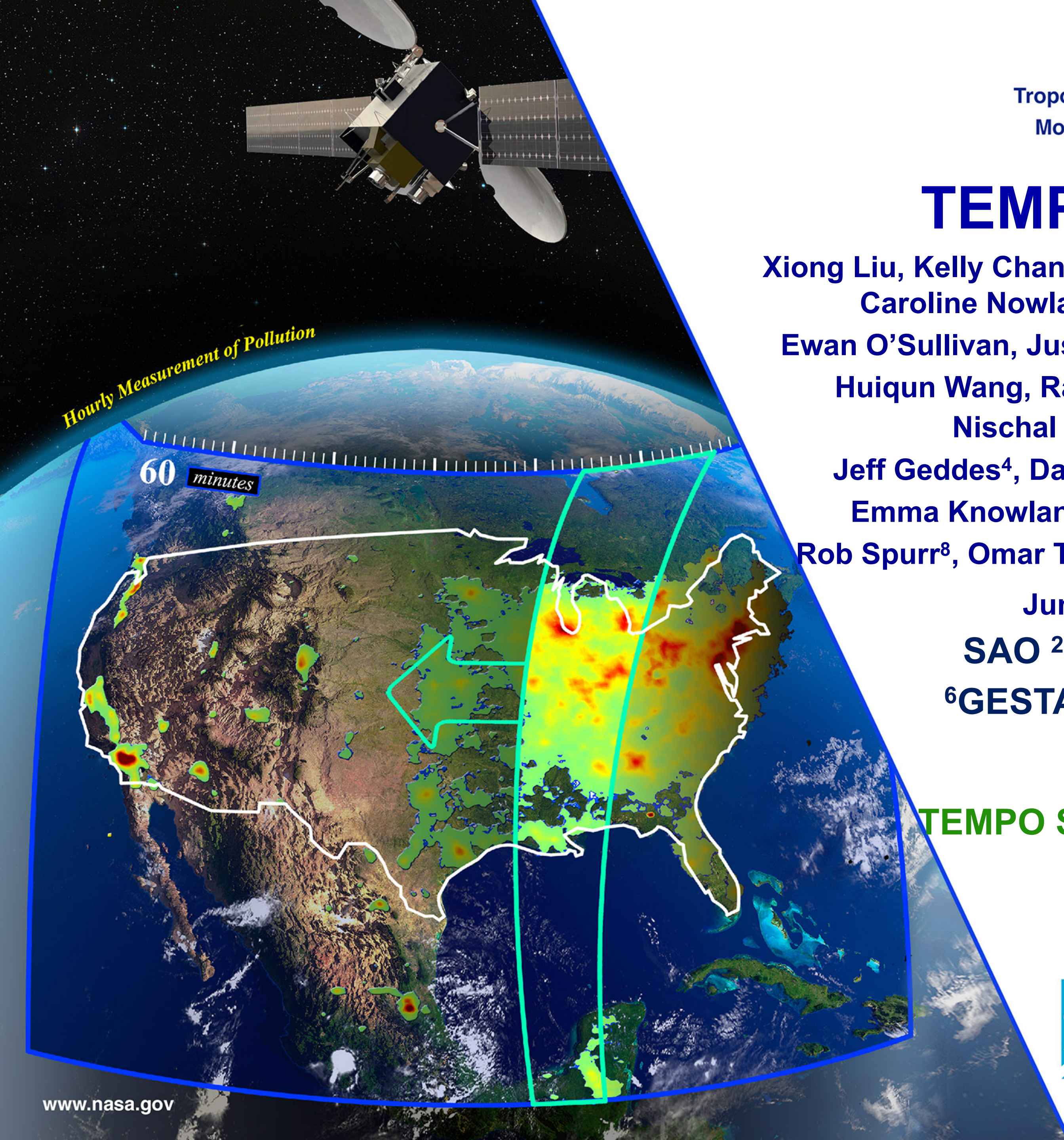

Tropospheric Emissions:
Monitoring of Pollution

TEMPO Algorithms

Xiong Liu, Kelly Chance, Gonzalo González Abad, Caroline Nowlan, John Houck, John Davis, Ewan O'Sullivan, Juseon Bak, Chris Chan Miller, Huiqun Wang, Raid Suleiman, Dave Flittner[2], Nischal Mishra[2], Zachary Fasnacht[3], Jeff Geddes[4], Dave Haffner[3], Joanna Joiner[5], Emma Knowland[6,5], Can Li[7,5], Wenhan Qin[3], Rob Spurr[8], Omar Torres[5], Alexander Vasilkov[3], Jun Wang[9] & The TEMPO Team

SAO [2]LaRc [3]SSAI [4]BU [5]GSFC [6]GESTAR [7]UMCP [8]RT Solution [9]Univ. Iowa

TEMPO Sci. Team Meeting 2022

May 31-June 2, 2022

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Outline

- Algorithm Overview (X. Liu)
  - Data products, retrieval teams
  - Algorithm development status and plan
  - TEMPO product distribution
- L0-1b processor (X. Liu)
- Ozone profile and tropospheric ozone algorithm (X. Liu)
- NO_2 and HCHO algorithms (C. Nowlan & G. Gonzalez Abad)
- O_2-O_2 cloud algorithm (H. Wang)
- SO_2 algorithm (C. Li)
- NRT production (P. Zoogman)
- Discussion

TEMPO Baseline Products (Variables) & Requirements

Species/Products	Required Precision	Temporal Revisit*
0-2 km O_3 (Selected Scenes) Baseline only	10 ppbv	2 hour
Tropospheric O_3	10 ppbv	1 hour
Total O_3	3%	1 hour
Tropospheric NO_2	1.0×10^{15} molecules cm^{-2}	1 hour
Tropospheric H_2CO	1.0×10^{16} molecules cm^{-2}	3 hour
Tropospheric SO_2	**1.0×10^{16} molecules cm^{-2}**	**3 hour**
Tropospheric $C_2H_2O_2$	**4.0×10^{14} molecules cm^{-2}**	**3 hour**
Aerosol Optical Depth	**0.10**	**1 hour**

* # of hourly measurements to be averaged to achieve required precision

- Mission duration: 20 months for baseline
- Spatial resolution: < 60 km^2 for baseline (4 native pixels coadded)

- **Aerosols, SO_2, $C_2H_2O_2$ were removed from baseline products during KDPC**
  - **Proposed to bring them back along with additional products and produce NRT/off-line products for some species, pending on funding from Science Needs Working Group (SNWG) in late 2022 or 2023.**
- **Cloud product (cloud fraction, cloud pressure): used in trace gas/aerosol retrievals**

TEMPO Data Products
(Inc. Proposed Additional & NRT Products)

Level	Product	Algorithm	Major Outputs	Res km^2 **	Freq/Size
L0	Digital counts	Raw to L0	Reconstructed/reformatted digital counts	2.0 x 4.75	Daily/hourly
L1-b	irradiance NRT	SAO L0-1	Calibrated & quality flags		daily
	radiance NRT	SAO L0-1	Geolocated,calibrated, viewing,geolocation&quality flags	2.0 x 4.75	Hourly, granule
L2	Cloud NRT	OMI O2-O2*	Cloud fraction, cloud pressure	2.0 x 4.75	Hourly, granule
	O_3 profile	SAO O3 profile	O3 profile, total/strat/trop/0-2 km O3 column, errors, a priori, AKs	8.0 x 4.75 ***	Hourly, granule
	Total O_3	TOMS V8.5	Total O3, AI, cloud fraction	2.0 x 4.75	Hourly, granule
	NO_2 NRT	SAO trace gas, BU strat/trop sep.	SCD, strat./trop. VCD, error, shape factor, scattering weights	2.0 x 4.75	Hourly, granule
	H_2CO NRT	SAO trace gas	SCD, VCD, error, shape factor, scattering weights	2.0 x 4.75	Hourly, granule
	$C_2H_2O_2$	SAO trace gas		2.0 x 4.75	Hourly, granule
	H_2O	SAO trace gas		2.0 x 4.75	Hourly, granule
	BrO	SAO trace gas		2.0 x 4.75	Hourly, granule
	Aerosol NRT	OMAERUV+UI AOCH	AAI, UVAOD, UVSSA, AOCH, VISAOD	8.0 x 4.75	Hourly, granule
	SO_2 NRT	OMSO2 PCA	SCD, VCD (PBL,TRL,TRM,TRU,STL)	2.0 x 4.75	Hourly, granule
	TEMPO/GOES-R Synerg. product	GOES-R products on TEMPO pixels	Radiance, aerosol, cloud & mask, fire/hotspot, snow/ice, rainfall, precipitable water, land/sea surface T, lightning	2.0 x 4.75	Hourly, granule
L3	Gridded L2	SAO L2-3	Same as L2	2 x 2 (?)	Hourly, scan
L4	UVB	GEMS UVB	UV irradiance, erythemal irradiance, UVI	TBD	Hourly, scan

*Algorithm changed from NASA GSFC's OMCLDRR to GSFC's new O_2-O_2 cloud algorithm combined with SAO's trace gas retrieval algorithm to retrieve O2-O_2 SCDs. ** Spatial resolution at center of FOR. *** Might be at 8 x 9.5km^2

Black: baseline, green/orange/purple: additional products (being proposed)

NRT: NRT products & off-line products (with additional NRT funding, otherwise produce 1 product within 3-6 hours except for O_3 profile)

TEMPO Algorithm Teams

Operational Algorithm	Personnel
Raw to L0	John Davis
L0-1b	John Houck, Xiong Liu, Dave Flittner, Weizhen Hou, Jim Carr, Chris Chan Miller
Ozone profile	Xiong Liu, Juseon Bak, Weizhen Hou
Total ozone	Dave Haffner, Joanna Joiner
Nitrogen dioxide	Caroline Nowlan, Gonzalo González Abad, Jeff Geddes, Chris Chan Miller
Formaldehyde	Gonzalo González Abad, Caroline Nowlan, Hyeong-Ahn Kwon, Chris Chan Miller
Glyoxal	Gonzalo González Abad, Hyeong-Ahn Kwon, Chris Chan Miller
Clouds	Huiqun Wang, Alexander Vasilkov, Eun-Su Yang, Joanna Joiner
Sulfur dioxide	Can Li, Nicolay Krotkov
Aerosols	Omar Torres, Jun Wang

Operational implementation and IT support @ SAO Science Data Processing Center (SDPC) by John Houck

TEMPO

Algorithm Development Status & Plan

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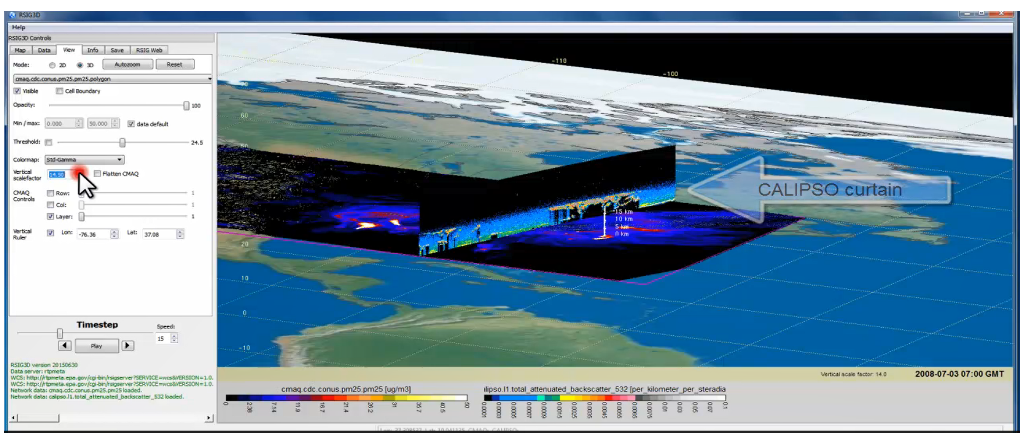
- SDPC V3 (launch ready) completed in Feb. 2022, verification almost done
- L0-1b updates: **T-dependent dark current correction, straylight correction based on 1-D PSF, INR using GOES-R**
- Major updates to L1-2 algorithms (O_3 profile, NO_2, HCHO, cloud, total O_3):
  - CLDO4[new]: SAO O_2-O_2 fitting + GSFC's O_2-O_2 cloud at ~477/466 nm (Huiqun Wang, Eun-Su Yang, Alexander Vasilkov)
  - NASA GMAO's GEOS-CF trace gas profiles and meteorology (Emma Knowland and GMAO)
  - Hourly resolved monthly mean Geometry-dependent Lambertian Equivalent Reflectivity (GLER) climatology (Christopher Chan Miller, Wenhan Qin, Zachary Fasnacht)
  - Interactive Multi-sensor snow & ice mapping systems (IMS) (Gonzalo Gonzalez Abad)
- Development of other products
  - CHOCHO, H_2O, BrO: will use SAO's trace gas algorithm
  - SO_2: OMI PCA SO_2 algorithm adapted for TEMPO/GEMS from synthetic/GEMS data (Can Li)
  - Aerosols: being adapted from OMI/TROPOMI AERUV algorithm (Omar's team), from EPIC/TROPOMI Aerosol Layer Height algorithm using O_2-A/B (Jun Wang's team)
- Continue to make minor updates to improve beyond V3
  - Further improvements using synthetic and GEMS data: destriping, radiance reference & background correction, cross section updates, empirical correction
  - Algorithm refinement/optimization during commissioning (Jun-Aug 2023) and nominal operation

TEMPO Data Products Distribution

- ❑ **TEMPO commissioning: ~L+105-L+195 (mid-May – mid August)**
- ❑ **Nominal operation: ~6 months after launch**
- ❑ **Plan to release initial L1b in ~4 mons, L2/3 in ~6 mons to the public after commissioning (i.e., Dec 2023 for L1b, Feb 2024 for L2/3).**
- ❑ **Provide data products to validation team priori to the public release via ASDC.**

❑ EPA RSIG3D Gateway

TEMPO data can be served directly through the EPA RSIG.
https://www.epa.gov/hesc/remote-sensing-information-gateway



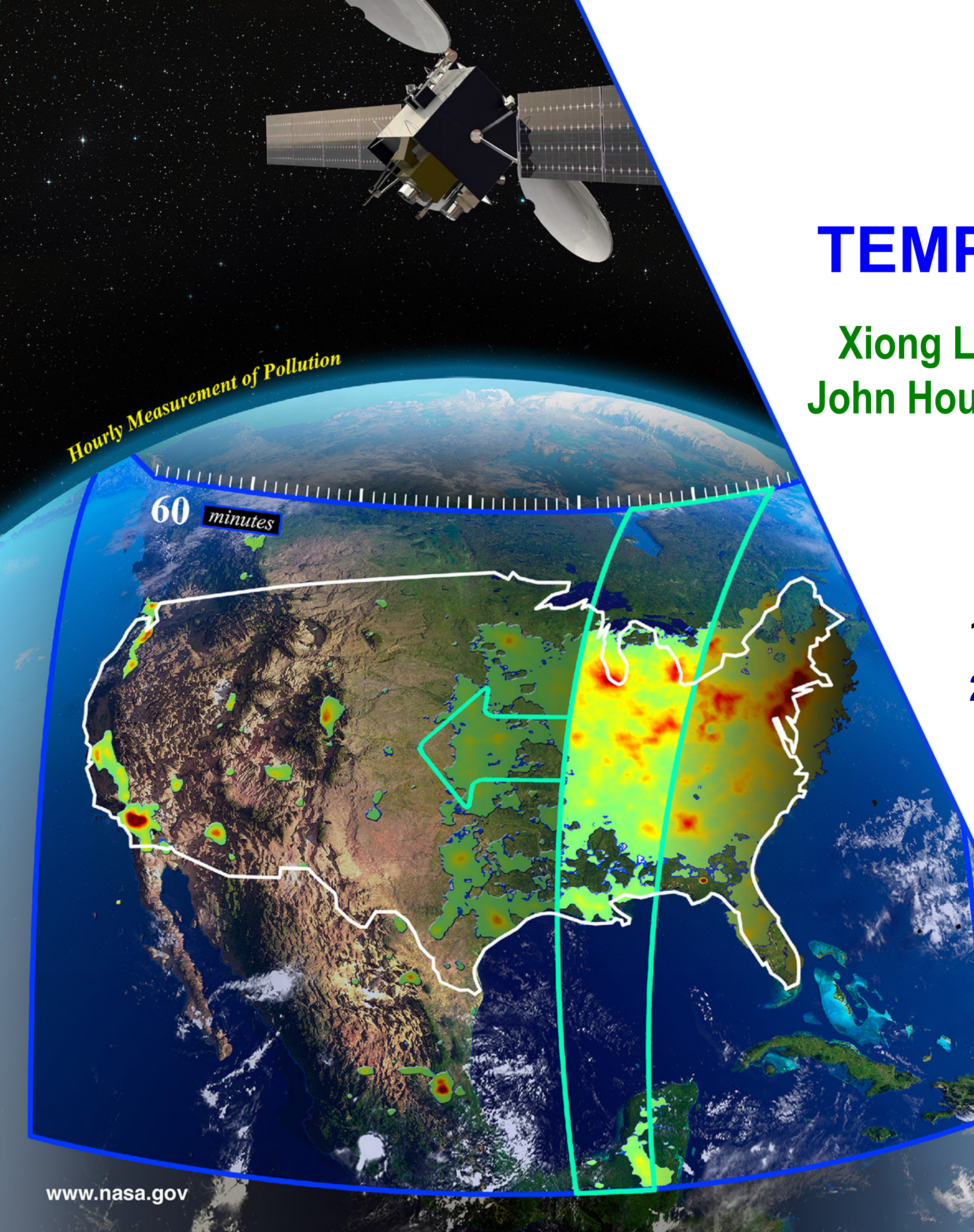
❑ ASDC Data Archival & Distribution: Tools and Services

- ✓ NASA Earthdata Search
  - CMR Search ∘ Metadata
- ✓ NASA WorldView
  - GIBS API ∘ visualization
- ✓ Harmony and OPeNDAP
  - ∘ transform ∘ subsetting
  - ∘ reformatting ∘ distribution
- ✓ HTTPS data access
  - ∘ datapool
  - ∘ permanent URL/direct access
  - ∘ enables scripts/workflow
- ✓ Geospatial Web Services
  - ∘ WCS ∘ WMS ∘ ArcGIS Image Service
- ✓ Example scripts
  - ∘ Python/Jupyter Notebook
  - ∘ R scripts
  - ∘ contributed tutorials/scripts

❑ User Support and Other Resources

Earthdata Login https://urs.earthdata.nasa.gov
Earthdata Forum https://forum.earthdata.nasa.gov/
ASDC User Support support-asdc@earthdata.nasa.gov

Slides from Jeff Walters, Tim Larson at TEMPO STM 2020 & EAWNov2021



Tropospheric Emissions:
Monitoring of Pollution

TEMPO

TEMPO L0-1b Processor

Xiong Liu[1], Dave Flittner[2], Kelly Chance[1], John Houck[1], Jim Carr[3], Chris Chan Miller[1] and the TEMPO Team

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1 Smithsonian Astrophysical Observatory
2 NASA Langley Research Center
3 Carr Astronautics

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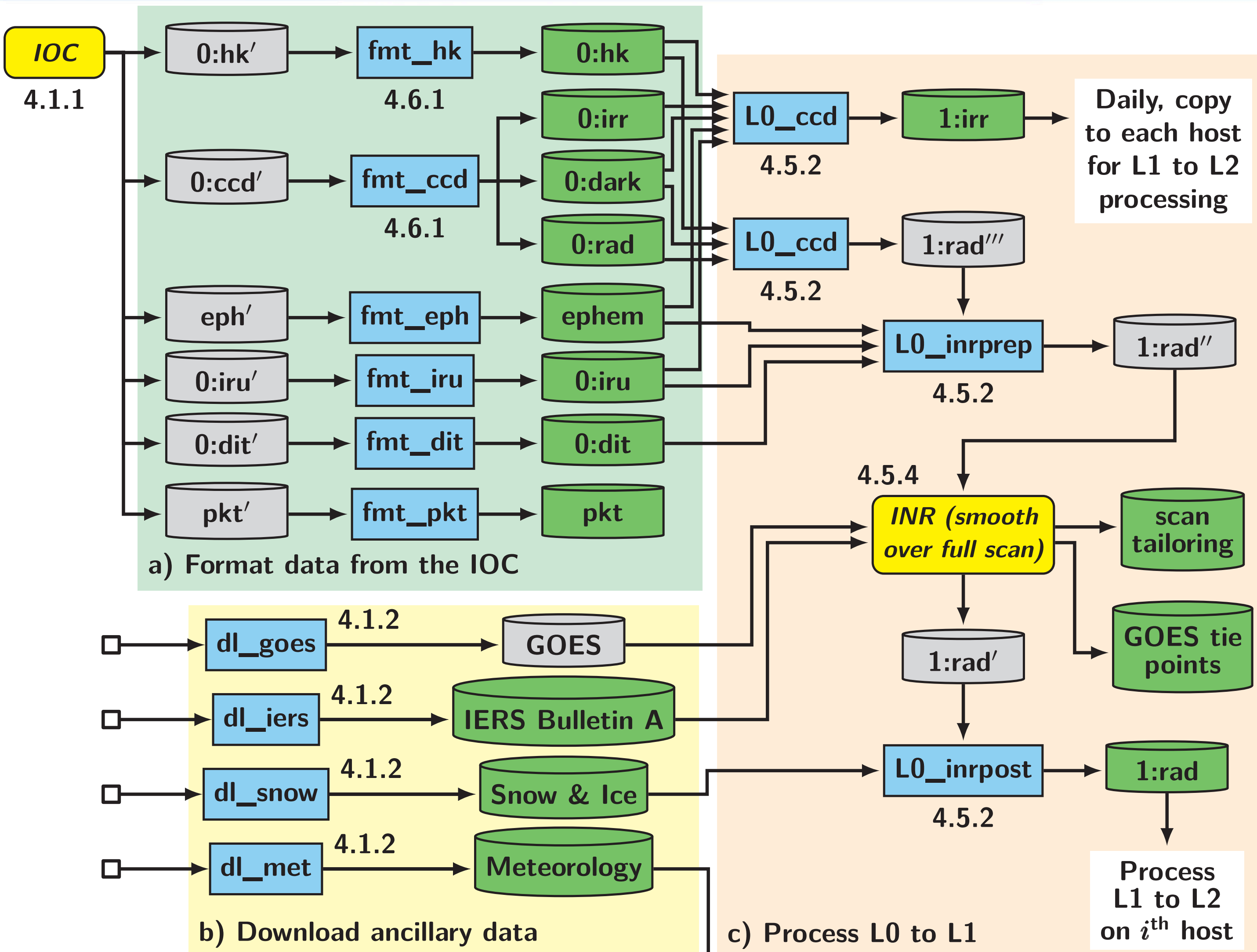
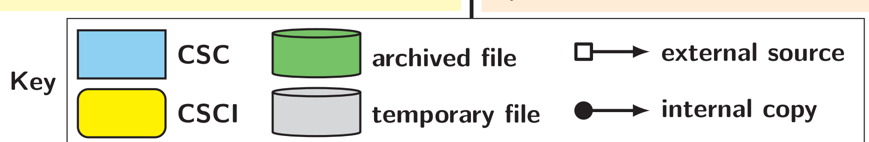
L0-1 Processor Overview



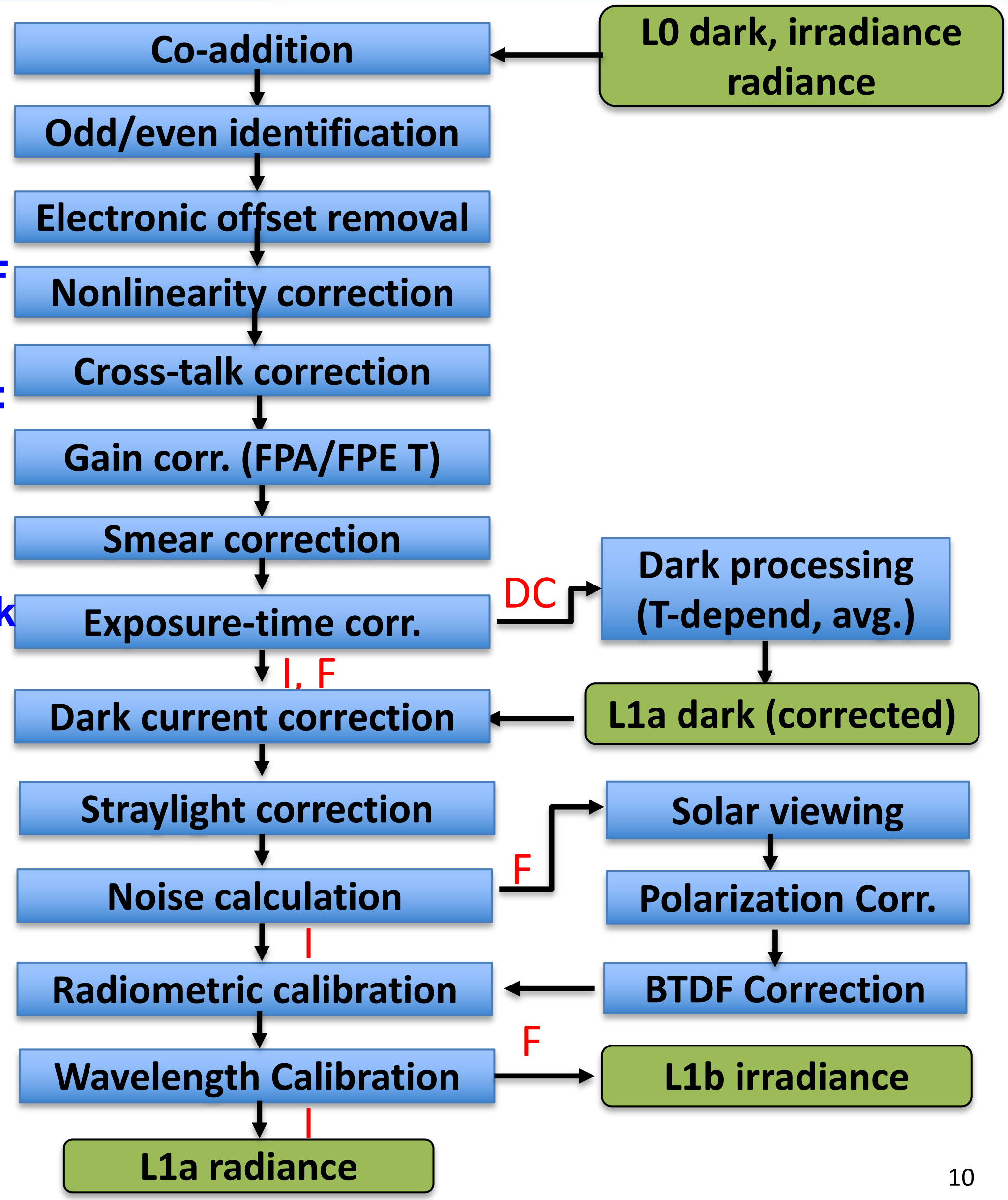


- Heritages from: OMI, TROPOMI, OMPS, GOME/GOME-2 SCIAMACHY GEOTASO
- TEMPO specifics
  - ➢ INR (geo-location) by Carr Astronautics
  - ➢ T-dependent dark current correction
  - ➢ Polarization correction

Requirements from SDPCRD [TEMPO-09-0003] labeled as 4.X.X

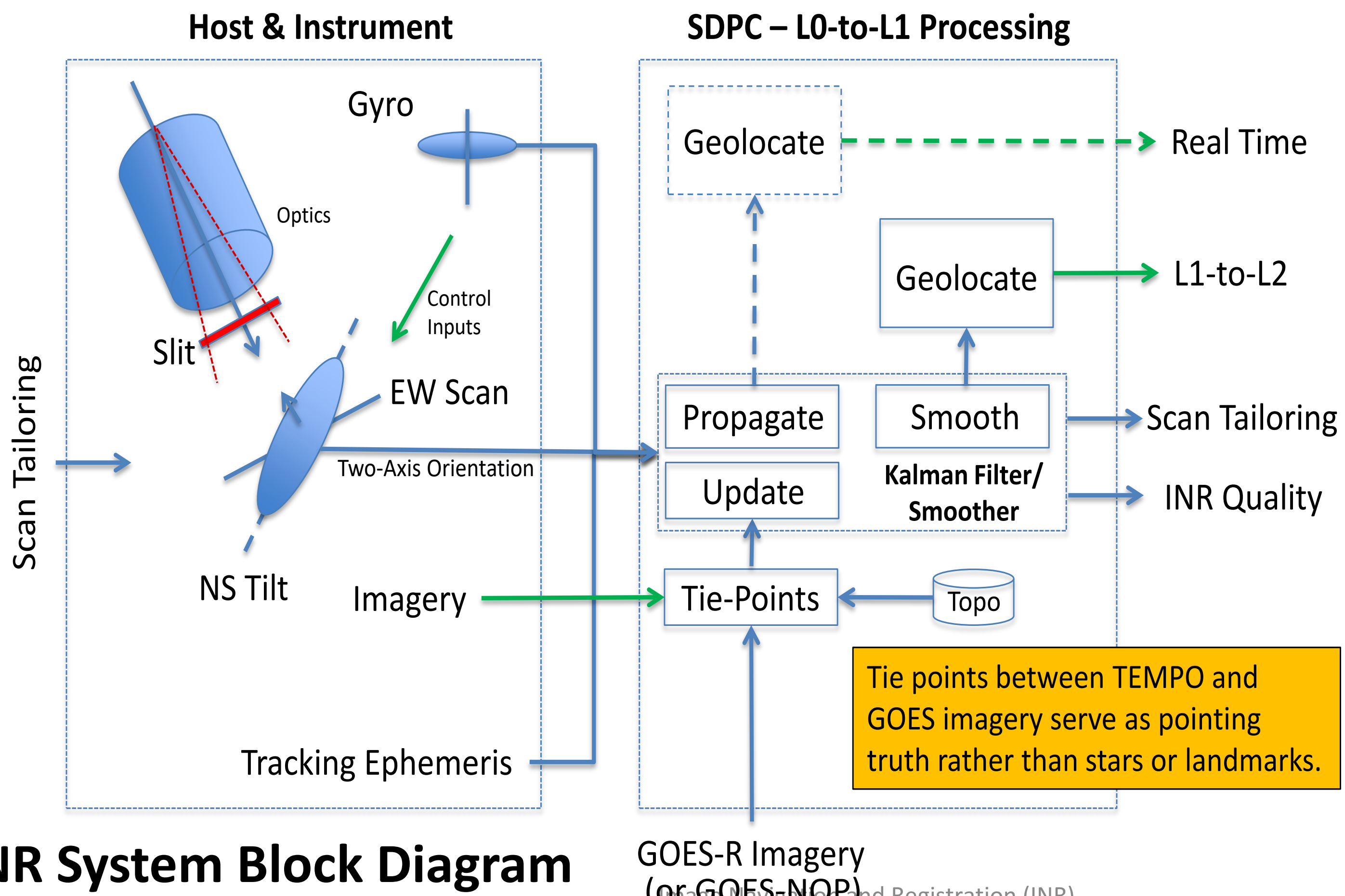
L0_ccd + L0_wavcal & In-flight Calibration

- T-dependent gain correction
- T-dependent dark current correction
- Straylight correction with 1-D spectral PSF due to much smaller spatial straylight (correction with mean 2-D PSF to be developed)
- Wavelength and slit function calibration: cross correlation with high-resolution solar reference & atmospheric absorption
- Quality flagging: Flag bad/RTS from dark current measurements, flag transient, saturated, missing pixels.
- Special solar measurements vs. integration time to derive ADC non-linearity via standard photon transfer methods.
- Trending solar measurements from working & reference diffusers to derive degradation in radiometric coefficients and diffuser BTDF.



INR, L0_inrprep, L0_inr

- L0_inrprep: add spacecraft position & scan mirror orientation
- L0_inr: provide geo-location coordinates to all spatial pixels by transferring GOES geo-location accuracy to TEMPO

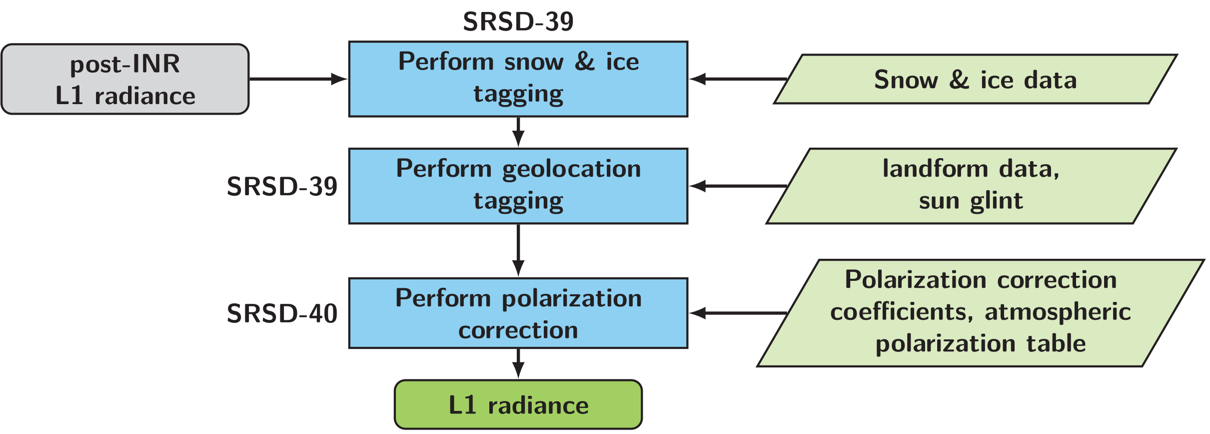


INR System Block Diagram

- Combine Earth orientation and spacecraft tracking to align tie points in the GOES imagery with TEMPO data
- Two-pass Kalman filter (smoothing at end of hourly scan)
- Archive tie points
- Provide scan tailoring parameters

L0_inrpost

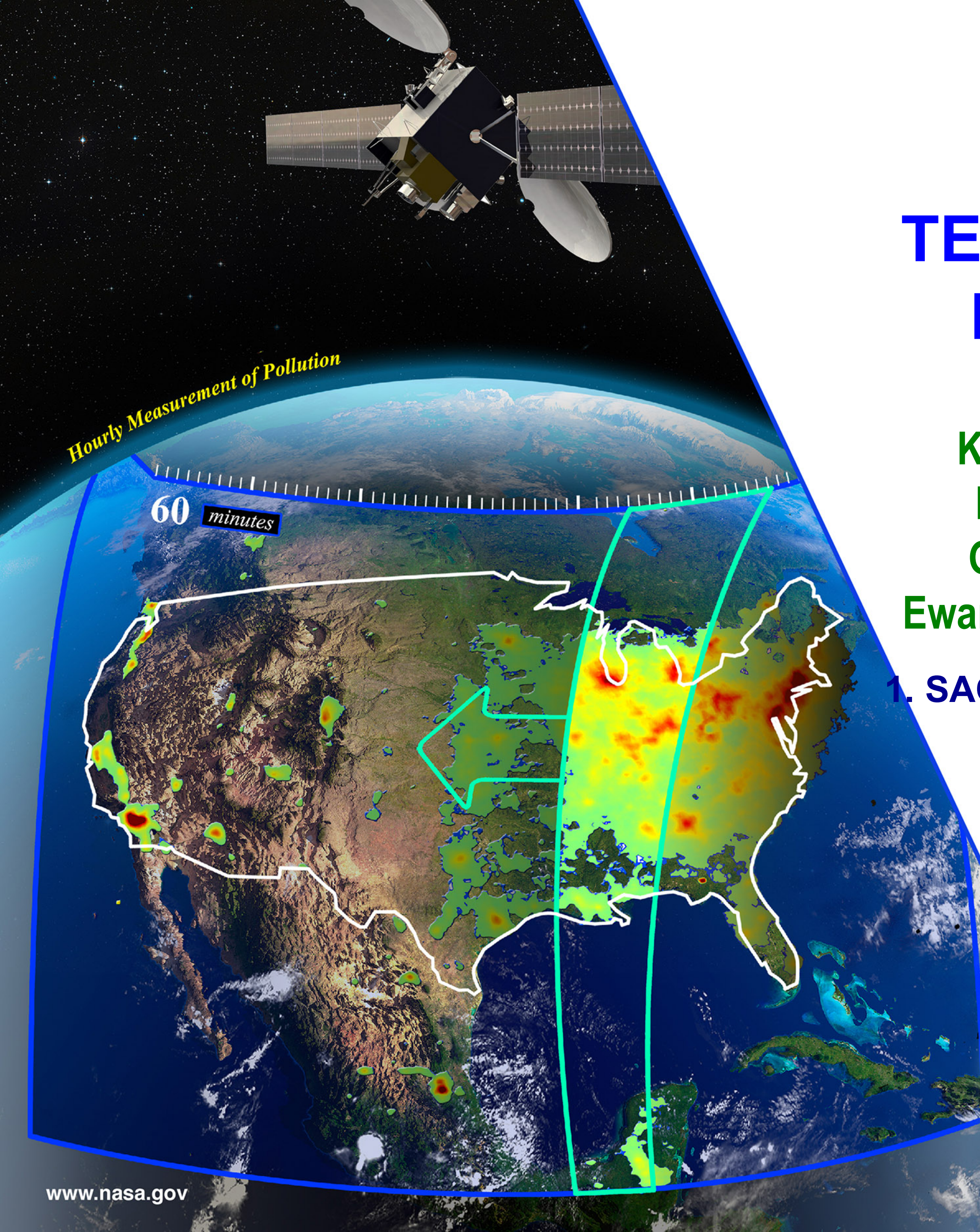
- L0_inrpost: additional processing after INR to derive the final radiance product
  - Calculate viewing geometry
  - Snow/ice from IMS
  - Flag pixels affected by sun glint
  - Terrain height (GMTED2010, 30 arc s)
  - MODIS land cover type product MCD12Q1 (17 classes, 500 m res.)
  - Correct for radiance error due to instrument polarization sensitivity



- Polarization correction: Combine instrument polarization sensitivity with quick estimate of atmospheric state & polarization (MLER/LER, clouds/surface albedo, total ozone) using LUTs

Verification and Validation Plan

- Verify/update image correction steps in the L0-1 during commissioning phase
- Assess wavelength scale & ILS: L0-1b, L1-2
- Assess geo-location methodology, INR (registers TEMPO granules against GOES-R/S/T visible images and other fiducial points in L1b) during commissioning phase
- Assess out of field stray light assessed using unilluminated spatial pixels from early morning/late afternoon scans of CONUS
- Assess spectral stray light in shortest UV channels using radiative transfer
- Multi-pronged approach to radiometric validation: internal assessment, L2, high resolution solar reference, satellite intercomparison, comparison with RTM simulation



Tropospheric Emissions:
Monitoring of Pollution

TEMPO

TEMPO Ozone Profile Retrieval Algorithm

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G. Gonzalez Abad[1], John Houck[1],
Ewan O'Sullivan[1], Matthew Johnson[3]

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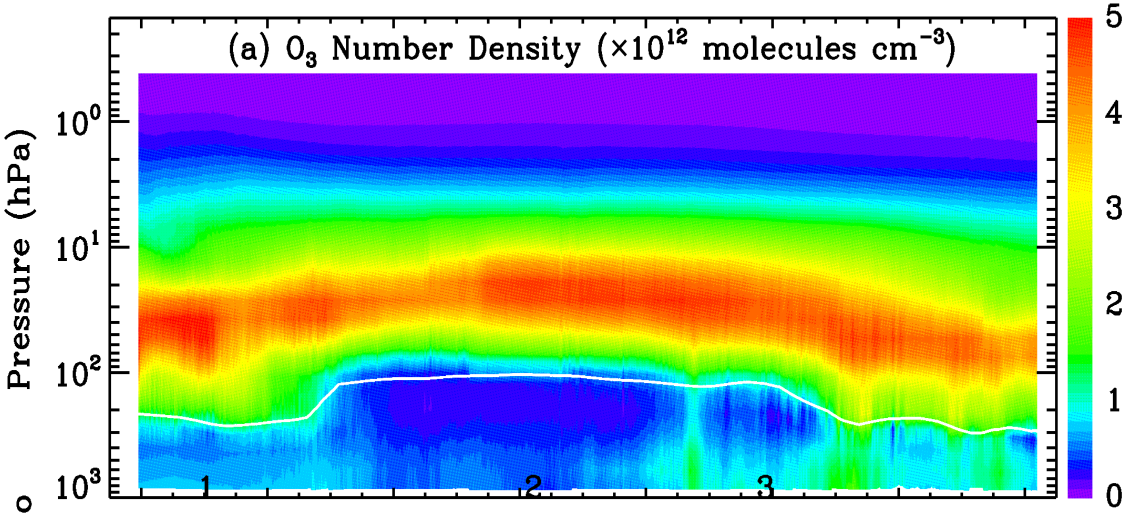
TEMPO Ozone Profile and Tropospheric O_3 Algorithm

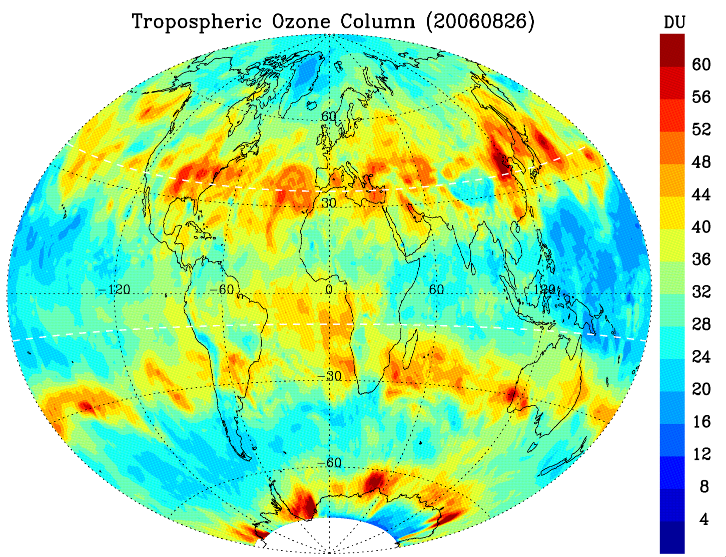
- **Adapted from OMI V2 (Liu et al., 2010; Bak et al., 2022): Spectral fitting + OE + VLIDORT**
- **Fitting windows: 293-340 nm, 540-650 nm**
- **OE constrained by O_3 profile apriori/climatology & measurement errors**

$$\chi^2 = \left\| \mathbf{S}_y^{-\frac{1}{2}} \{\mathbf{K}_i(\mathbf{X}_{i+1} - \mathbf{X}_i) - [\mathbf{Y} - \mathbf{R}(\mathbf{X}_i)]\} \right\|_2^2 + \left\| \mathbf{S}_a^{-\frac{1}{2}} (\mathbf{X}_{i+1} - \mathbf{X}_a) \right\|_2^2$$

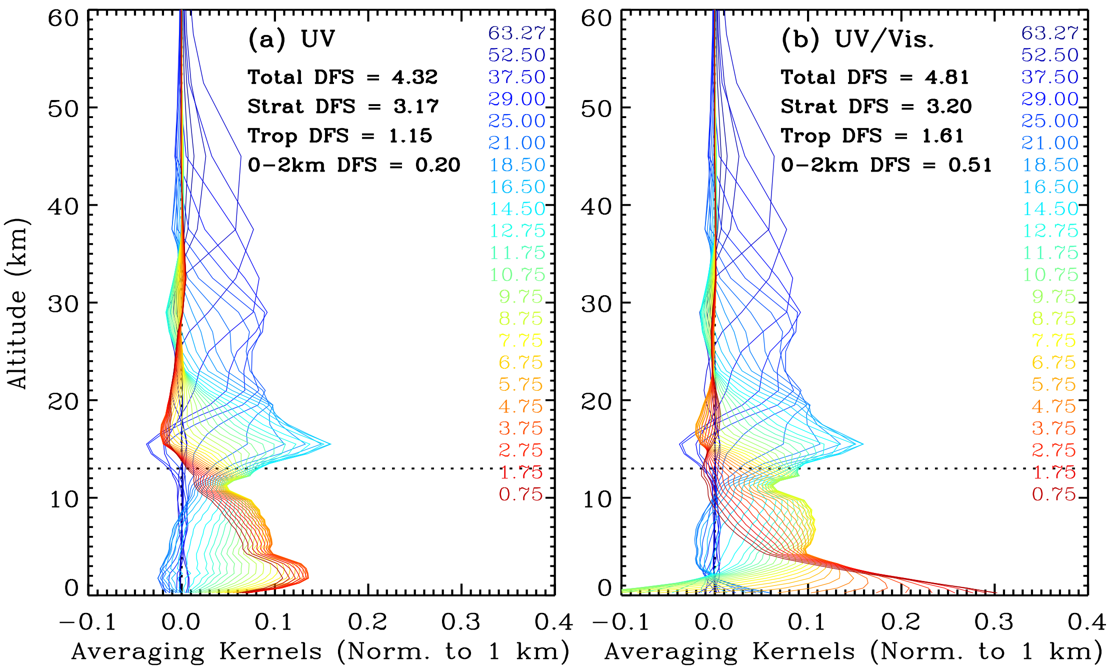
$$\mathbf{X}_{i+1} = \mathbf{X}_i + (\mathbf{K}_i^T \mathbf{S}_y^{-1} \mathbf{K}_i + \mathbf{S}_a^{-1})^{-1} \{\mathbf{K}_i^T \mathbf{S}_y^{-1} [\mathbf{Y} - \mathbf{R}(\mathbf{X}_i)] - \mathbf{S}_a^{-1} (\mathbf{X}_i - \mathbf{X}_a)\}$$

- **Retrieve partial O_3 columns at ~24 layers as well as total, stratospheric, tropospheric, and 0-2 km O_3 columns, other trace gases, and auxiliary parameters. Output includes retrieval a priori, retrieval error and its covariance matrix, averaging kernels.**





TEMPO Ozone Profile and Tropospheric O3 Algorithm



- This example: SZA=25, VZA=45, AZA=86, SNR with 4 pixels coadded
- Adding visible improves retrieval sensitivity in the lower trop. and help separate free trop. O_3 from boundary layer O_3
- Under ideal conditions (4-pixel coadded): 3-5 total DFS with up to ~1.5 in the troposphere, and up to ~0.5 DFS in 0-2 km
- Challenge: weak VIS O_3 signal, strong interferences from surface, aerosol, clouds, requires accurate radiometric calibration in UV/VIS

- Climatological a priori: a combination of tropopause-based climatology (Bak et al., 2013) with diurnally-resolved GEOS-CF O_3 data
- Combine GLER climatology (MODIS/SCIA. BRDF database over land, glint kernel over ocean) at high spatial res. with existing spectral albedo libraries (e.g., ASTER, USGS) to improve characterization pf surface albedo spectra
- Time consuming due to on-line radiative transfer calculations: perform retrievals with 4-8 pixels with spatial resolution of 8.0 x 4.75-9.5 km2
- Continue to optimize, speed up visible with LUT correction, derive empirical calibration after launch

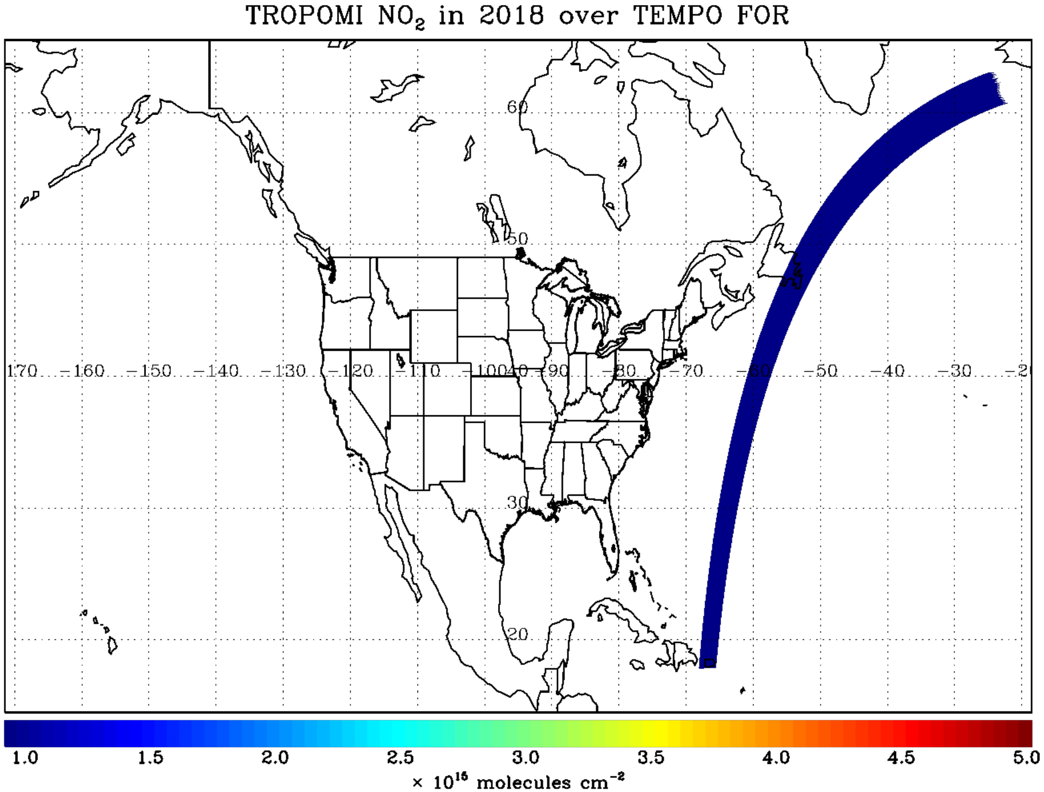
Ancillary Inputs Used in O3 Profile and Total O3 Algorithms

Input	Ozone profile algorithm	Total ozone algorithm (TOMSV8.5)
Cloud-top pressure	TEMPO O_2-O_2 cloud product Defaults to a cloud pressure climatology (OMI-derived) if cloud retrieval is unavailable.	TEMPO O_2-O_2 cloud product Defaults to a cloud pressure climatology (OMI-derived) if cloud retrieval is unavailable.
Cloud fraction	Iteratively retrieved based on the MLER. If fc <=0 or >=1, it is set to 0 or 1, R_s or R_{cld} is retrieved instead.	Retrieved based on the MLER. If fc <=0 or >=1, it is set to 0 or 1, R_s or R_{cld} is retrieved instead.
Ozone profiles apriori	Tropopause-base climatology + GEOS-CF	TOMS V8 climatology (total ozone dependent, monthly / 10° zonally mean)
Surface albedo	Initialized with GLER climatology at 0.05, also iteratively retrieved	15% or directly retrieved as R_s if f_c=0
Temp. profiles	GEOS-CF	TOMS V8 climatology (monthly / 10°zonally mean)
Tropopause P	GEOS-CF	N/A
Surface Pressure	GEOS-CF, adjusted to terrain height	Climatology at 1/3° x1/3° from the TOMSV8.5
Snow/ice fraction	IMS data	Climatology at 1° x1° from the TOMS V8.5
Terrain height	L1b (GMTED2010)	L1b (GMTED2010)
Aerosols	Not explicitly treated	Not explicitly treated, but an aerosol correction is included

Back up slides

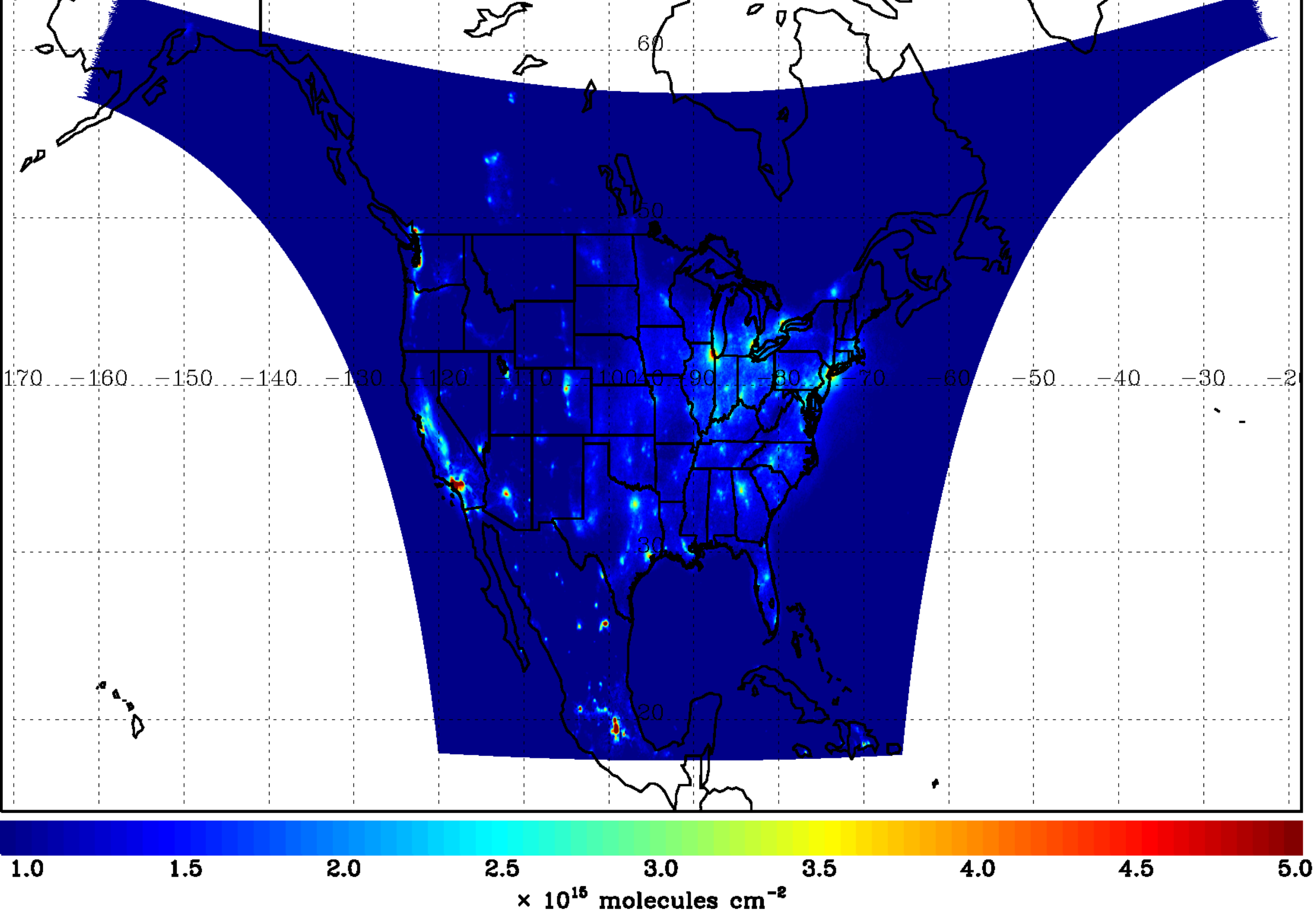
TEMPO Nominal Hourly Scan and Special Scans (GEO@91W)

❑ **Operate on geostationary communications satellite Intelsat 40e (IS-40e) at 91.1 ° W**



- Field of regard is optimized to cover both Puerto Rico and Canadian tar sands.
- S5p-TROPOMI NO2 product oversampled by Kang Sun.

- **Nominal:** Scan FOR in 1 hour with 10 granules
- ~ 2K N/S pixels x 1226 steps/hr, ~ 2.5 M pixels/hr, # spatial pixels ~TROPOMI
- 2 x 4.75 km^2 @center of FOR, from 8 km^2 at Mexico City to 21 km^2 at Canadian Tar Sands
- FOR: N/S +/-210 pixels,
  E/W +230/160 pixels
- **Optimized scan:** in the early morning and late afternoon, daylight portion of FOR, higher temporal resolution
- **High-time scan (up to 25%):** selected portion of FOR at higher temporal resolution (e.g., <= 10 mins)



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- Boresight: 33.7°N, 91°W
- ~ 2035 good N/S pixels
- ~ 1226 steps/hr
- ~ 2.5 M pixels/hr
- # spatial pixels ~TROPOMI
- 2 x 4.75 km^2 @center FOR
- FOR: N/S +/-210 pixels,
  E/W +230/160 pixels

- Field of regard is optimized to cover both Puerto Rico and Canadian tar sands.
- S5p-TROPOMI NO2 product oversampled by Kang Sun.

Research Products

- TEMPO research products will greatly extend science and applications
  - OClO, IO, HNO_2, volcanic (SO_2 plume height and VCD)
  - Additional/improved cloud with O_2-O_2 bands / O_2-B bands
  - Additional aerosol products from hyperspectral spectra, O_2-B and O_2-O_2-bands, and TEMPO + GOES-R synergy at @U Iowa, NOAA, GSFC
  - Vegetation products: solar Induced fluorescence (SIF)
  - Diurnal out-going shortwave radiation and cloud forcing
  - Night lights: allows discrimination between lightning types
  - Higher-level products: Near-real-time pollution/AQ indices

NRT vs. Off-line Trace Gas Products

- Implementing both NRT and off-line trace gas products (e.g., NO_2, HCHO) for NO_2, HCHO, aerosol, SO_2, cloud in two separate processing pipelines
- Major potential differences between NRT and offline products

	NRT	Off-line
Trace gas profiles/Met data	GEOS-CF	GEOS-CF Replay
Surface	GLER climatology	MODIS/VIIRS albedo/BRDF products
Spectral fitting	Normal spectral fitting	Improve radiance reference & cross-track correction, different fitting windows
L1B	Default Pol. Correction	Improved pol. correction with L2 retrievals (?), improved dark current (AM&PM dark current)
RTM	Look-up tables	On-line radiative transfer?
Aerosol correction	None	Improved aerosol fields?

L1b Requirements

- L1b products: Spectral Radiance, Irradiance and Uncertainty, Spectral Scale, Geo-location (lat/lon)
- PLRA: no requirement for radiance or irradiance, geolocation accuracy < 4km
- Instrument design & performance requirements were derived from L2 precision req.
  - Signal to Noise Ratio (SNR) was the dominate factor for radiance performance
  - Radiometric Uncertainty: < 4% (1-sigma) for both irradiance & radiance
  - Albedo uncertainty: wavelength independent < 2%, dependent < 1%
  - Long-term (20 months) radiometric drift detection: < 0.9%
  - Nonlinearity: <2% of 98% well response, and knowledge (after corr.) < 0.5% from 2-98% of well response
  - Pre-launch Wavelength mapping uncertainty: < 0.02 nm
  - Spectral stability (within 24 hours): < 0.1 nm for radiance & irradiance
  - Spectral co-registration error: < 0.7 pixel between 2 bands, < 0.4 pixel within UV or visible bands

Table of SNR req. and with Beginning of Life (BOL) as-built performance (4 Pixels coadded)

Earth-View TEMPO Signal to Noise Ratio (SNR) Verification Summary

Req Number	Requirement			BOL SNR		EOL SNR	
	Atmospheric Constituent	Wavelength (nm)	SNR Requirement e- / e-	As-Measured SNR	Margin	Predicted EOL SNR	Margin
	O3	290	19.6	N/A	N/A	N/A	N/A
	O3	300	46.1	49	5.4%	45	-2.4%
	O3	305	161.9	191	17.8%	178	10.1%
	O3	310	377	471	24.9%	447	18.5%
	O3	320	1220	1664	36.4%	1621	32.8%
	O3, H2CO	330	2003	2829	41.2%	2779	38.7%
IRD-320 TSS-59	O3, H2CO, Cloud	340	2013	2867	42.4%	2827	40.4%
	H2CO, Cloud	350	1414	2717	92.1%	2685	89.9%
	NO2	420	836	2138	155.8%	2127	154.4%
	NO2	430	675	1681	149.0%	1670	147.4%
	NO2	450	733	1875	155.8%	1865	154.4%
	Cloud	490	1176	1886	60.4%	1879	59.8%
	O3	540	1109	1813	63.5%	1806	62.9%
	O3	600	987	1577	59.8%	1571	59.1%
	O3	650	898	1383	54.0%	1376	53.2%
	Cloud	690	820	1195	45.8%	1188	44.9%