kCARTA : Fast pseudo line-by-line Radiative Transfer Algorithm for Allsky Infrared Sounding

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Outline

- Motivation
- Line-by-Line codes (eg monoRTM, UMBC-LBL) *many minutes/hours*
- Pseudo Line-by-Line codes (eg kCARTA, LBLRTM, σ-IASI) *seconds to minutes*
- Fast Codes (eg SARTA, PCRTM, OSS) *milliseconds*
  - Flux (OLR) codes eg RRTM, ecRad *milliseconds*
- Applications (Weather and climate)
- Conclusions

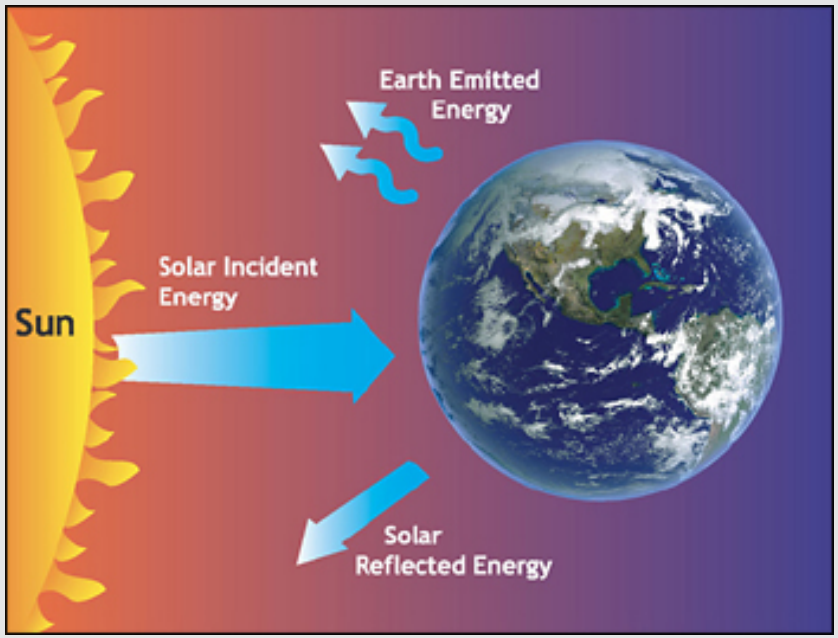
Motivation

- New generation sounders : low noise, high spectral resolution sounders
  - NASA Atmospheric Infrared Sounder (AIRS) 09/2002-
  - ESA Infrared Atmospheric Sounding Interferometer (IASI) 06/2007-
  - NOAA Cross Track Infrared Sounder (CrIS) 03/2012-
- Designed to make observations for Numerical Weather Prediction
  - long/overlapping timespans allow for 40+ year record for climate studies
- Need fast, accurate RTA to fully exploit millions of daily observed radiances
  - accurate spectroscopy
    - ⋆ latest line parameters eg HITRAN or GEISA databases
    - ⋆ accurate lineshapes : voigt or line mixing or ....
  - accurate radiative transfer : clear sky or allsky
  - esoteric needs (Non-Local Thermodynamic Equilibrium) NLTE
  - jacobians for retrievals
  - flux calculations for Outgoing Longwave Radiation (OLR) studies

Two Temperatures to describe Sun-Earth

Sun provides our energy

Earth Radiation budget balances incoming (shortwave) solar and outgoing terrestrial (longwave) radiation

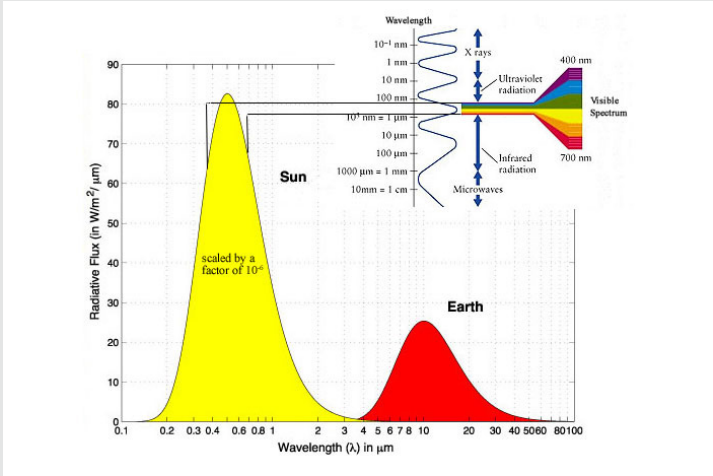


T_{sun}, T_{earth}

$$P_{in} = \sigma A_{sun} T_{sun}^4 = f 4\pi r_{sun-earth}^2$$

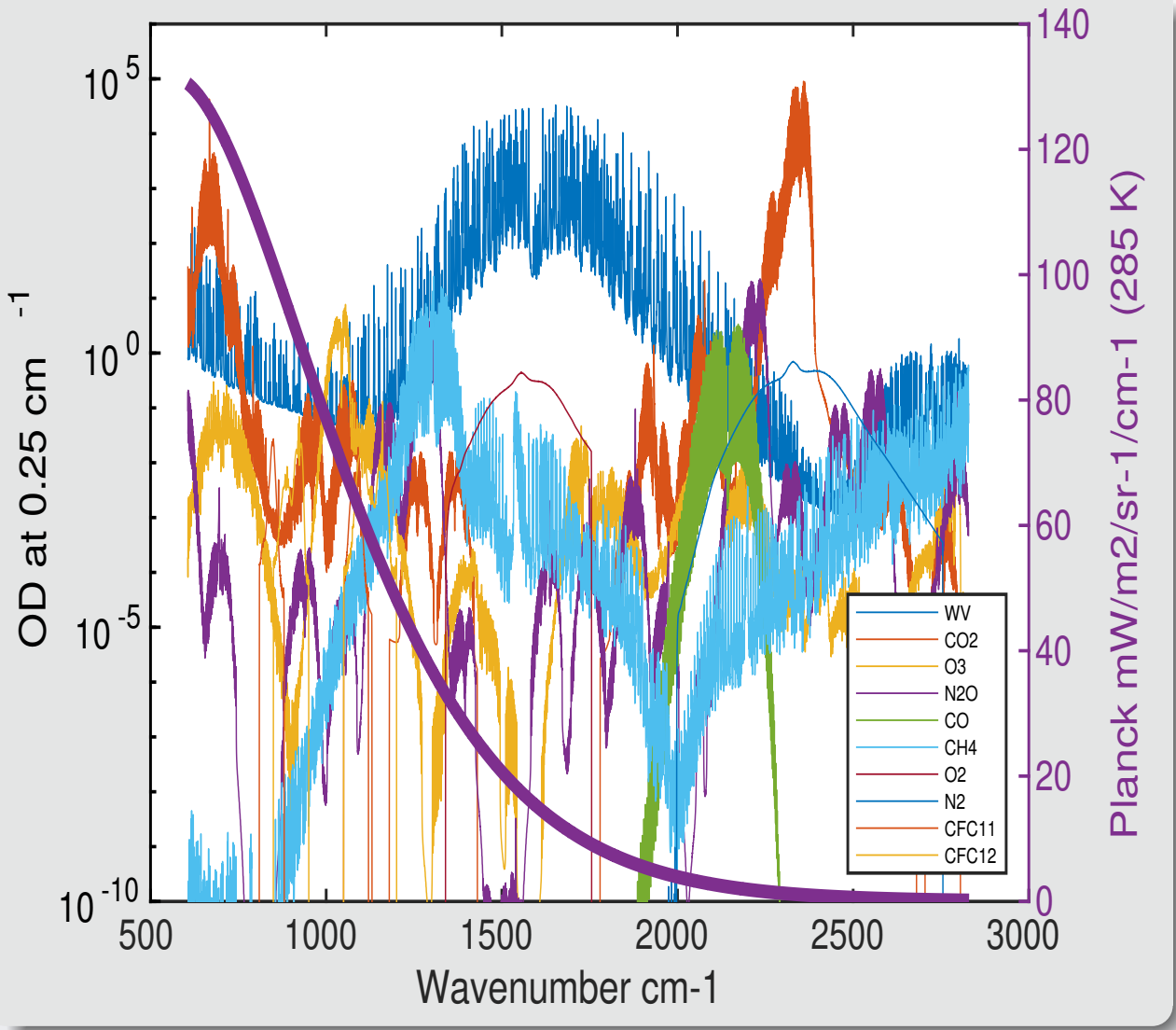
$$P_{out} \rightarrow f \pi R_{earth}^2 (1 - a) = 4\pi R_{earth}^2 \sigma T_{earth}^4$$

$T_{sun} = 5600$ K $T_{earth}^{radiating} = 255$ K
$T_{earth}^{surface} = 285$ K $f = 1360$ W/m2 at TOA



Importance of the infrared to studying Earth Atmosphere

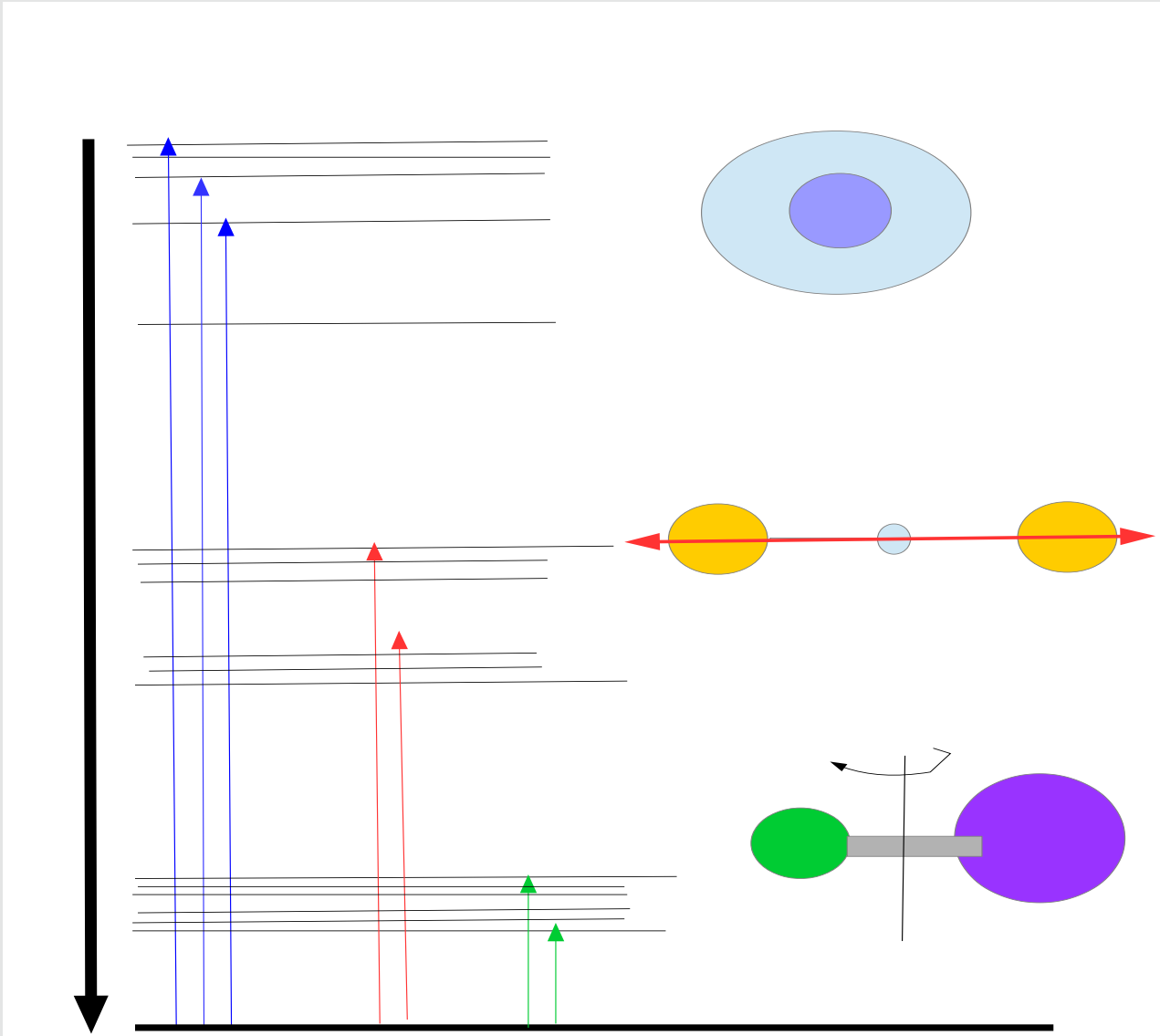
- Terrestrial Planck function peaks in infrared $\rightarrow$ OLR studies
- Greenhouse Gases (GHG) such as H_2O, CO_2, O_3, CH_4, CFCs have spectral signatures; also have temperature effects
- Clouds & large aerosols ($\geq 4\ \mu m$) impact infrared, 24/7
- Radiative Transfer Equation : height sensitivity



Spectroscopy

https://asl.umbc.edu/pub/packages/lbl.pdf

Simple Energy Level Sketch



Simple models

Electronic

VISIBLE

$\frac{1}{\lambda} = R(\frac{1}{n_2} - \frac{1}{m^2})$

Vibrational

INFRARED

$E_n = (n + \frac{1}{2})h\nu$

Rotational

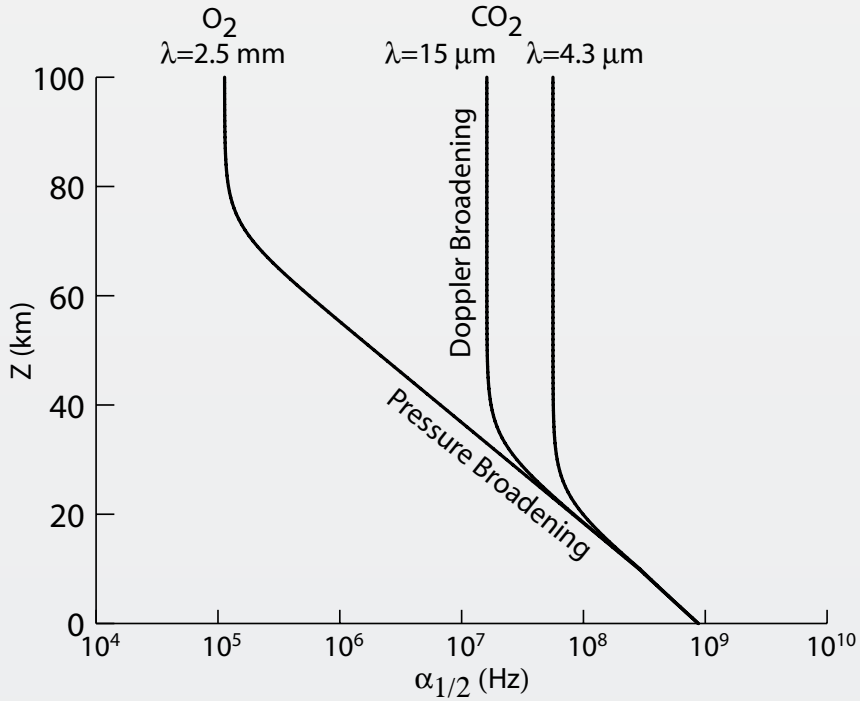
MICROWAVE

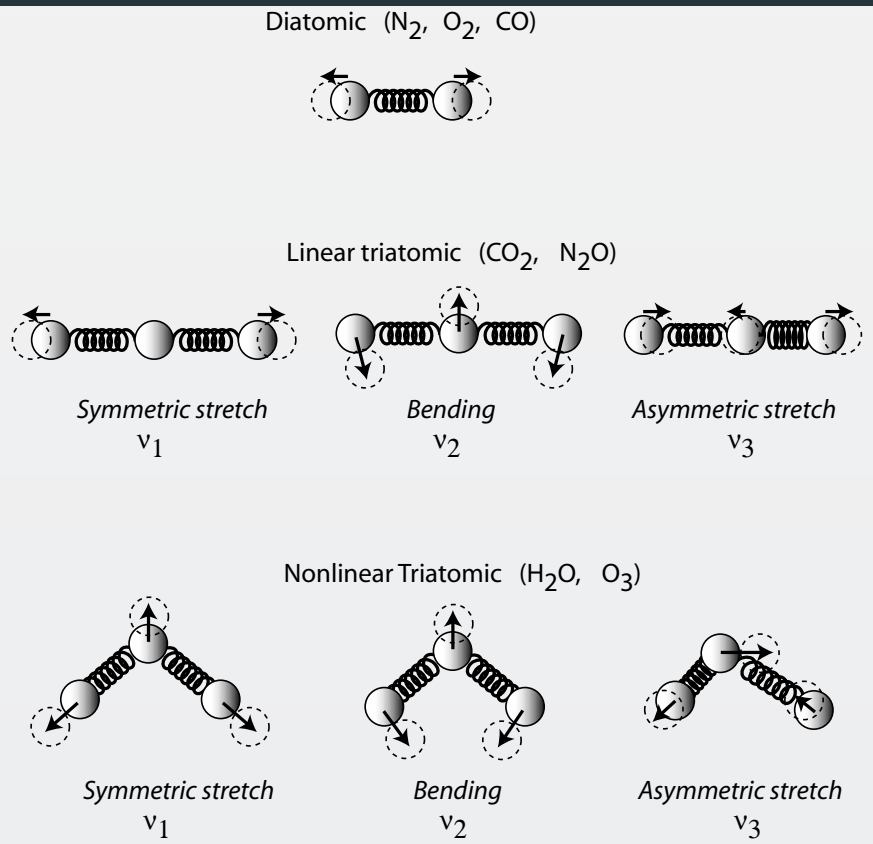
$E_j = j(j+1)\frac{h^2}{8\pi^2 cI}$

$E = E_{elec} + E_{vib} + E_{rot}$

Quantum selection rules obeyed

Atomic and molecular Spectroscopy - Basics 2





Spectroscopic databases

- Publicly available spectroscopic databases include HITRAN and GEISA
- Line strengths, Line centers, Line widths
- Lineshape (typically voigt, though water/CO2 more complicated)

Infrared Atmospheric Spectroscopy

Literature

Introduction to Molecular Spectroscopy : Gordon Barrow

First Course in Atmospheric Radiation : Grant Petty

GENLN2 : https://opensky.ucar.edu/islandora/object/3A3407

UMBC LBL : https://asl.umbc.edu/pub/packages/lbl.pdf

Ideal Gas Law

L = length of Gas cell

P, PS_g = total pressure, gas partial pressure

T = temperature (K)

R = molar gas constant (8.31 J/mol/K)

$PS_g/P = mr_g$ = mixing ratio

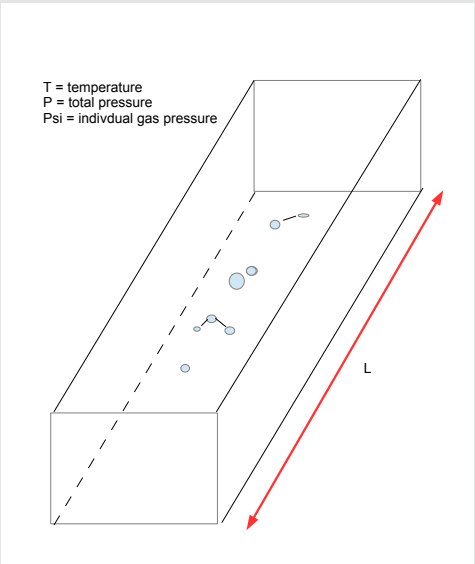
$$pV = nRT \rightarrow Q_g = \frac{n}{V}L = CF\frac{PS_g \times L}{R \times T}$$

CF = conversion to eg molecules/cm2

Gas Cell

Find optical depth of all gases

$k(\nu, P, T) = \sum_g k_g(\nu, Q_g, P, PS_g, T_g)$



OD = linestrength(T) $\times$ (gas amount $\times$ pathlength) $\times$ lineshape

$$\{cm-1/(molecules/cm2)\}\{molecules/cm3 \times cm\}\{1/cm-1\}$$

$$k_g^l(\nu,\nu_0) = S(T) \times Q_g \times f_{lineshape}(\nu,\nu_0^l)$$

$$k(\nu,P,T) = \sum_g k_g(\nu,Q_g,P,PS_g,T_g)$$

Master Equation for Spectroscopy

$$k(\nu,P,T) = \sum_g^{all\ gases} \sum_l^{all\ lines} k_g((\nu,Q_g,P,PS_g,T_g),(lineshape^l(\nu_0^l,\gamma^l)))$$

Key idea

$$k_g(\nu,Q_g,P,PS_g,T_g) = Q_g \times S(T) \times f_{lineshape}(\nu,P,PS_g,T) = Q_g\sigma(\nu,T,P,PS_g)$$

Line Strength S(T)

Partition fraction $Z(T)$ gives population stats for a given line

line center shift due to pressure $\nu_0(P) = \nu_0(0) + \lambda P$

line strength $S(T) = S(296K)\frac{Z(296K)}{Z(T)} \times f(exp^{-hcE/kT})$

Line Broadening : Lorentz vs Doppler

$\gamma_L = (PS \times sbroad + (P - PS) \times fbroad) \times (296/T)^n$

$\gamma_L^{air}(P,T) \sim \gamma_0^{air}\frac{P}{P_{ref}}(\frac{T_{ref}}{T})^n \sim 0.1\frac{P}{P_{ref}}$ cm^{-1}

$\gamma_D(T) = \nu_0(\frac{kT}{m})^{1/2} \sim \sqrt{T/m}$

Lineshape

Typically use Voigt lineshape for IR Note : H_2O, CO_2, CH_4 more complicated

$f_{lorentz} = \frac{1}{\pi}\{\frac{\gamma_L}{(\nu-\nu_0)^2+\gamma_L^2}\}$

$g_{doppler} = \frac{1}{\gamma_D(T)}(\frac{ln2}{\pi})^{1/2}e^{-(ln2(\frac{\nu-\nu_0}{\gamma_D(T)})^2)}$

$f_{voigt} = f_{lorentz} \bigotimes g_{doppler}$; $f_{voigt} \rightarrow f_{lorentz}$ as pressure increases

$k(\nu) = Qf_{voigt}(\nu)S(T)$

HITRANonline Logged in as Sergio DeSouza-Machado | Logout

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Line-by-Line Search

4. Select or Create Output Format

Select an output format or create a new one, then 5. Start Data Search >

Available Output Formats

- .par (160 chars)
- test2

Create New Output Format

Output Format Description

.par (160 chars)

The 160-byte fixed-width format used since HITRAN 2004 - see Table 1 in Rothman et al., *JQSRT* **96**, 139 (2005).

Field separator: [no separator], Line endings: Windows (CR LF)
This output format has variable-width fields and no header line.

Parameter	Units	C | Fortran Format	Err	Ref
Molecule ID		I2		
Isotopologue ID		I1		
ν	cm^{-1}	F12.6	✓	✓
S	$cm^{-1}/(molec \cdot cm^{-2})$	E10.3	✓	✓
A	s^{-1}	E10.3		
γ_{air}	$cm^{-1} \cdot atm^{-1}$	F5.4	✓	✓
γ_{self}	$cm^{-1} \cdot atm^{-1}$	F5.3	✓	✓
E''	cm^{-1}	F10.4		
n_{air}		F4.2	✓	✓
δ_{air}	$cm^{-1} \cdot atm^{-1}$	F8.6	✓	✓

Line-by-Line codes

https://asl.umbc.edu/pub/packages/lbl.pdf

UMBC-LBL

Basics

- Matlab based
- input : gasID,(T,P,PS,Q),($\nu_{start}, \nu_{end}, d\nu$),(preset parameters)
- output : $\nu = (\nu_{start} : d\nu : \nu_{end} - d\nu), k(\nu)$; d$\nu = 0.0025$ cm^{-1};
- Reads in HITRAN/GEISA spectral database line parameters
- Loops over lines, applying voigt lineshape to each line (Fortran Mex)
- Does H_2O (without basement, HDO, continuum) and CO_2 (line mixing)

Size/Timings

- 40 molecular gases H_2O,CO_2,O_3,CH_4 plus HDO, self+foreign continuum
- 40 cross section gases CFCs
- 100 layers : 1100 mb $\geq$ Pressure $\geq$ 0.005 mb (0 km $\leq$ z $\leq$ 82 km); thickness 250 m at GND, 4 km at TOA); span 605-2830 cm^{-1} in 25 cm^{-1} chunks
- Takes a long time to compute ODs for one atmosphere

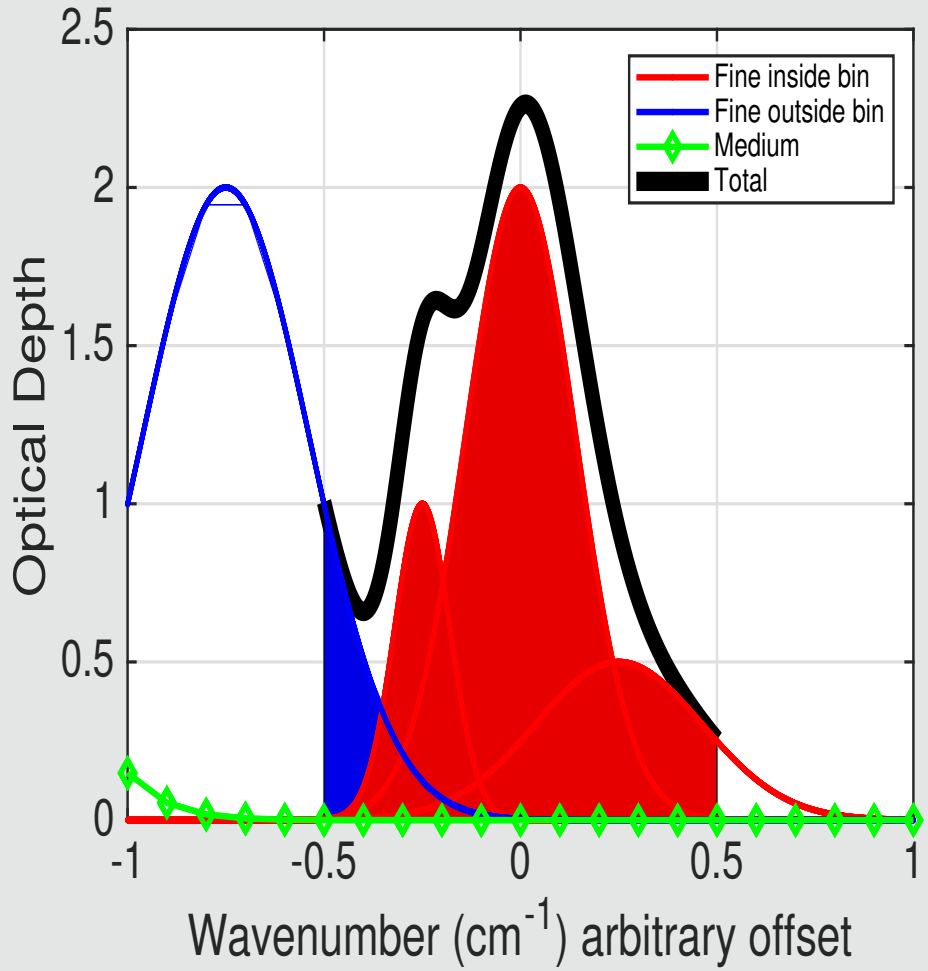
How to speed up parts of the code

The "preset parameters" in the previous slide include *nbox* = number of points to boxcar integrate, and width of "near","medium","far" intervals

Algorithm

- 1 cm^{-1} chunks, $d\nu/nbox$ resolution
- bin lines : "near" "medium" "far"
- "near " within $\pm$ 1 cm^{-1} of the bin : OD at fine resolution $d\nu/nbox$ (red), box car integrate to $d\nu$
- "medium" within $\pm$ 1-2 cm^{-1} of the bin : OD at resolution 0.1 cm^{-1}, interpolate to $d\nu$ (green)
- "far" within $\pm$ 2-25 cm^{-1} of the bin : OD at resolution 0.5 cm^{-1}, interpolate to $d\nu$ (not shown)
- repeat at next 1 cm^{-1} interval

Figure 1 of AMT kCARTA paper



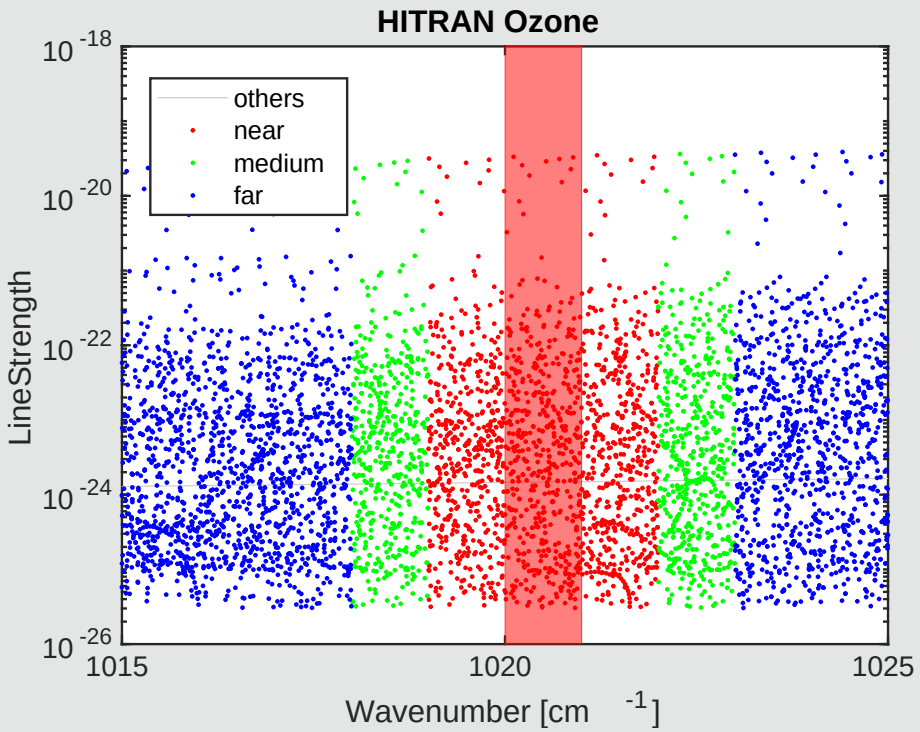
Example : Ozone lines from HITRAN 2020

Some numbers

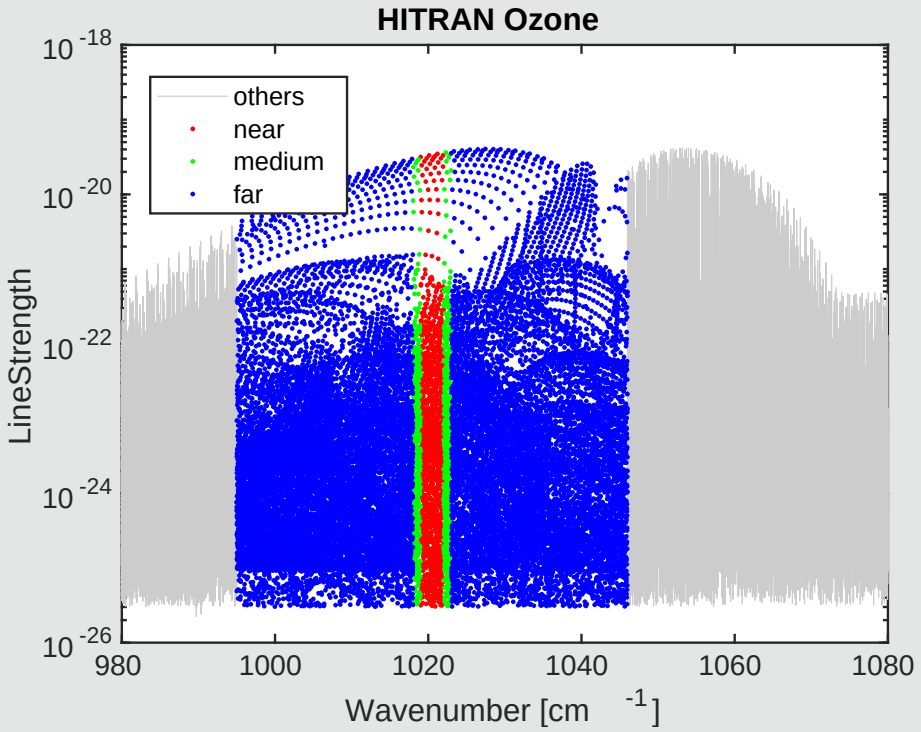
46985 lines In the 980-1080 cm^{-1} interval; choose the 1020-1021 cm^{-1} bin

- 1629 lines in the fine bin [1019,1022] cm^{-1}
- 1099 lines in the medium bins [1018,1019] cm^{-1} and [1022,1023] cm^{-1}
- 23194 lines in the far bins [0995,1018] cm^{-1} and [1023,1046] cm^{-1}

Zoom in



Zoom out



Pseudo Line-by-Line codes : kCARTA

https://asl.umbc.edu/pub/packages/kcarta1.22.pdf

How to speed this up

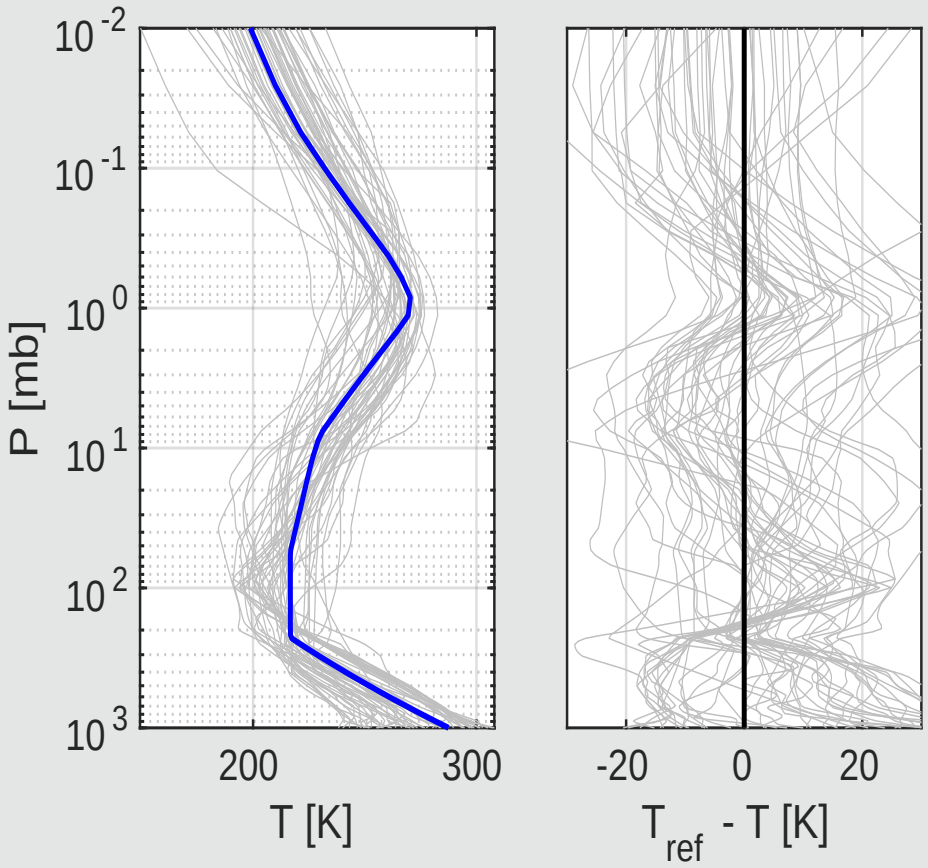
Some challenges

- About 8 seconds for 1 cm^{-1}, about 36 seconds to do 25 cm^{-1}, for one layer
- Need 100 layers so about 60 minutes to do 25 cm^{-1}; to span 605-2830 cm^{-1} would take 89 chunks = 89 hours
- We have 80 gases so about .....
- It's not so bad, there are about 6 main HITRAN gases; not all gases have so many lines, in every spectral region
- Very Accurate! Too slow to be practical for remote sensing applications!

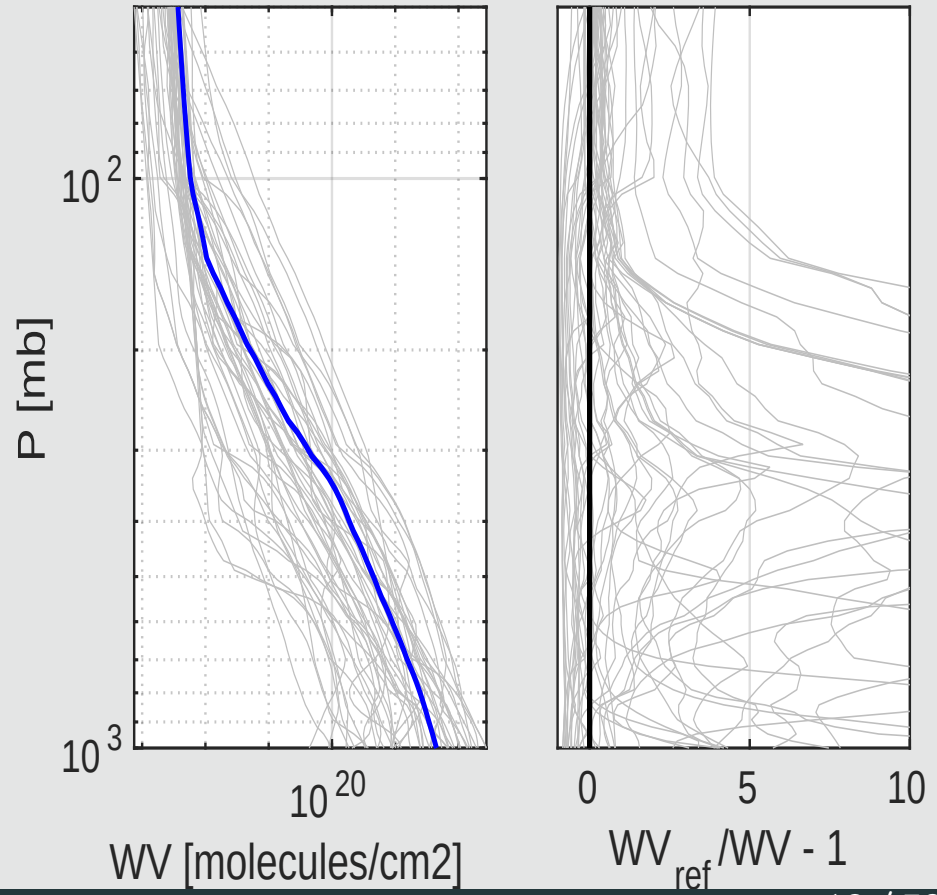
T and Q profiles

49 AFGL regression profiles, including Tropical, Mid Lat Summer, Mid Lat Winter, Sub Arctic Summer, Sub Arctic Winter (cold/hot and dry/wet)

Temperature



Water Vapor



How to speed this up A

Idea A : Make a database

- $$k_g(\nu, T) = Q_g \sum_{l}^{all\ lines} S_l(T) f_{voigt}(l, \gamma(P, PS_g, T)) = Q_g k_g(T)$$
- Make database in term of $T_{USStandard}(z)$, $Q_{USStandard}(g, z)$ for all 80 gases
- Use 10 K temperature offsets from US Standard (reference) profiles : $T_{ref}(z) - 50, T_{ref}(z) - 40, ... T_{ref}(z), ... T_{ref}(z) + 40, T_{ref}(z) + 50$
- Will take time to generate, but when saved can find optical depths for arbitrary profile (T(z),Q(g,z))
  - n = -5 : 1 : +5 (11 temperature offsets)
  - interpolate in temperature $k_g^{ref}(\nu, z, T), Q_g^{ref}(z)) = interp(T_{ref}(z) + n * 10, k_g^{ref}(\nu, T_{ref}(z) + n * 10, Q_g^{ref}, z), T(z))$
  - scale with gas amount $k_g(\nu, z, T) = k_g^{ref}(\nu, z, T), Q_g^{ref}(z)) \frac{Q(z)}{Q_g^{ref}(z)}$

How to speed this up B

Idea B : Reduce Database Size!

- The raw database is huge : (80 gases) $\times$ (89 chunks of 25 cm^{-1} at 0.0025 cm^{-1} spacing) $\times$ (100 layers) $\times$ (11 T offsets)
- There are spectral features : use Singular Value Decomposition to compress
- $k_g(\nu, T, P) \rightarrow k_g^{compressed}(\nu, T, P)$
- We call this the kCompressed database
  - check compression by running radiative transfer and ensuring errors in TOA brightness temperature are less than 0.1 K
- Generated using H1998, H200,H2004, H2008, H2012, H2016, H2020, ... (and also GEISA 2015)
- Also have done (FIR) 10-605 cm^{-1} and (NIR,Vis,UV) 2830-44000 cm^{-1} (making sure point spacing dν changes with central wavenumber); but older H2004,H2008

Raw database

- Use UMBC-LBL to compute ODs for $\sim$ molecular gases and $\sim$ cross section gases, using US Standard Temperature and gas profiles
  - for H_2O we use 5 different variable water widths to account for self broadening of water
  - We use LBLRTM (v12.8) to generate CO_2 and CH_4 since they have more recent line mixing coefficients
- 25 cm^{-1} chunks at 0.0025 cm^{-1} resolution (10000 points per chunk) spanning 605-2830 cm^{-1} (89 chunks)
- 100 Pressure layers spanning 1100 mb (surface) to 0.005 mb (TOA)
- 11 Temperature offsets from the US Standard Temperature profile : 0 K, $\pm$ 10 K, $\pm$ 20 K, ..., $\pm$ 50 K
- For each gas, each 25 cm-1 chunk $k_g(\nu, T, P) = (100 \times 11) \times 10000$
- Takes about a week to grind out on a HPC
- Database size $\sim$ 60 Gb

SVD compressed database

- $m \times n$ **Matrix** of absorption coefficients K ($m = 100 \times 11, n = 10000$)

$$K_{ij} = U\Sigma V^T = \sum_{l=1}^{L} U_{il}\Sigma_l V_{jl} + \sum_{l=L+1}^{n} U_{il}\Sigma_l V_{jl}$$

- **Many** of the singular values are small ... drop the second term.
  $U = m \times n, \Sigma = n \times n, V = n \times n \rightarrow U = m \times L, \Sigma = L \times L, V = n \times L.$
  $L \simeq 30 - 40$ for H_2O, CO_2 $\quad$ $L_{avg} \simeq 5$ for rest of gases

$$K = U\Sigma V^T \simeq \hat{U}\hat{K} \quad \hat{K}_{ij} = \sum_{l=1}^{L} \Sigma_l V_{jl}$$

- **Reconstructing** the absorption coefficients for the m-th layer

$$K_{m(g)}(\nu) = \frac{q_{m(g)}}{q^{ref}_{m(g)}} \sum_{l=1}^{L} \hat{k}_{l(g)}(T_m, m) \;\; \hat{u}_l$$

  $\hat{u}_l$ are basis vectors, $\hat{k}_{l(g)}(T_m)$ are interpolated coeffs from $\hat{K}(T)$

- Database $\sim$ 776 Mb (200 Mb (H_2O), 76 Mb (CO_2), 500 Mb (other gases))

kCARTA Radiative Transfer

https://asl.umbc.edu/pub/packages/kcarta1.22.pdf
https://amt.copernicus.org/articles/13/323/2020/

Add on a Radiative Transfer Algorithm

Clear Sky

- After you have the optical depths, add in : solar source term, emissivity, reflectivity, ray tracing and do Radiative Transfer
- kCARTA : the k-Compressed Atmospheric Radiative Transfer Algorithm
- Analytic jacobians, can do flux calculations
- Takes about 30-45 seconds to uncompress and calculate TOA (or ground) infrared radiances $R(\nu)$ (605-2830 cm^{-1}) for an arbitrary profile
  - convolve with appropriate instrument Spectral Response Function
  - $R_i^{calc}(\nu) = \int d(\nu) R(\nu) SRF_i(\nu)$
- Takes about x3 longer to do 100 layer analytic jacobians dBT/dT(z),dBT/dQ(z),dBT/dST
- WARNING Since we use 0.0025 cm^{-1} resolution throughout the (605-2830 cm^{-1}) spectral range
  - noticeable differences when you compare with LBLRTM since that uses variable (higher) spectral resolution
  - but after you convolve with an instrument SRF, these differences are very small

Clear Sky

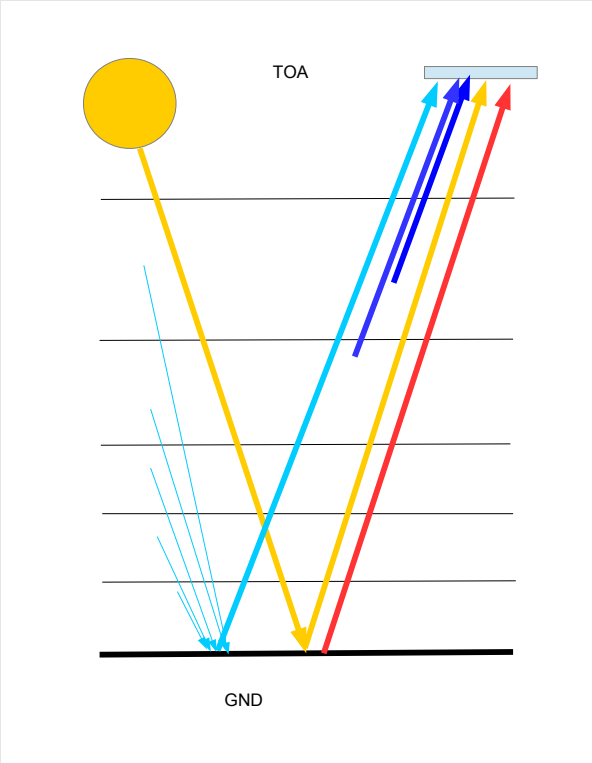
At steady state, 1D radiative transfer (RT) described by Schwartzchild equation (ignoring solar and background contributions)

$$\mu \frac{dI(\nu,\theta)}{\kappa_e dz} = -I(\nu,\theta) + J(\nu)$$

- $\mu = cos(\theta)$, dz is the vertical coordinate
- κ_e is the total extinction (due to gases, clouds etc)
- $\kappa_e dz = dk$ is the optical depth
- $I(\nu,\theta)$ is the radiance intensity
- J is the source function
  - Clear Sky, in LTE : $J = B(\nu, T)$
  - Clear Sky, in NLTE : $J = rB(\nu, T)$

kCARTA 1D Radiative Transfer

Schematic



Details

$$R(\nu,\theta) = R_{surface} + R_{atmospheric\ emission} + R_{background\ thermal} + R_{solar}$$

- $R_{surface}(\nu,\theta)$ = surface to TOA at angle θ
- $R_{atmospheric\ emission}(\nu,\theta)$ = thermal emission from each angle at angle θ
- $R_{background\ thermal}(\nu,\theta)$ = downward thermal radiation from all angles, reflected at surface at angle θ
- $R_{solar}(\nu,\theta,\theta_{sun})$ = downward solar radiation at θ_{sun} reflected at surface at angle θ

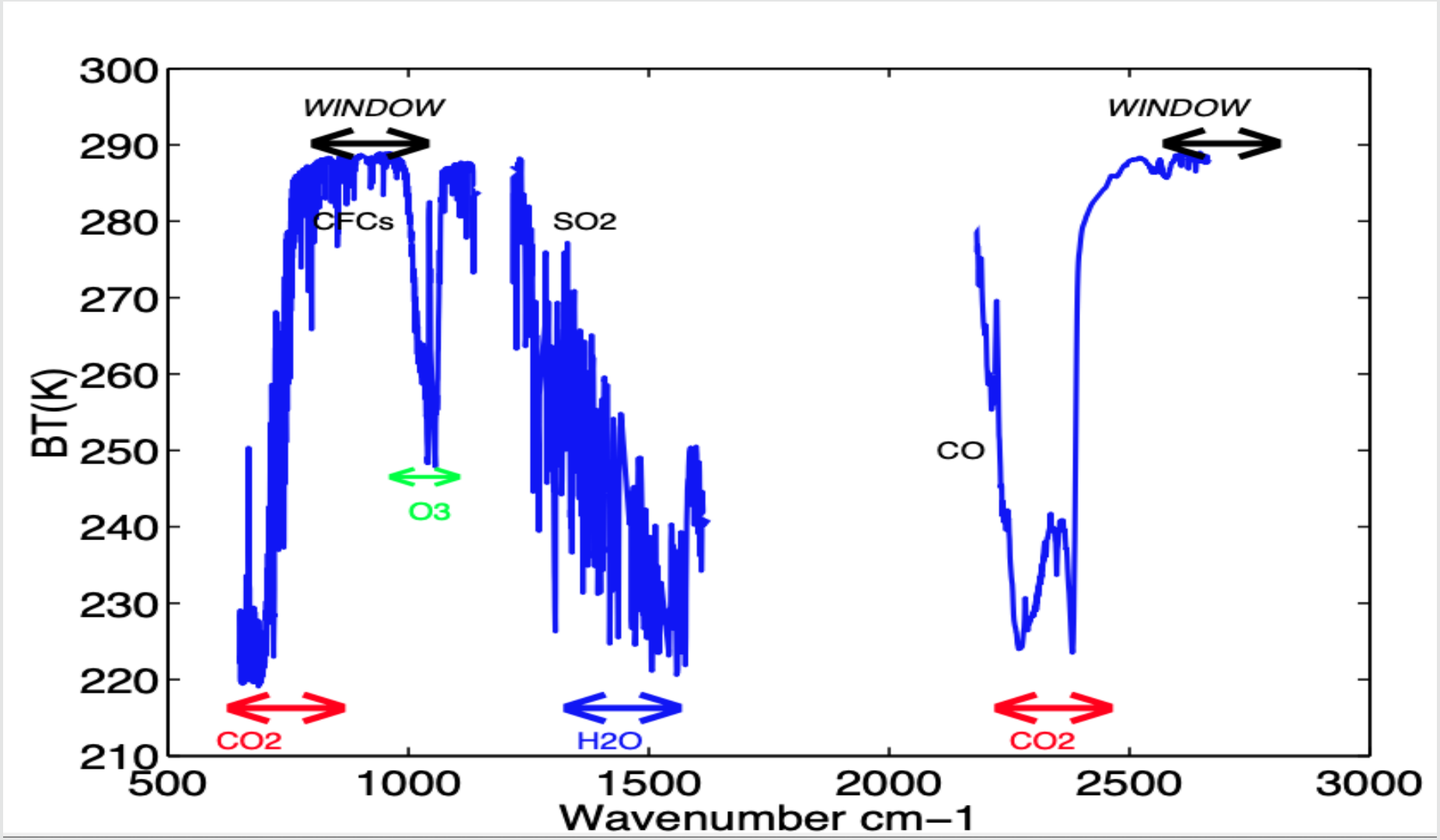
Soln to Schwartzchild Eqn

$$
\begin{aligned}
R(\nu,\theta) = & \epsilon_s(\nu)B(\nu,T_s)\tau_{atm}(\nu,\theta) + \\
& \int_{surface}^{TOA} B(\nu,T(z))\frac{\partial\tau(\nu,\theta)}{\partial s}ds + \\
& \frac{1-\epsilon_s(\nu)}{\pi}\tau_{atm}(\nu)\int d\Omega^{+}\int_{TOA}^{surface} B(\nu,T(s))\frac{\partial\tau(\Omega)}{\partial s}cos(\theta)ds + \\
& \rho_s(\nu)B_{\odot}(\nu)cos(\theta_{\odot})\tau_{atm}(\nu,\theta_{\odot})\tau_{atm}(\nu,\theta)
\end{aligned}
$$

Layer by Layer Iterative Solution

- Surface Emission : $R_s(\nu) = \epsilon_s(\nu)B(\nu,T_s)\tau_{GND\rightarrow TOA}(\nu,\theta)$
- Layer Emission : $R_{\mathbf{lay}} = \sum_{i=1}^{i=N} B(\nu,T_i)(1.0-\tau_i(\nu))\tau_{i+1\rightarrow TOA}(\nu,\theta)$
- Background thermal :
  $R_{th}^{surface}(\nu) = \pi\rho_s\sum_{i=N}^{i=1} B(T_i)\left[\tau_{i-1\rightarrow ground}(\nu,\theta_{diff}) - \tau_{i\rightarrow ground}(\nu,\theta_{diff})\right]$
  We speed up the integral over hemispheres by using layer by layer/spectrally varying effective diffusive angles; see AMT paper
- Solar reflected : $R_{\odot}(\nu) =$
  $\rho_s(\nu,\theta,\phi)B_{\odot}(\nu)cos(\theta_{\odot}) \times \tau_{N\rightarrow ground}(\nu,\theta_{\odot}))\tau_{ground\rightarrow TOA}(\nu,\theta))\Omega_{\odot}$

Typical AIRS spectrum (KCARTA convolved with AIRS SRFs)



Jacobians

$$R(\nu) = \epsilon_s B(T_s,\nu)\tau_{1\rightarrow TOA}(\nu) + \Sigma_{i=1}^{i=N} B(T_i,\nu)(1.0-\tau_i(\nu))\tau_{i+1\rightarrow TOA}(\nu)$$

Differentiation with respect to the m-layer variable s_m, (gas amount or layer temperature $s_m = q_{m(g)}$, T_m) yields

$$\begin{aligned}\frac{\partial R(\nu)}{\partial s_m} = & \left[\epsilon_s B(T_s)\tau_{1\rightarrow TOA}\right](-1)\frac{\partial k_m(\nu)}{\partial s_m} + \\ & \left[\sum_{i=1}^{m-1}(1.0-\tau_i(\nu))B_i(\nu)\tau(\nu)_{i+1\rightarrow TOA}\right](-1)\frac{\partial k_m(\nu)}{\partial s_m} + \\ & \left[(1.0-\tau_m(\nu))\frac{\partial B_m(\nu)}{\partial s_m} - B(T_m,\nu)\frac{\partial \tau_m(\nu)}{\partial s_m}\right]\tau_{m+1\rightarrow TOA}(\nu)\end{aligned}$$

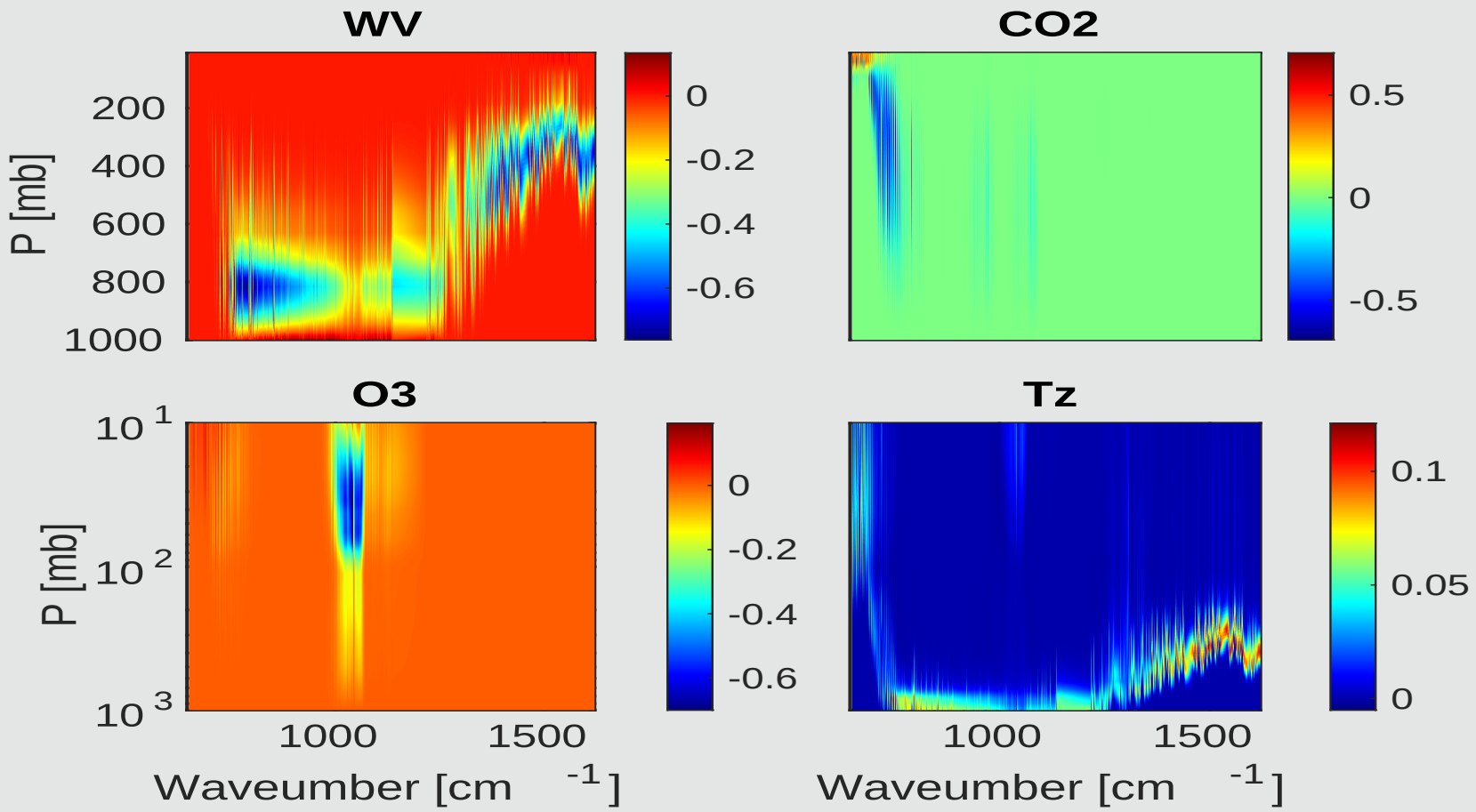
Individual jacobian terms $\frac{\partial k_m}{\partial s_{m(g)}}$ are as follows

- gas amount derivative is $\frac{\partial k_m}{\partial q_{m(g)}} = \frac{k_m}{q_{m(g)}}$ (with added complexity for water, to account for self broadening),
- temperature derivative $\frac{\partial k_m}{\partial T}$ cumulatively obtained *while* performing the temperature interpolations during individual gas database uncompression.

Tropical Jacobians (kCARTA convolved with AIRS SRFs)

Gas Jacobians are dBT/d(log(Q(p))) in K

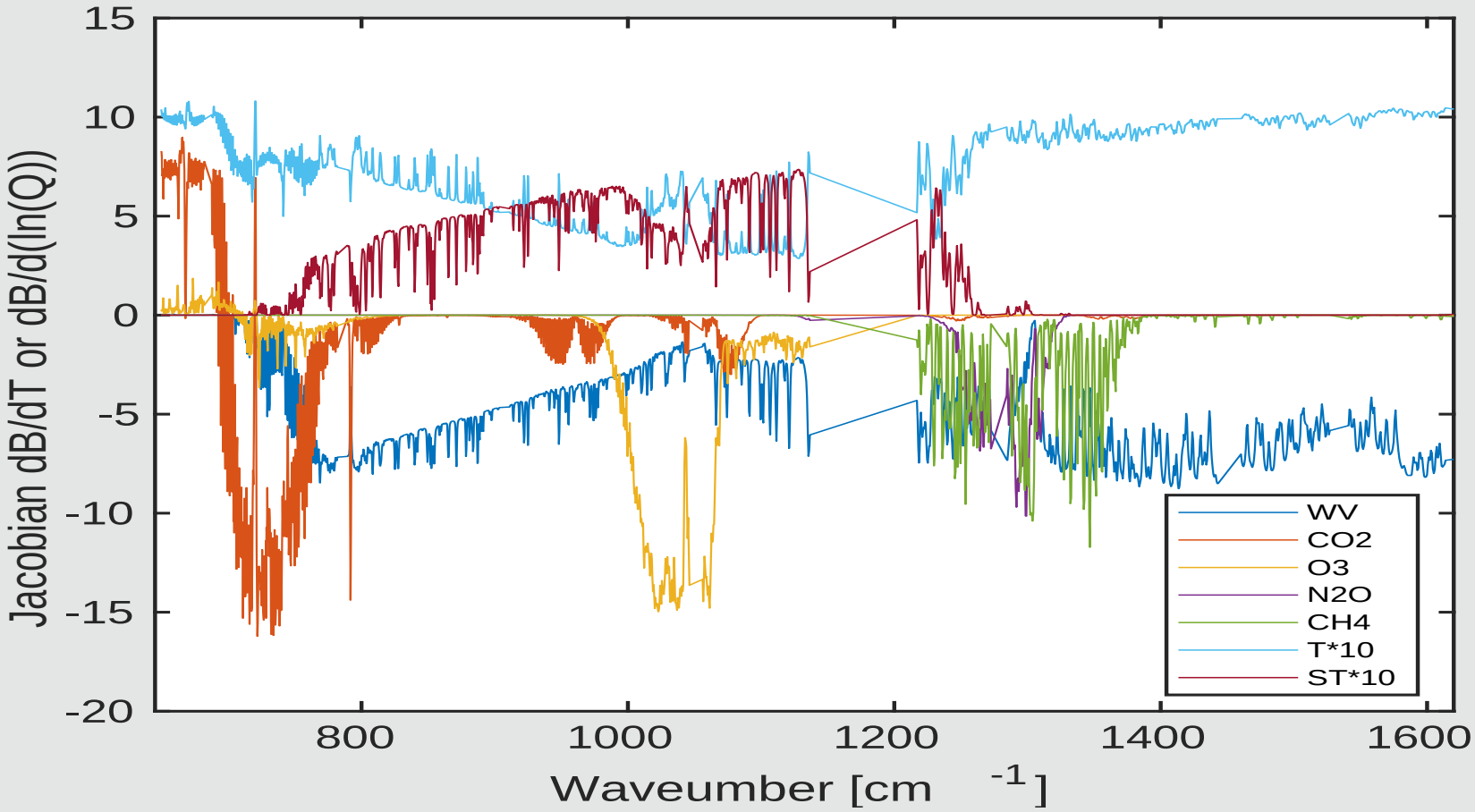
Temperature Jacobian is dBT/dT(p) in K/K



Column Tropical Jacobians (kCARTA convolved with AIRS SRFs)

Gas Jacobians are dBT/d(log(Q(p))) in K

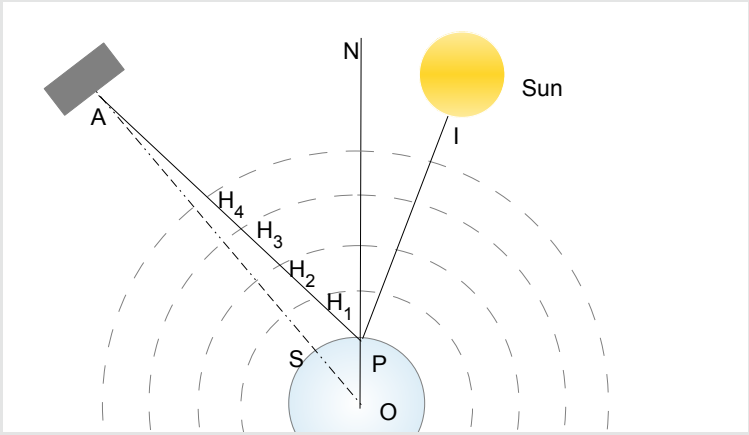
Temperature Jacobian is dBT/dT(p) in K/K



kCARTA 1D Radiative Transfer

Variation in local zenith angle

- Can use plane parallel atmosphere
- Default is to slowly vary angle as ray propagates through spherical layers



Viewing geometry for the sounders modeled by kCARTA. A is the satellite and point P is being observed by the satellite, while I is the sun

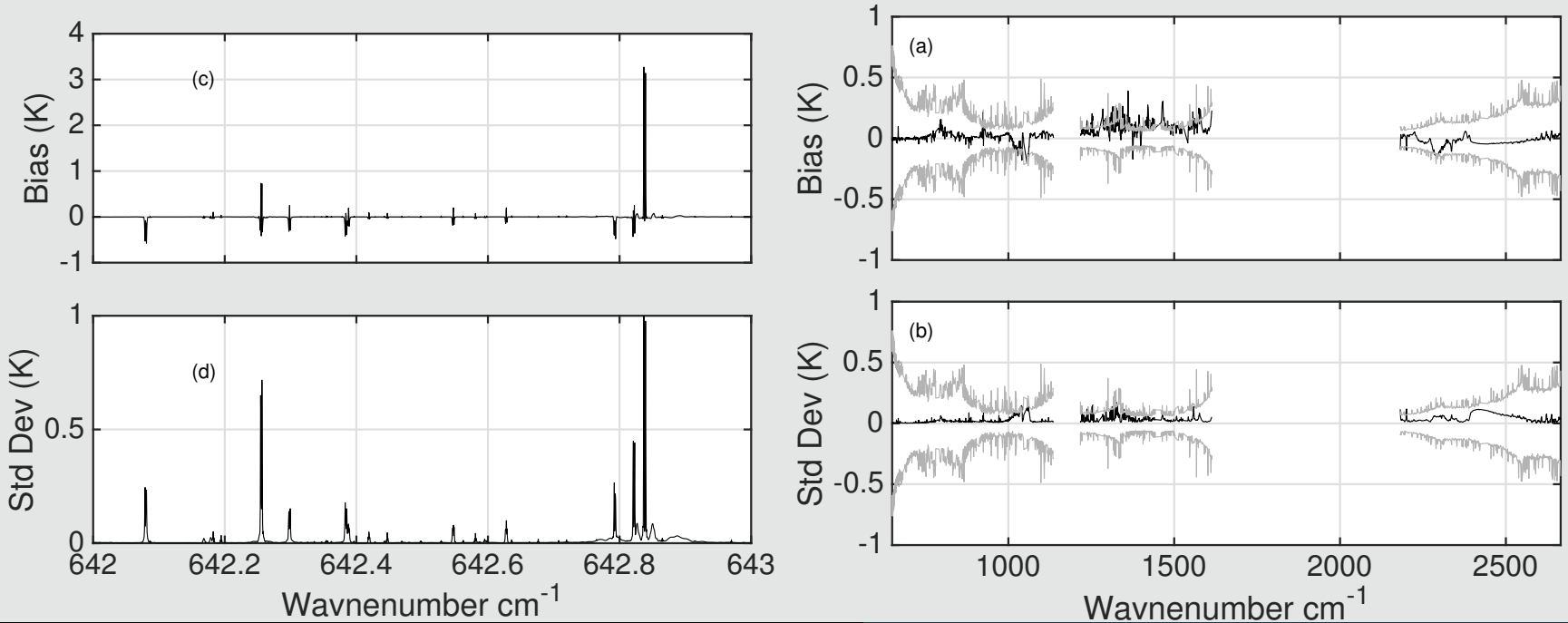
Variation in layer temperature with optical depth

- Default : constant layer temperature
- eg LBLRTM use linear-in-tau variation of temperature; let $\tau(\nu) = e^{-K(\nu)}$

$$I(\nu) = I_0(\nu)\tau + (1-\tau)\left\{B_{av}(\nu) + (B_u(\nu) - B_{av}(\nu))\left(1 - 2\left(\frac{1}{K} - \frac{\tau}{1-\tau}\right)\right)\right\}$$

Comparisons to LBLRTM

- kCARTA uses fixed resolution 0.0025 cm^{-1}
- LBLRTM varies spectral resolution with wavenumber
- (L) kCARTA less accurate on line centers at larger wavelengths (3K errors at 15 um); improves as wavelengths decrease (0.1 K errors at 10 um)
- (R) After convolution with instrument SRFs, on average kCARTA-LBLRTM within NeDT. Plots averaged over 49 profiles.



NLTE Computation

- Daytime Solar radiation is preferentially absorbed by some CO_2 and O_3 bands
- This gives higher kinetic energies and hence vibrational temperatures than other bands/other molecules for $z \geq 40$ km
- Nadir sounders (AIRS/CrIS/IASI) : 10 K effect at 4.3 um T(z) sounding region
- Due to the Planck function $\ll$ in 15 um (limb sounders see effect)
- Manuel Lopez Puertas (U. of Granada, Spain) has given AIRS team CO2 vibrational temperatures as function of solar angle and temperature profile
- Some bands remain in LTE, others go into NLTE
- UMBC has developed a line-by-line model for kCARTA to make a fast model for SARTA
- Lorenzo Cassini (UniBas) currently visiting UMBC to develop a NLTE model using LBLRTM for σ-IASI
- GENLN2, KOPRA and RFM also have NLTE models

kCARTA 1D Radiative Transfer

NLTE : Basic Idea

- LTE : compute ODs as usual (contribution "in-between" lines, using local kinetic temperature $T(z)$)
- NLTE : 'laser" effect (enhanced OD and Planck emission) mostly "on top of lines/line centers" using vibrational temperature $T^i_{vib}(z)$

OD Modification

- $\tau_{NLTE}(\nu)$: needs additional factor β
- As solar angle $\theta_{\odot}$ increases beyond 90°the factor $\alpha_{NLTE}(\nu, \theta_{\odot}) \rightarrow 1$
- In reality there is a "dusk" effect ($\theta_{\odot}$ between 90°and 120°) which we have difficulty modeling accurately
- Nadir low earth orbit sounders such as AIRS, CrIS, IASI have
  - $\theta_{\odot}$ between 10-60 °in tropics and mid latitude regions
  - $\theta_{\odot}$ above 60 °in polar regions
  - Plus there can be aurora events in the polar regions

$$\eta(\nu, \theta_{\odot}) = \sum_{LTE} \tau_{LTE}(\nu) + \sum_{NLTE} \alpha_{NLTE}(\nu, \theta_{\odot}) \tau_{NLTE}(\nu)$$

kCARTA 1D Radiative Transfer

NLTE : Planck Modification

As solar angle $\theta_{\odot}$ increases beyond 90°the factor $\beta_{NLTE}(\nu, \theta_{\odot}) \rightarrow 1$

$$B_{NLTE}(\nu, \theta_{\odot}) = B_{Planck}(\nu, T)\beta_{NLTE}(\nu, \theta_{\odot})$$

NLTE : Rad Transfer Modification

$$\begin{array}{lll} dz_{NLTE} & = dz\ \eta(\nu, \theta_{\odot}) & \\ \frac{dI(\nu,\theta,\theta_{\odot})}{dz_{NLTE}} & = & -I(\nu, \theta, \theta_{\odot}) + \beta(\nu, \theta_{\odot})B_{Planck}(\nu, T) \end{array}$$

NLTE : Quick summary

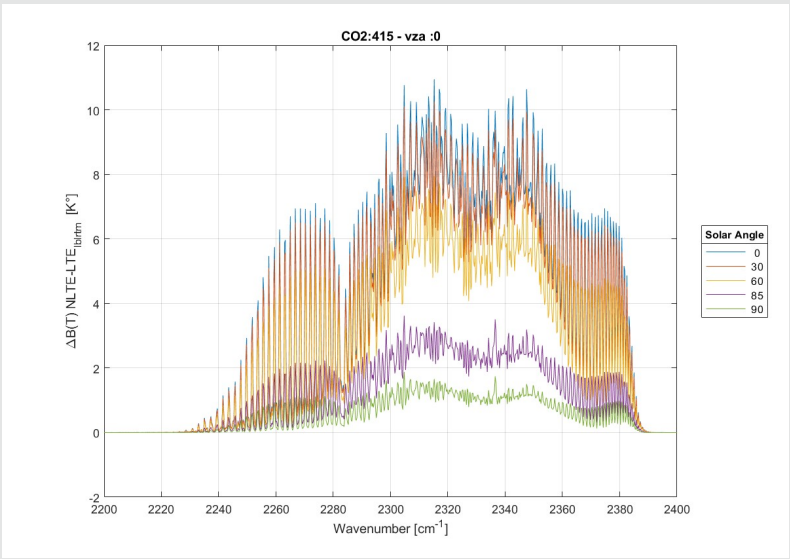
- Daytime solar : some bands of CO_2 can be in NLTE above 40 km
- Need to modify the optical depth and the planck function
- Between 0-30 km, do usual LTE calc for radiative transfer
- Above 30 km, do NLTE calc for radiative transfer
- But you need the vibrational temperatures to be able to do this

kCARTA 1D Radiative Transfer

Work done by Lorenzo Cassini (for future use in σ-IASI)

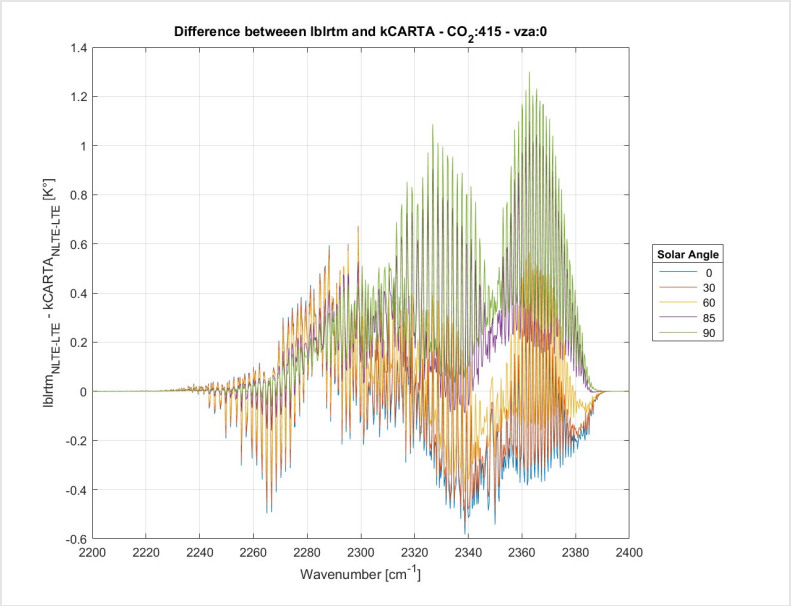
NLTE - LTE : (LBLRTM)

- function of solar zenith angle
- 415 ppmv for CO_2. Very small changes as CO_2 changes (0.25 K/40 ppmv)
- Largest effect is at solzen = 0°, $\rightarrow$ 0 as solzen becomes 90°



NLTE - LTE : LBLRTM - KCARTA

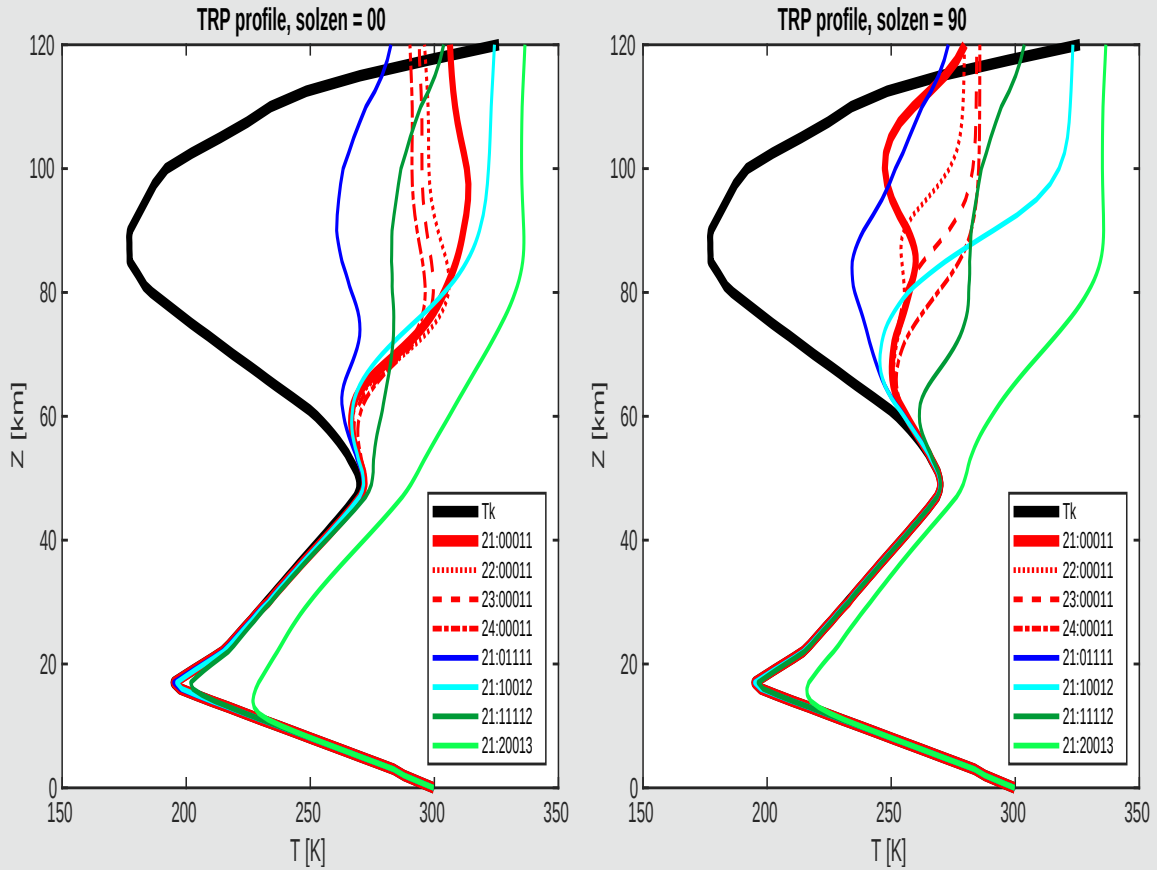
- KCARTA : NLTE line mixing coeffs made in 200
- LBLRTM : Niro et. al (2012)
- US Standard Profile, 415 ppmv
- Other profiles show similar results



Tvib vs Tkin

TRP profile; Solzen = 0 and Solzen = 90

Tvib → Tk as day → night



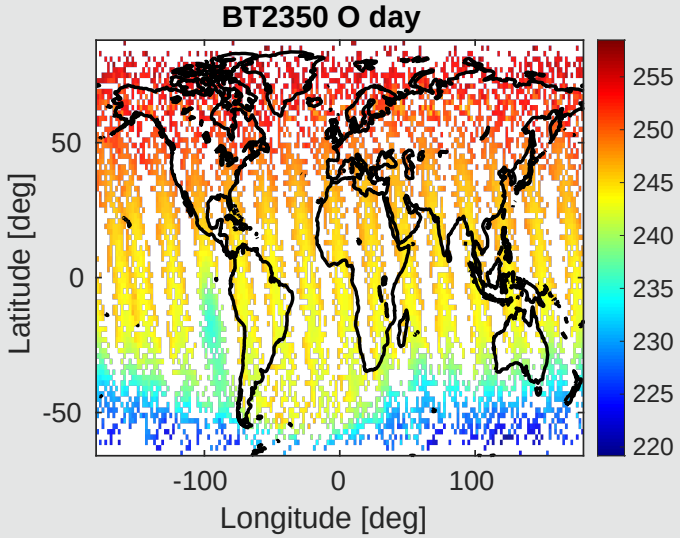
Modelling for SARTA

- 3 models since 2005
- Manuel has tweaked Tvib collisional model
- We tweaked our fitting parameters
- Have not fitted latest 2025 data
- O-C Bias (AIRS) has oscillated between about ± 1 K

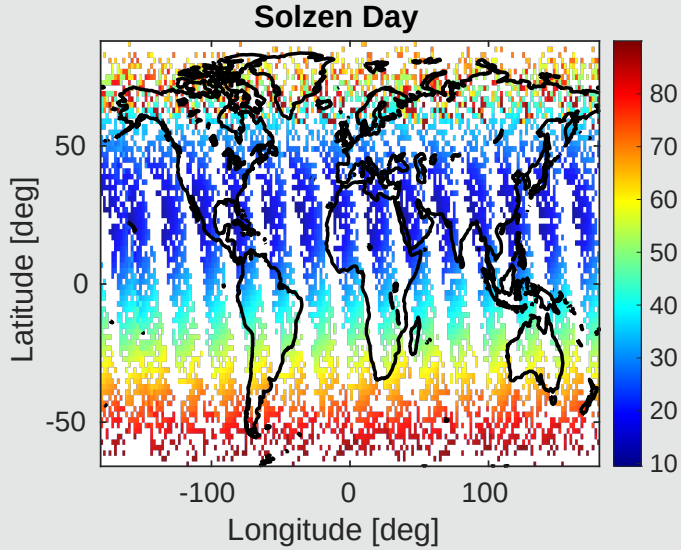
kCARTA 1D Radiative Transfer

June 2019 Random observations, 2350 cm^{-1} channel

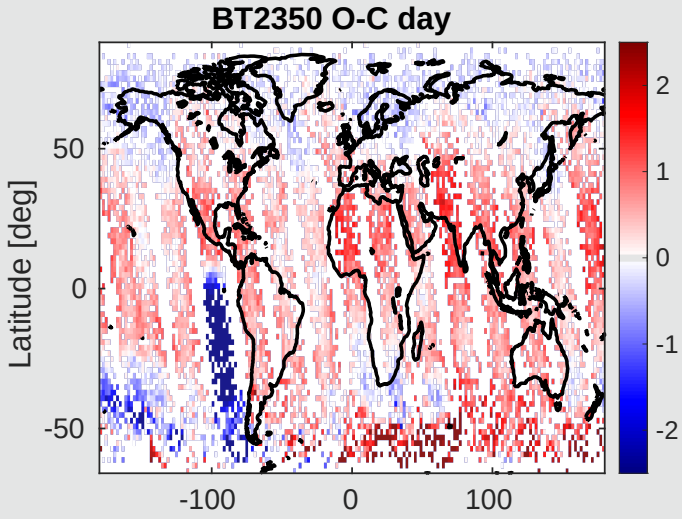
Observations



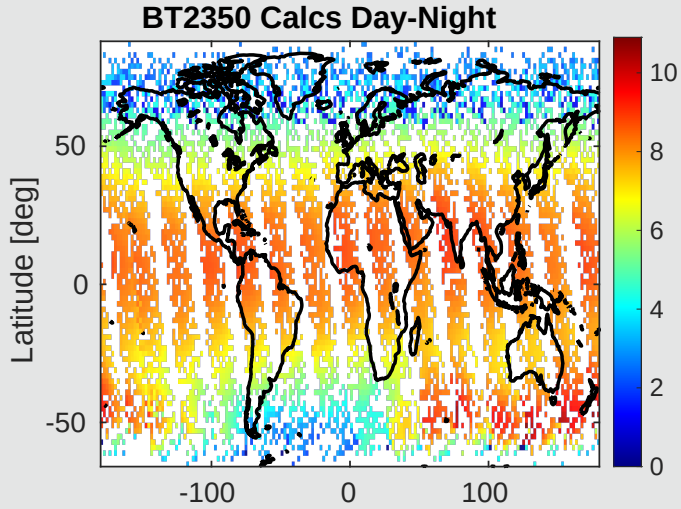
Solzen



Bias

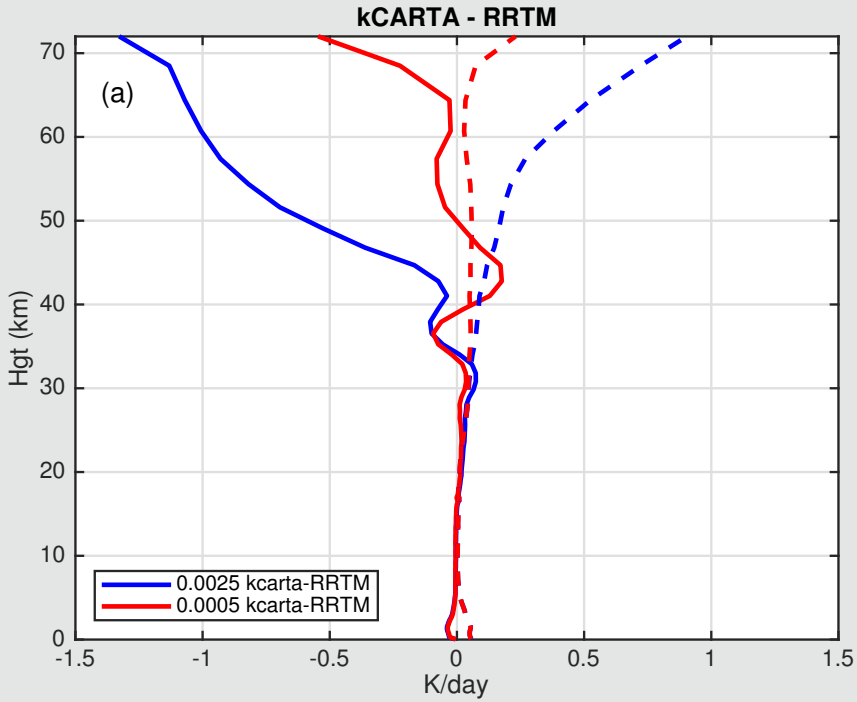


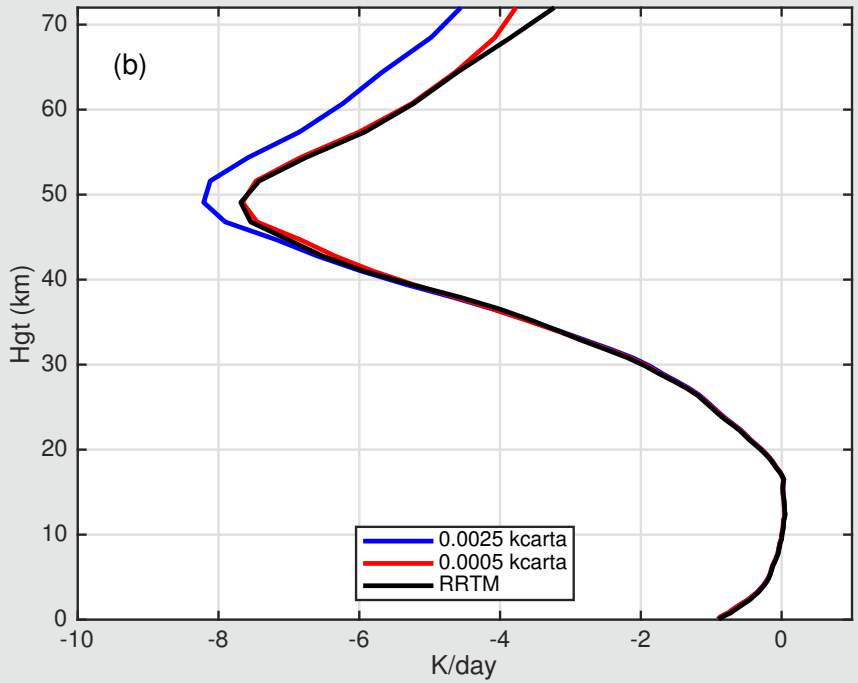
Simulations



Flux Computation

- Default : 0.0025 cm^{-1} resolution is acceptable for integration with SRFs
- Limitations become evident when you integrate over wavenumber to get fluxes and/or heating rates
- When we use 0.0005 cm^{-1} reolution, we approach LBLRTM heating rates and fluxes (but this slows down our code)





kCARTA 1D Radiative Transfer

All Sky

$$\mu \frac{dI(\nu)}{dk_e} = -I(\nu) + B(\nu, T)(1-\omega_0) + \frac{\omega_0}{2}\int_{-1}^{+1} I(\nu, k_e, \mu\prime)P(\mu, \mu\prime)d(\mu\prime) + \frac{\omega_0}{4\pi}\pi I_{sun} P(\mu, -\mu_{sun}) e^{-k_e/\mu_{sun}}$$

- $\omega = k_s/k_e = 1 - k_a/k_e$ is the single scattering albedo (0 for no scatter)
- $P(\mu, \mu')$ is probability of scattering from μ' into μ
- $P(\mu, -\mu_{sun})$ is probability of scattering from μ_{sun} into μ

- Can interface to DISORT or to PCLSAM to do scattering calculations
- This also has analytic jacobians for the PCLSAM version
  - Have also put in a correction (by G.Tang and P.Yang)
- Mie scattering for water clouds and aerosols, have Ping Yang/Bryan Baum scattering database for cirrus (different habits)

kCARTA 1D Radiative Transfer

DISORT

- Solves integro-differential equation by using a number of streams (2,4,8, ...)
- Can be "slow" for line-by-line applications, especially if you also try to use it to do the RT for the clear sky part
- Stamnes, K., Tsay, S.-C., Wiscombe, W., and Jayaweera, K.: Numerically Stable Algorithm for discrete ordinate method Radiative Transfer in multiple scattering and emitting layered media, Appl. Opt., 27, 2502–2509, 1988

PCLSAM

- More accurate in cases where single scattering albedo much smaller than 1
- Effective scattering of cloud and aerosol becomes very similar to an effective cloud optical depth $k_{total}(\nu) = k_{gas}(\nu) + k^{eff}_{cloud}(\nu, \omega)$
- Radiative Transfer now like earlier slides (fast/analytic jacobians)
- Chou, M.-D., Lee, K.-T., Tsay, S.-C., and Fu, Q.: Parameterization for Cloud Longwave Scattering for use in Atmospheric Models, J. Climate, 12, 1999
- G. Tang and P.Yang (2018) : Improvement of the simulation of cloud longwave scattering in broadband radiative transfer models, JAS (75)

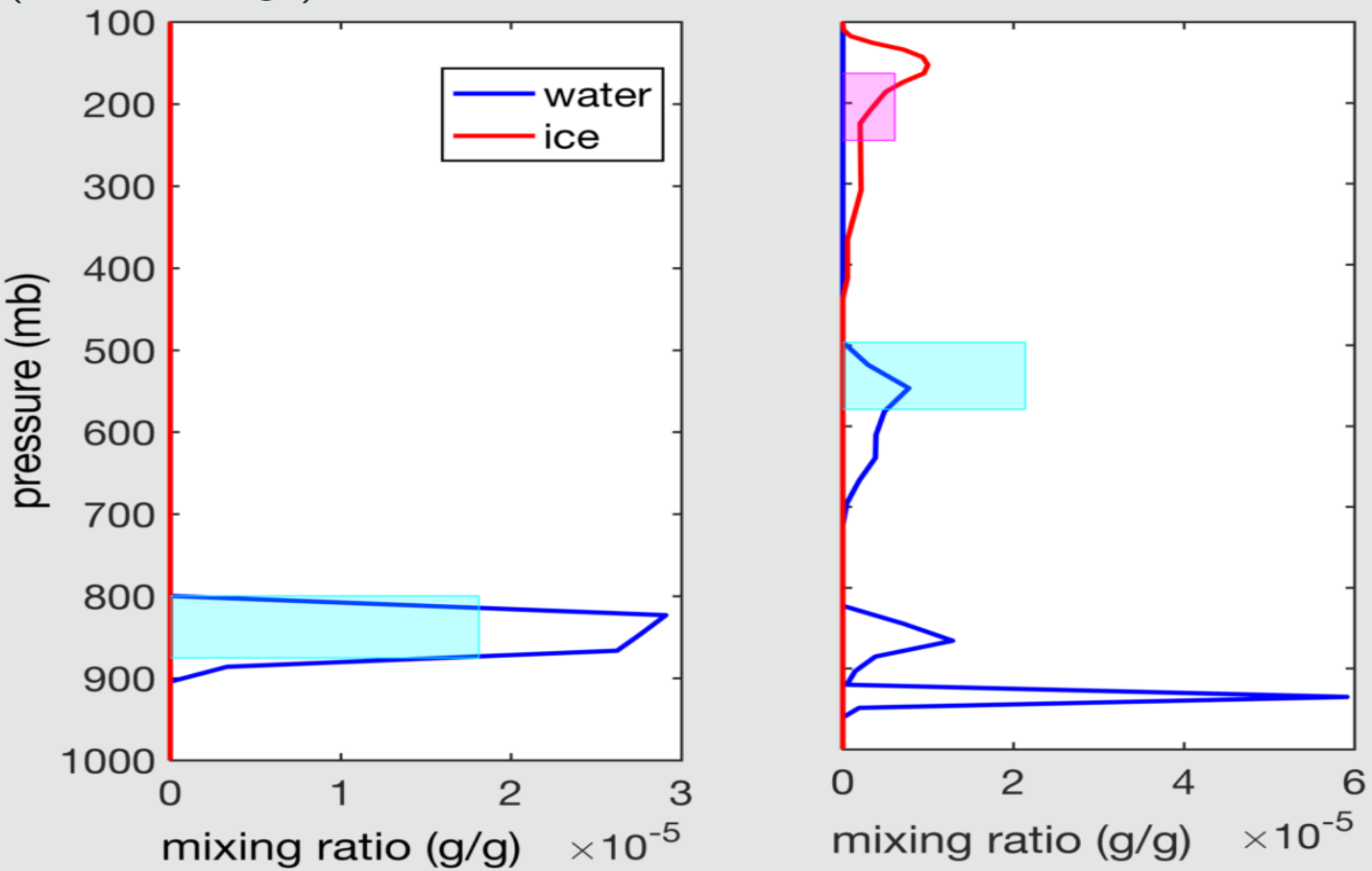
kCARTA 1D Radiative Transfer

Two Slab Clouds

- NWP models have ice/water cloud profiles (91 levels); but there are typically very few deg of information in IR radiances
- UMBC has developed a Two Slab Cloud approximation to reduce these profiles to two randomly overlapping clouds, using NWP information
  - Cloud/Aerosol 1 : type, fraction, amount, effective particle size, cloud top/bottom
  - Cloud/Aerosol 2 : type, fraction, amount, effective particle size, cloud top/bottom
  - Cloud Overlap fraction (random)
- Slab placement can be adjusted "as high as possible" "median of distribution" to get better agreement with eg DISORT based RTAs
- DeSouza-Machado, Strow, Tangborn, X. Huang, X. Chen, X. Liu, W. Wu, Q. Yang, "Single-footprint retrievals for AIRS using a fast TwoSlab cloud-representation model and the SARTA all-sky infrared radiative transfer algorithm", AMT 2018

Example

Cloud vertical profiles, reduced to one or two slabs. The red and blue curves come from the NWP model, while the cyan and magenta are the resulting locations (and loadings) for the slabs.



Fast RTA codes : SARTA

https://asl.umbc.edu/pub/packages/sarta.html

Fast Models

Need more speed

- Pseudo LBL codes are fast eg kCARTA (30 seconds), σ-IASI (0.8 seconds) per 0.0025 cm^{-1} spectrum
- New generation sounders (AIRS, CrIS, IASI) 2-3 million spectra daily
- The sounders make observations with finite number of channels (eg AIRS has 2378 channels, IASI has about 8400 channels)

Fast Models

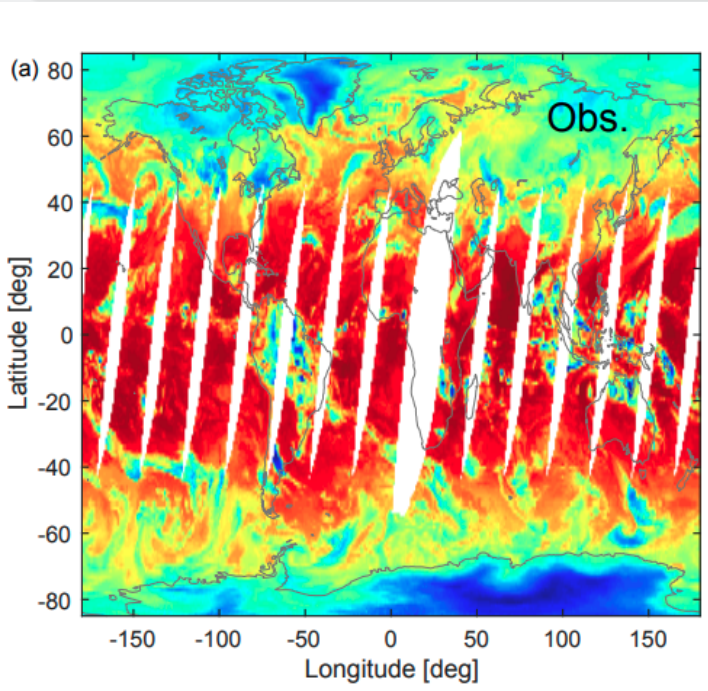
Basic Idea

- We use 49 regression profiles spanning Earth's typical temperature/H_2O/O_3 and other trace gases (eg CO_2,CH_4) to produce convolved layer-to-space transmittances for each instrument channel
  $\tau_{L2S}(i,l) = \int_{dv} e^{-\sum_{j=l+1}^{N}(K(\nu,j)/cos(\theta))} SRF_i(\nu)$
- We then fit these convolved transmittances using linear combinations of gas amounts, temperatures, view angles such as
  $\tau_{L2S}(i,l) = a_l T(l) + a_{l+1} T(l+1) + ... + a_N T(N) + q_l Q_g(l) + s_l sec(\theta)$
  $\tau_{L2S}(i,l) = Predictors(T(l), T(l+1), ...T(N), Q_g(l), \theta) \times Coefficents$
- Then $k_{eff}(i,l) = -log(\tau_{L2S}(i,l))$ and we can do clear sky/all sky radiative transfer exactly as for kCARTA, also with analytic jacobians
- SARTA = Stand Alone Radiative Transfer Algorithm takes about 0.02 seconds/AIRS spectrum; also has Two Slab Cloud Scattering
- Can then use this SARTA Fast Model in AIRS L2 operational retrievals at NASA or NOAA

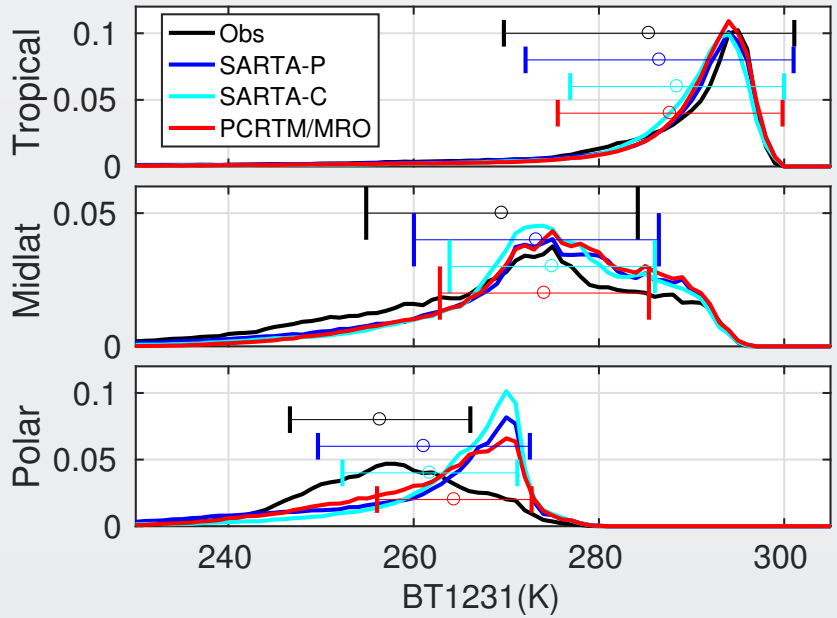
SARTA TwoSlab Examples

The i-th channel all-sky radiance $r_i(\nu)$ is computed using four weighted radiance streams : f_{clr} is clear fraction, $c_{overlap}$ is cloud overlap, $cx1, cx2$ are exclusive cloud fractions $c_i - c_{overlap}$

$$r_i(\nu) = f_{\text{clr}} r_i^{\text{clr}}(\nu) + c_{\text{overlap}} r_i^{(12)}(\nu) + cx_1 r_i^{(1)}(\nu) + cx_2 r_i^{(2)}(\nu)$$



BT1231 for nighttime 03/11/11 AIRS observations



BT PDFS ocean 1231 cm^{-1} channel for the 03/11/2011 AIRS observations

Conclusions

Conclusions

- Accurate Radiative Transfer needed for weather and climate
  - number of layers (more layers, more accurate, slower)
  - spectroscopy (most gases : voigt; CO_2, CH_4 needs line mixing)
  - new line shapes being used (speed dependent voigt)
- Monochromatic line-by-line codes are very accurate
  - Accuracy does depend on the lineshape used
  - Can take minutes/gas for a 25 cm^{-1} interval
- Pseudo line-by-line codes are quite accurate
  - kCARTA optimized to be accurate enough for current generation high spectral sounders $R_i^{calc}(\nu) = \int d(\nu) R(\nu) SRF_i(\nu)$
  - Monochromatic inaccuracies versus eg LBLRTM (0.0025 cm^{-1} spacing) can easily be reduced by using eg 0.0005cm^{-1} database (but slows down code)
  - takes about 30-45 seconds to run 605-2830 cm-1
  - can do analytic jacobians, fluxes, all sky scattering
- Sounders provide millions of daily radiance spectra
  - SARTA Fast Model takes 0.02 second/2378 channel AIRS spectrum
  - can do analytic jacobians, all sky scattering, fluxes (eg RRTM, ecRad)
- Applications to weather and climate

Public code repositories

UMBC

Matlab UMBC LBL : https://github.com/sergio66/UMBC_LBL

Matlab kCARTA : https://github.com/sergio66/kcarta

F90 kCARTA : https://github.com/sergio66/kcarta_gen

F90 SARTA : https://github.com/strow/sarta

AER

LBLRTM : https://github.com/AER-RC/LBLRTM

RRTM : https://github.com/AER-RC/RRTMG_LW

ECMWF

RTTOVS

ecRad : https://github.com/ecmwf-ifs/ecrad

NOAA GFDL

pyLBL : https://github.com/GRIPS-code/pyLBL

GRTcode : https://github.com/NOAA-GFDL/GRTCODE

and many others (eg PCRTM, OSS etc) ...

Thanks

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AIRS Science Team

Chris Hepplewhite, Steve Buczkowski

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