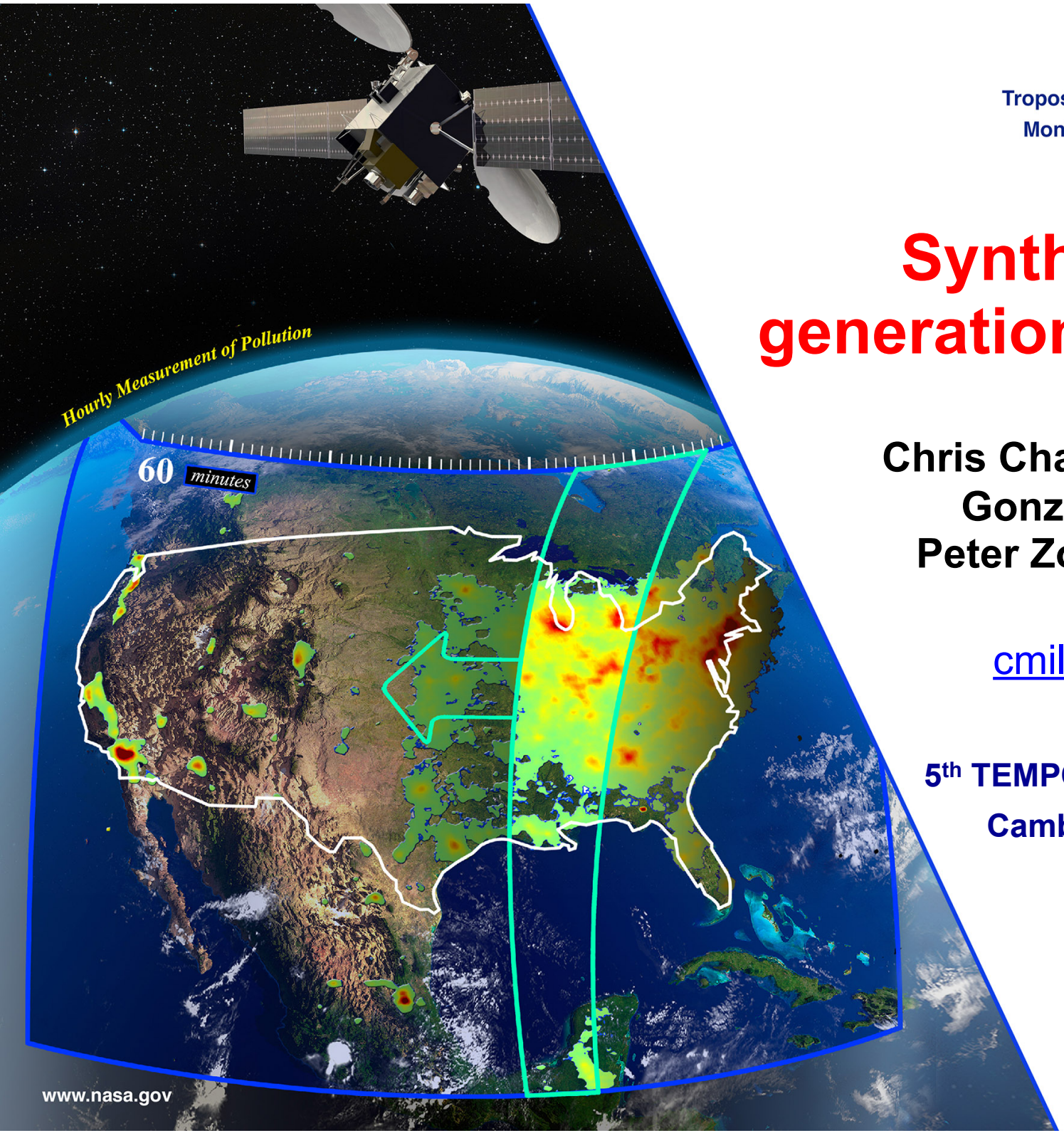


Tropospheric Emissions:
Monitoring of Pollution

Synthetic spectra generation for TEMPO

Chris Chan Miller, Xiong Liu, Gonzalo Gonzalez Abad, Peter Zoogman, Rob Spurr

cmiller@cfa.harvard.edu

5th TEMPO Science Team Meeting

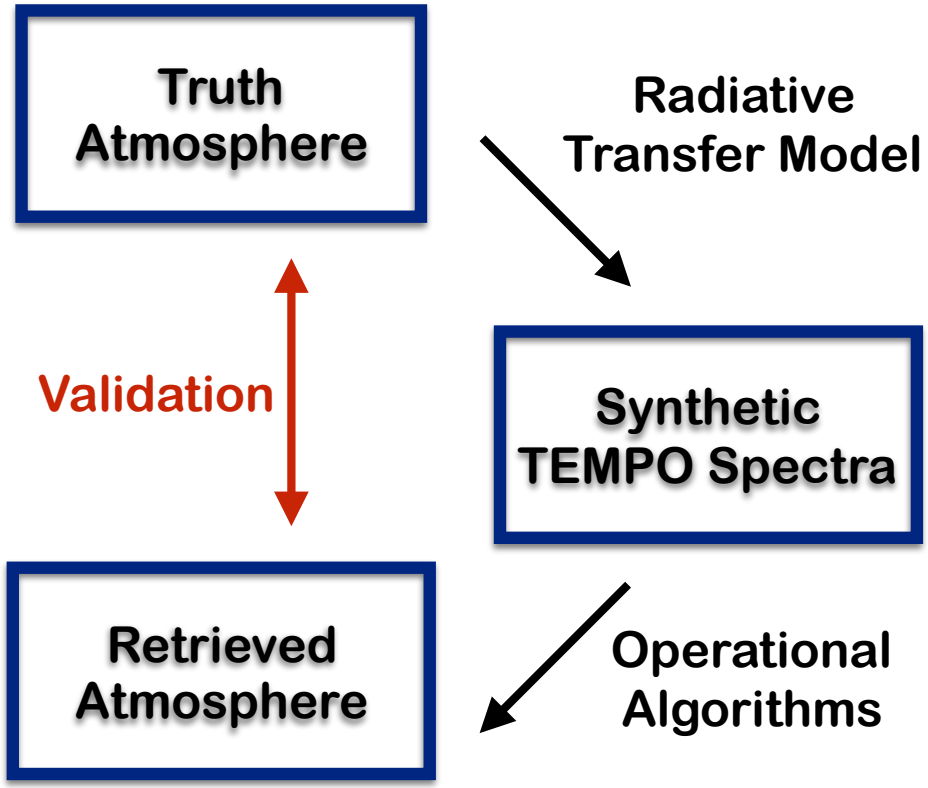
Cambridge, MA, May 31, 2016

Smithsonian

Why do we need synthetic spectra?

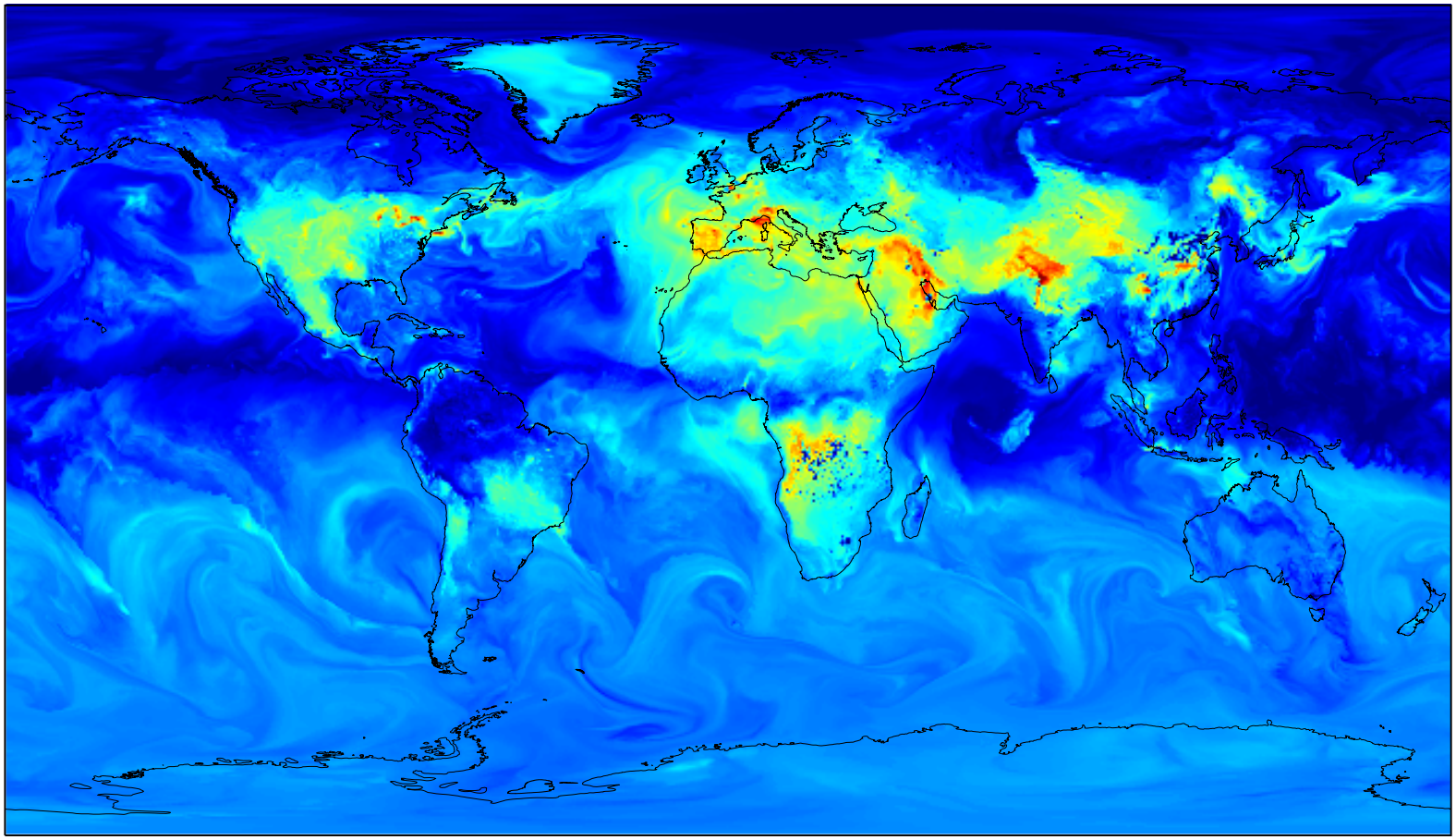
(1) To test the Science Data Processing Center Pipeline

(2) To validate TEMPO retrieval algorithms



GEOS-5 Truth Atmosphere

Surface Ozone - 20130715 - 13:00 EST



"G5NR" - GEOS-Chem coupled to the GEOS-5 GCM run globally at ~12x12 km^2 resolution

Courtesy of Christoph Keller

Construction of truth atmosphere

G5NR

Python Sampling Tool

Truth Atmosphere

Construction of truth atmosphere

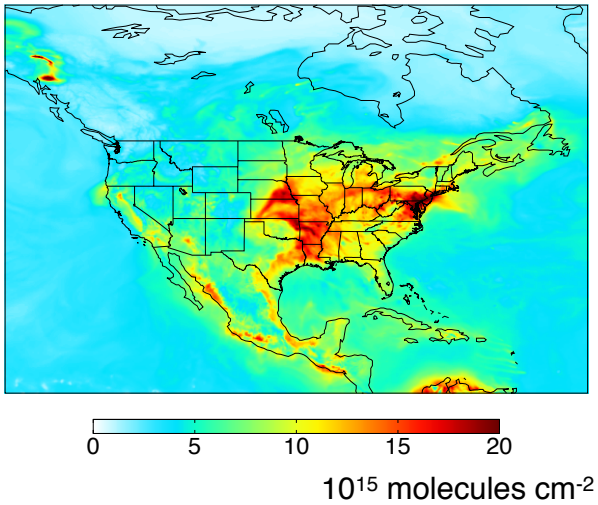
G5NR

Sampled Fields:

- Trace Gases
- Aerosols
- Pressure
- Temperature
- Relative Humidity
- Winds (u,v)
- Cloud fraction & Optical depth
- Snow fraction & depth

Python Sampling Tool

Example: G5NR HCHO



Truth Atmosphere

Construction of truth atmosphere

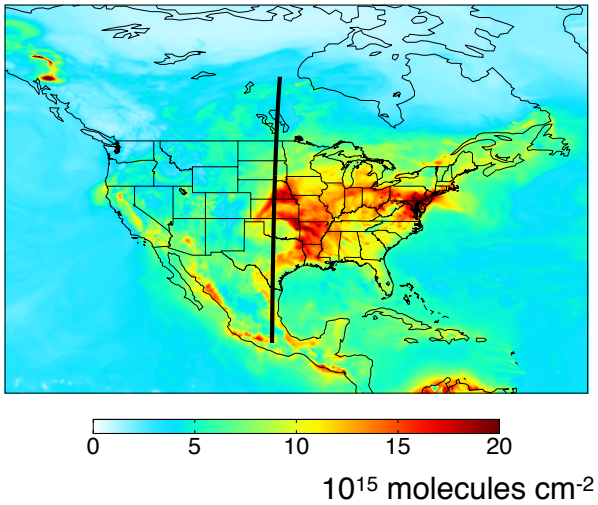
G5NR

Spacecraft Orbit (Carr Astronautics)

"Proxydynamics" simulation of spacecraft orbit + pitch/yaw/roll

Python Sampling Tool

Example: G5NR HCHO



Truth Atmosphere

Sample G5NR fields based on simulated geolocation

Construction of truth atmosphere

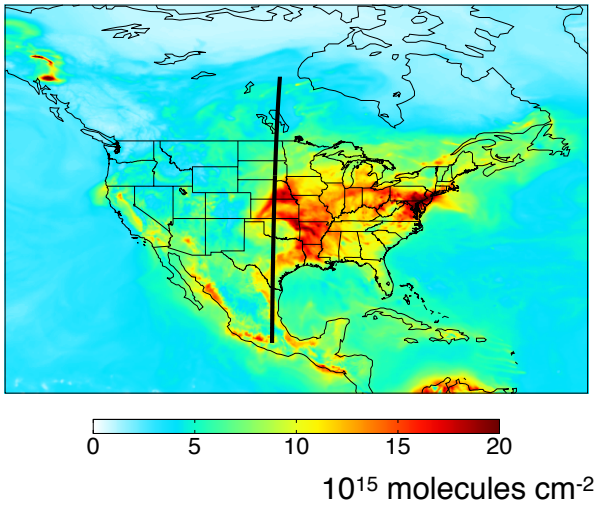
G5NR

Spacecraft Orbit (Carr Astronautics)

"Proxydynamics" simulation of orbit + spacecraft pitch/yaw/ roll

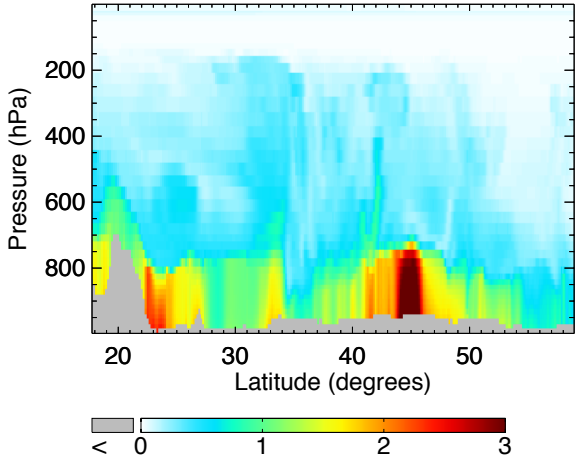
Python Sampling Tool

Example: G5NR HCHO



Truth Atmosphere

Sampled HCHO Field



Sample G5NR fields based on simulated geolocation

Construction of truth atmosphere

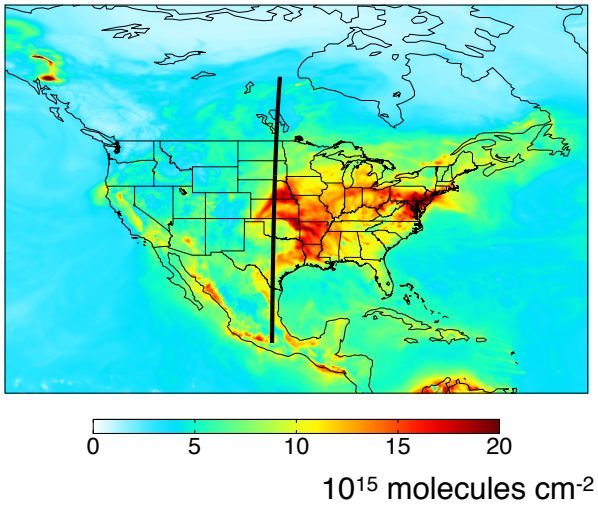
G5NR

Spacecraft Orbit (Carr Astronautics)

"Proxydynamics" simulation of orbit + spacecraft pitch/yaw/ roll

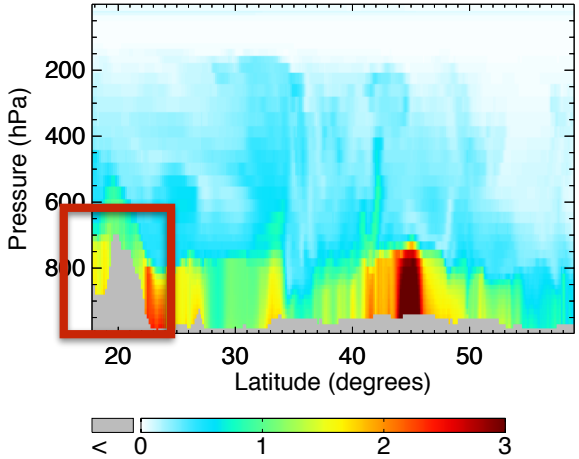
Python Sampling Tool

Example: G5NR HCHO



Truth Atmosphere

Sampled HCHO Field



Sample G5NR fields based on simulated geolocation

Construction of truth atmosphere

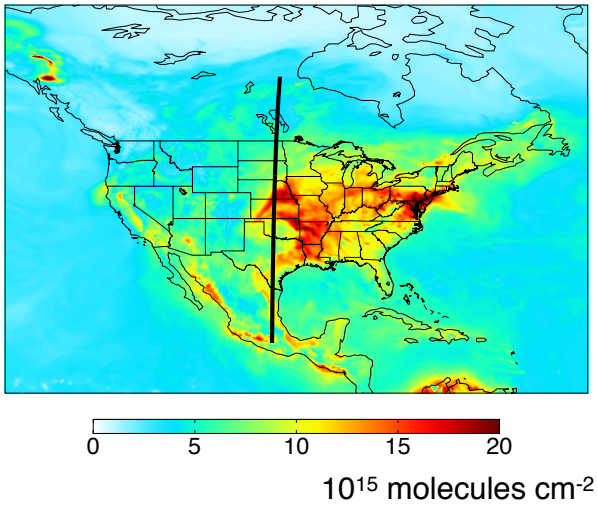
G5NR

Spacecraft Orbit (Carr Astronautics)

"Proxydynamics" simulation of orbit + spacecraft pitch/yaw/ roll

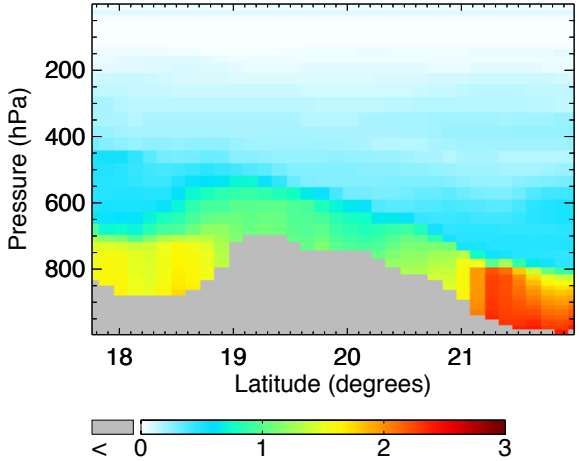
Python Sampling Tool

Example: G5NR HCHO



Truth Atmosphere

Sampled HCHO Field



Construction of truth atmosphere

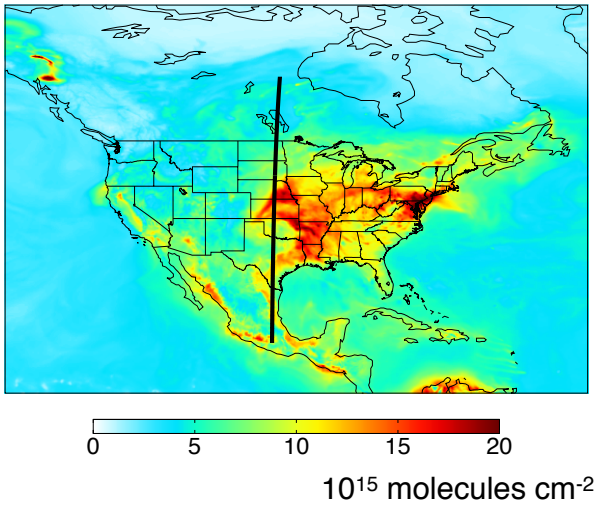
G5NR

Spacecraft Orbit (Carr Astronautics)

GMTED DEM Database

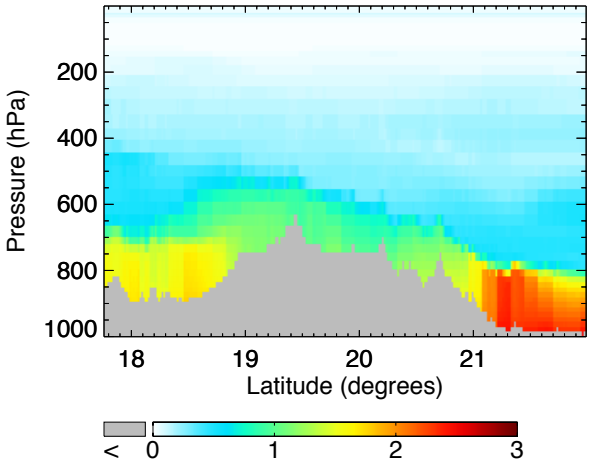
Python Sampling Tool

Example: G5NR HCHO



Truth Atmosphere

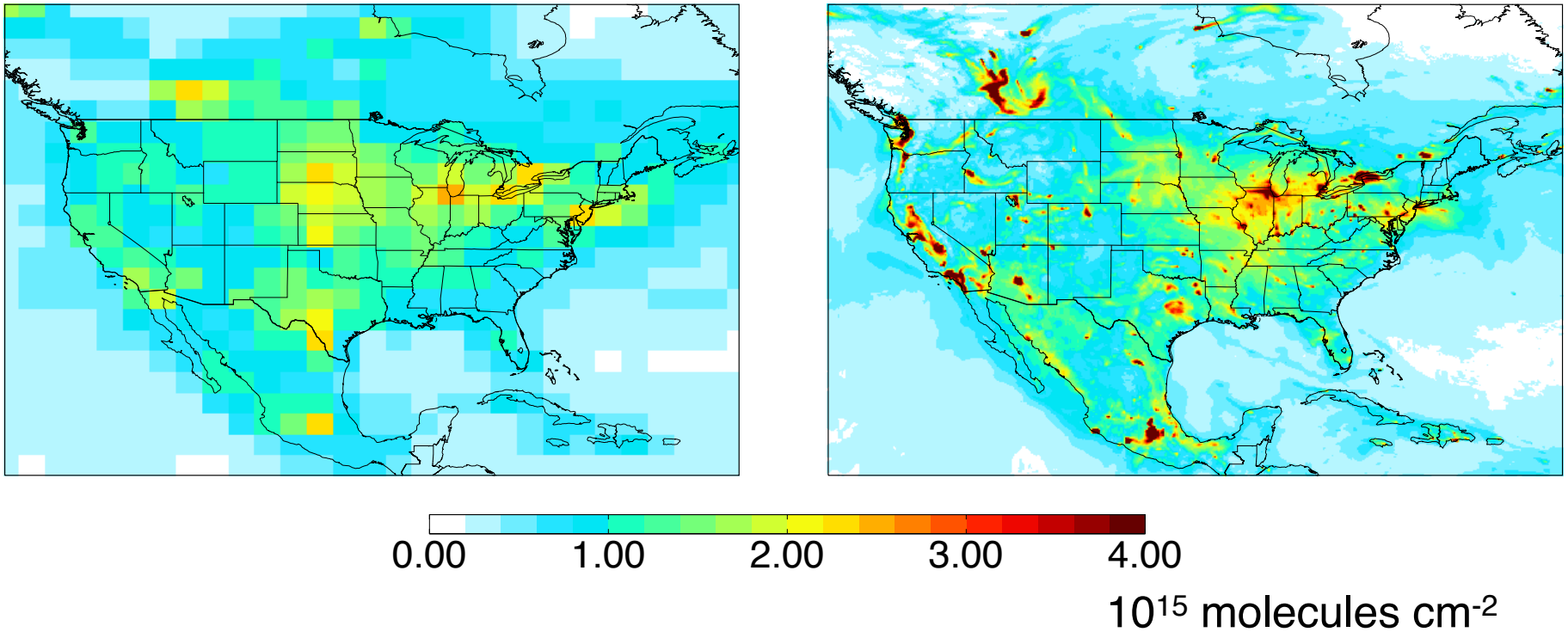
Sampled HCHO Field



Profiles adjusted for subgrid altitude variation using GMTED2010 7.5 arc second digital elevation database

Comparison with previous truth atmosphere

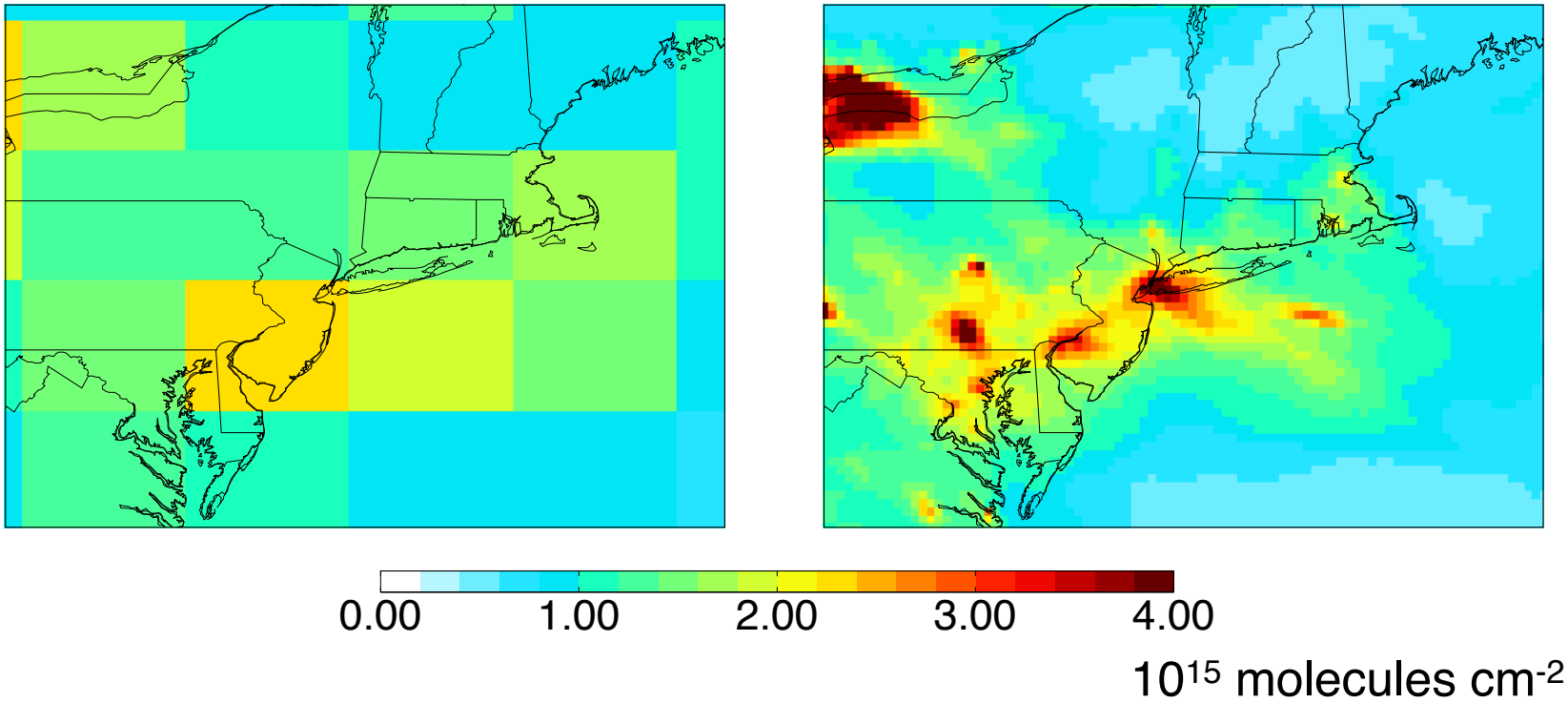
Tropospheric NO2 Column - 15/7/13 1pm EST



G5NR appears adequate for resolving range of trace gas concentrations expected for TEMPO

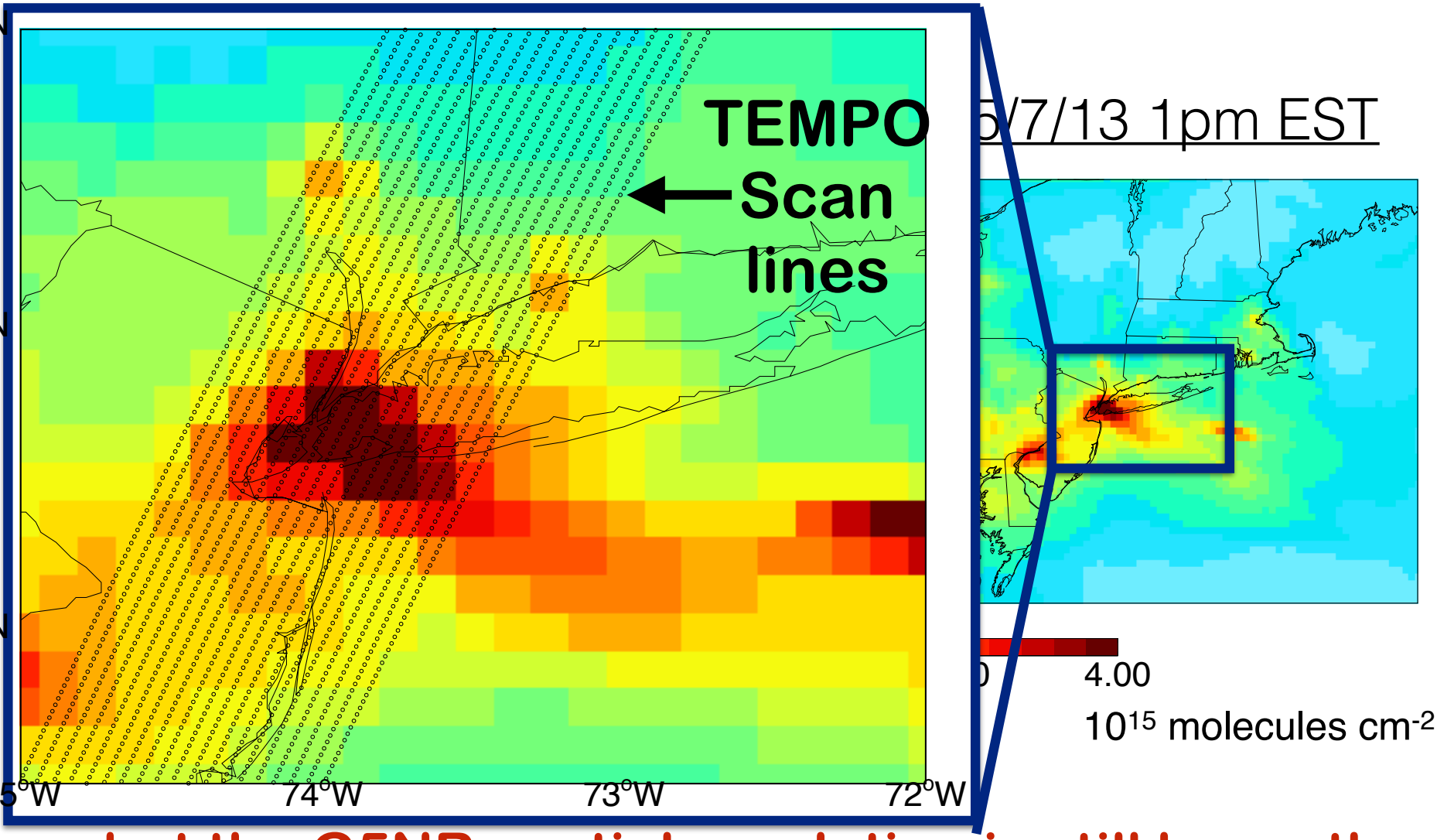
Comparison with previous truth atmosphere

Tropospheric NO2 Column - 15/7/13 1pm EST



G5NR can resolve filamented plumes from urban emissions

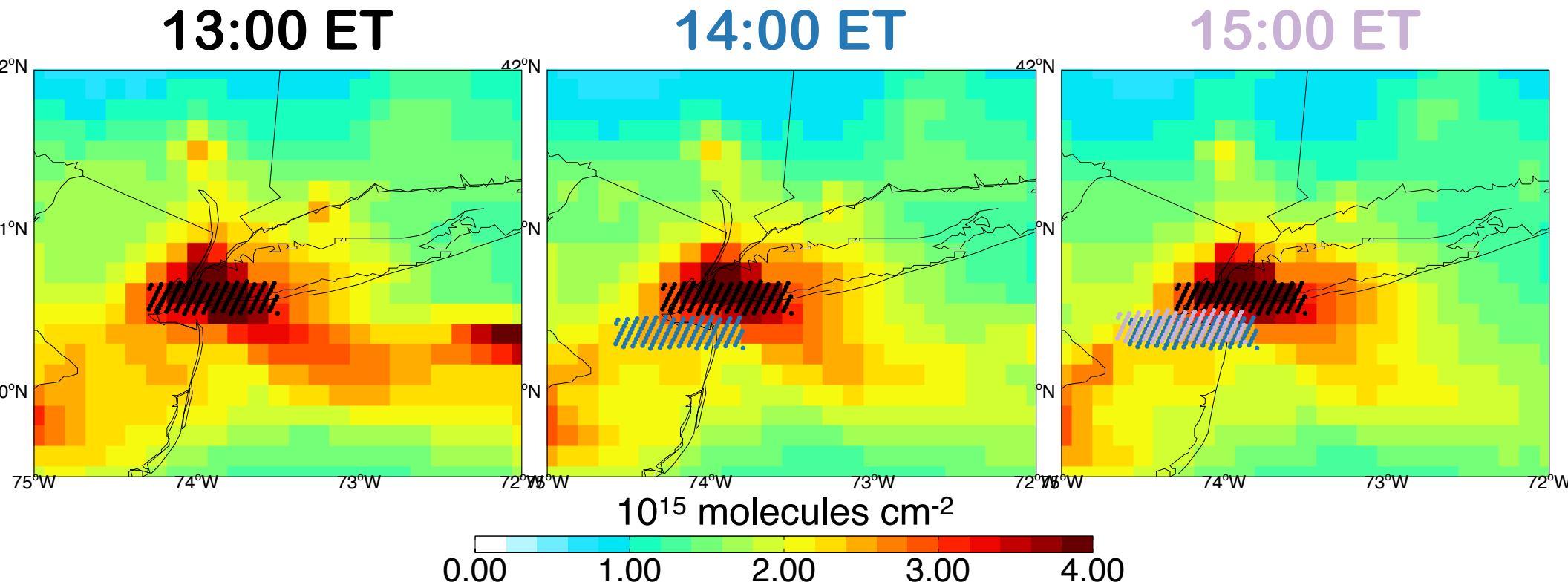
Comparison with previous truth atmosphere



… but the G5NR spatial resolution is still lower than the TEMPO pixels

Hour-to-hour pointing variation

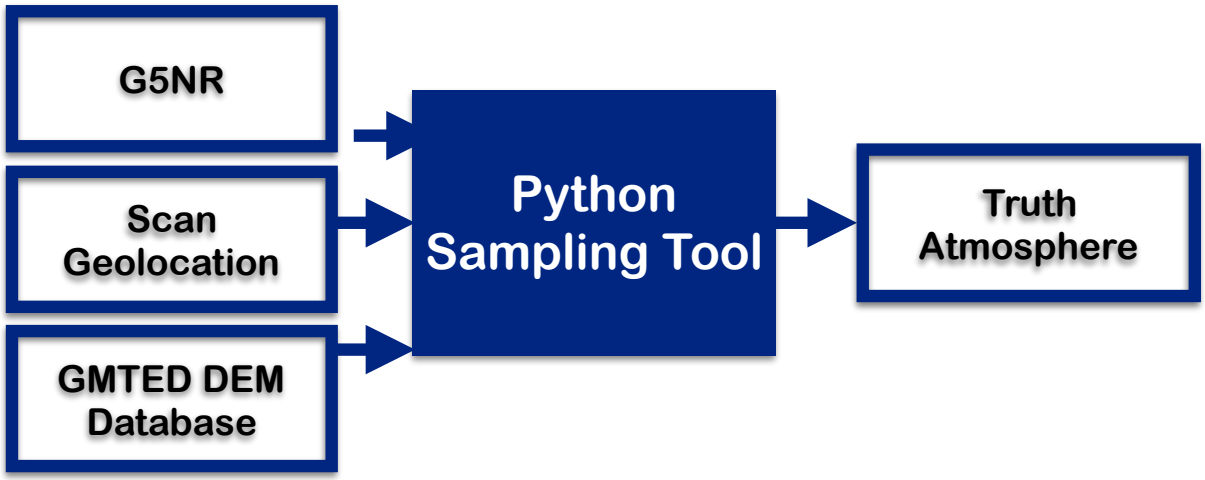
Tropospheric NO2 Column - 15/7/13



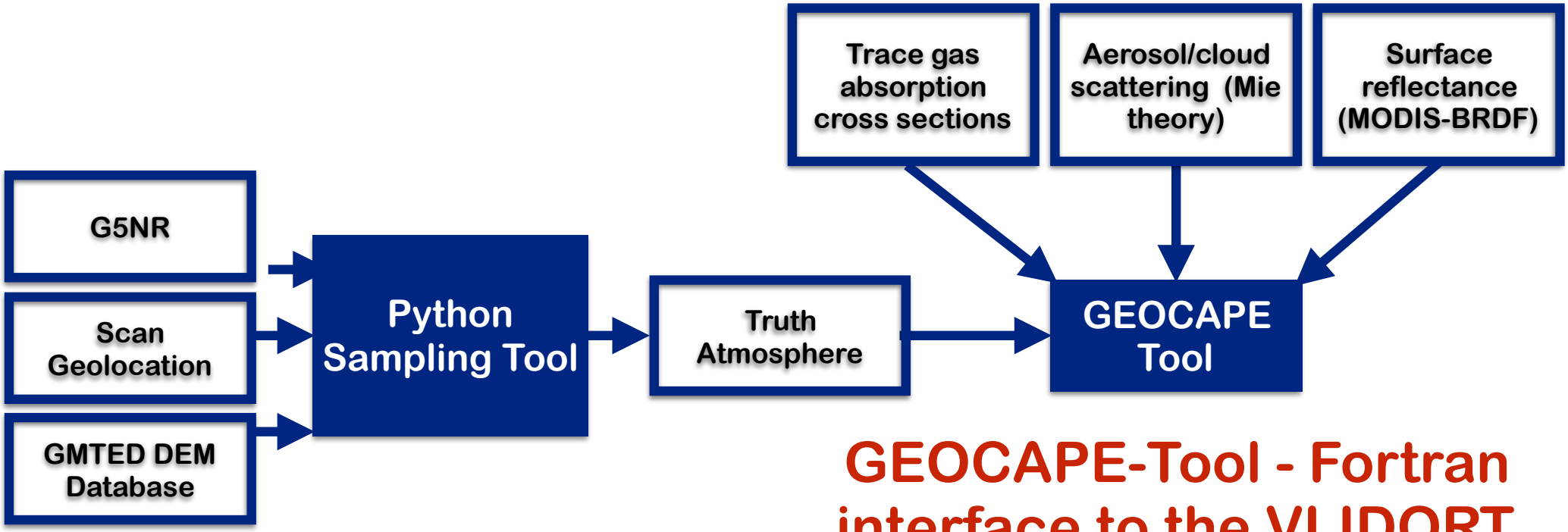
Expected hour-to-hour jitter >> pixel dimension

Implications for oversampling?

Simulation of TEMPO Spectra

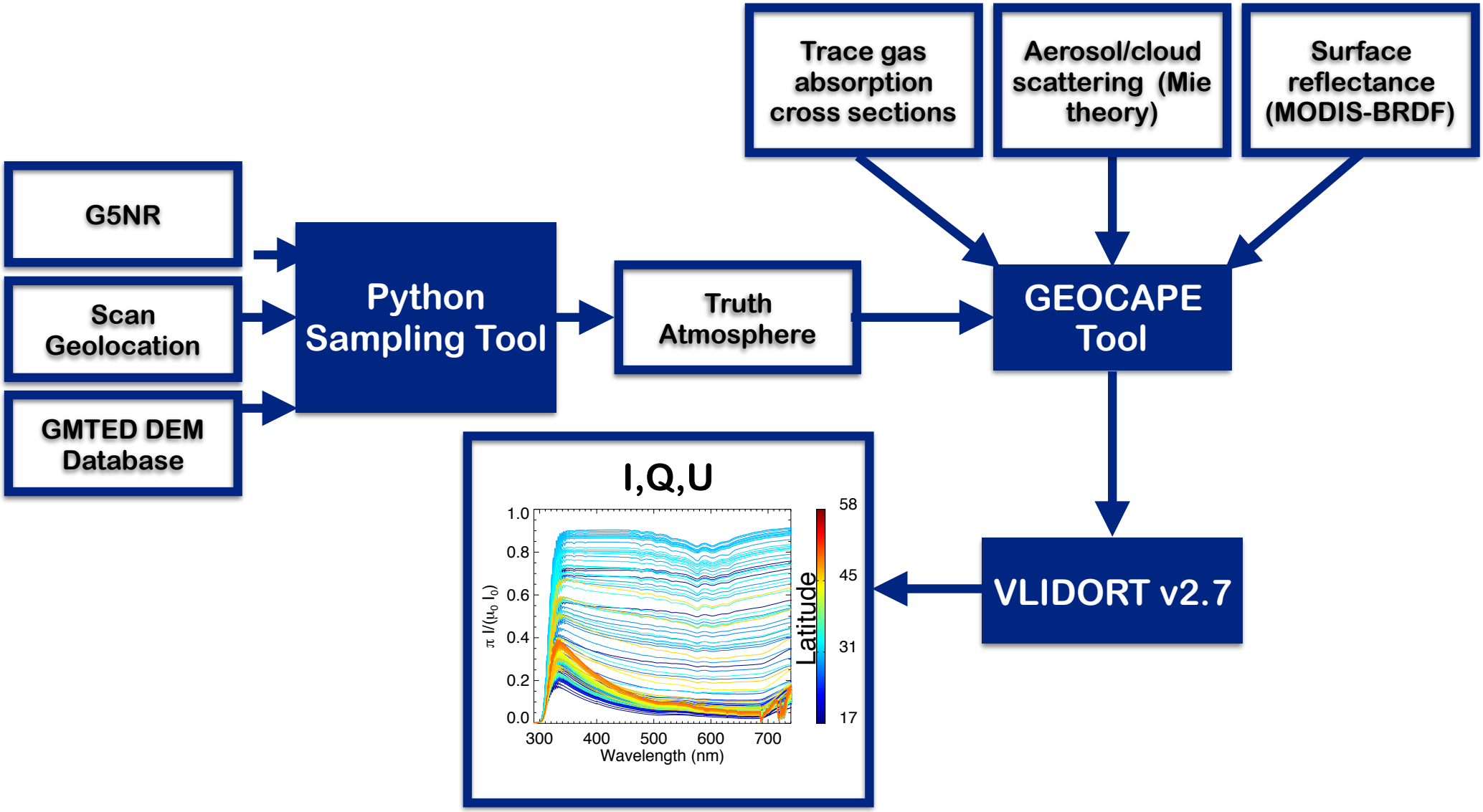


Simulation of TEMPO Spectra

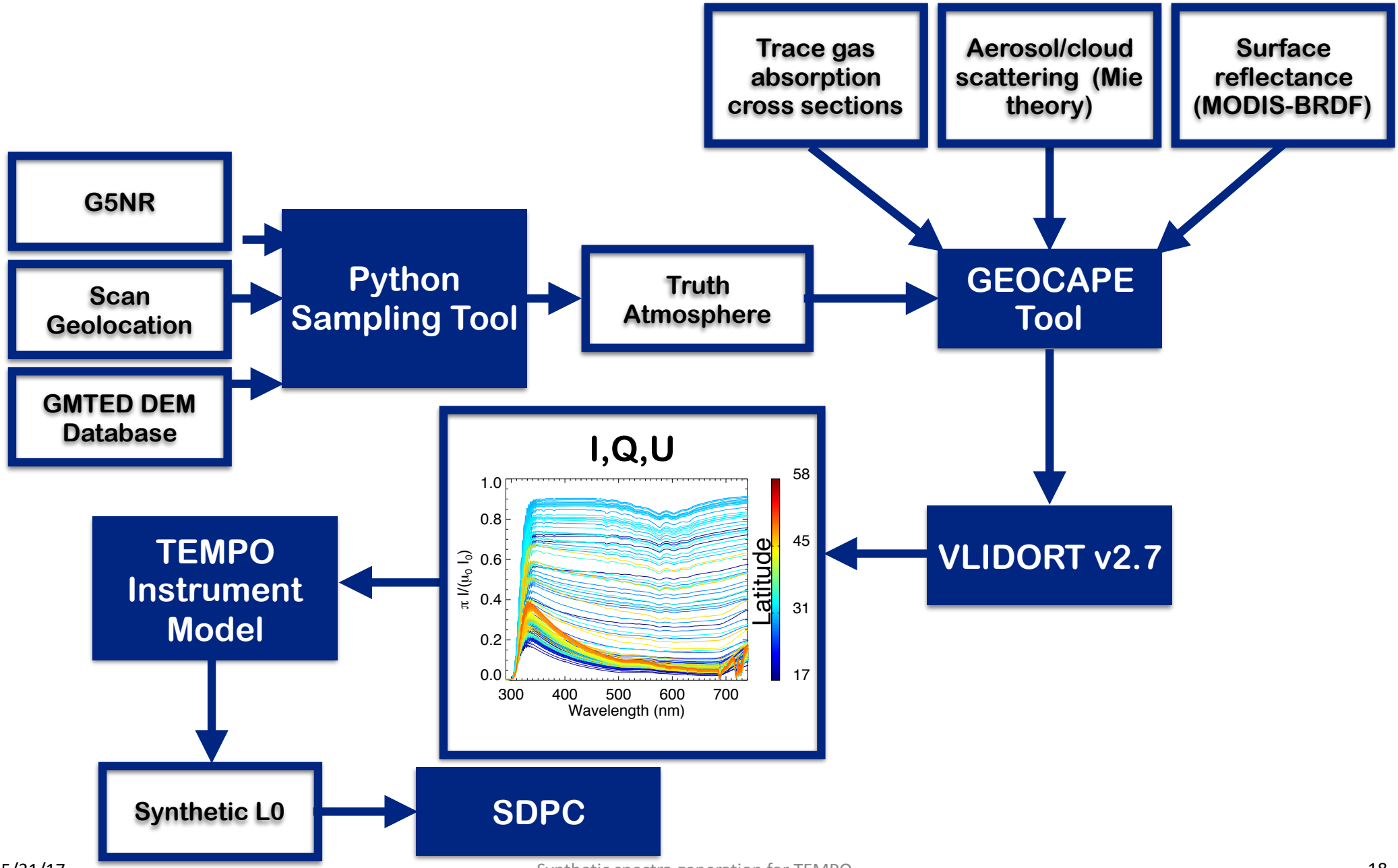


GEOCAPE-Tool - Fortran interface to the VLIDORT RT Model

Simulation of TEMPO Spectra

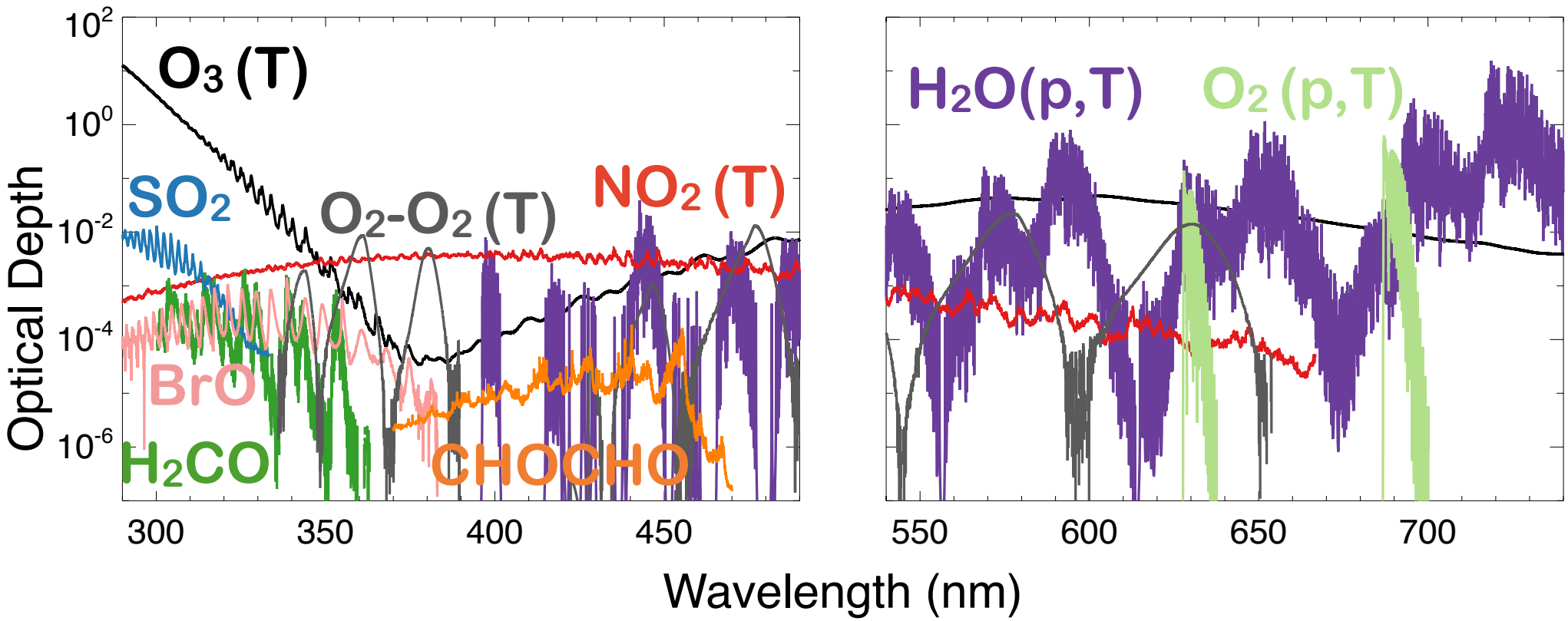


Simulation of TEMPO Spectra



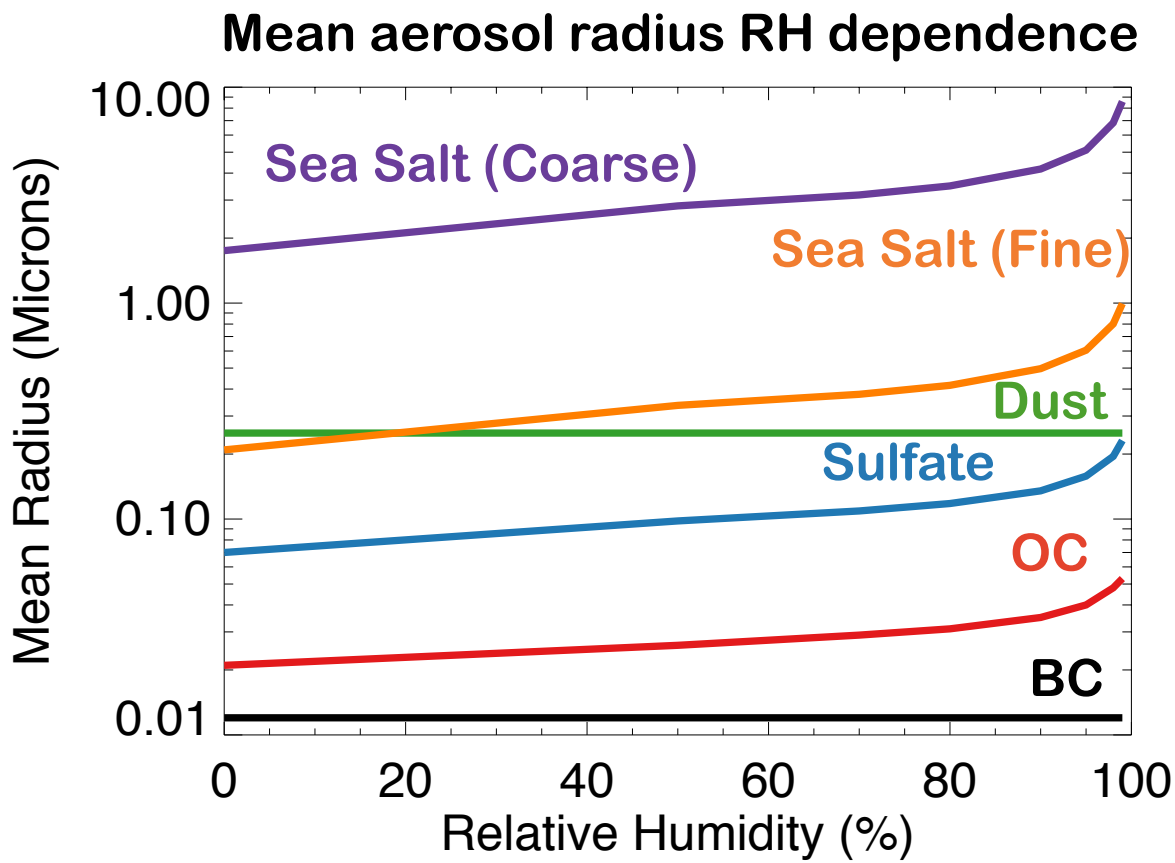
Trace gas absorption

Typical optical depths for simulated species



Scattering by aerosols

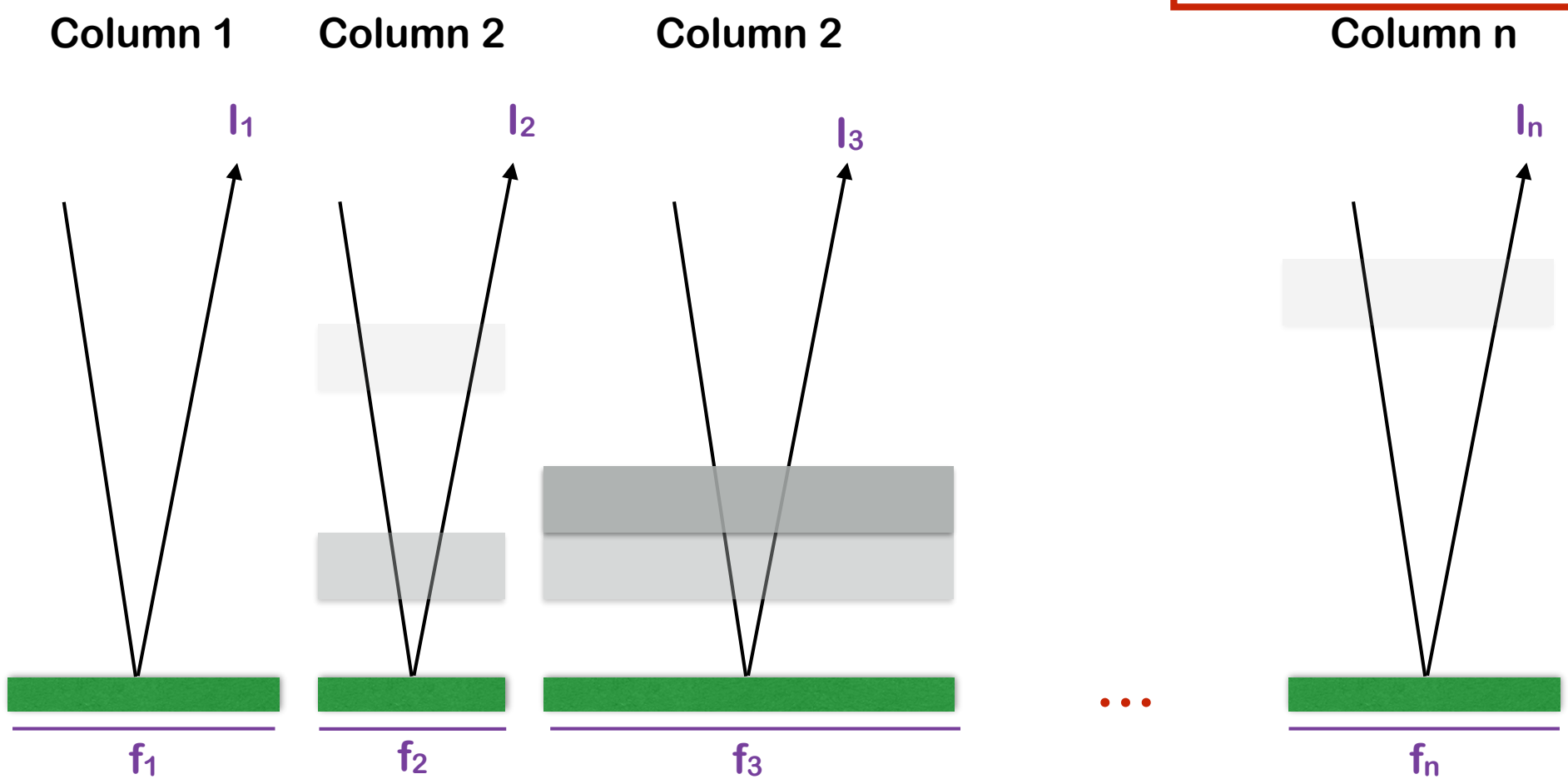
- Aerosol cross sections/ phase functions calculated from Mie theory
- Aerosol refractive indices and size distribution from GADs
- The RH dependence of sea salt, sulfate and organic carbon optical properties is accounted for



Scattering by clouds

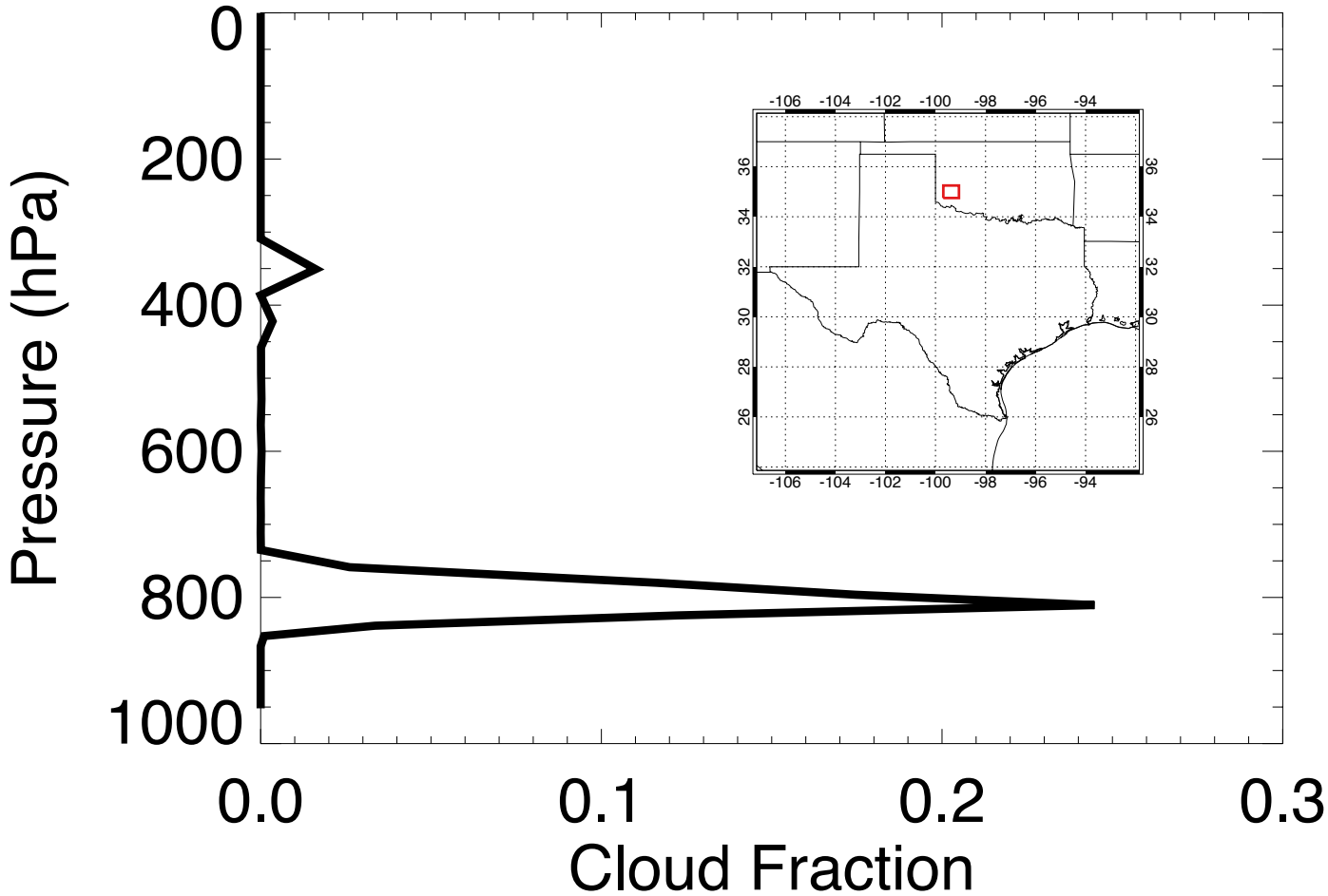
Clouds modeled using the independent pixel approx.

$$I(\lambda) = \sum_{j=1}^{n} f_j I_j(\lambda)$$



Cloud scattering is explicitly simulated (i.e. no lambertian surface approximation)

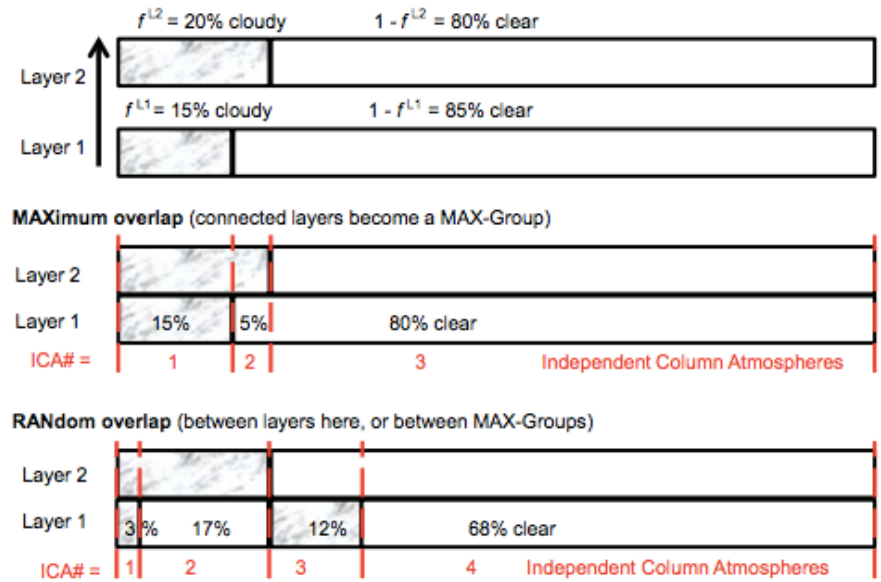
Cloud downscaling



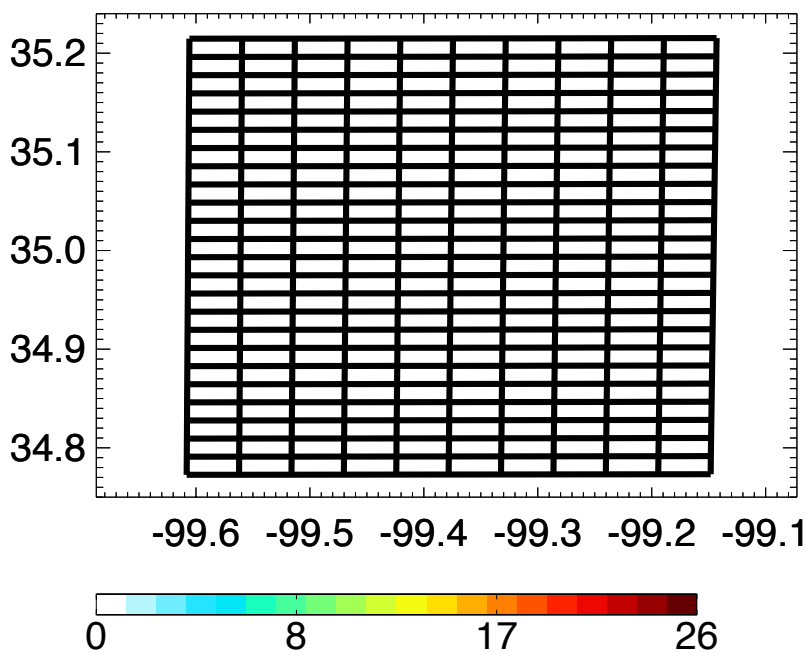
How do we infer cloud subpixels from an aggregate cloud profile?

Cloud downscaling

The simulated radiance will be sensitive to cloud overlap assumptions

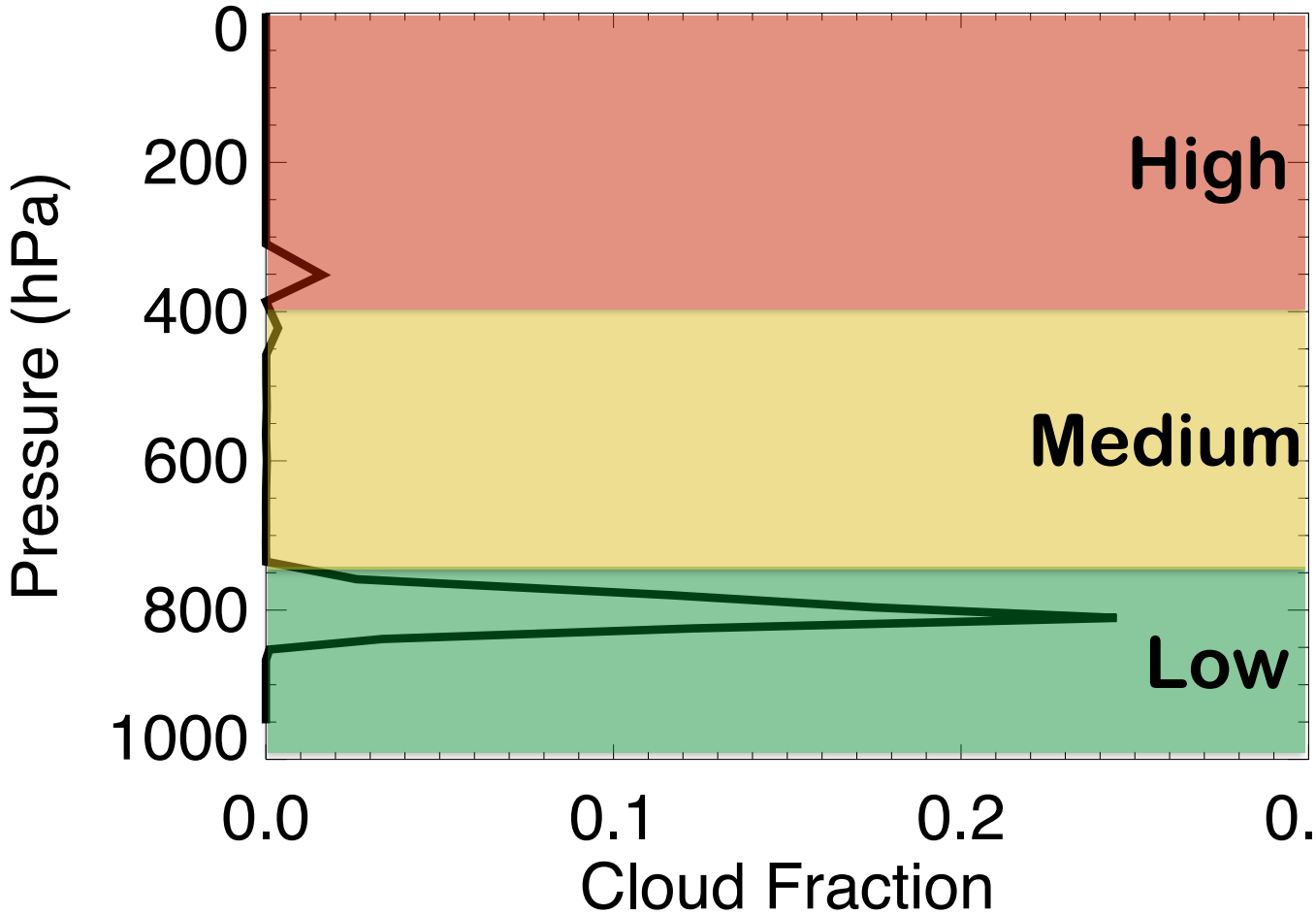


Prather (2015)



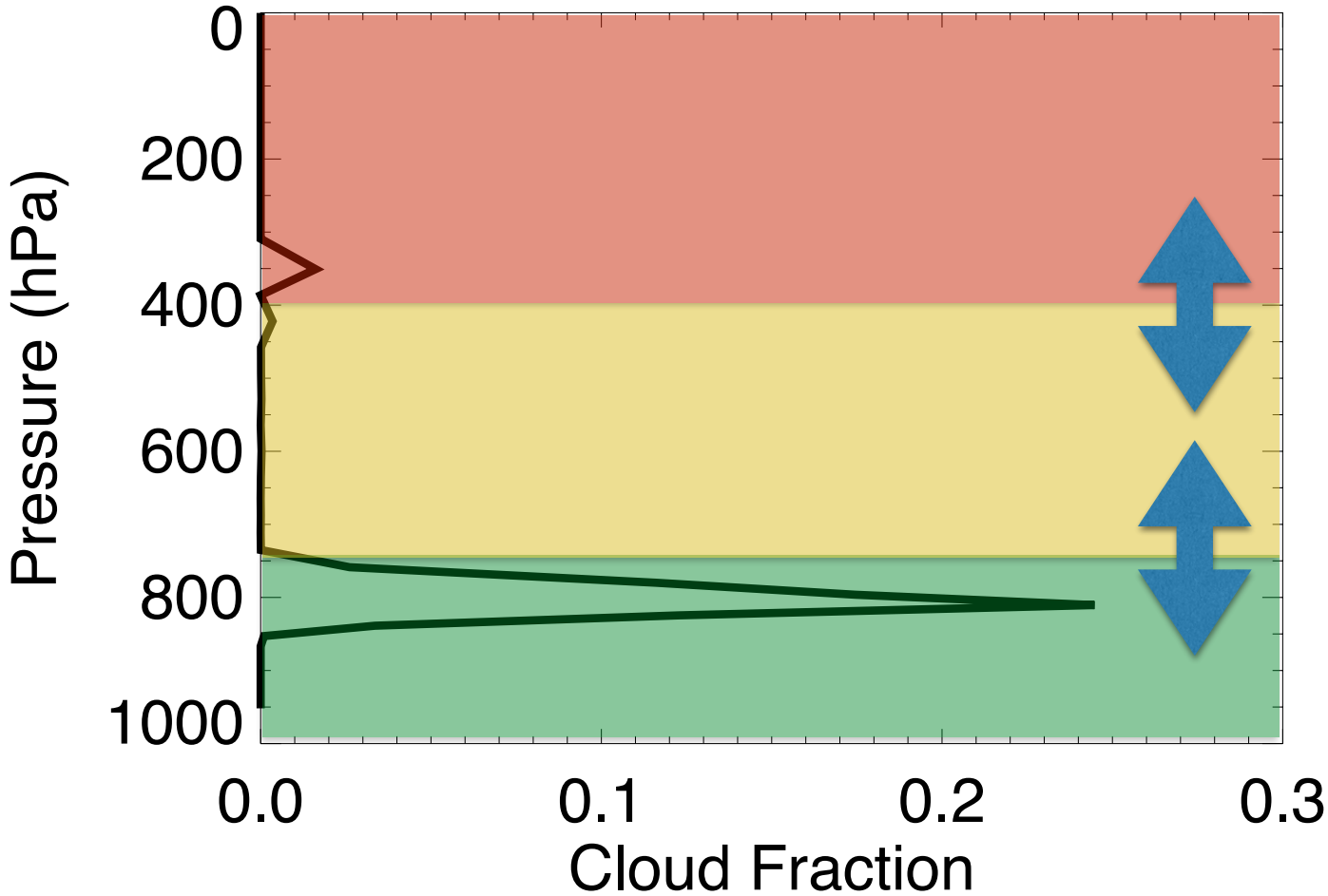
Clouds are archived on a 0.5x0.625 grid. This is an order of magnitude larger than a TEMPO pixel

Approximate MRAN Overlap



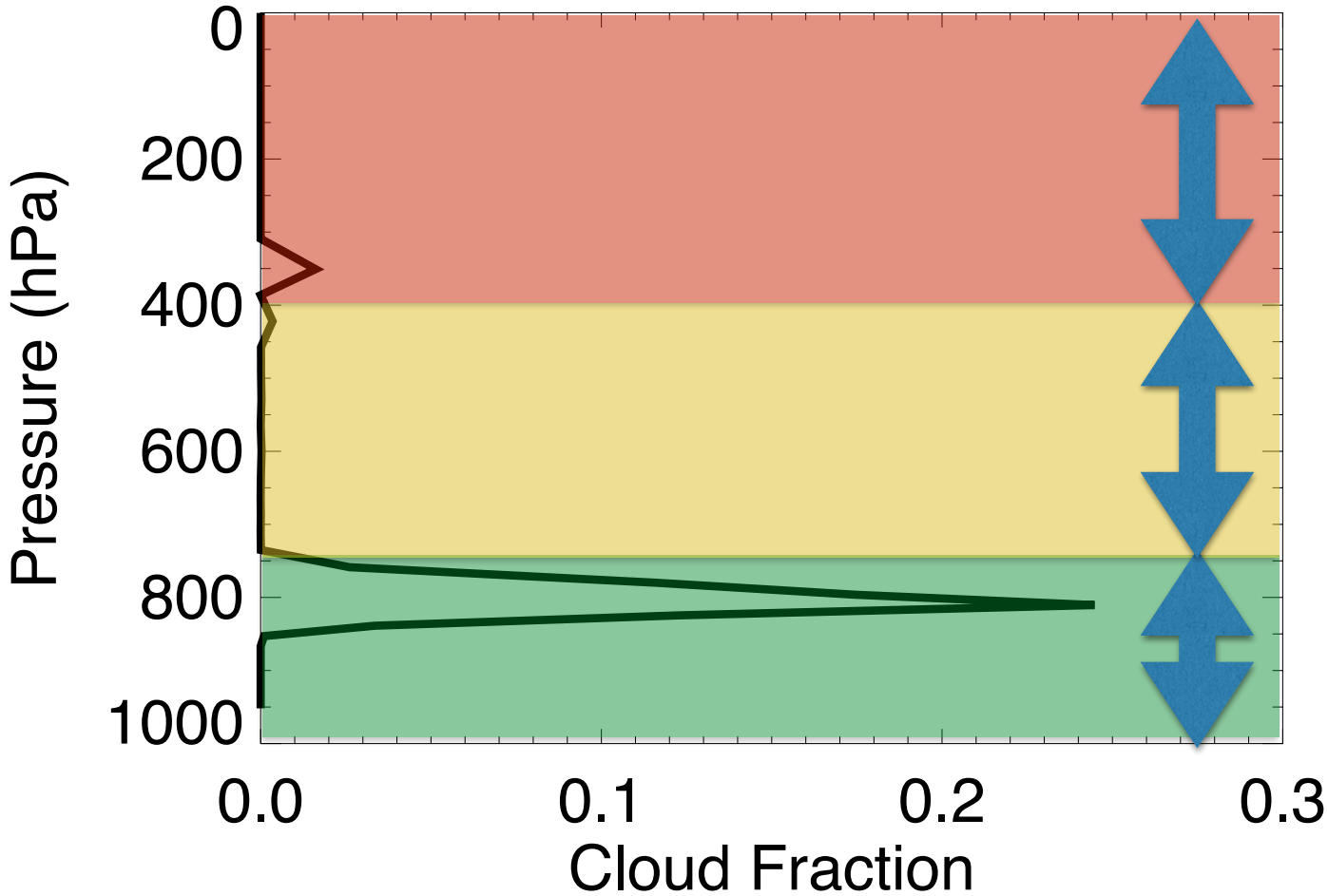
(1) Divide clouds into low medium and high altitude type layers

Approximate MRAN Overlap



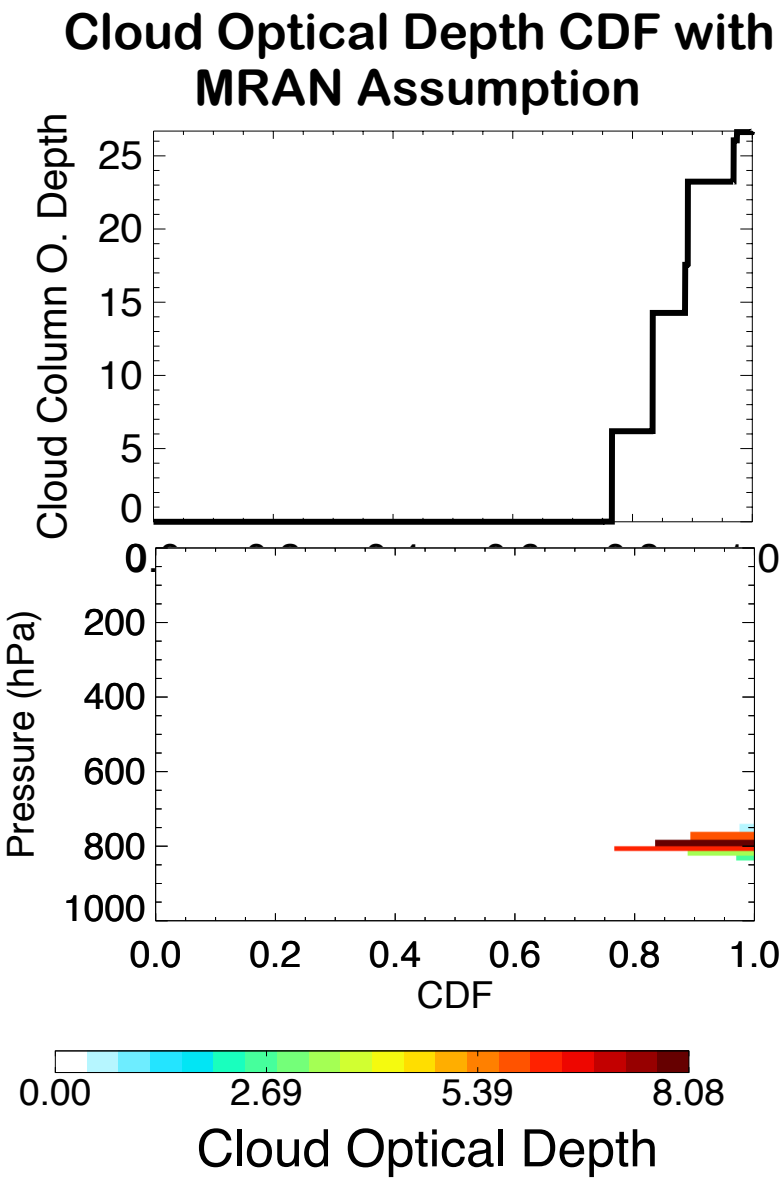
(2) Assume clouds randomly overlap between each coarse layer

Approximate MRAN Overlap

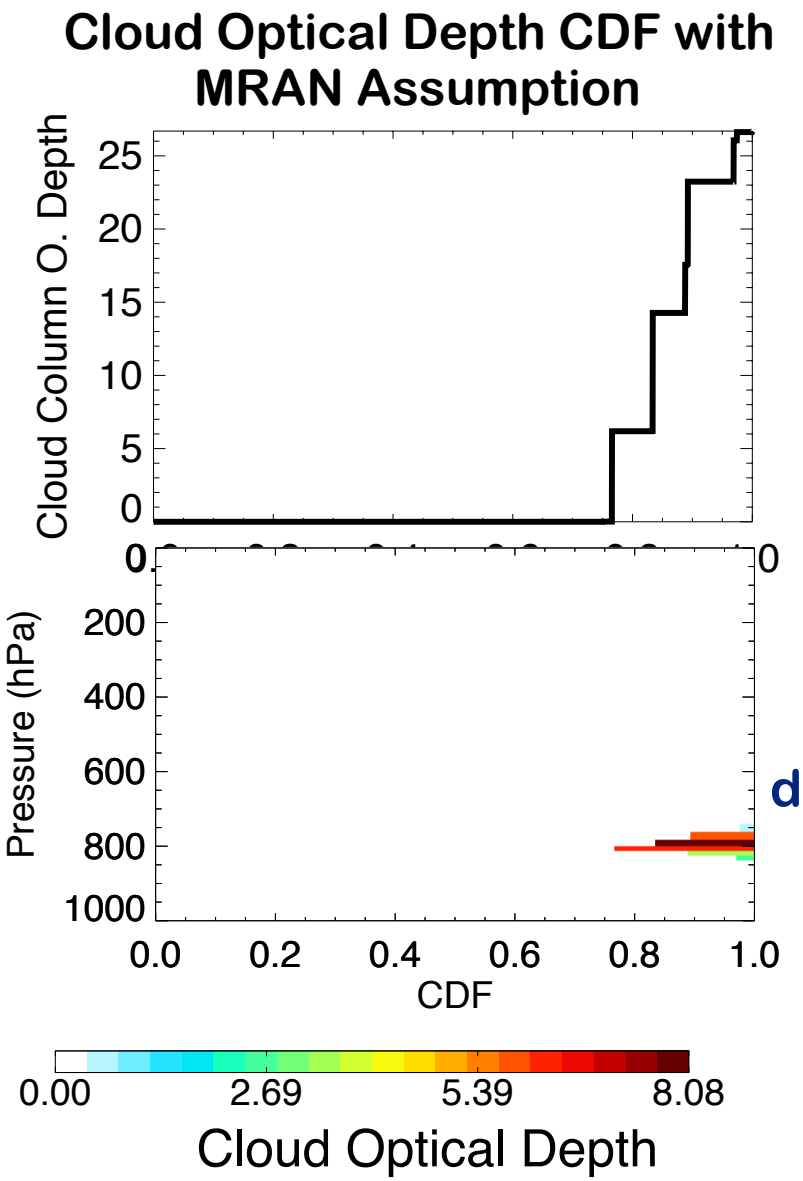


(3) Assume clouds are maximally overlapped within each layer

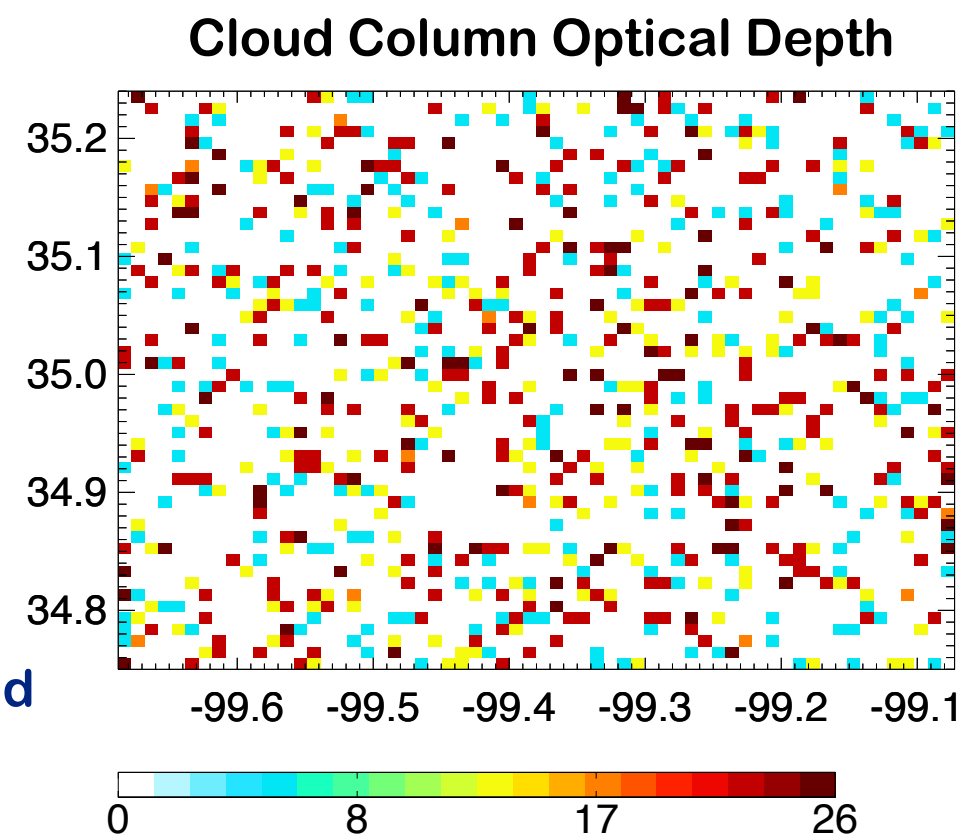
Stochastic column generation



Stochastic column generation

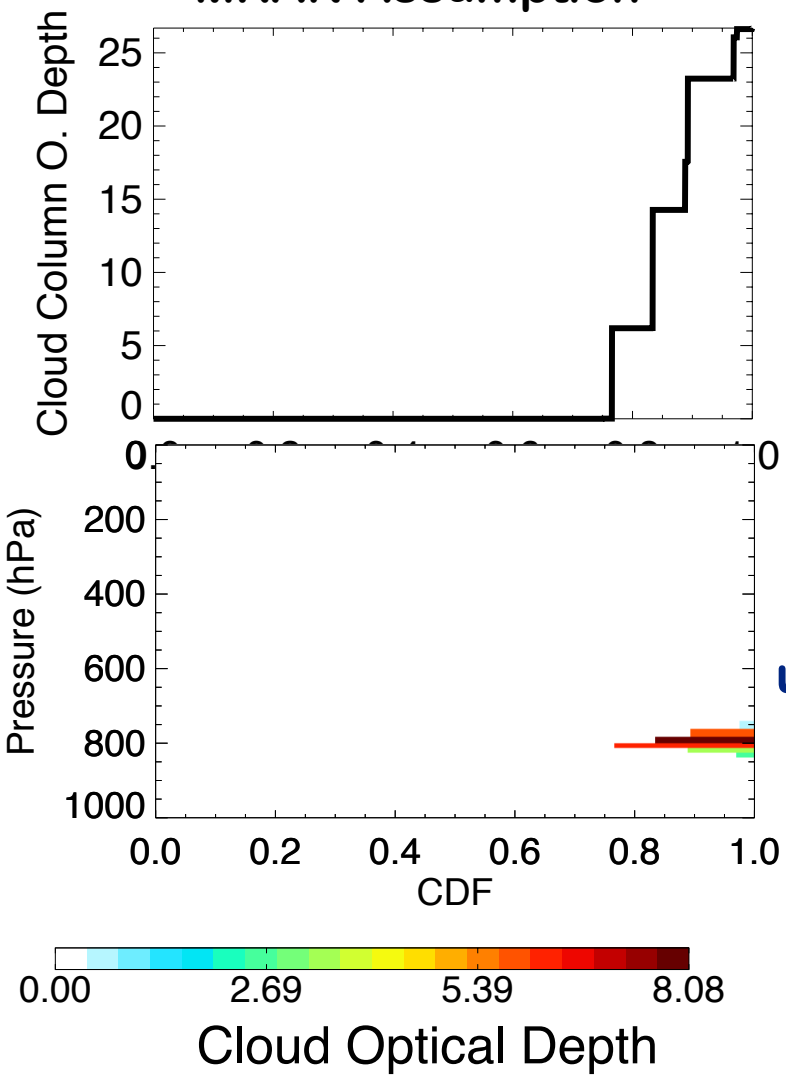


Sample CDF onto 0.1x0.1 degree sub grid



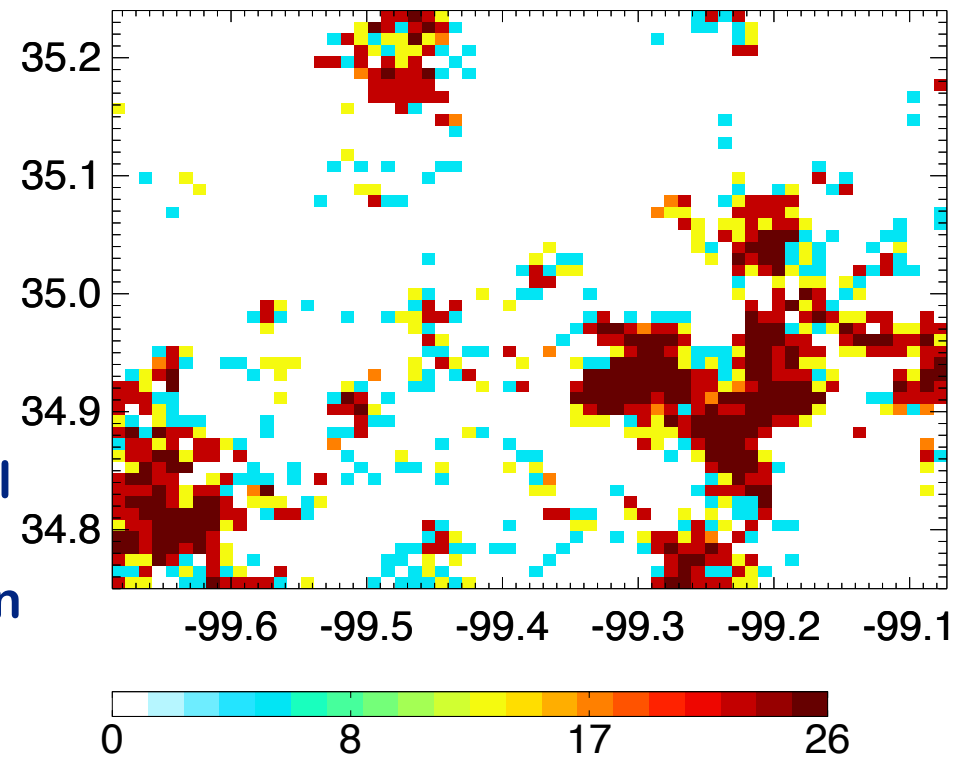
Stochastic column generation

Cloud Optical Depth CDF with MRAN Assumption



Impose spatial correlation using Gaussian Copula (Wind et al. 2013)

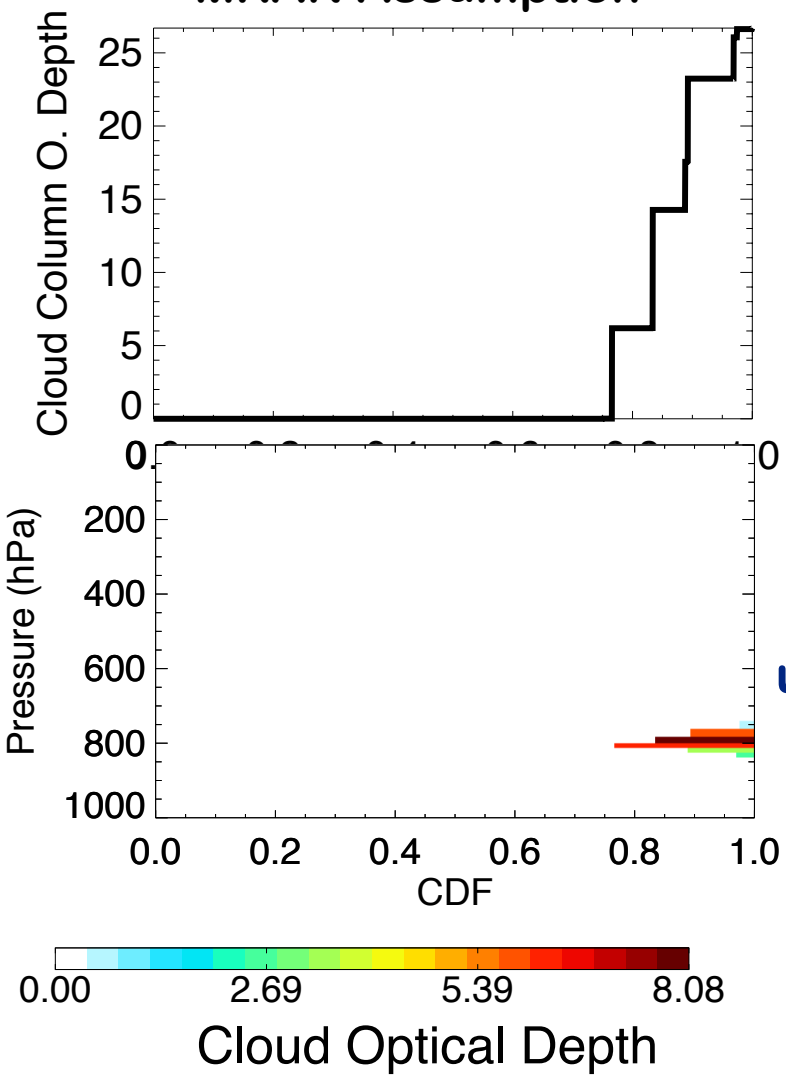
Cloud Column Optical Depth



Not accounting for spatial correlation between pixels will underestimate the number of cloud free pixels

Stochastic column generation

Cloud Optical Depth CDF with MRAN Assumption



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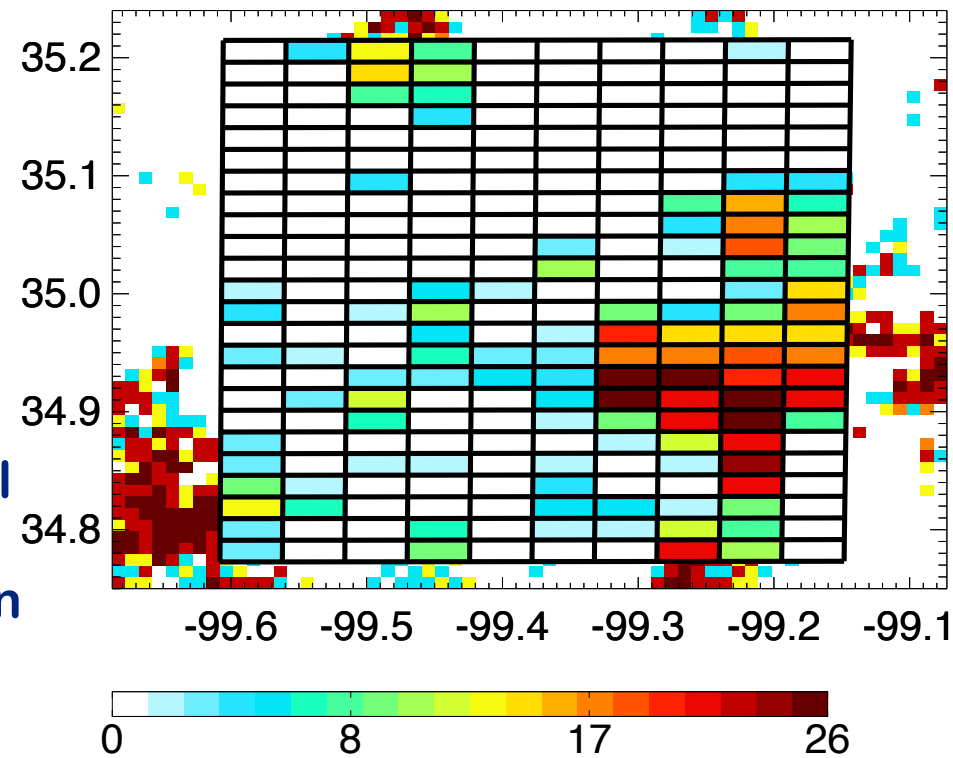
Cloud Column Optical Depth

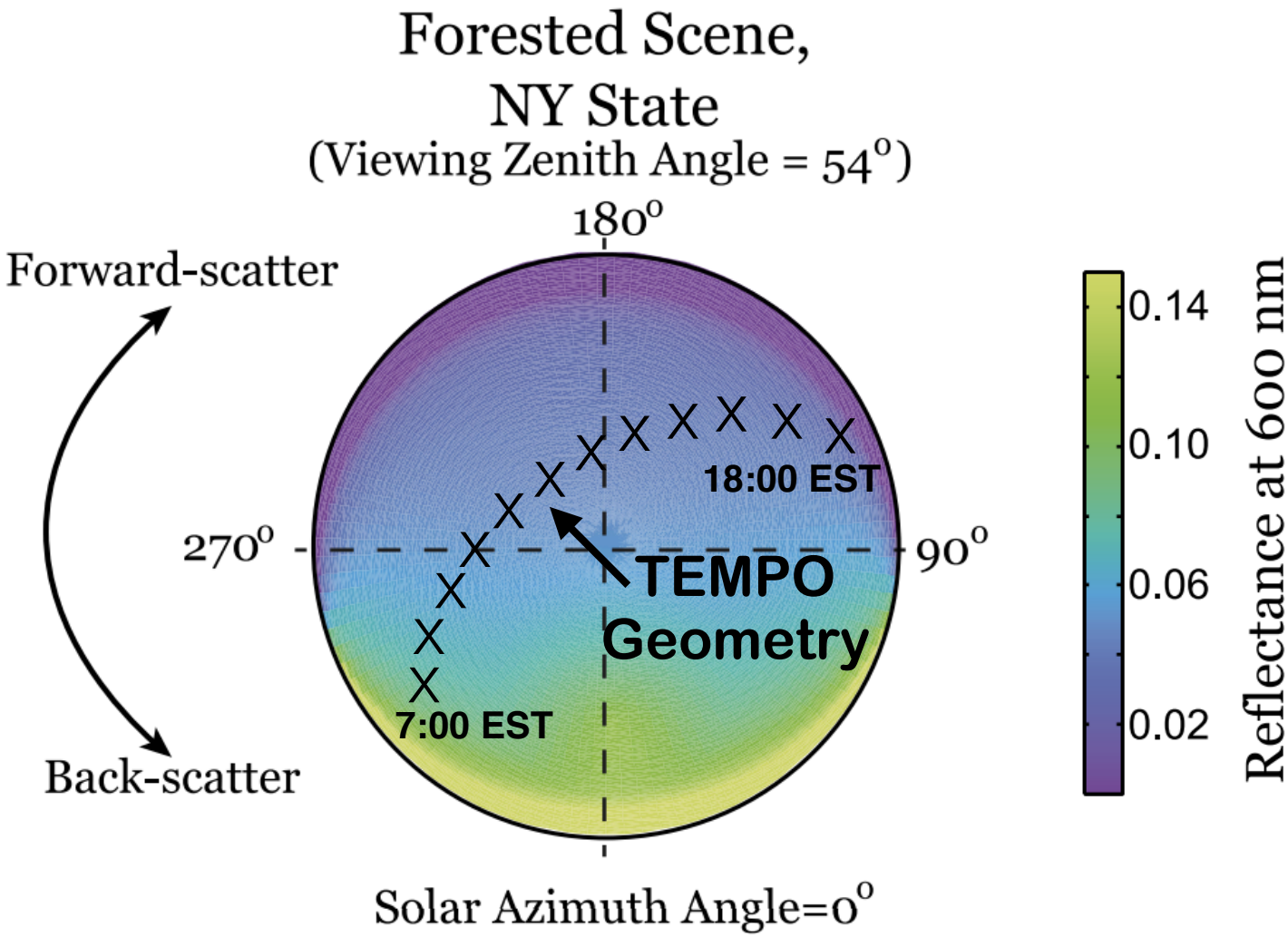


Sample clouds to TEMPO grid

Surface reflection

Snow Free Land	MODIS BRDF with EOF-Interpolation
Snow Covered Land/ Sea Ice	GISS GCM Snow parameterization
Ocean	Cox-Munk ocean BRDF

Diurnal variation in surface reflectivity



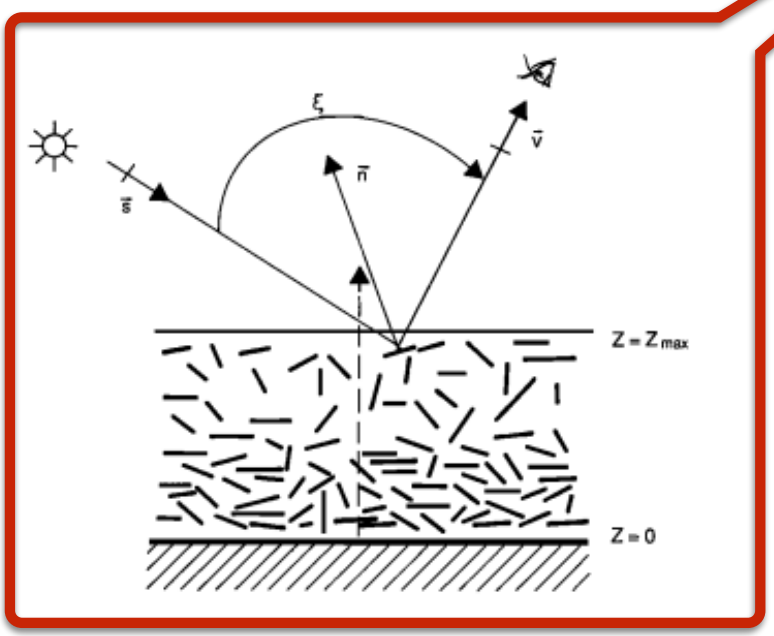
Zoogman et al. (2016)

Large variations over the course of a day

MODIS BRDF

MODIS uses a 3 Kernel BRDF approximation:

$$f_r(\lambda, \vec{\omega_i}, \vec{\omega_f}) = f_{iso}(\lambda) + f_{vol}(\lambda) K_{vol}(\vec{\omega_i}, \vec{\omega_f}) + f_{geo}(\lambda) K_{geo}(\vec{\omega_i}, \vec{\omega_f})$$



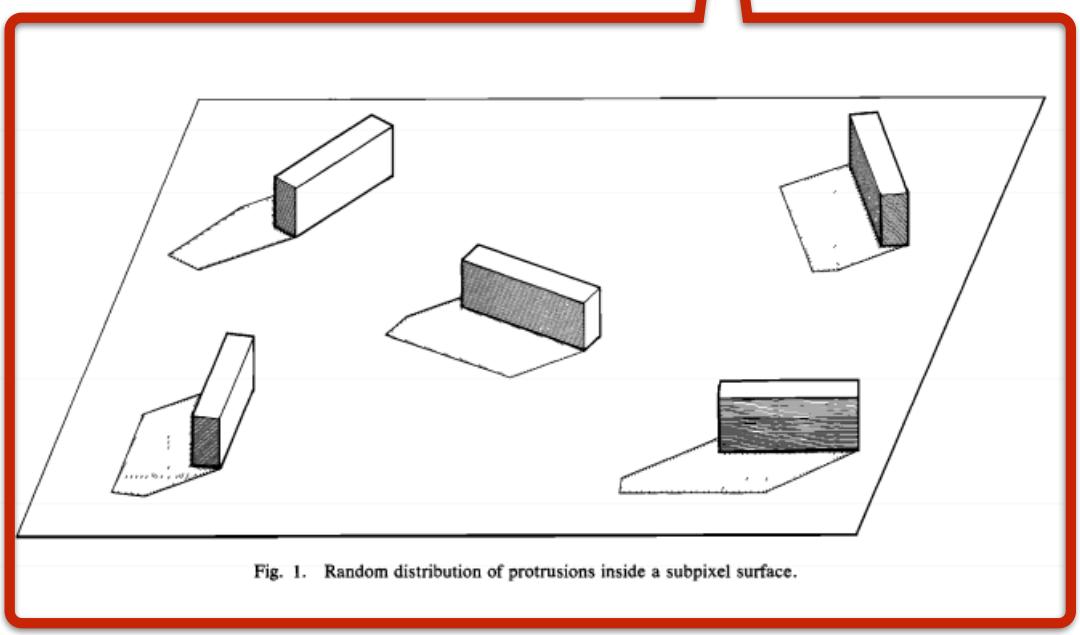
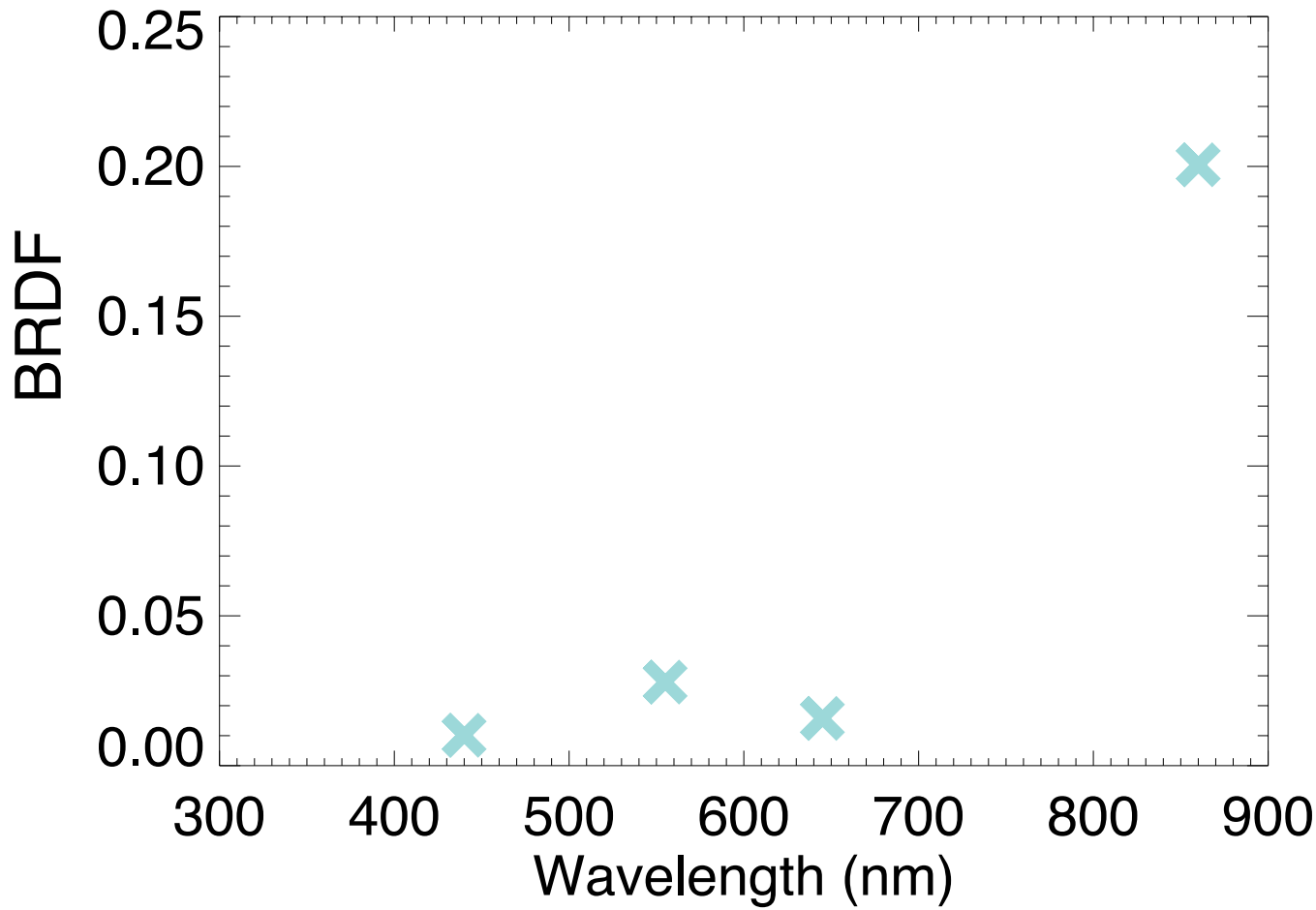


Fig. 1. Random distribution of protrusions inside a subpixel surface.

MODIS BRDF

Consider reflectance for one geometry (w_i,w_f):

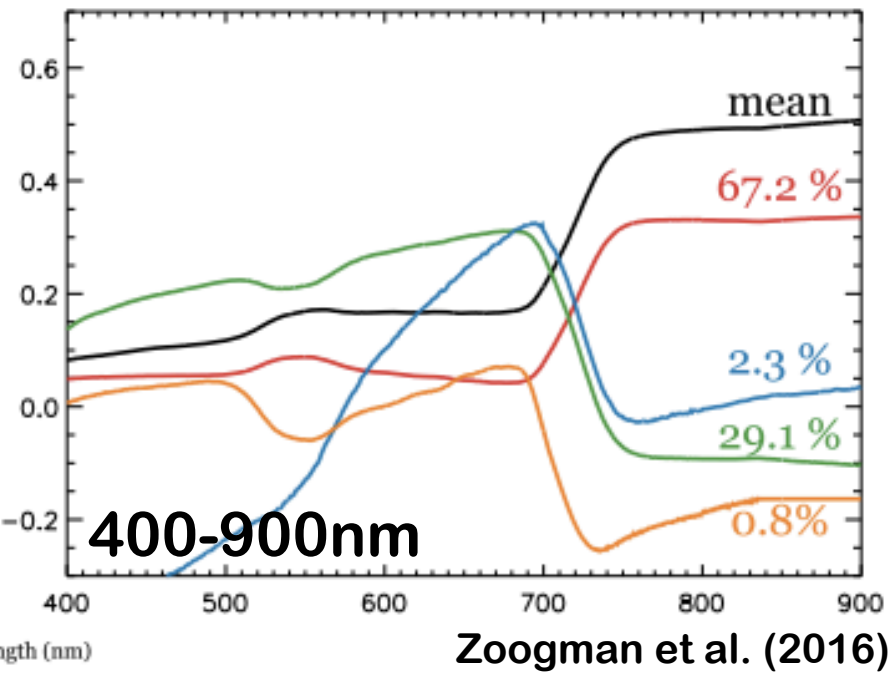
$$f_r(\lambda, \vec{\omega_i}, \vec{\omega_f}) = f_{iso}(\lambda) + f_{vol}(\lambda) K_{vol}(\vec{\omega_i}, \vec{\omega_f}) + f_{geo}(\lambda) K_{geo}(\vec{\omega_i}, \vec{\omega_f})$$



Issue - Sparse wavelength coverage

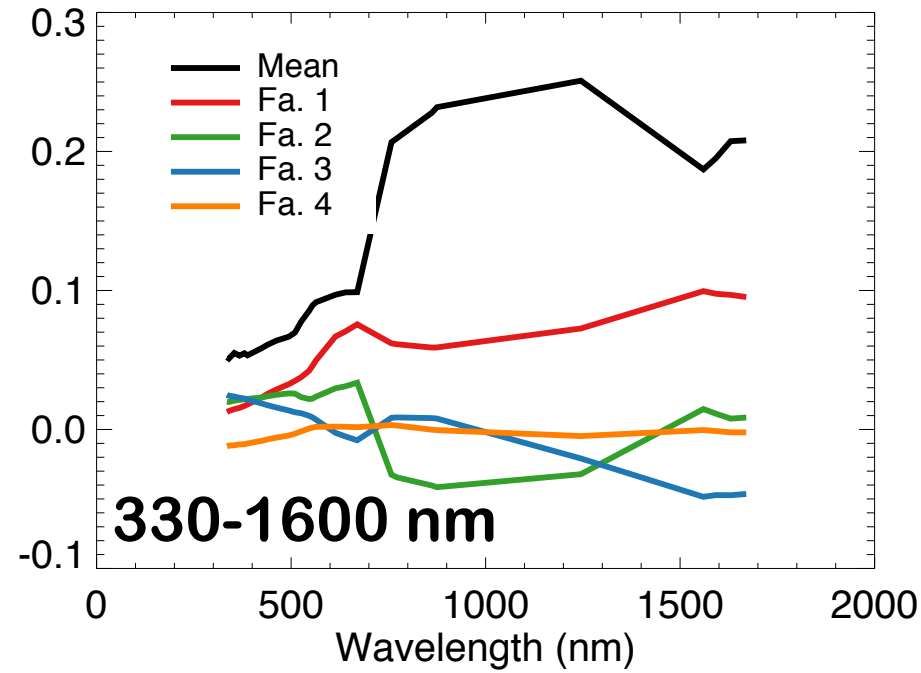
Decomposition of reflectance databases

EOFs derived from USGS/ASTER databases



Zoogman et al. (2016)

Factor loadings derived from snow free SCIAMACHY LER observations

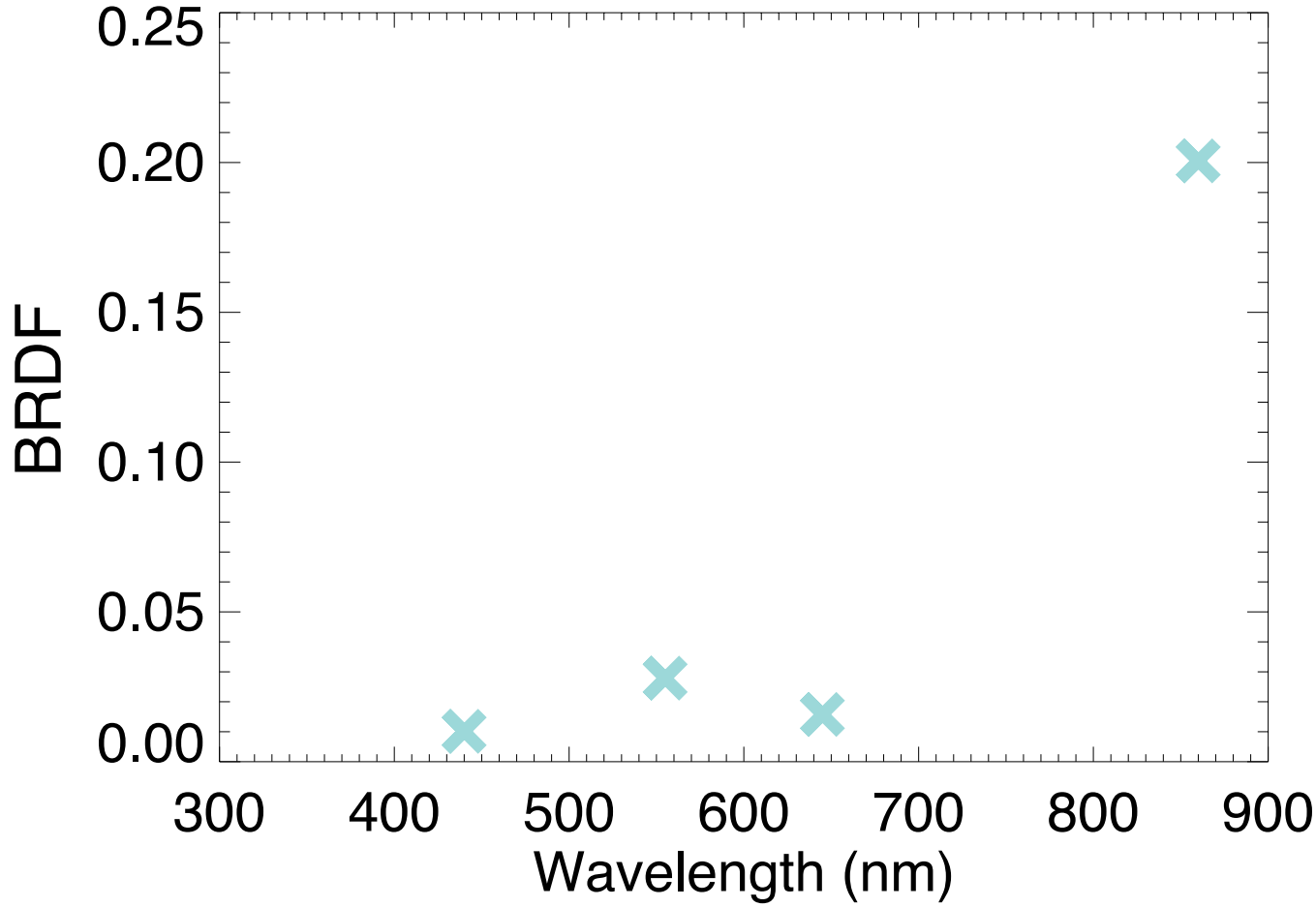


Tilstra et al. (2017)
Chan Miller et al. (In prep)

Both loading vectors can explain >99% of variability in their respective datasets

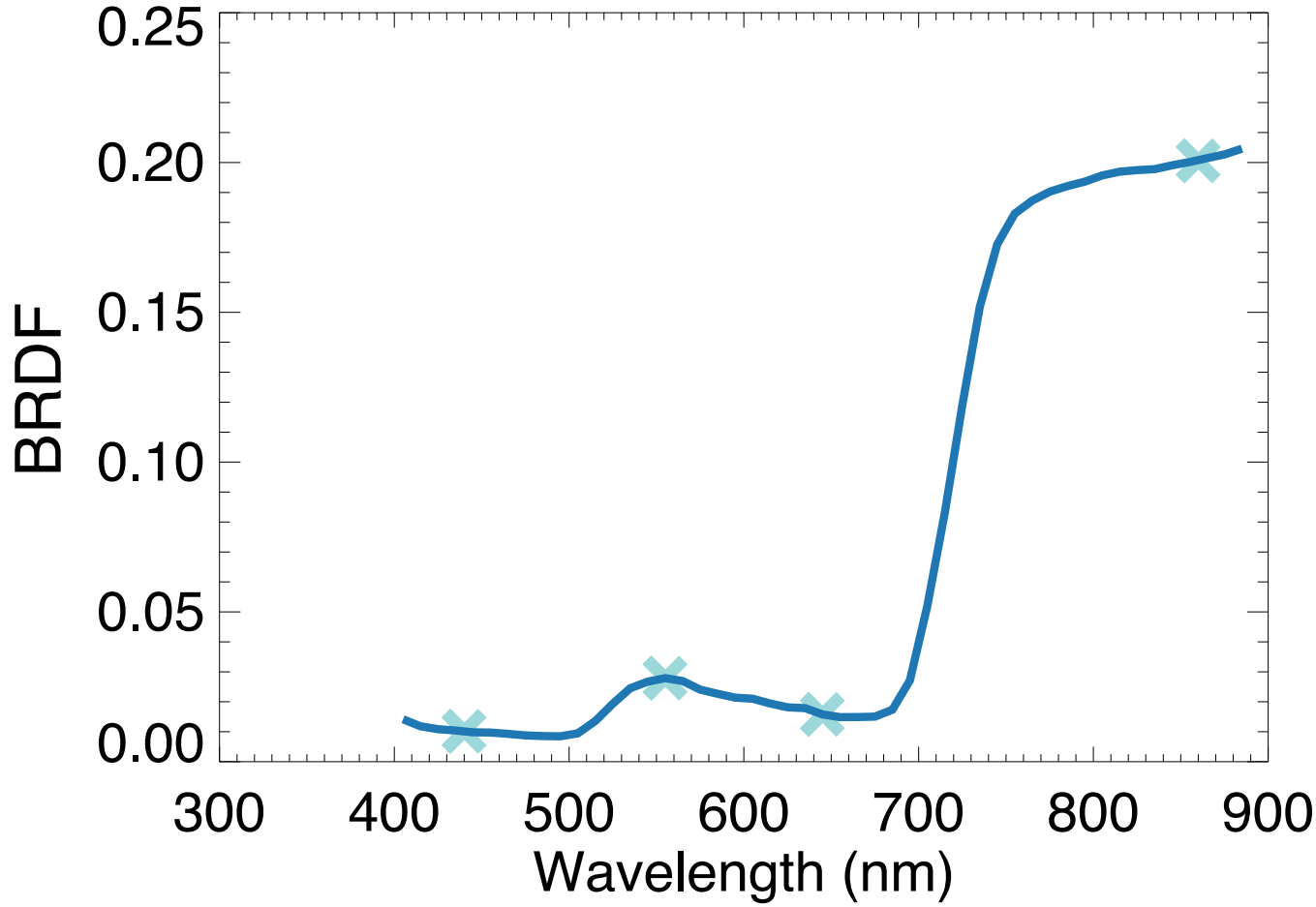
Interpolation of MODIS BRDF

Consider reflectance for one geometry(w_i,w_f):



Fitting EOFS

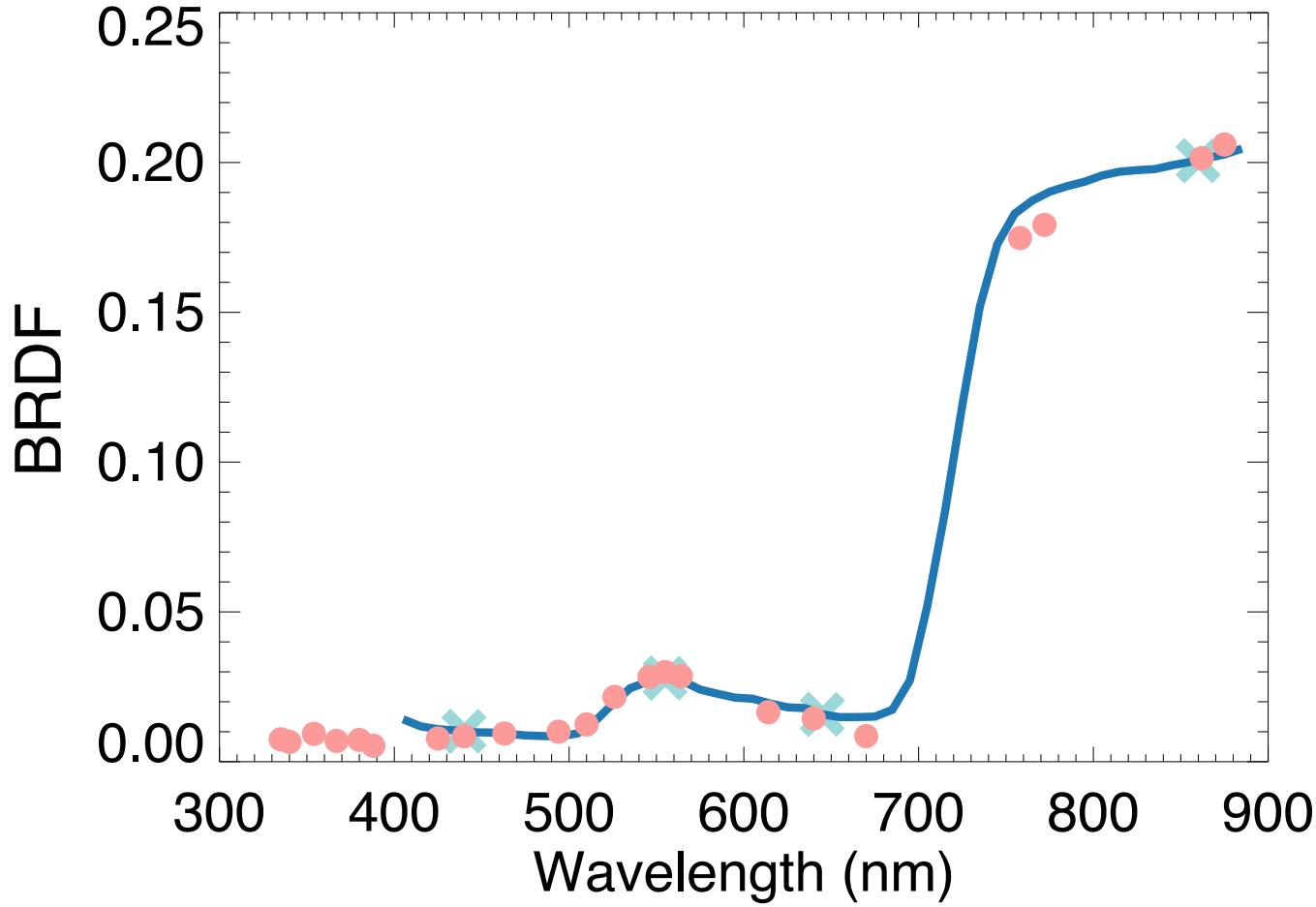
Consider reflectance for one geometry(w_i,w_f):



Fit database EOFs (Zoogman et al.) over 400-900 nm

Fitting EOFS

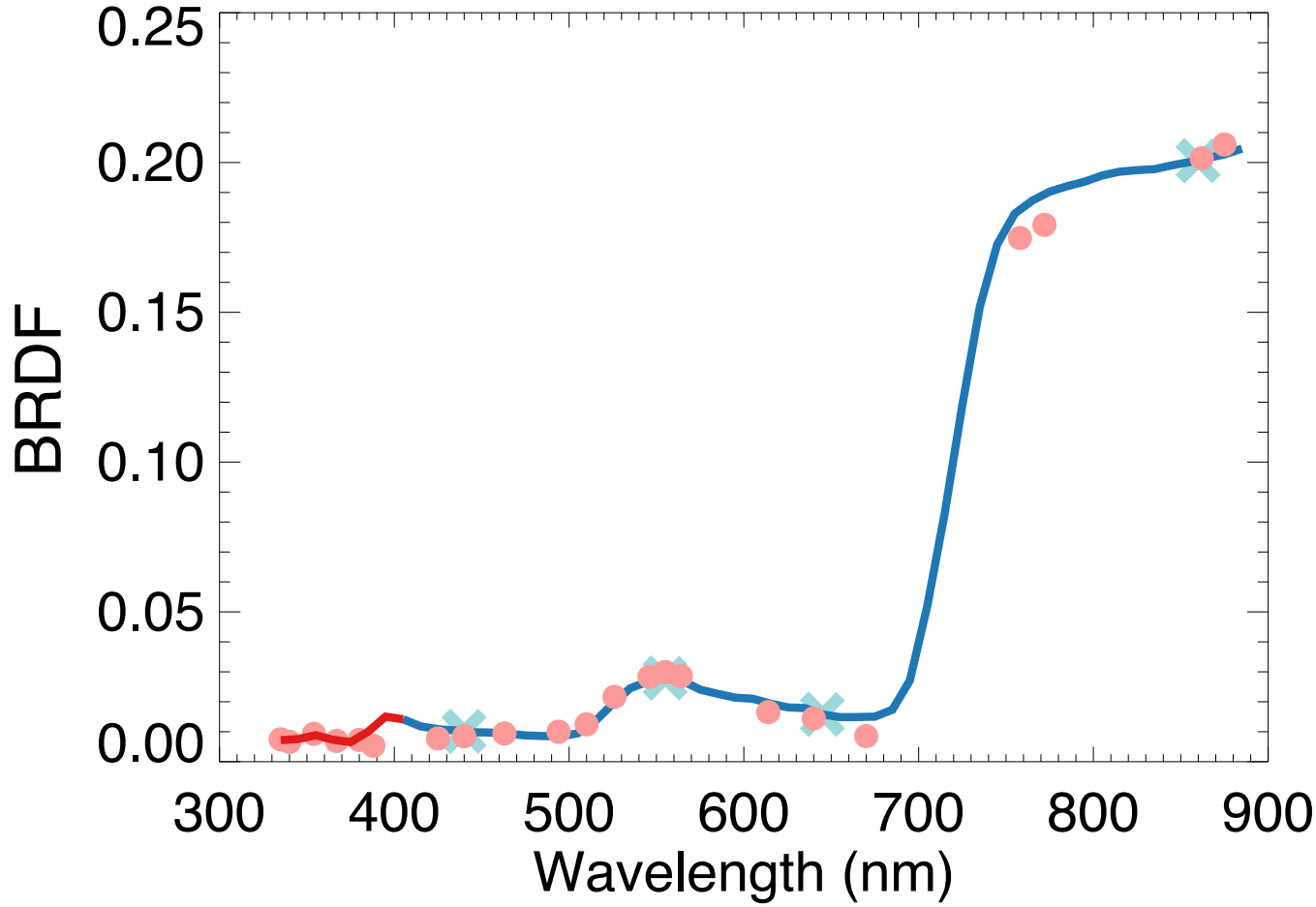
Consider reflectance for one geometry(w_i,w_f):



Perform least squares fit of SCIAMACHY factor loadings between 400 - 900 nm to predict reflectances < 400 nm

Fitting EOFS

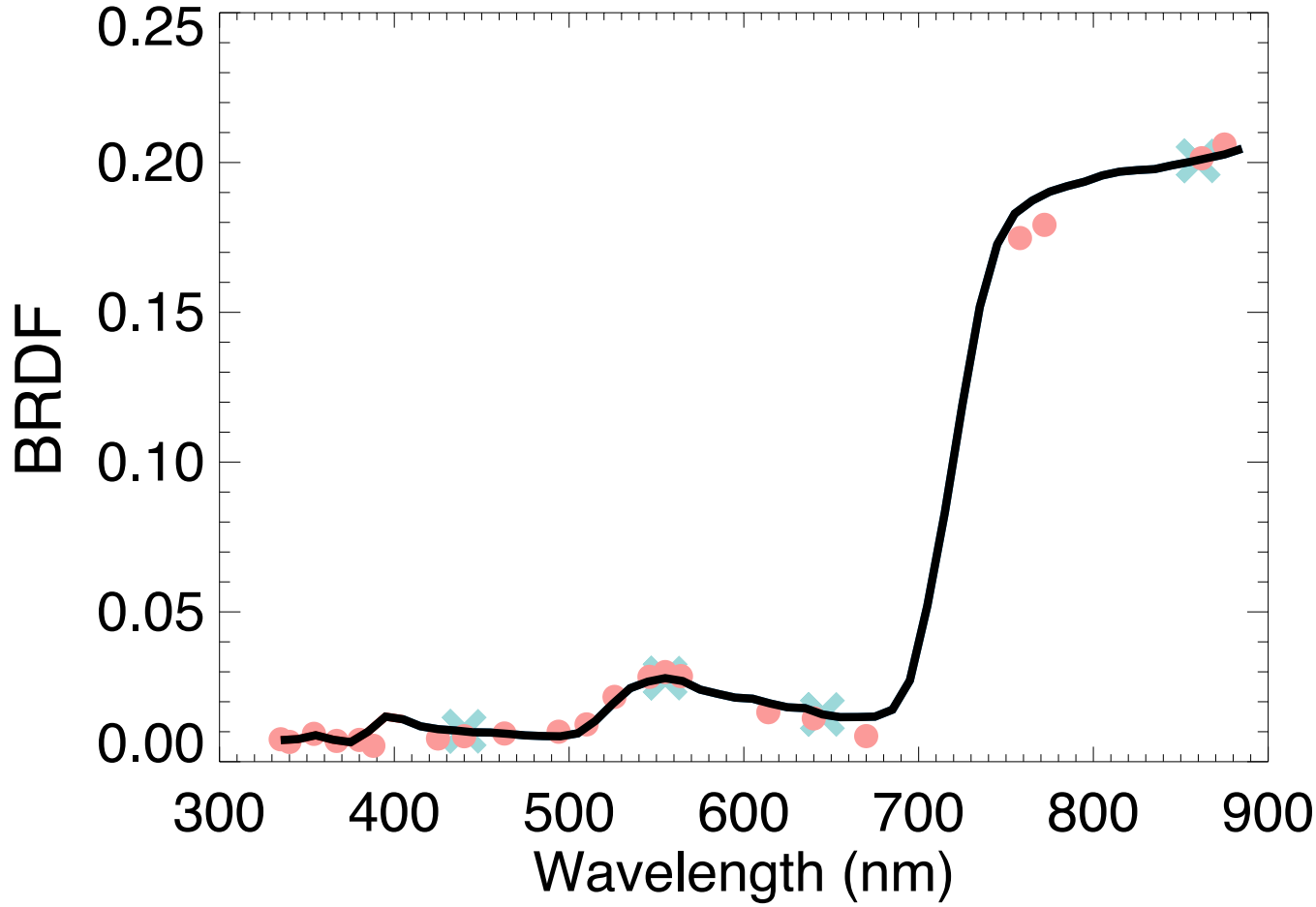
Consider reflectance for one geometry(w_i,w_f):



Interpolate values below 400nm using a smoothed spline to reduce potential discontinuity at 400nm

Fitting EOFS

Consider reflectance for one geometry(w_i,w_f):



Interpolate values below 400nm using a smoothed spline to reduce potential discontinuity at 400nm

The synthetic view from TEMPO

Courtesy of J. Carr

Thank you!

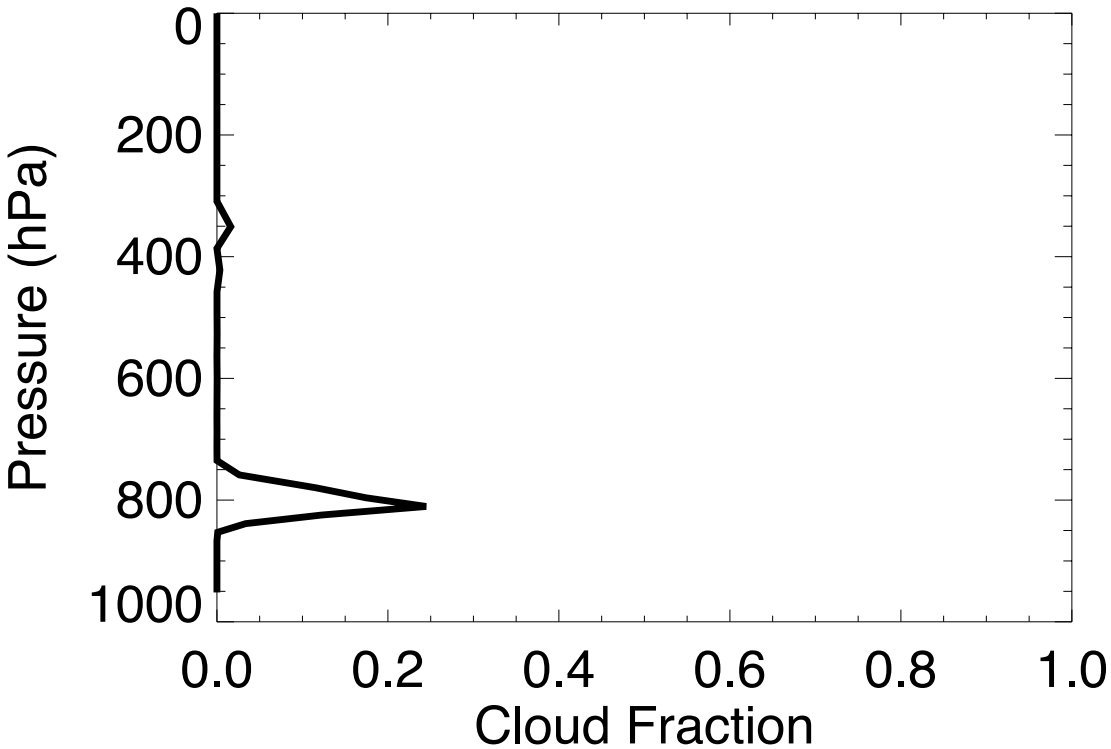
Future improvements

- RRS approximation using VLIDORT jacobians
- Chlorophyll fluorescence
- Liquid Water + Chlorophyll Absorption in ocean
- More trace gases - HONO, OCIO, IO, Methylglyoxal, ….

Requests?

EXTRA SLIDES

MRAN Stochastic column generator



(1) Sample 3 numbers from a uniform distribution corresponding to the cloud layers

$$r_l, r_m, r_h \sim \mathcal{U}(0,1)$$

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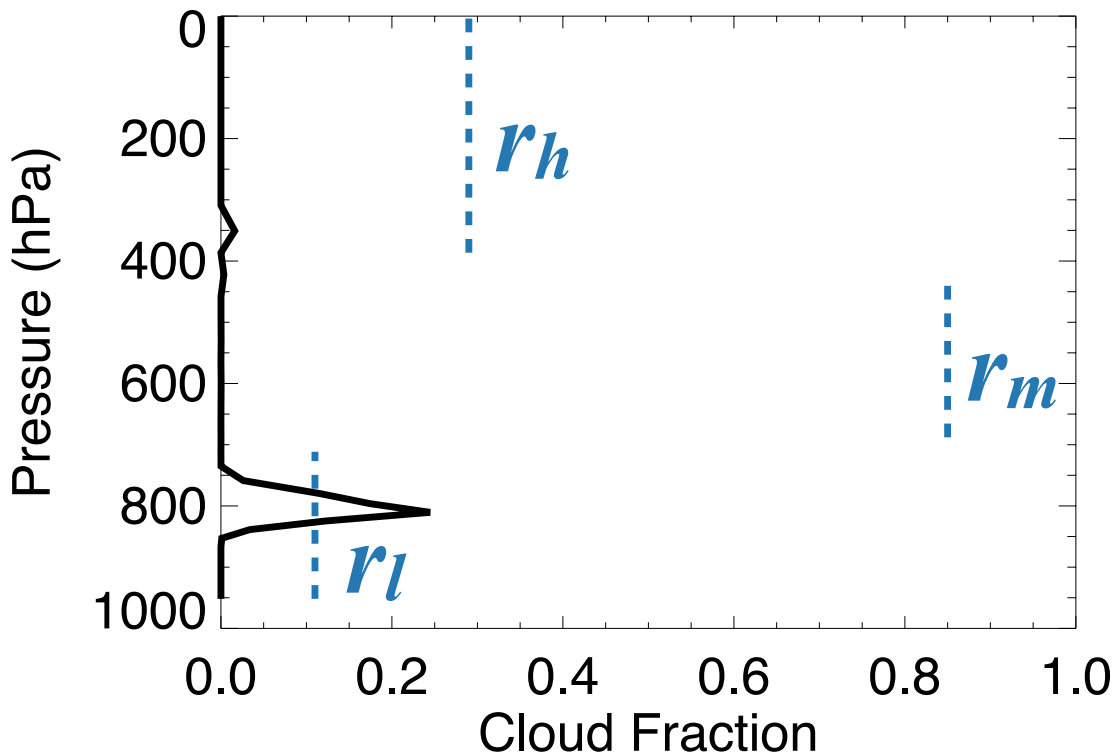

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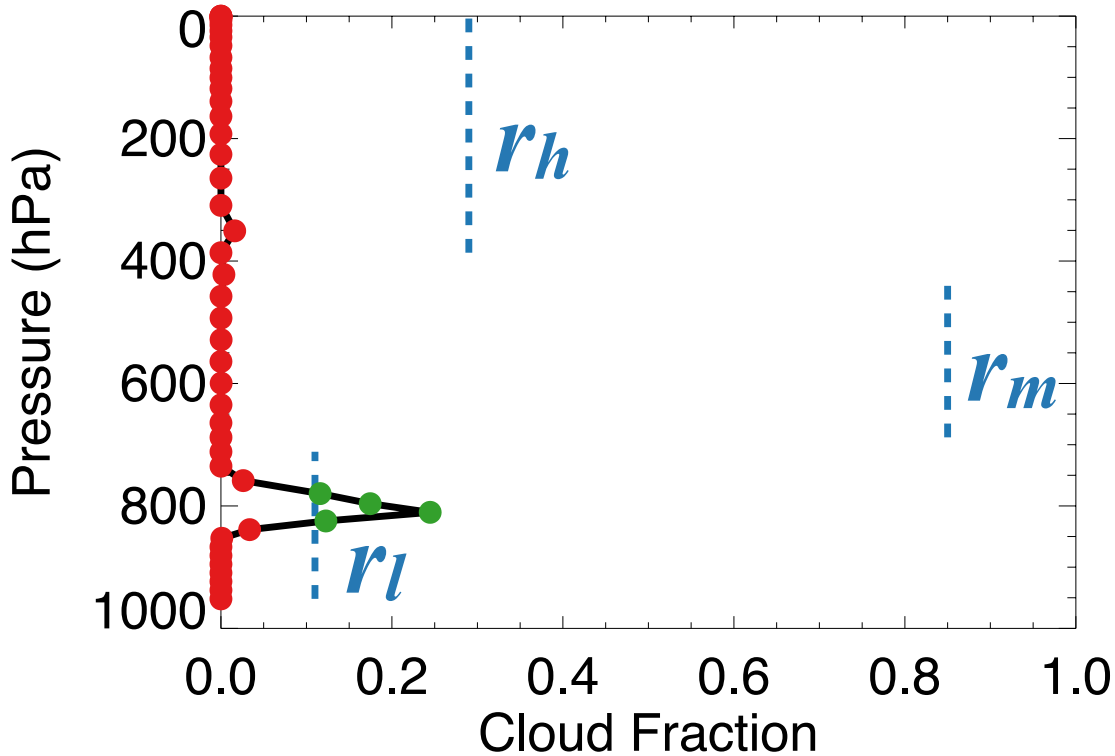
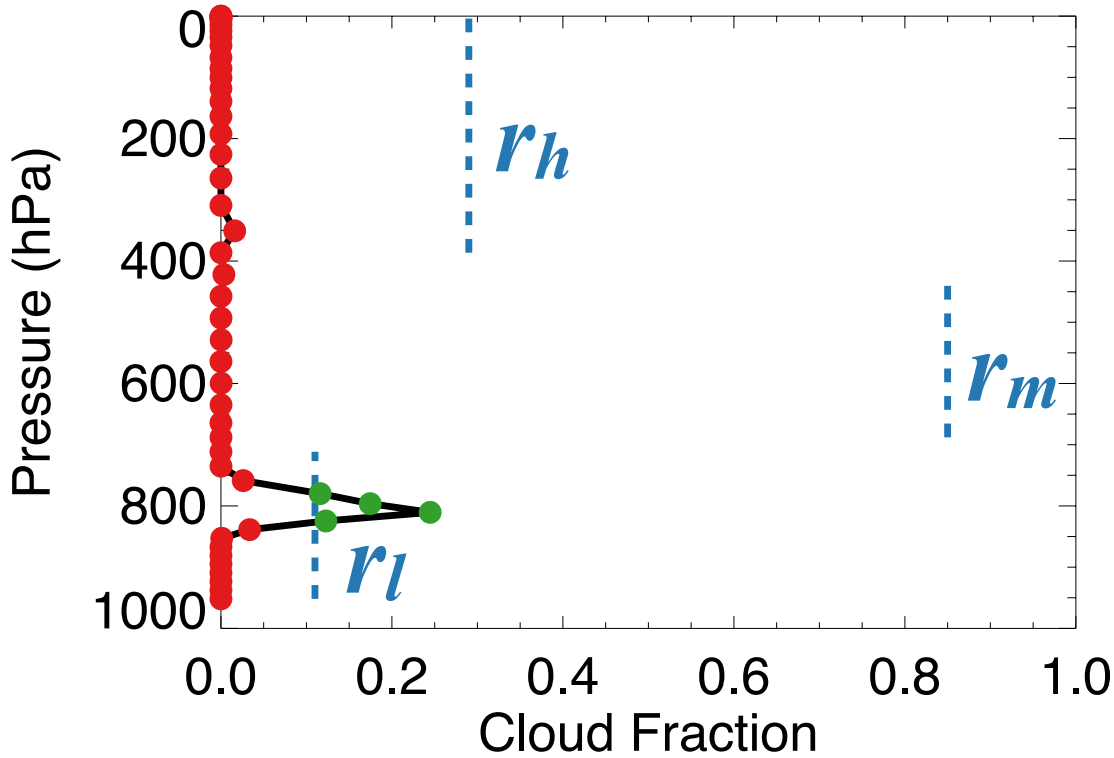
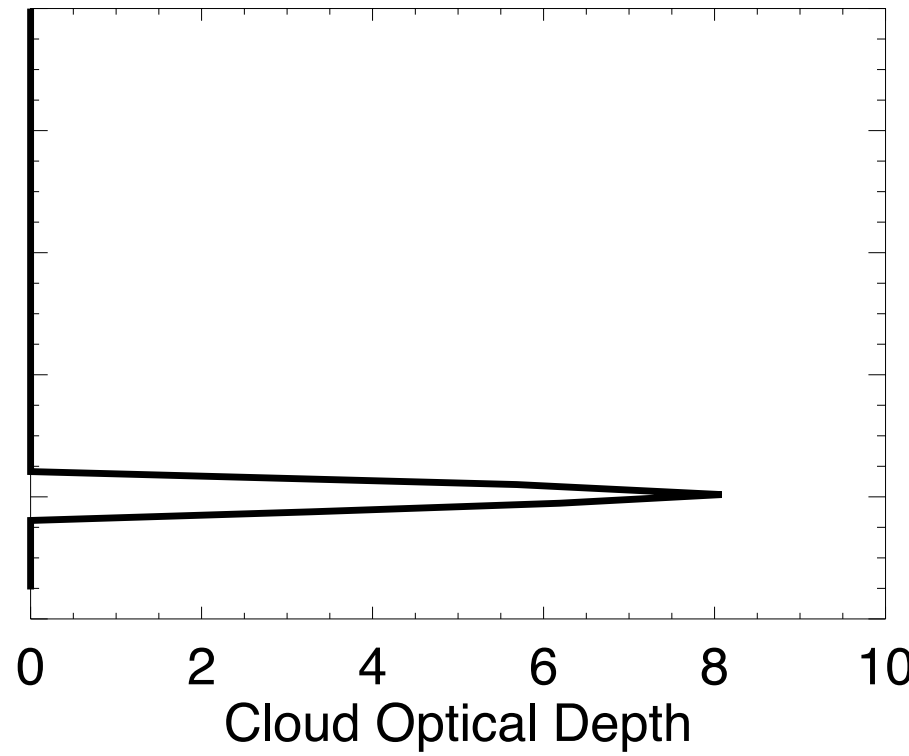


(2) Layer is cloudy if cloud fraction > r

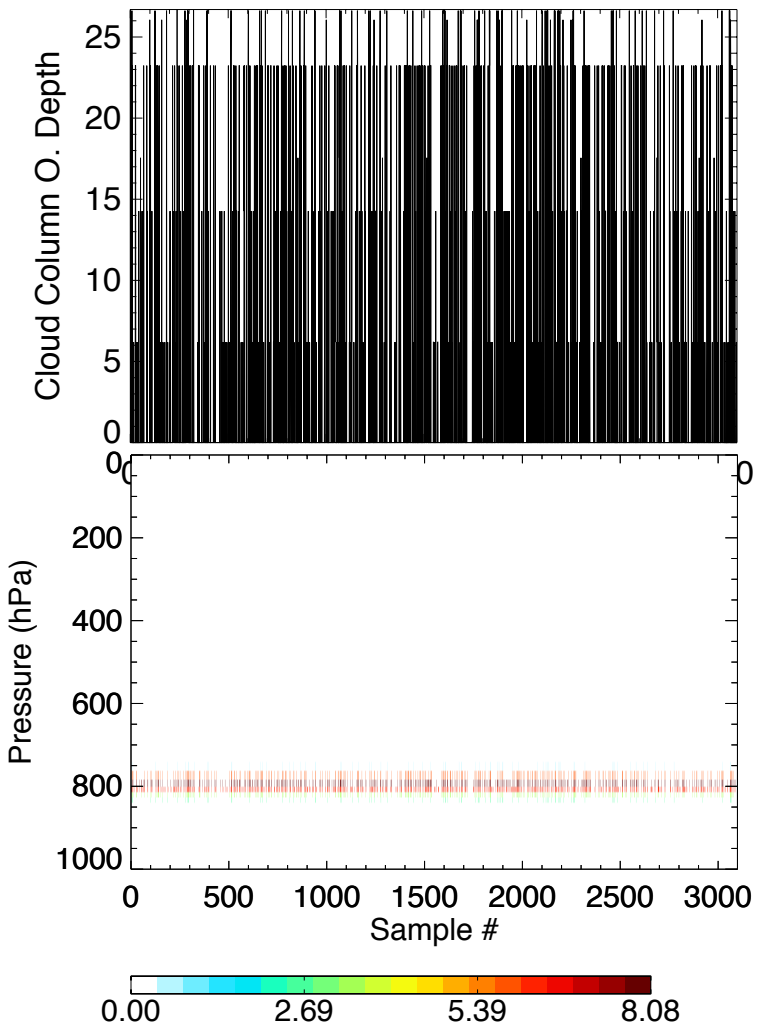
MRAN Stochastic column generator

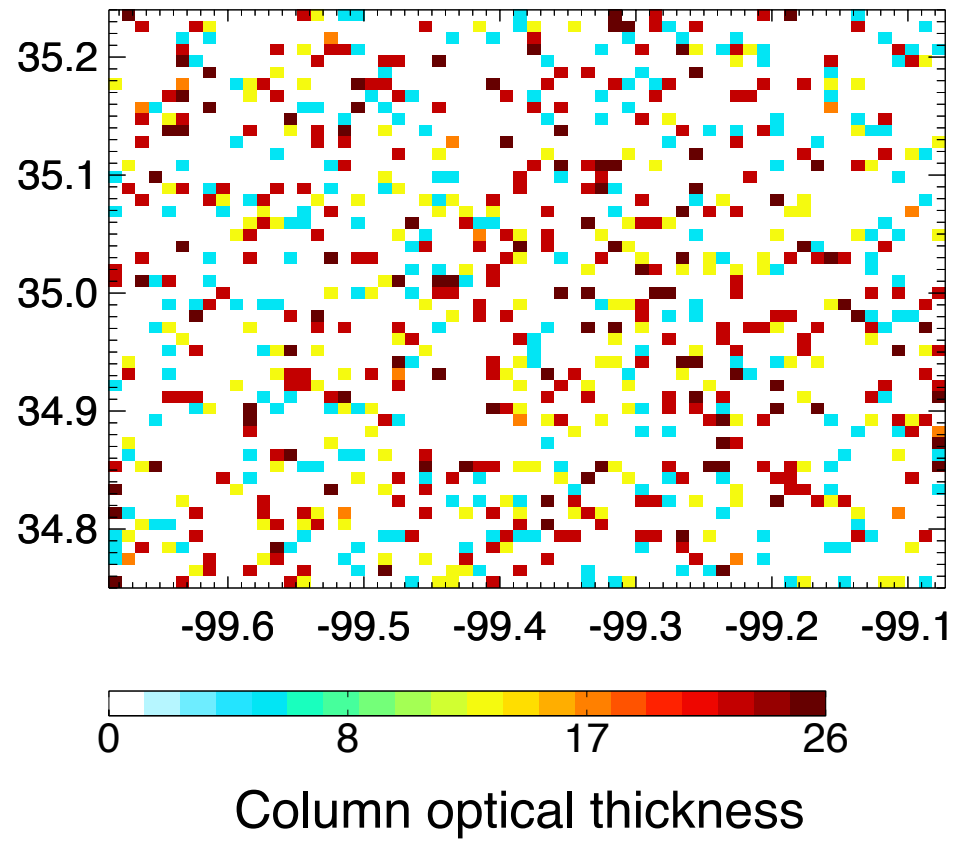




(3) Sample cloud optical depths for layers classified as cloudy

Stochastic column generation

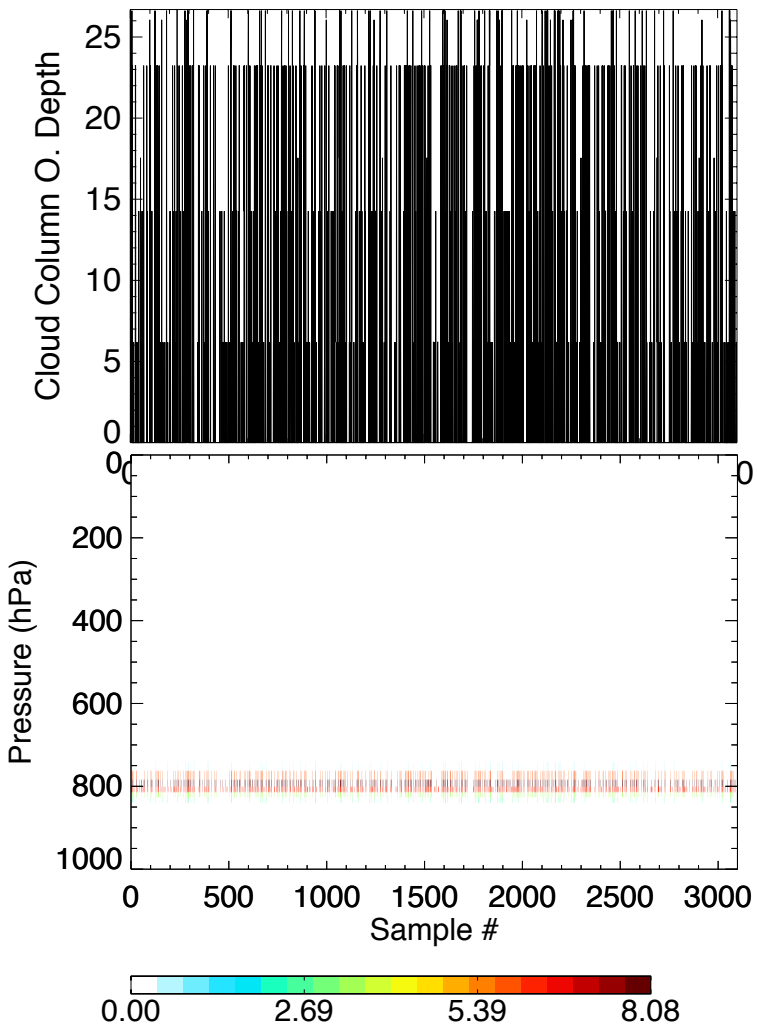


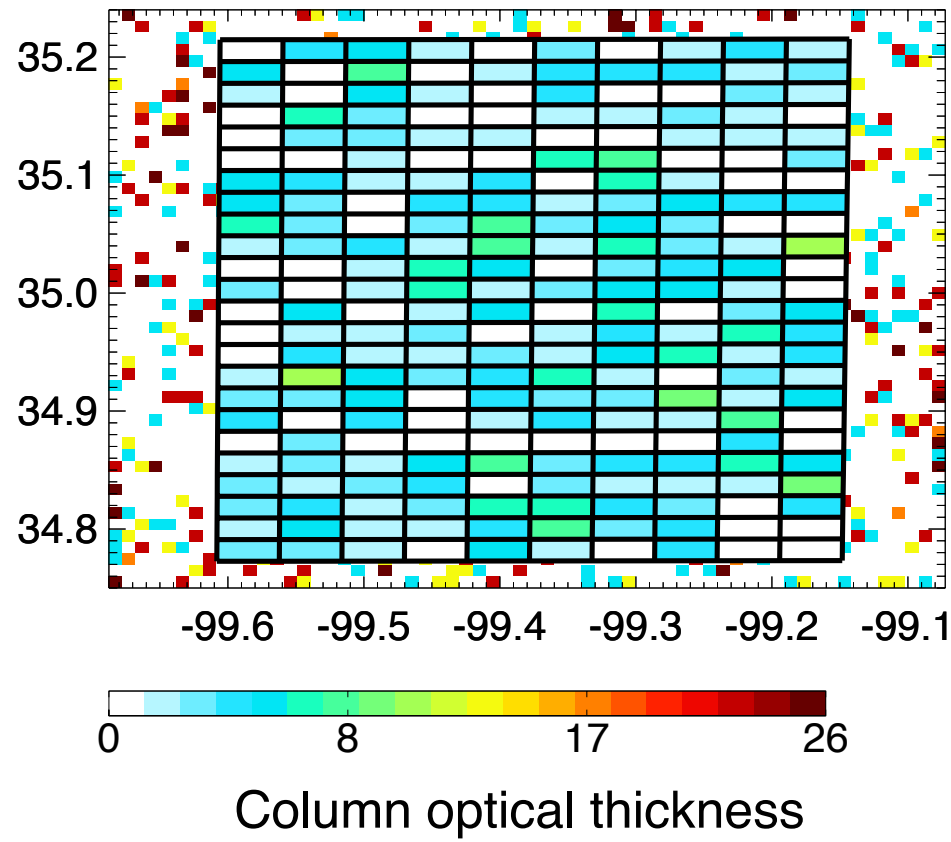


(1) Generate cloud subcolumns using stochastic column algorithm with MRAN assumption

(2) Distribute on 0.1x0.1 sub grid

Stochastic column generation

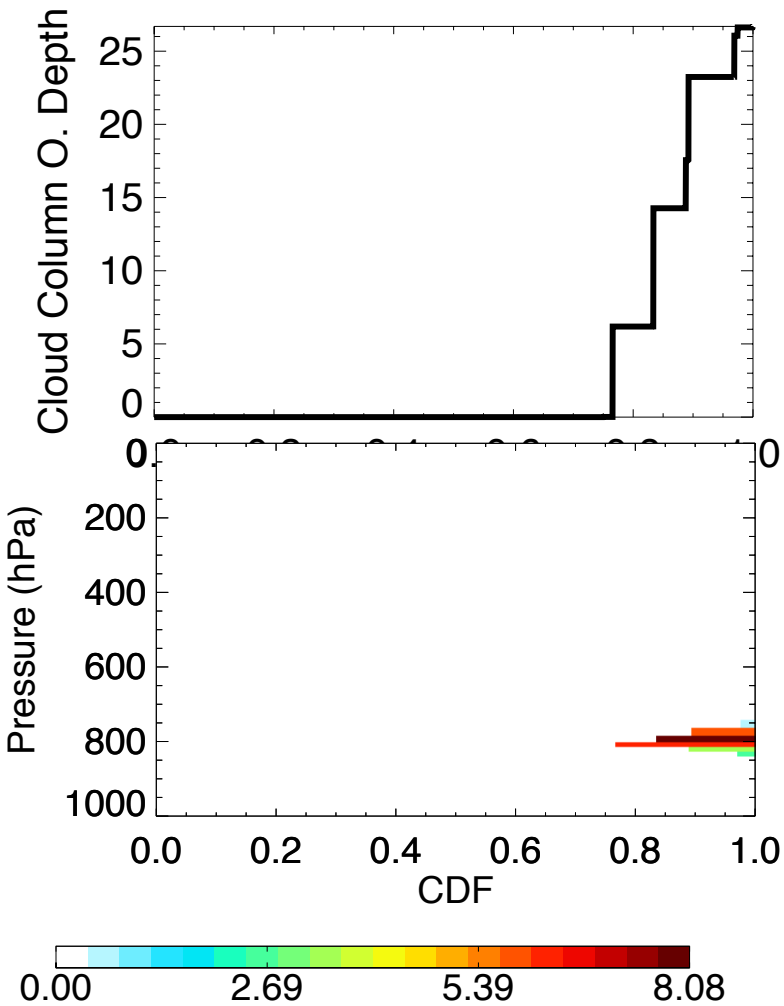




(3) Sample columns for each TEMPO pixel

NB - This implicitly assumes no spatial correlation between pixels on the downscaled grid - and likely underestimates the fraction of clear TEMPO pixels

Stochastic column generation



(1) Sort columns by optical depth to create marginal CDF

Wind et al. (2013)

Downscaled grid

x_7	x_8	x_9
x_4	x_5	x_6
x_1	x_2	x_3

$$\vec{x} \sim \mathcal{N}(\vec{0}, \mathbf{S})$$

Distance between xi and xj

$$S_{i,j} = \exp\left(-\frac{d_{i,j}}{d_c}\right)$$

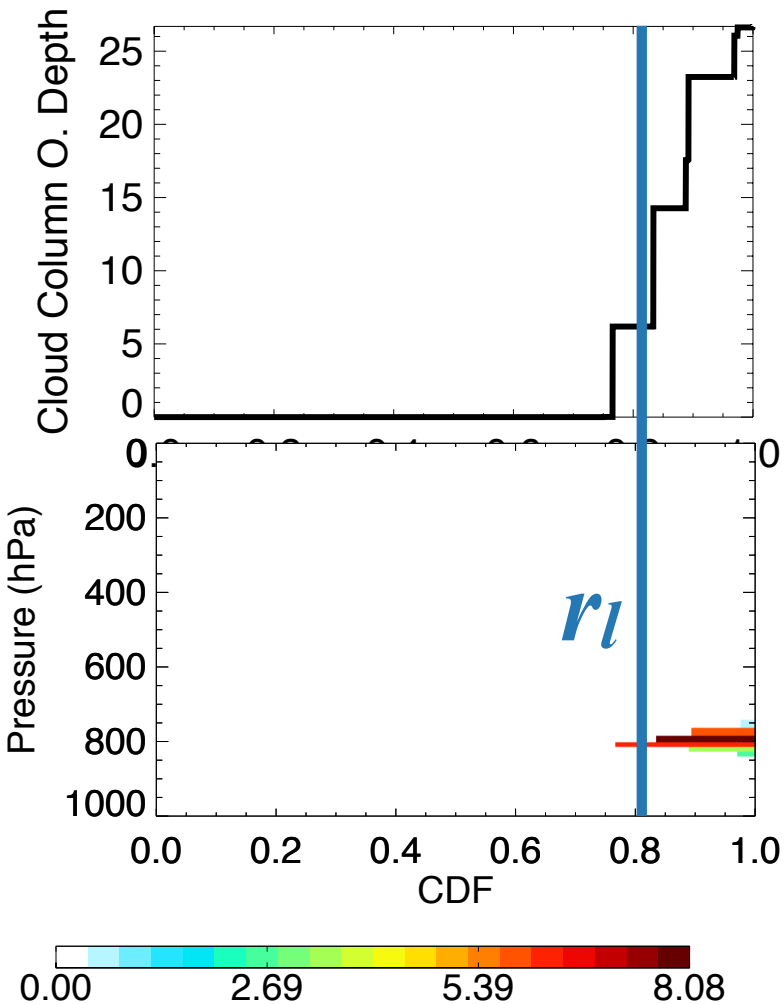
Correlation length scale

(2) Use gaussian copula to specify relationship between cloud fields

$$r_i = \frac{1}{2}(1 + \mathrm{erf}(\frac{x_i}{\sqrt{2}})) \qquad r_i \in [0, 1]$$

(3) Compute inverse transform for each x_i and sample marginal CDF

Stochastic column generation



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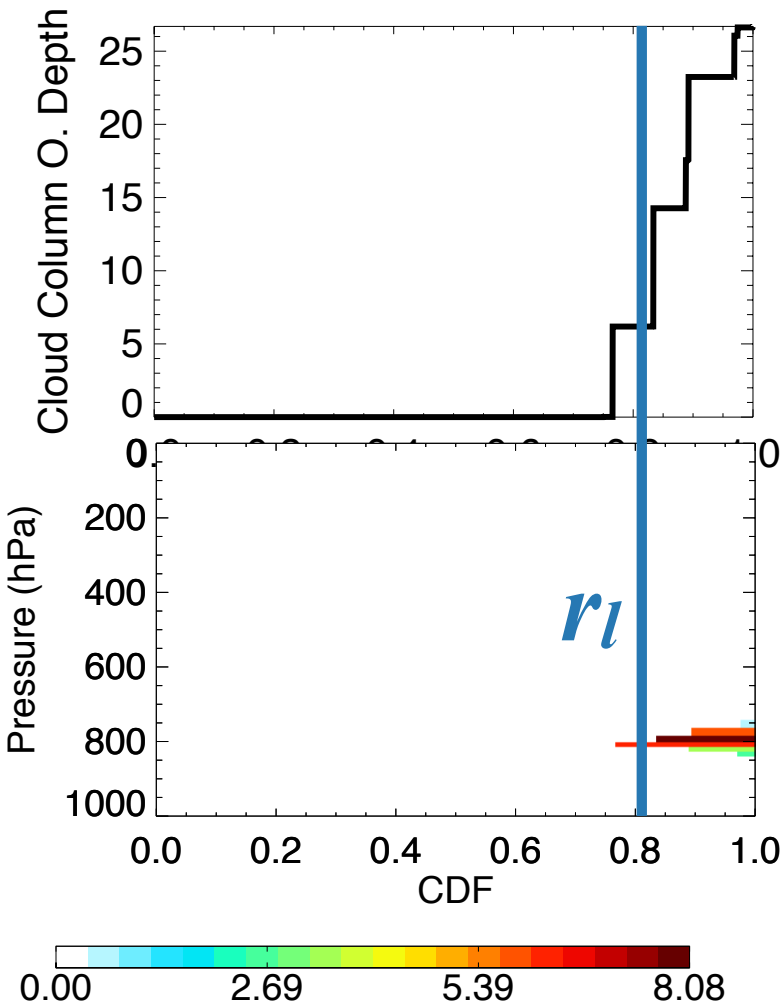

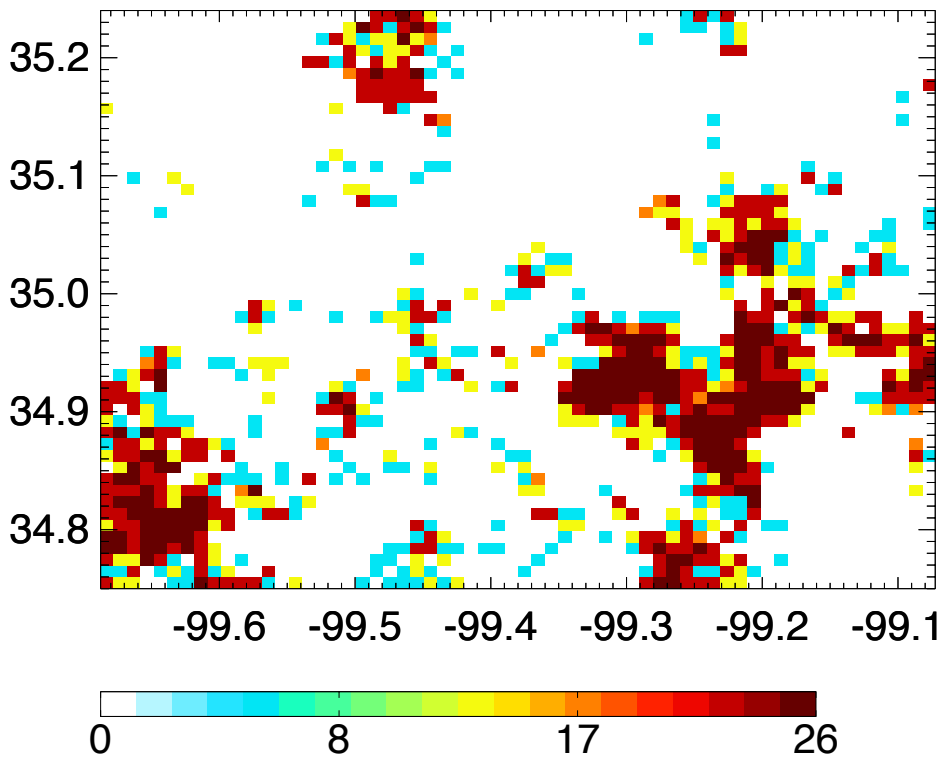

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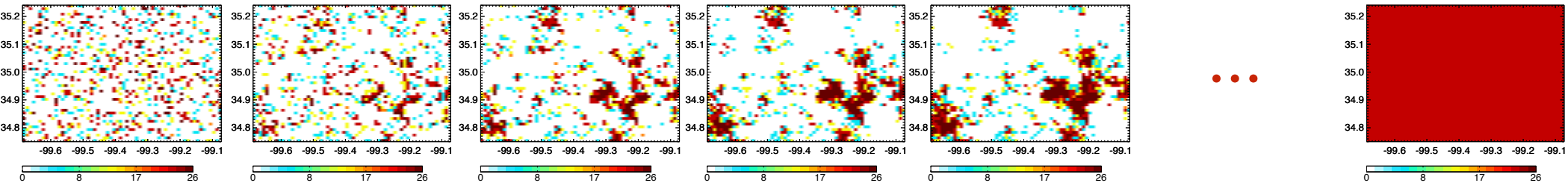
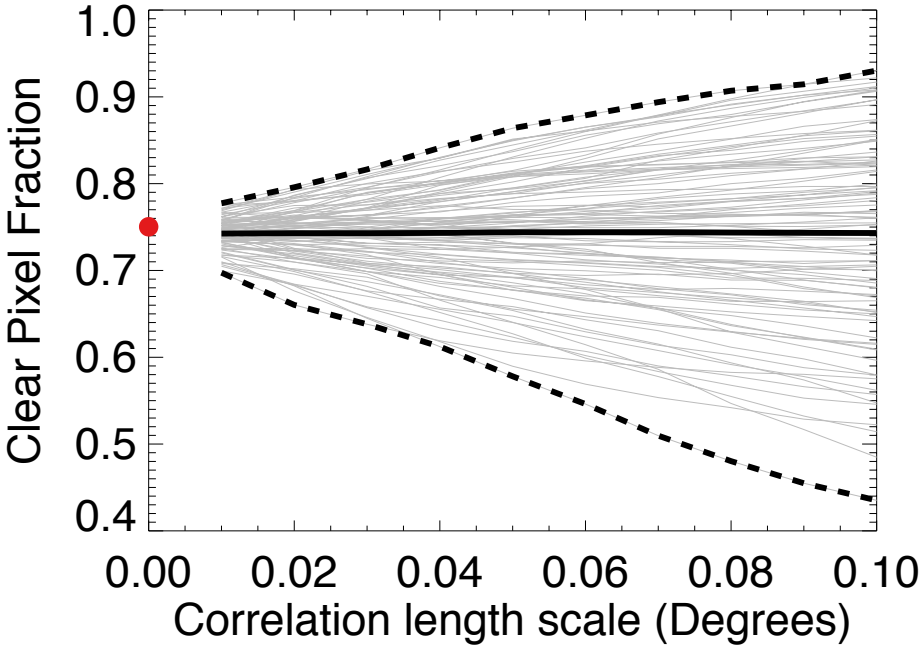
Effect of correlation length scale

d=0

d=\inf





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