Near-Real-Time Processing Plans for Aura MLS Data for Use in Data Assimilation

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Data Assimilation Systems

- Estimate the state of the atmosphere at a given time from:
  - Measurements and covariances
  - Prior information and covariances
  - Problem solution
    - Variational (4D-VAR, 3D-VAR)
    - Sequential (Kalman Filter, Direct inversion)
- Estimate biases
  - Between model and observations
- Numerical Weather Prediction (NWP)
  - General Circulation Model based:
    - Can include appropriate feedback of dynamical, photochemical, radiative components
- Chemical Transport Model (CTM)
  - Driven by offline-NWP analyses or short-term forecasts
    - Allows more detailed chemistry schemes

Practical benefits of assimilation of research satellite data

e.g. height-resolved ozone from limb sounders

- Improvements in the analysed ozone fields
  - Less dependent on background error covariance
- Improvements in the temperature, radiation and heating fields internal to the model
- Improvements in air quality prediction through the estimation of tropospheric ozone
- More accurate regional and global forecasts of surface UV radiation
- Provide chemical constraints for unobserved constituents
- Better description of stratospheric dynamics
- Better planning and support of large coordinated atmospheric measurement campaigns

Motivation for assimilation of Aura MLS data

- Achieve a decrease in the mean analysis error and standard deviation for the assimilated fields
  - Improve the operational forecast skill
    - Weather, stratosphere, water vapor in the UTLS
  - Decrease the residuals of the assimilated operational satellite radiance data sensitive to ozone
  - Improve the temperature analyses by providing the radiation scheme with more accurate heating rates
  - Improve wind analyses indirectly in the upper troposphere and lower stratosphere through improvements in tracer fields

Motivation for assimilation of Aura MLS data

- Strong interest in the availability of a Near-Real-Time Data Stream from Aura MLS
  - e.g. several partners within the Joint Center for Satellite Data Assimilation (JCSDA) and elsewhere at the UK Met Office and University of Edinburgh/ECMWF

- Goal is to provide an end-to-end processing capability for Aura MLS NRT measurements of ozone, temperature and humidity
  - Appropriate accuracy, precision and vertical resolution
  - Low latency with realistic processing requirements of a few CPUs

Retrieval of MLS standard data products

- MLS limb radiance measurements are inverted using an optimal estimation retrieval
  - Level-2 operational processing
  - Current standard production stream is version 2.2
- Standard MLS processing suite is not practical for processing a NRT data stream
  - Large demands on computational resources
  - Inherent latency of a few days

Retrieval of MLS NRT data products

- "Reduced Level-2 algorithm" NRT data processing
  - Fast linearized forward model
  - Uses tabulated coefficients

- Preliminary results from a current project with the GMAO: *"Towards a real-time capability for MLS data using GEOS-5"*
  - Examine feasibility of providing a Level-2 NRT processor using modified retrieval algorithms for a subset of the Aura MLS data products

Retrieval of MLS NRT Ozone

- Ozone is measured in several microwave bands
  - Investigate the appropriate band to use for NRT retrievals
  - Standard product is from R3 240 GHz
  - Other possible bands are R2 190 GHz, R4 640 GHz, R5 2.5 THz
  - Experiment with various optical depth cut-offs to select radiances from channels / heights which are not too non-linear
- Preliminary Ozone NRT retrieval is from R3 240 GHz
  - Band 7 (25-channel) and B33 (4-channel)
  - Fast linear forward model
  - 1D homogeneous line-of sight

Retrieval of MLS NRT Ozone

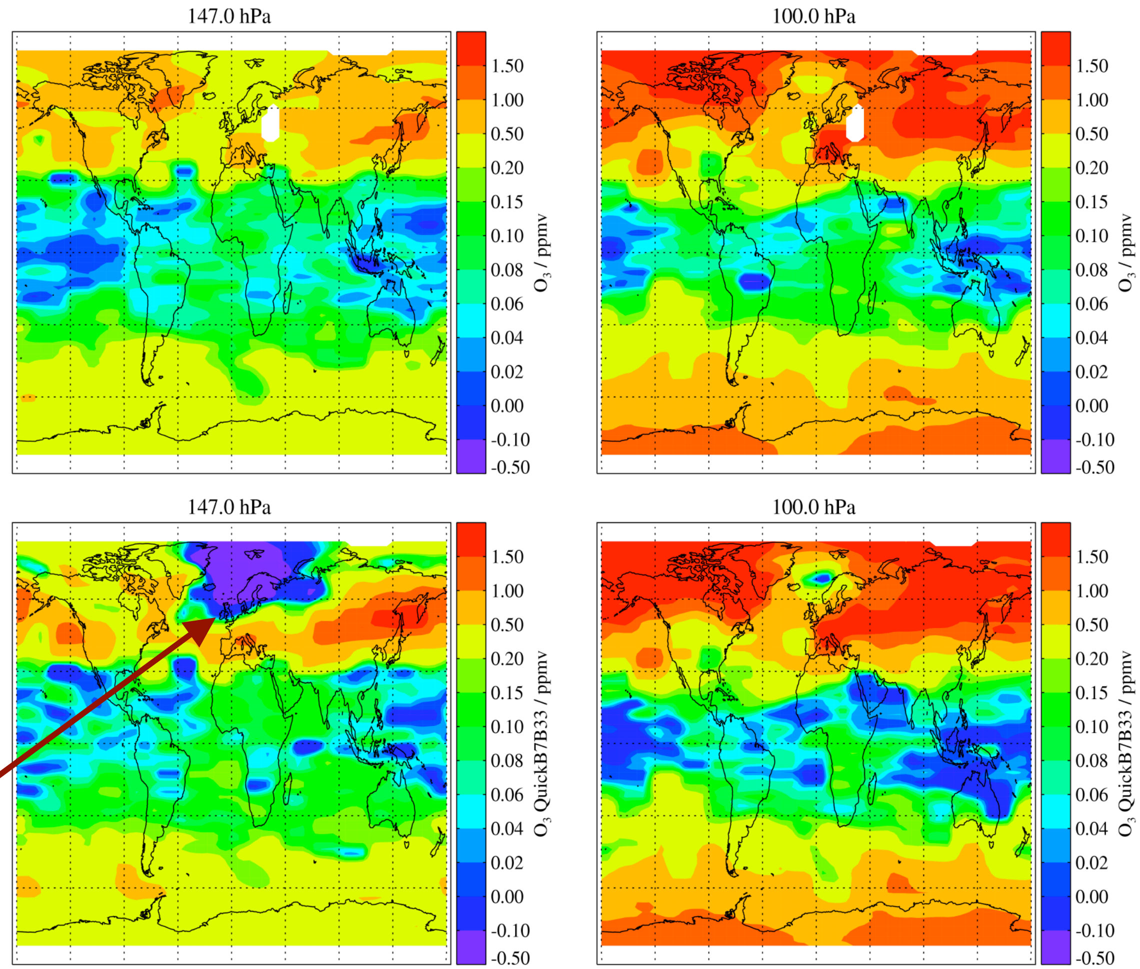
Quick MLS retrievals include (mainly) Temperature/P_{tan} and Ozone

Preliminary "Quick O_3" fields (bottom) from std. MLS O_3 band(s) show a lot of similarities with standard (validated) MLS v2.2 O_3 (top).

2005 Jan. 28 results are shown here.

Larger departures seen at high lats. & lowest altitudes - starting mainly at 147 hPa.

Results for 215 hPa (not shown here) are worse … but we expect to improve upon this.



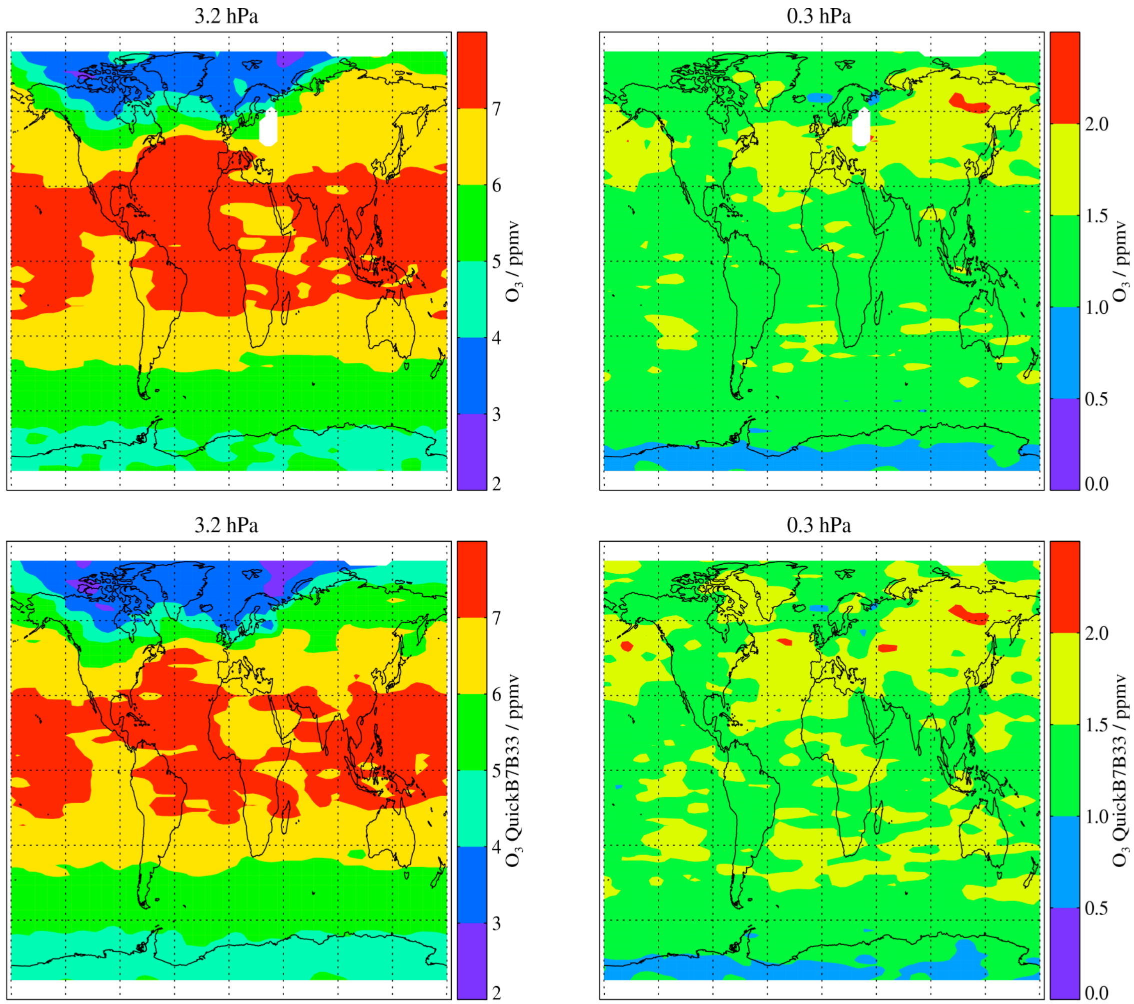
v2.2 O_3

Quick O_3

Retrieval of MLS NRT Ozone

MLS "quick ozone" results track the standard MLS product very well into the upper stratosphere and lower mesosphere (top useful sensitivity near ~ 0.1 hPa).

Results for 3 hPa (left) and 0.3 hPa (right) shown here.



v2.2 O_3

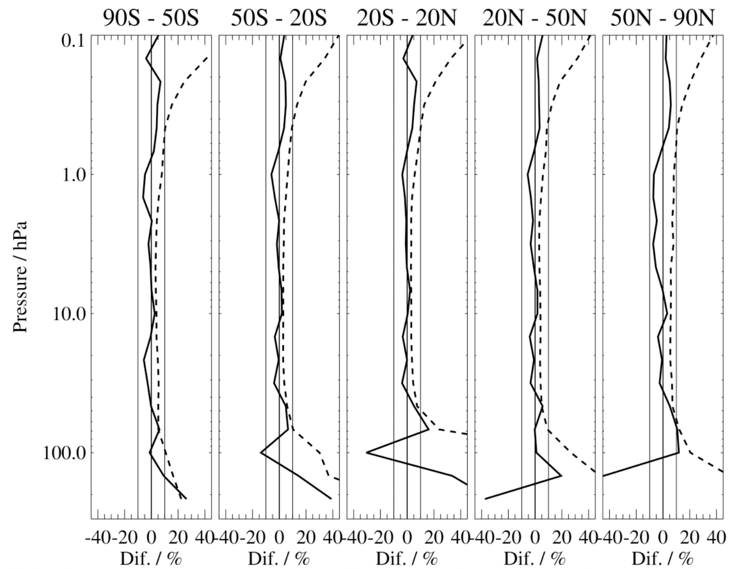
Quick O_3

Retrieval of MLS NRT Ozone

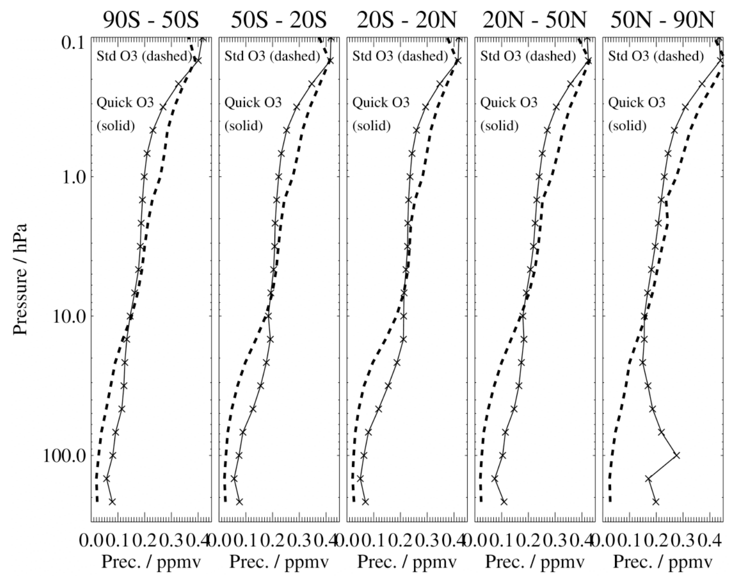
Differences between Quick O_3 and standard MLS (v2.2) O_3 for 2005 Jan. 28.

Avg. Differences: solid

Std. Deviations: dashed



Expected Precision for Quick O_3 is somewhat worse (by > factor of two) than std. MLS product in lower stratosphere.



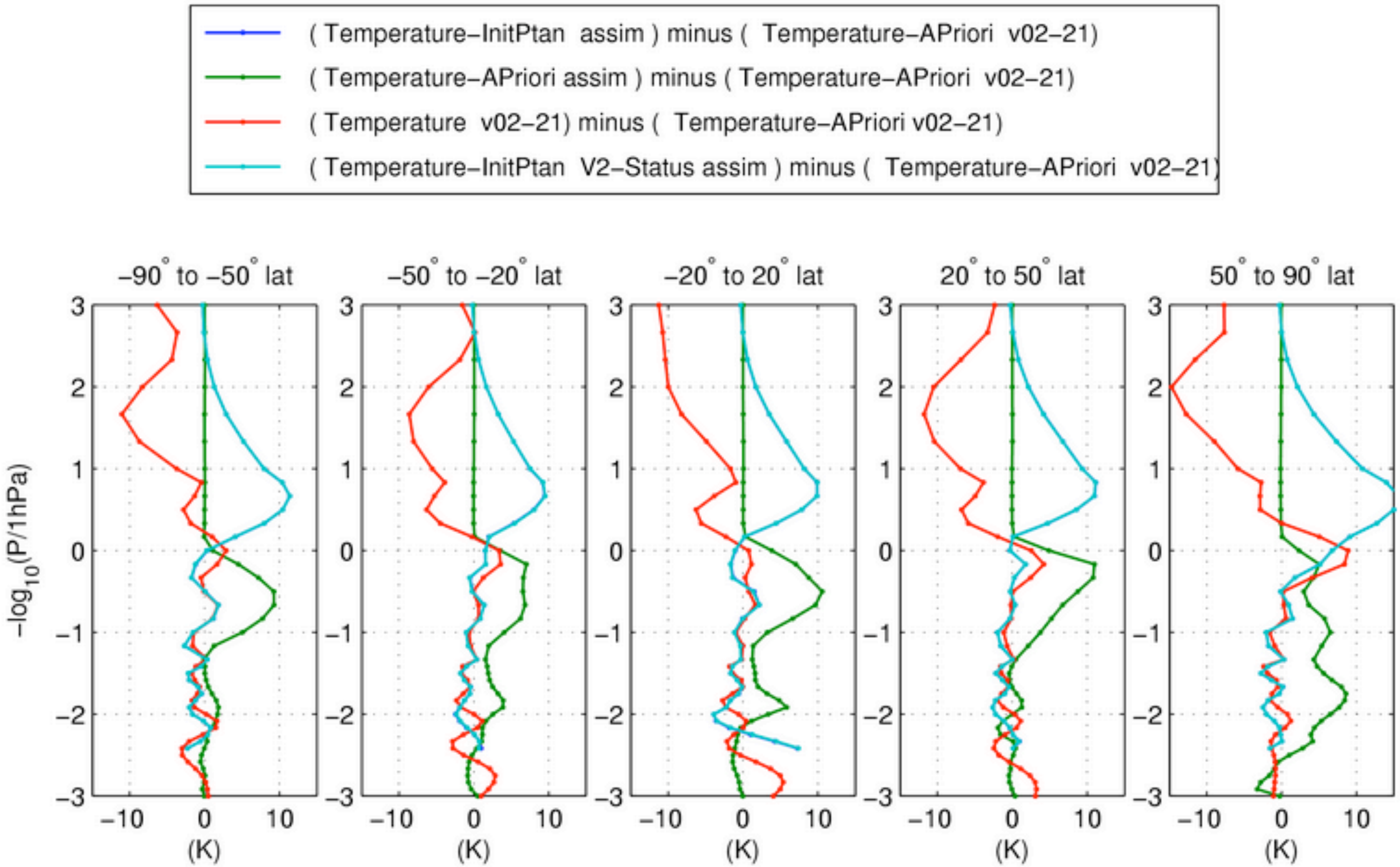
Retrieval of MLS NRT Ozone

- Quick retrievals (near-real-time) for MLS O3 are very promising
  - Within 5-10% of standard MLS product in most of stratosphere and lower mesosphere
- Need some improvements to be viable globally at 150 and 215 hPa

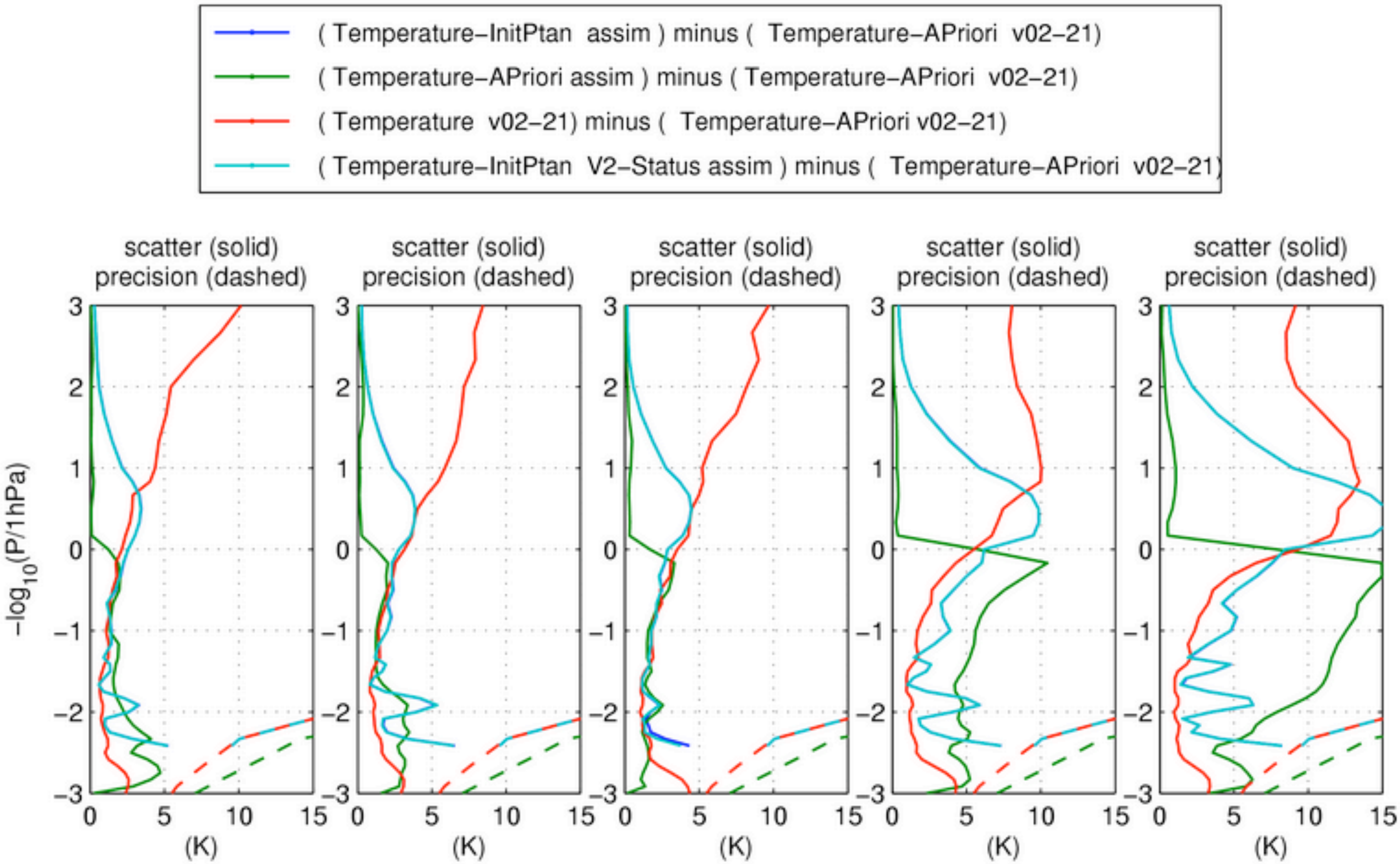
Retrieval of MLS NRT Temperature

- Preliminary temperature and geopotential height NRT retrievals are from the R1A and R1B 118 GHz
  - Band 1 (25-channel), band 32 (4-channel), band 34 (4-channel)
  - Fast linear, un-polarized forward model
  - 1D homogeneous line-of sight
  - Top retrieval height is limited to the lower mesosphere because the narrow-band Digital Autocorrelator Spectrometer (DACS) is not included (band 22)

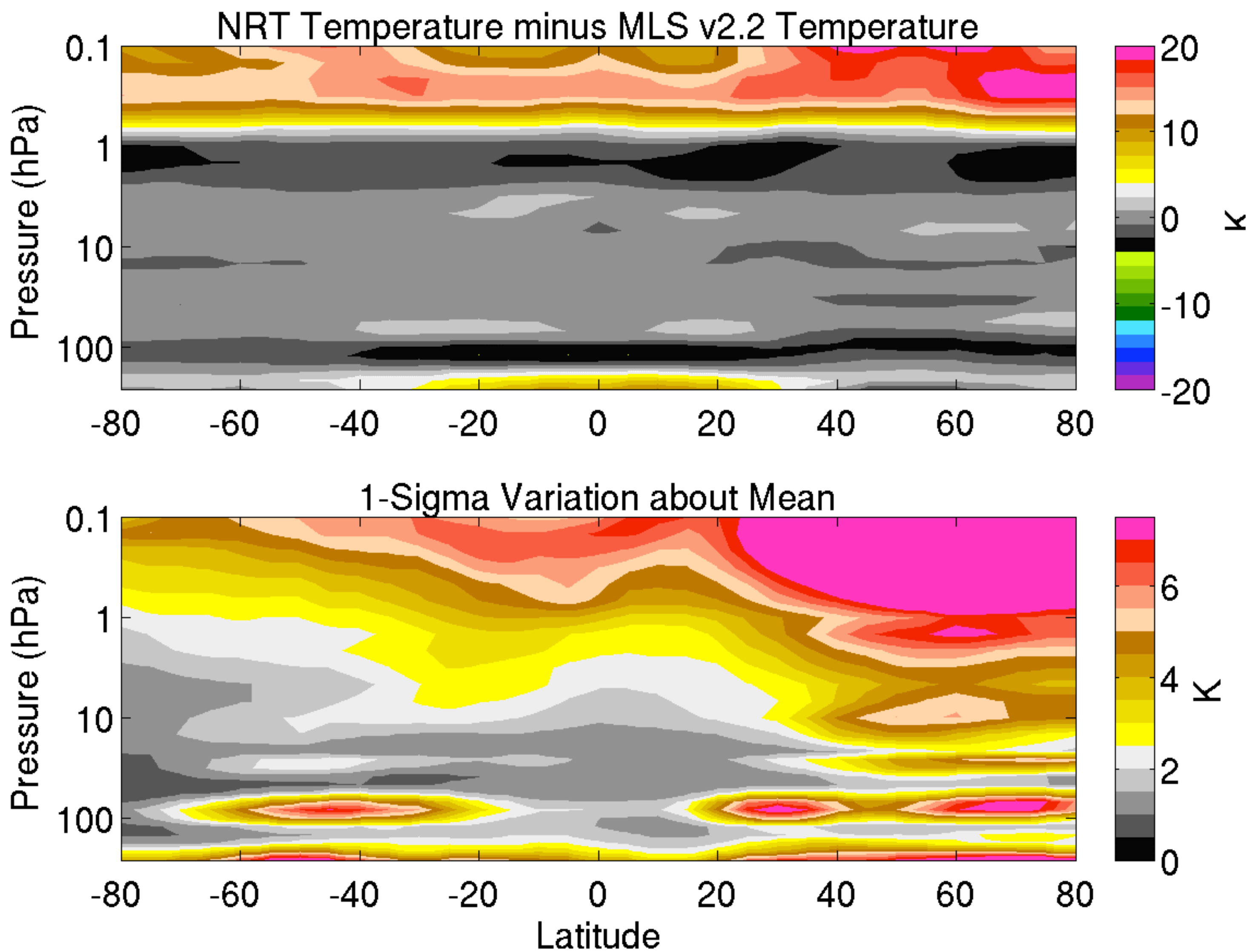
Retrieval of MLS NRT Temperature



Retrieval of MLS NRT Temperature



Retrieval of MLS NRT Temperature



Retrieval of MLS NRT Temperature

- Quick retrievals (near-real-time) for MLS temperature
  - Within 2K of standard MLS product in most of stratosphere
  - 1D retrievals lead to artifacts in the presence of large line-of-sight temperature gradients
- Need some improvements to be viable globally at 150 and 215 hPa

- Upper Stratosphere – Lower Mesosphere (USLM)
  - For pressures less than 0.3 hPa the Zeeman split O_2 spectral line requires the polarized forward model for greater accuracy

Aura MLS Data Processing System

- Science Computing Facility (SCF)
  - Provides services and resources for algorithm development
  - Processing software development
  - Investigation of quality control
  - Scientific data analysis

- Science Investigator-led Processing System (SIPS)
  - Interfaces to GES-DAAC
  - Software developed on SCF is run in the operational environment
  - One incoming processing and two re-processing data streams

Modifications for NRT Processing

- Additional interface to GES-DAAC – MLS SIPS
  - New NRT Level-0 data product
    - Constructed from satellite and instrument Rate Buffered Data (RBD)
    - Handling of time-gaps, glitches and repeated data records
    - Sub-divide the orbit contacts (100 mins) into Level-0 NRT files with a granularity of about 15 minutes each
  - Use predictive ephemeris and orbit / attitude data

Modifications for NRT Processing

- Modifications to produce a Level-1 NRT processor
  - Only calibrate selected GHz radiances needed for NRT products
  - Ingest NRT Level-0 and orbit/ephemeris data
  - Output Orbit and Attitude data
  - Output GHz radiance data

- Modifications to produce a Level-2 NRT processor
  - Ingest NRT Level-1 GHz radiances and orbit/attitude data
  - Addition of fast second-order forward model
  - Output the NRT Level-2 products

Future improvements to the fast forward model

- 1^{st} order linear scheme
  - Tabulated coefficients as function of:
    - Time (Monthly bins)
    - Latitude (7.5 degree bins)
    - First-order derivatives of forward model radiances with respect to atmospheric constituent mixing ratios, temperature, and tangent pressure
- 2^{nd} order scheme
  - Create tabulations of the second-order derivatives
  - More accurate radiance calculation
  - Relatively little cost in terms of execution time
  - Requires significant algorithm coding changes and testing

Hardware Requirements for Processing Platform

- Based on the production of 2 months of preliminary NRT test data
  - One 3.06 GHz processor will take 7 minutes to process a 15 min data chunk
  - Add overhead of 6 minutes for the Level-1 processor and data i/o
    - Processing time = 13 minutes per 15 min data chunk
  - Latency (measurement time to ingestion by NRT processor) would typically be about 2 hrs
  - If line-of-sight homogeneity can be assumed then the data chunk can be sub-divided and run on multiple processors
    - Limit would still be the 6 minute overhead per data chunk
  - Memory
    - 4 Gb is adequate
  - Storage requirements on the processor
    - Approx 40 Gb for the tabulated coefficients
    - Space per job is less than 1 Gb
    - NRT-products occupy about 10 Gb per year

Schedule for release of the MLS NRT Processor

- Phase I (6 months): Algorithm development and validation
  - Level-1 NRT
  - Level-2 NRT
  - Arrange and test new NRT data feeds and interfaces
- Phase II (6 months): Create and test the configuration for the NRT ozone retrieval
  - Produce a one month test data set, validate and deliver
  - Assess the impact of horizontal homogeneity along the line-of-sight
    - (1D vs 2D retrievals)
  - Assess the data quality control metrics
  - Produce a one year test data set, validate and deliver
  - Provide a data quality description document
  - Package and release an end-to-end NRT processor
- Repeat Phase II for the temperature and humidity retrievals

Summary of MLS NRT Processing Plans

- Develop, test and validate an end-to-end processing capability for Aura MLS Near-Real-Time measurements of ozone, temperature and humidity
  - Time scale for delivery
    - 1 yr for ozone
    - 1.5 yrs for temperature
    - 2 yrs for humidity
- Preliminary results for ozone and temperature are encouraging
  - Further work required
    - Improve the fast forward model accuracy