TEMPO PCA SO_2 Algorithm: Introduction and Preliminary Results

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Background and Motivation

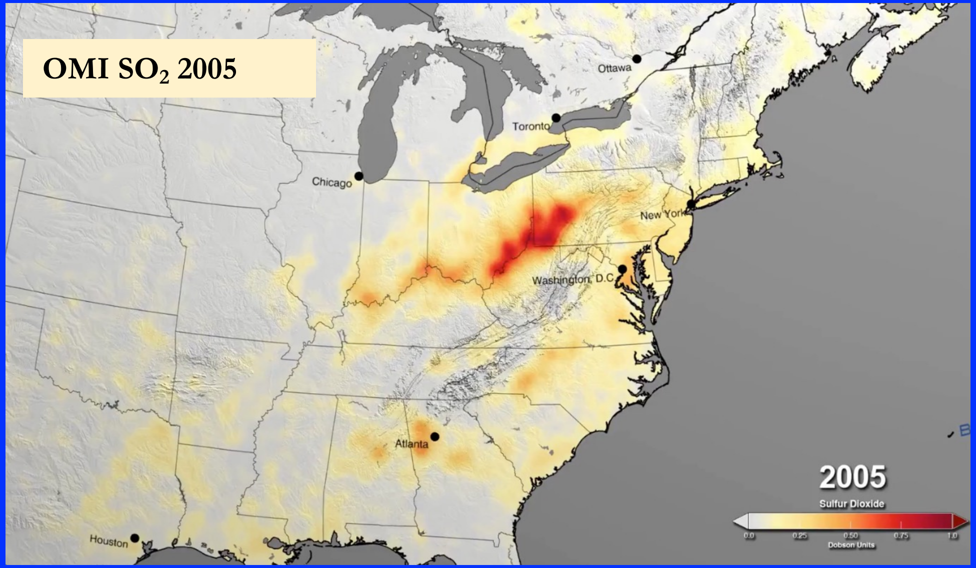
SO_2 plays an important role in global/regional environment:

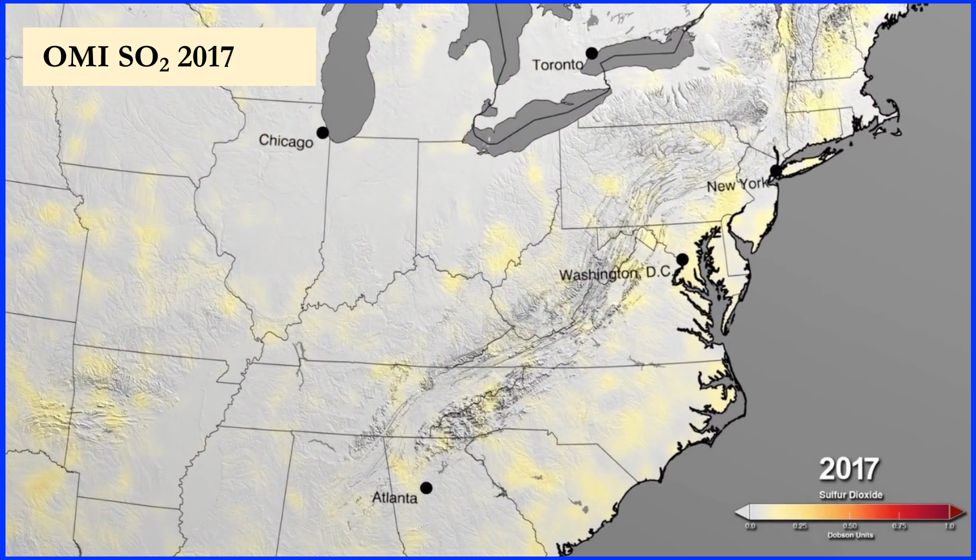
- A designated air pollutant.
- A precursor to sulfate aerosols (haze/acid deposition/climate).
- Helps to track volcanic plumes for aviation safety.

Hourly, high resolution measurements by TEMPO will greatly enhance capabilities of SO_2 monitoring over North America.

But there are also challenges:

- Anthropogenic SO_2 emissions from the U.S. have seen substantial reductions – requires algorithms with good sensitivity.
- TEMPO data volume > 10x larger than OMI – necessitates fast algorithms, especially for near-real-time (NRT) applications.





Featured in 2018 EPA Air Trends Report

GSFC Principal Component Analysis (PCA) Spectral Fitting Algorithm

The data-driven PCA spectral fitting algorithm:

- A PCA technique is applied to the measured radiance spectra to extract spectral features (principal components, PCs);.
- The PCs represent various interfering geophysical processes and instrumental factors.
- They are used in spectral fitting to reduce the interferences in SO_2 retrievals.

Measured Sun-normalized radiance spectrum

SO_2 column amount

$$N(\omega, \Omega_{\mathrm{SO_2}}) = \sum_{i=1}^{n_v} \omega_i v_i + \Omega_{\mathrm{SO_2}} \frac{\partial N}{\partial \Omega_{\mathrm{SO_2}}},$$

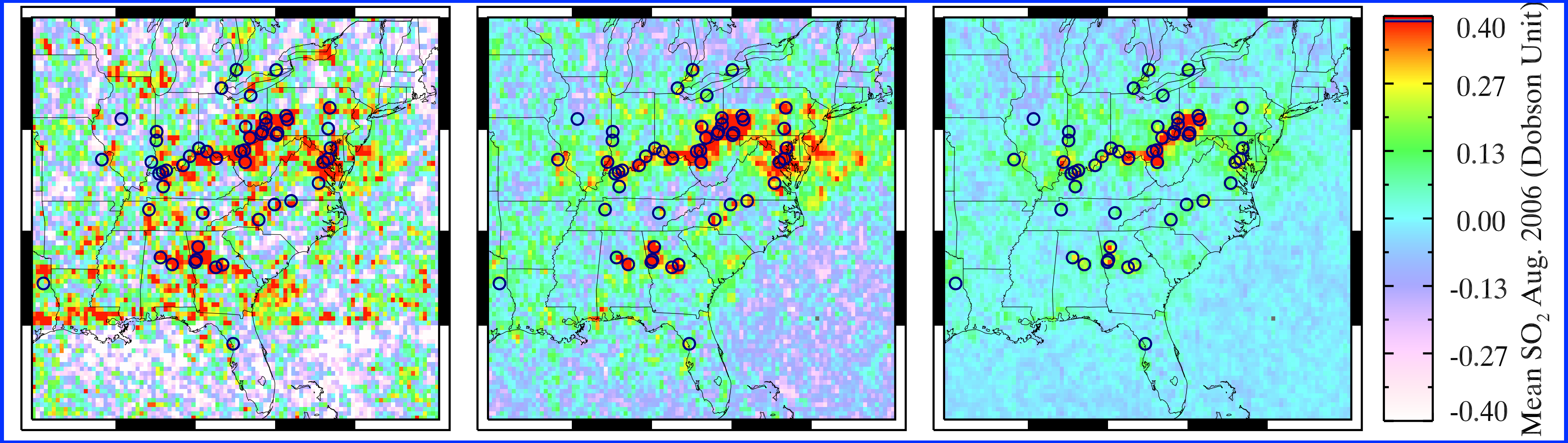
PCs from SO_2-free regions associated with processes (O_3 absorption, surface reflectance, RRS, measurement artifacts, *etc*.) **other than SO_2 absorption**

Pre-calculated SO_2 Jacobians (with assumed/retrieved O_3 profile, cloud fraction/pressure, surface reflectivity, *etc.*)

Fitting of the right hand side to the spectrum on the left hand side -> SO_2 column amount and coefficients of PCs (see [*Li et al.*, 2013; 2017; 2020] for details).

Evolution of the Operational OMI Anthropogenic SO_2 Product

(a) Early version, before PCA (b) PCA, fixed Jacobians (c) Latest PCA, updated Jacobians



1 DU = 2.69×10^{16} molecules/cm^2

(Circles: points sources > 70 kt/year)

Public Release: 2014

Public Release: 2020 (PCA-based volcanic SO_2 product released in 2017)

The PCA-based algorithm significantly improves the quality of the operational OMI SO_2 product.

Highly efficient – spectral fitting takes ~3-4 min for an entire OMI orbit (single CPU).

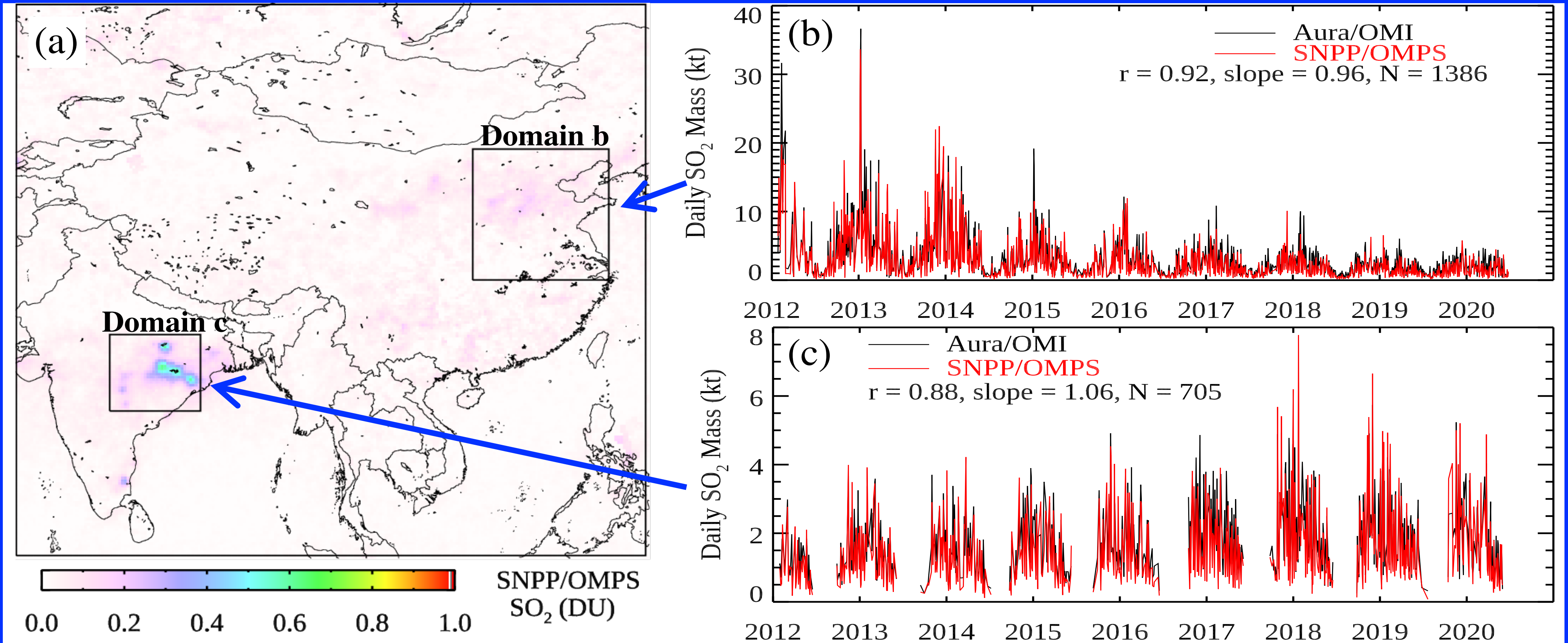
Straightforward implementation – easily adapted for different sensors:

- ✓ Current operational algorithm for OMI and SNPP/OMPS (a variant also implemented by the GEMS team).
- ✓ NRT and direct readout implementations with OMI/OMPS.
- ✓ Demonstrated for TOMS, GOME, SCIAMACHY, TROPOMI, N20/JPSS-1/OMPS.

Consistent Retrievals between OMI and SNPP/OMPS

SNPP/OMPS Annual Mean SO_2 for 2020

OMI/OMPS Daily SO_2 Mass over N China and NE India

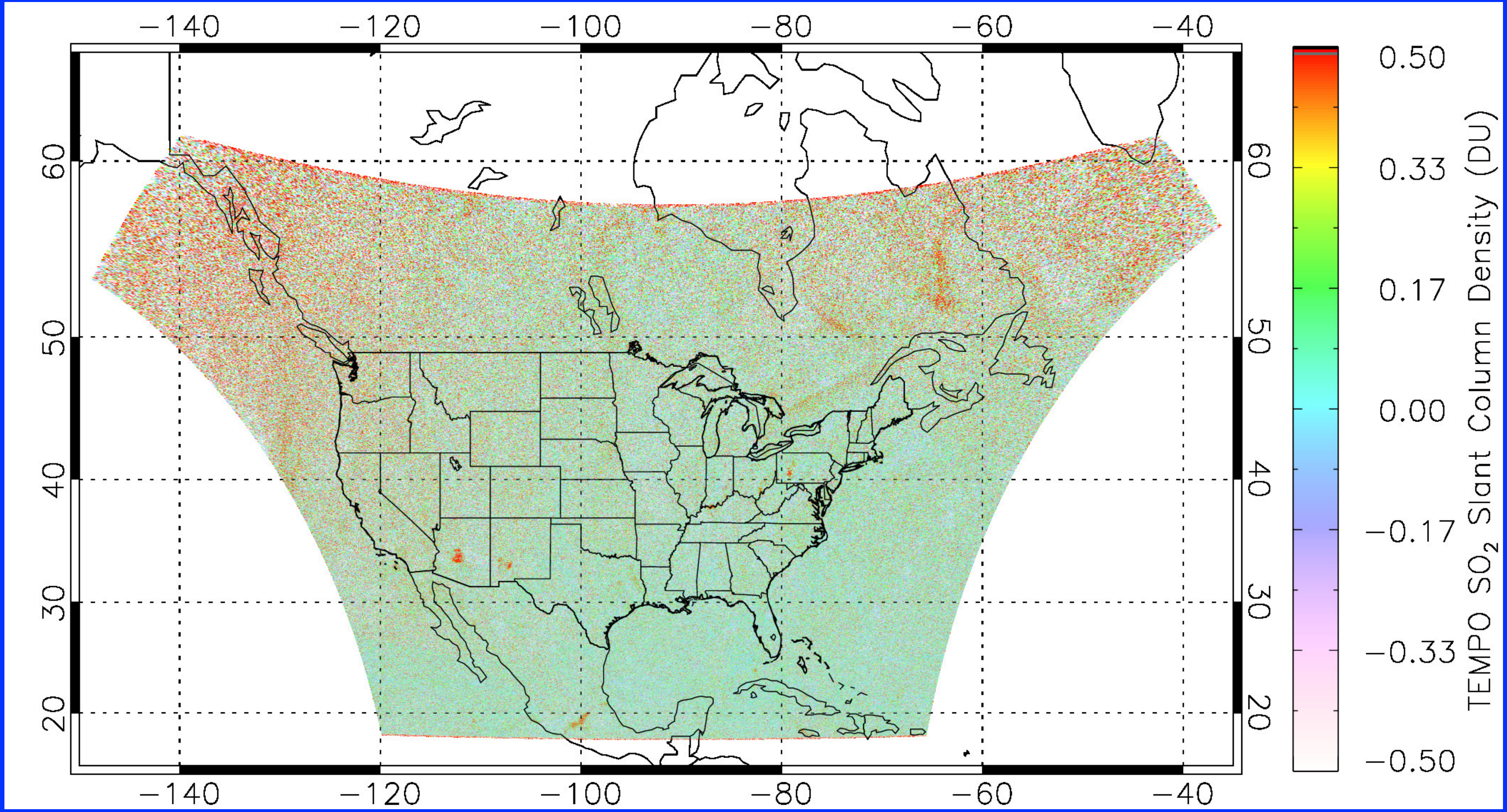


*Coverage gap due to cloud cover during the Indian summer monsoon

Data source: *Version 2 OMI and SNPP/OMPS standard SO_2 products publicly released in 2020.*

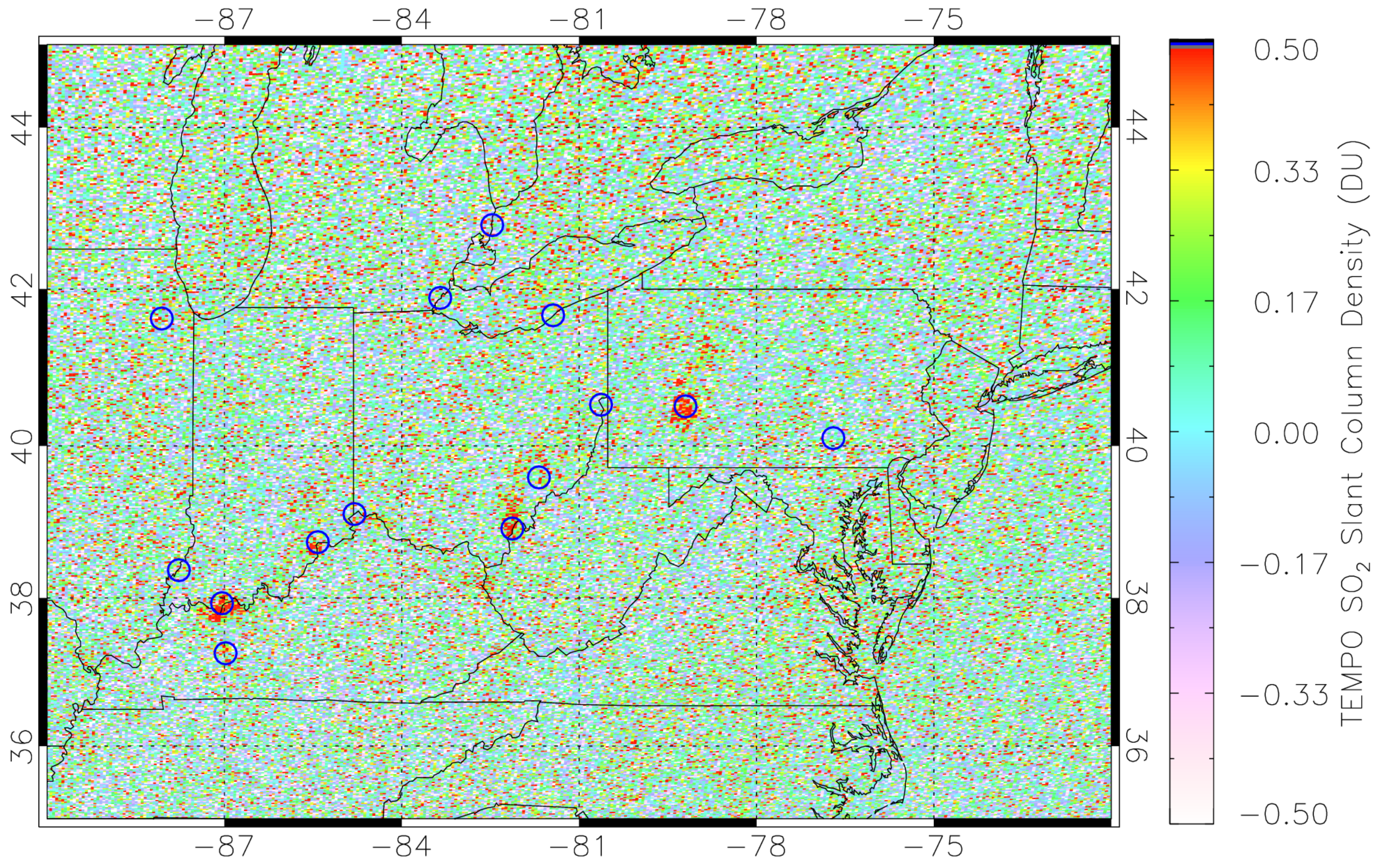
Implementation with TEMPO: Plan and Preliminary Results

- Each row (cross-scan-position) of the spatial (north – south) dimension of the detector processed separately.
- Retrievals limited to SZA < 75° and VZA < 80° for now.
- Can process data on a granule-to-granule basis or process the entire hourly scan at once (processing time: ~20 min).
- A table lookup approach similar to that for OMI/OMPS algorithms will be employed for Jacobian/AMF calculations.



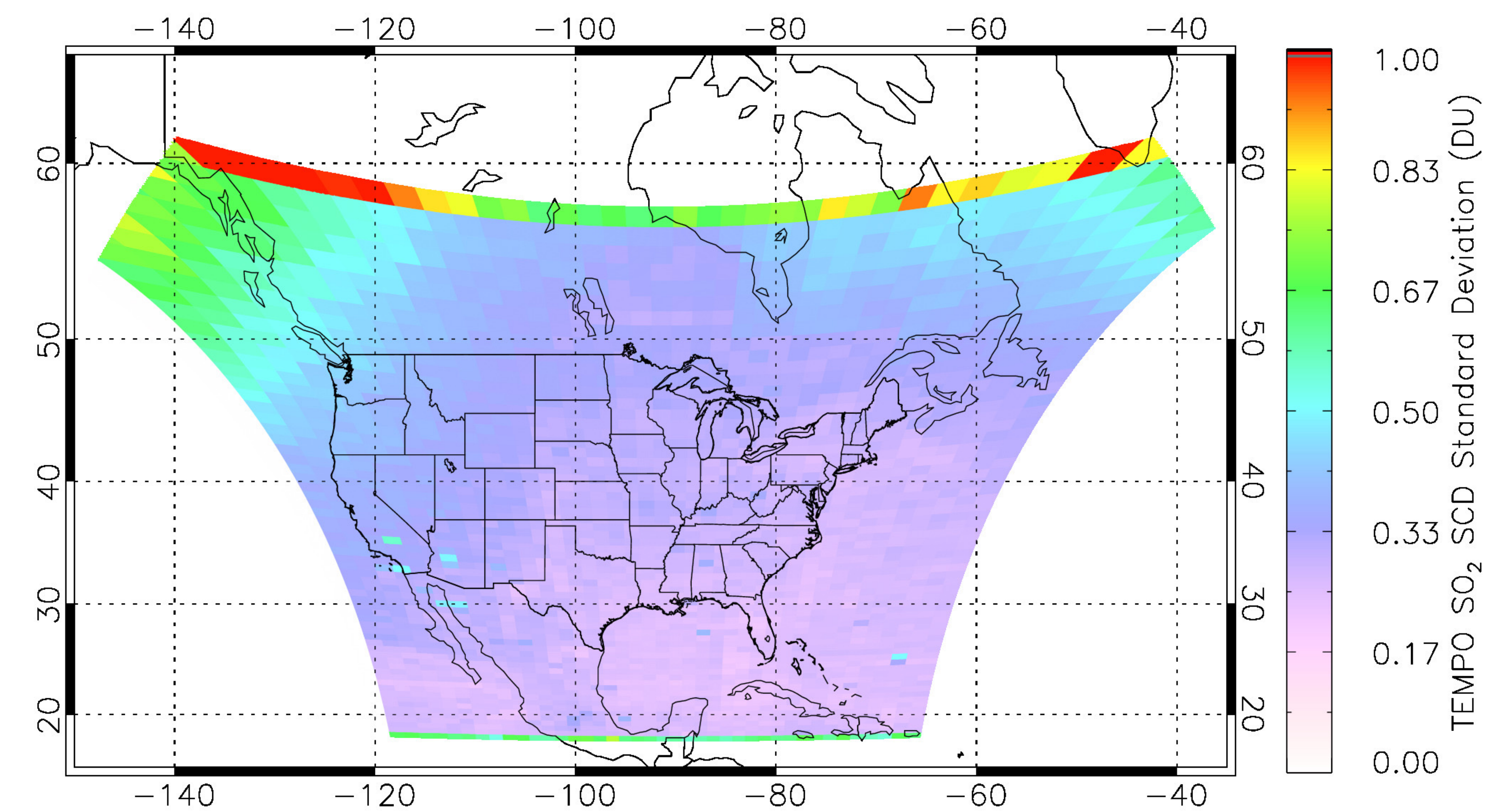
TEMPO SO_2 SCDs retrieved from synthetic radiance data for 07/01/2013.

Preliminary Results: Ohio River Valley and W Pennsylvania



Blue circles: sources > 30 kt/year based on OMI estimates between 2012 and 2015.

Preliminary Results: Standard Deviation of SO_2 SCDs



- Standard deviation calculated for blocks of 30 × 32 pixels.
- Dependence on SZAs and VZAs.
- For most of the CONUS, standard deviation is ~0.2-0.3 DU, greater than that of OMI over the Pacific (~0.15-0.3 DU), but TEMPO has much finer spatial resolution.

Next Steps and Potential Applications

- Next Steps:
  - Finalize prototype algorithm for slant column densities, including input/output and data format.
  - Adapt OMI/OMPS lookup tables and schemes for TEMPO Jacobian/AMF calculations.
  - Further testing of TEMPO algorithm using GEMS data.

- Potential Applications
  - Emissions – expect further improvement in source detection due to enhanced spatial and temporal resolution.
  - Diurnal changes in SO_2 sources.
  - Near-real-time volcanic hazard monitoring.
  - Synergy between LEO and GEO, for example, for transboundary transport.