12

Notes: 1. The SBUV/2 has a 180 km X 180 km cross-track by along-track FOV. It makes its 12 measurements over 24 Samples (160 km



V8Pro Validation



- Validation concept
 - Validation is concentrating on comparisons to ozone profile ozone retrievals from other ozone profile satellite instruments (e.g., SBUV/2 and MLS) and to ground-based records from Umkehr, Microwave and Ozone Sondes.
 - Products have been validated by the NOAA JPSS Ozone Team for the first four years of S-NPP data from the V8Pro offline records.