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The MODTRAN6 Line-By-Line Option: Band Model Validation and High Resolution Emitted and Scatter Radiance

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Presentation Outline

- MODTRAN Overview
- Line-By-Line (LBL) Motivation
- General LBL Approaches
- **MODTRAN Hybrid LBL Approach**
- **Validation against LBLRTM (AER Inc.)**
- **Validation of MODTRAN Correlated-k Algorithm**
- Radiative Transfer Details of MODTRAN LBL
- Conclusions / Continuing Activities

MODTRAN5 General Description

- Atmospheric Radiative Transfer Algorithm for computing IR / Vis / UV Transmittances, Radiances, Fluxes, … using a *Statistical* Band Model
- 0.2, 2.0, 10.0 or 30.0 cm^{-1} Spectral Resolution
  - From 0.1, 1.0, 5.0 or 15.0 cm^{-1} Band Model Bins, respectively
- Stratified Molecular / Aerosol / Cloud Atmosphere
  - Standard and Auxiliary Molecular Species
  - Standard and User-Specified Particulate Optical Properties
- Solar and Thermal Scattering
  - 2-Stream, 2-Stream scaled to DISORT, and DISORT N-Stream
  - *Statistical* Correlated-*k* Algorithm
  - Diffuse Transmittances and Spherical Albedo
- Spherical Refractive Geometry
- Multiple Spectral Convolution and Filtering Options
- Many Applications: Remote Sensing, Scene Simulation, Algorithm Development, Measurement / Data Analyses, Climate Forecasting, …

Line-by-Line (LBL) MODTRAN Motivation

- Difficult to isolate sources of discrepancies when validating MODTRAN against independent LBL models
  - Requires consistent inputs and methods
    - ✓ Pressure, temperature and density profiles
    - ✓ Column density calculations
    - ✓ **Continuum** and particular data
    - ✓ Spectral convolutions
    - ✓ …
  - Internal LBL option will provide *"common elements"*
- Many benefits
  - Accurate band model error budget estimates
  - Insight into approaches for refining the band model
  - Laser application simulations

MODTRAN6

- Primary Objective: Modernization of MODTRAN code
  - *Retain the full functionality of MODTRAN5.3 DOE*
    - *Mod5.3DOE = Mod5.3 with local gas clouds*
  - *Provide a modern architecture to improve accessibility to scientists and engineers*
    - *Modularize MODTRAN components*
    - *Improve I/O & interface including an API and full documentation*
    - *Provide parallel computing options*
  - ***Upgrade physics including adding LBL capability***

Highest Fidelity LBL (e.g. LBLRTM)

Map lineshapes out 25 cm^{-1} from line center for each molecular transition and path segment

- Molecular continua model contribution from distant lines
- Sum molecular optical depths at each spectral grid point
  - Fine gridding of Voigt function near line center
  - Coarse gridding with interpolation of Lorentzian tails
  - >10,000 lines typically contribute at each spectral point
- Sum segment optical depths to compute transmittances
- Advantages: Most accurate
  Arbitrarily fine spectral resolution
- Disadvantages: Slow
  Seldom include scattering

"Memory is Cheap" LBL Approach

Pre-compute a spectral grid of absorption cross-sections, $\sigma(\nu_i, P_j, T_k)$, for each molecular absorber

- Avoids on-the-fly access of molecular line data
- Interpolate absorption coefficients between pressure and temperature grid points
- Advantages: Very fast
- Disadvantages: Fixed spectral resolution
  Large pressures range interpolations
  Approximate Lorentz self-broadening

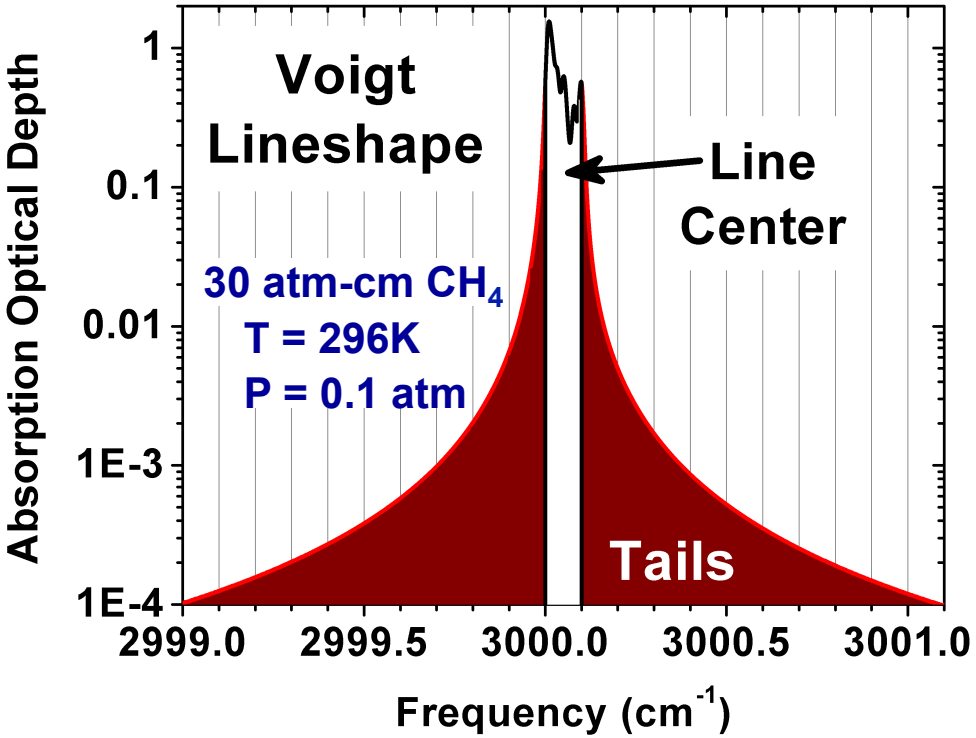
$$\gamma_L = \gamma_L^{air}\left(P - P_{self}\right) + \gamma_L^{self} P_{self} = \gamma_L^{air}\left[P + \left\langle \frac{\gamma_L^{self}}{\gamma_L^{air}} - 1 \right\rangle P_{self}\right] \equiv \gamma_L^{air} P_L$$

MODTRAN 0.1 cm^{-1} **Band Model** Absorption Components

- Since MODTRAN is a narrow band model, a large fraction **(red)** of the absorption arising from molecular transitions fall outside of the central spectral bin
- MODTRAN partitions molecular absorption contributions into 3 components:

$$t_{mol} = t_{cen}\ t_{tail}\ t_{cont}$$

- t_{cen} lines centered within the spectral bin
- t_{tail} lines centered outside of the spectral bin but less than 25 cm^{-1} from line center
- t_{cont} distant lines, centered >25 cm^{-1} from line center



MODTRAN Band Model
Line Tail Padé Fits

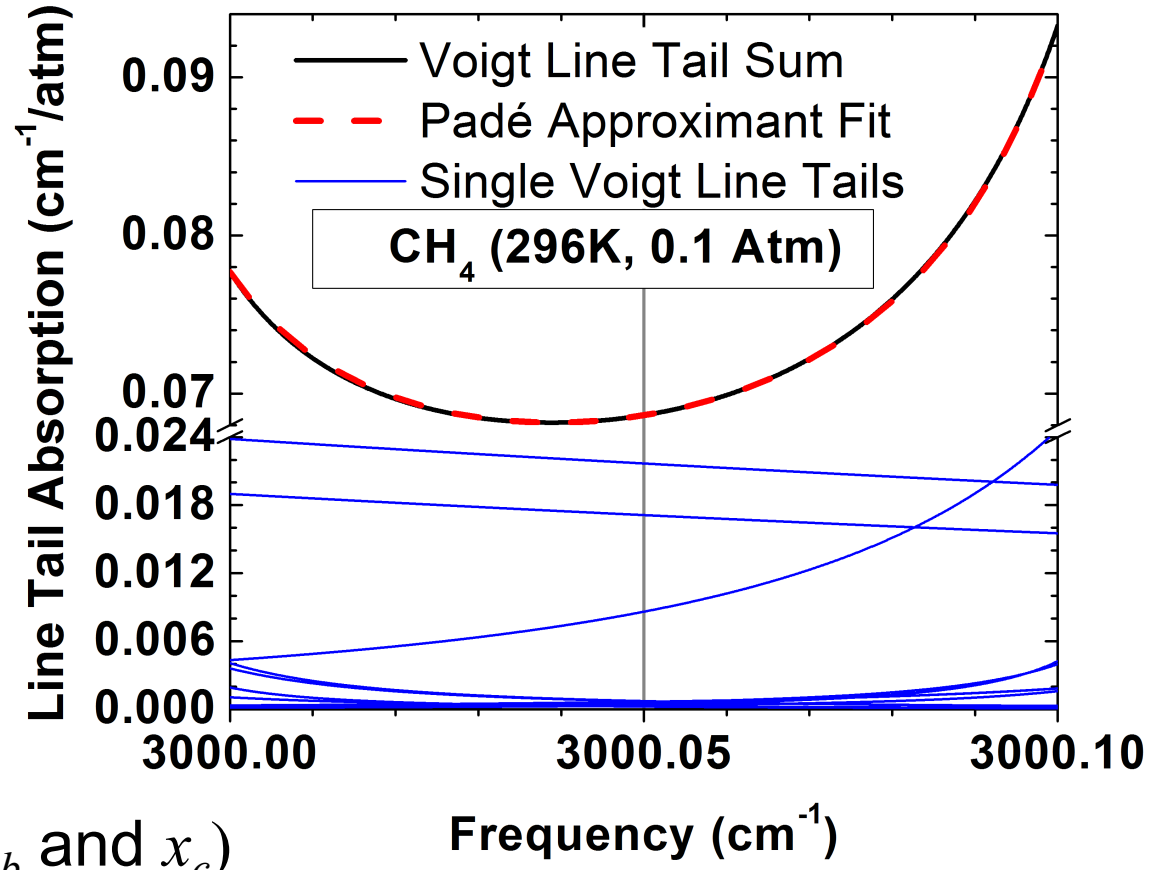
- Line tail cross-section fit to a [2,2] Padé approximant

$$\sigma_{\delta_\nu} = \frac{\sigma_a + \sigma_b\,\delta_\nu + \sigma_c\,\delta_\nu^{\,2}}{1 + x_b\,\delta_\nu + x_c\,\delta_\nu^{\,2}}$$

$$\delta_\nu \equiv \frac{\nu - \bar{\nu}}{\Delta\nu/2}$$

Centers offset from edge

Store $\sigma_{\delta\nu}$ over pressure



- 5 P,T dependent Padé parameters (σ_a, σ_b, σ_c, x_b and x_c) determined from calculated values for σ_0, $\sigma_{\pm1}$, σ_0', $\int_{[-1,1]} \sigma\, d\delta_\nu$

At most one minimum; excellent spectral fits; exact for single Lorentz.

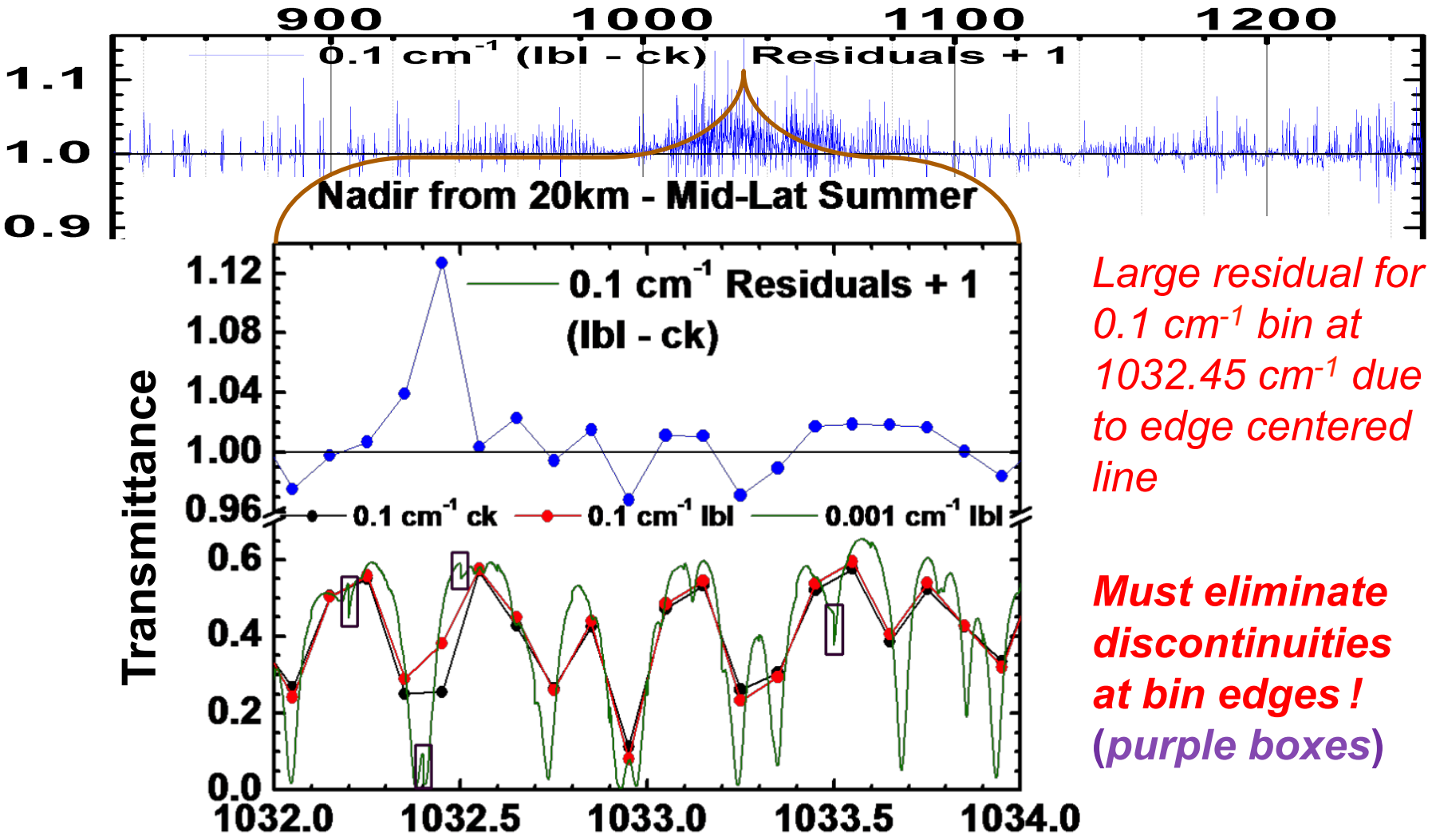
MODTRAN Hybrid LBL Approach

Compute LBL spectrum one 0.1 cm^{-1} bin at a time

- Use highest fidelity approach for *line center* contributions
- Use analytic Padé fits for *line tail* contributions
  - User specified spectral resolution, i.e. number of sub-bin points (default = 100)
  - Pre-store all candidate lines for each bin (up to ~4,400 lines) including pressure and temperature line center shifting
- ***Anticipated*** Advantages: Fast with LBLRTM accuracy
  Full suite of MODTRAN outputs
  DISORT scattering option
- ***Possible*** Disadvantages: Spectral discontinuities at 0.1 cm^{-1} boundary

MODTRAN LBL Option

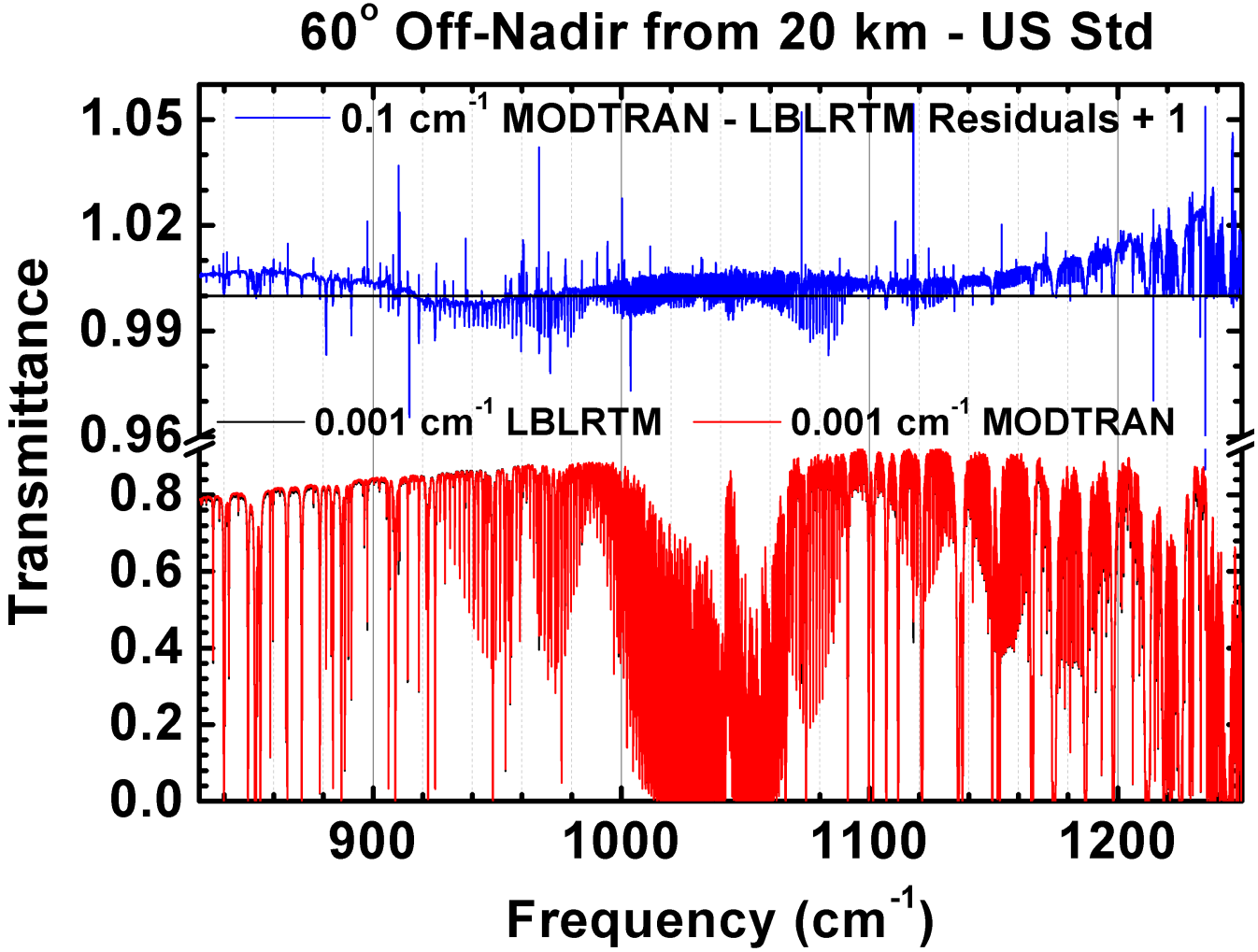
Initial Implementation



Large residual for 0.1 cm^{-1} bin at 1032.45 cm^{-1} due to edge centered line

Must eliminate discontinuities at bin edges ! ***(purple boxes)***

MODTRAN LBL Option
Validation against LBLRTM



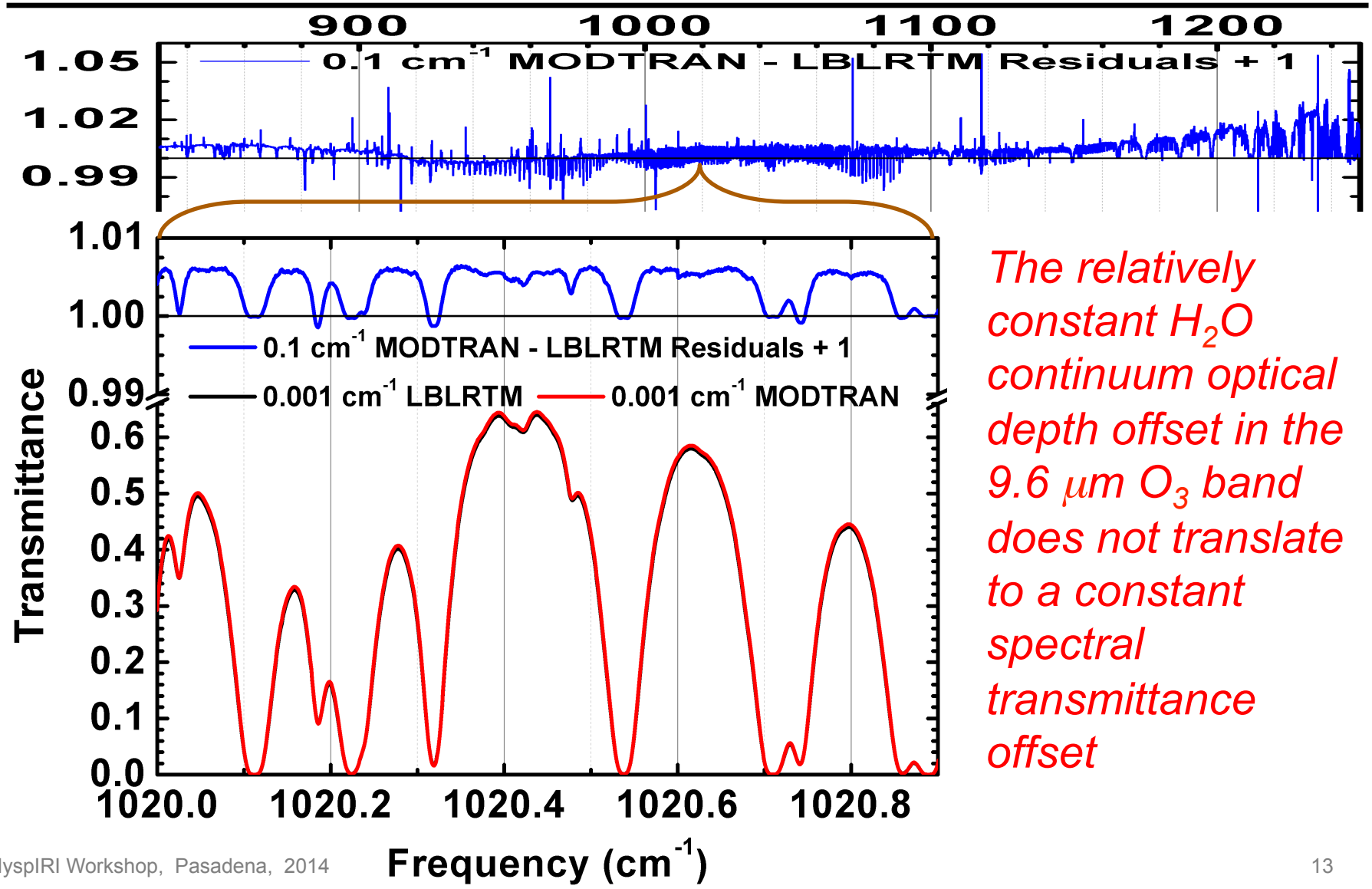
Differences in H_2O continuum lead to baseline discrepancies

Questions:

- *What is the source of the hash in the 9.6 μm O_3 band?*
- *What is the source of the spikes?*

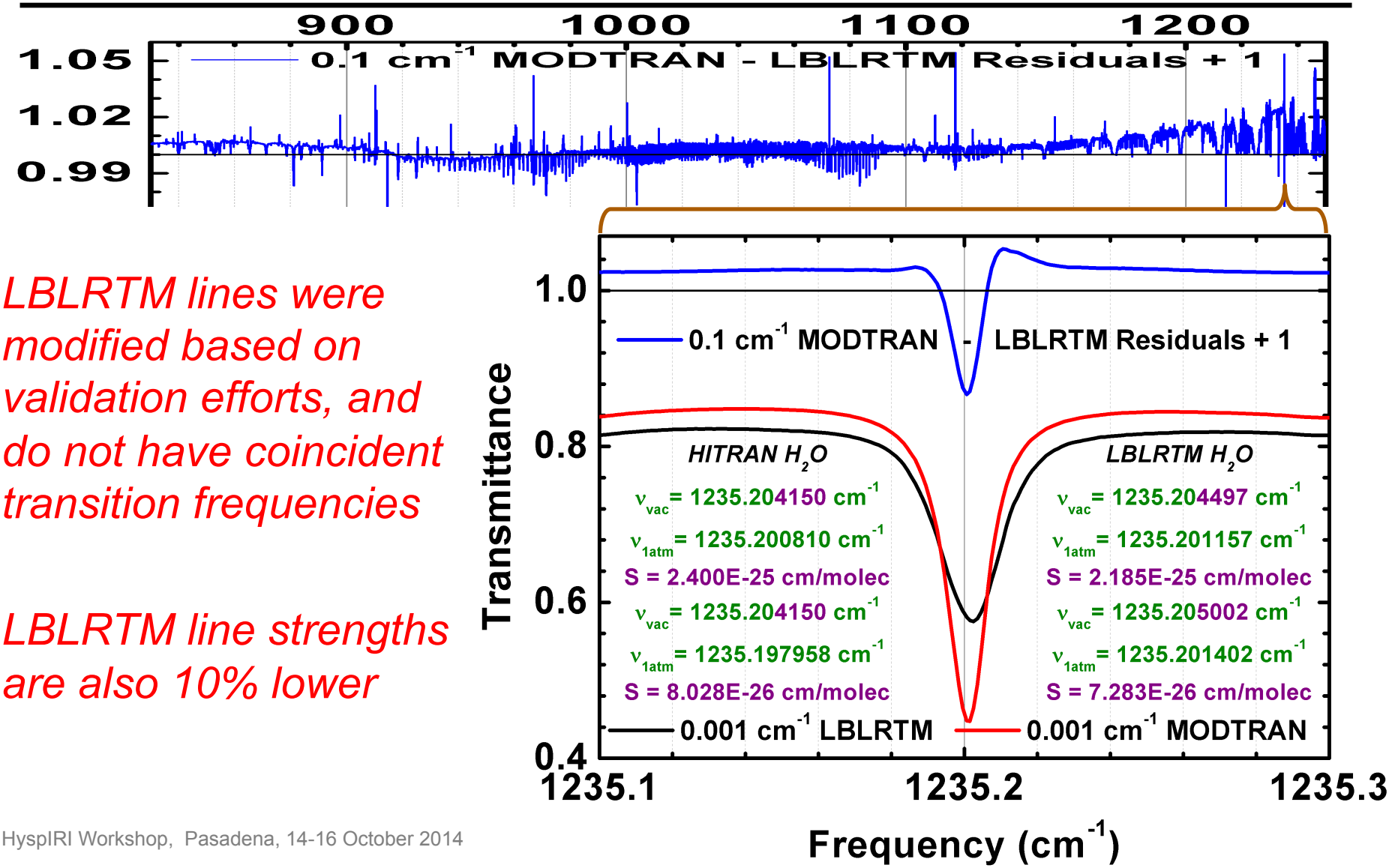
MODTRAN LBL Option

Validation against LBLRTM



The relatively constant H_2O continuum optical depth offset in the 9.6 μm O_3 band does not translate to a constant spectral transmittance offset

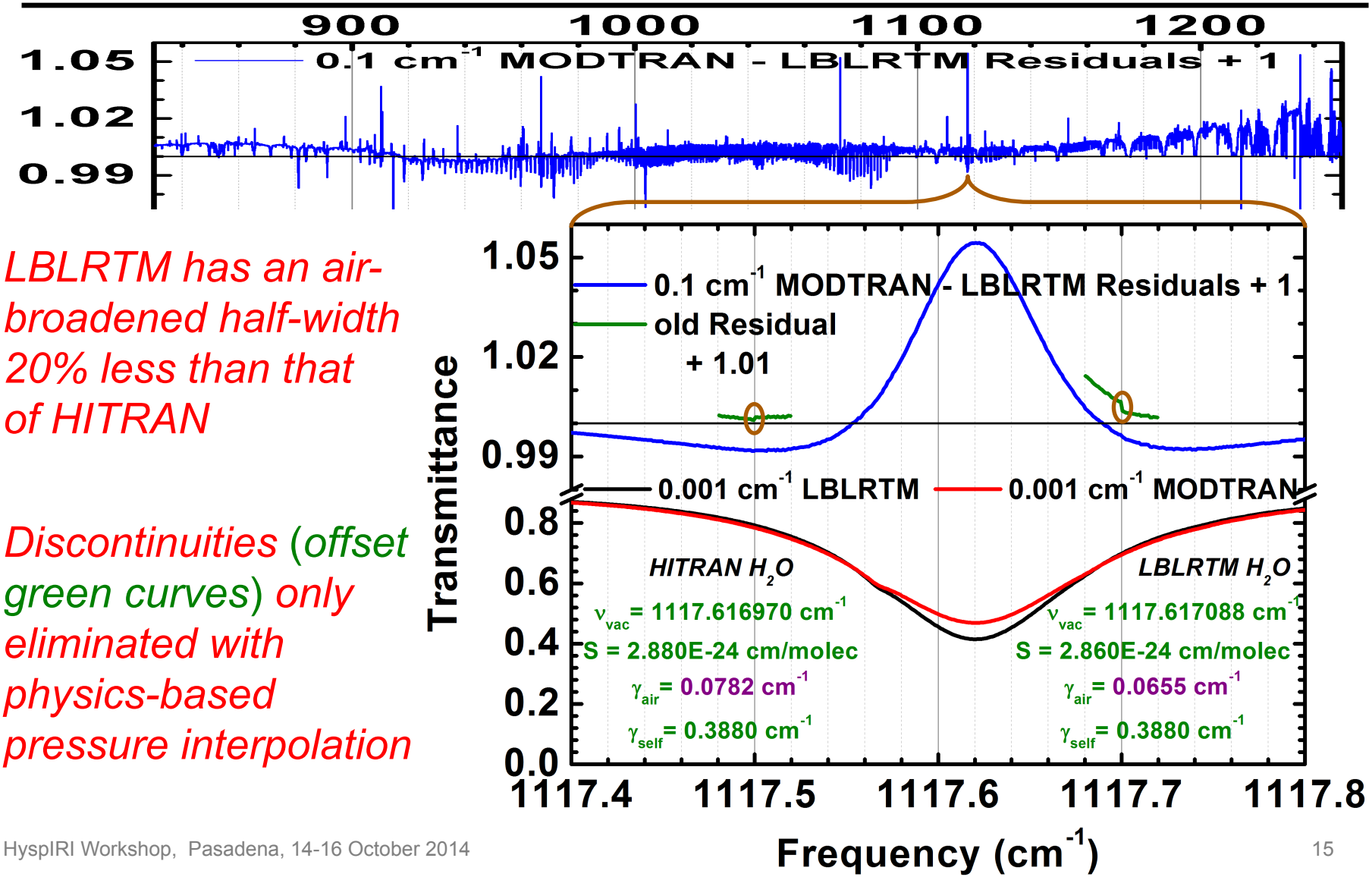
MODTRAN LBL Option
Validation against LBLRTM



LBLRTM lines were modified based on validation efforts, and do not have coincident transition frequencies

LBLRTM line strengths are also 10% lower

MODTRAN LBL Option
Validation against LBLRTM

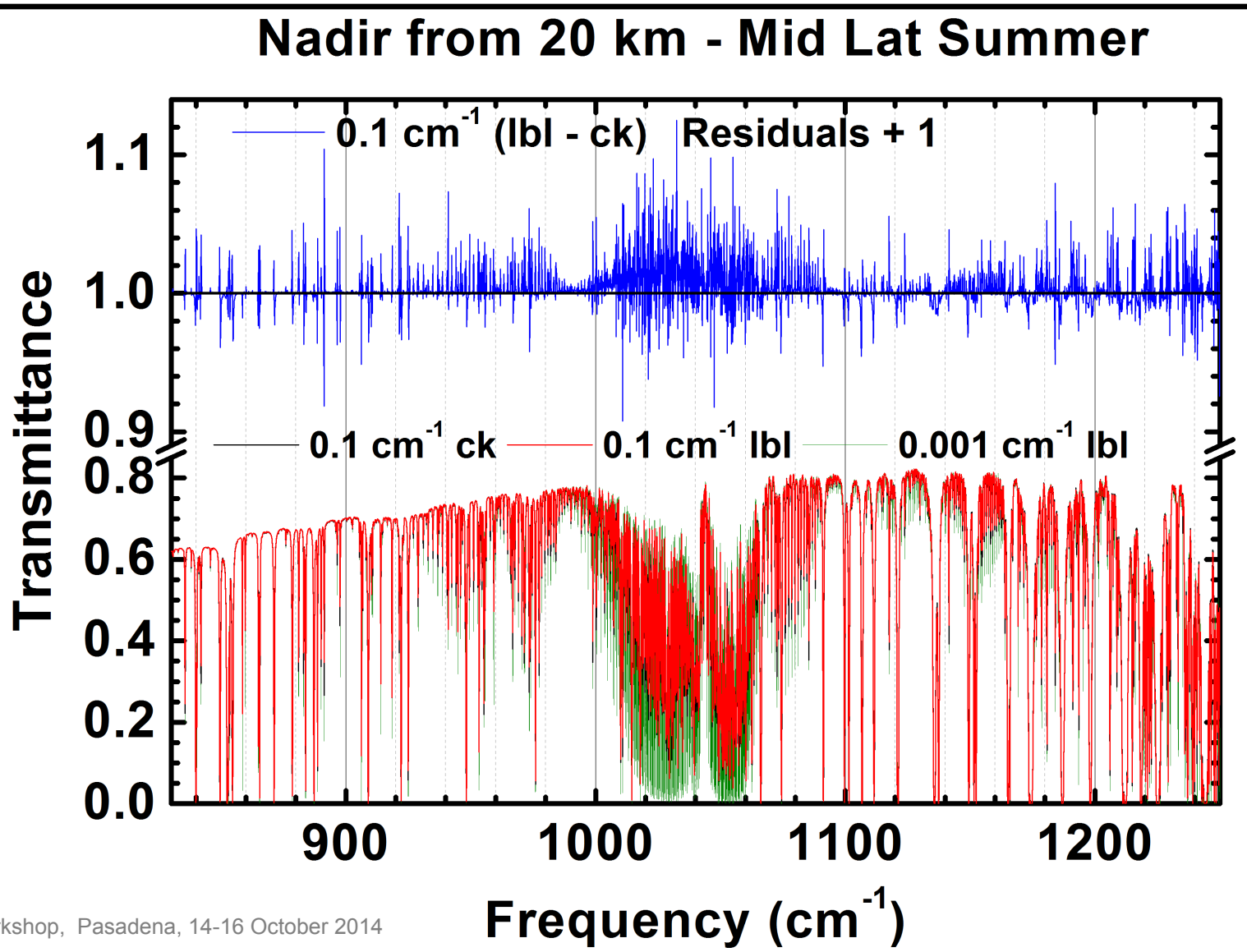


LBLRTM has an air-broadened half-width 20% less than that of HITRAN

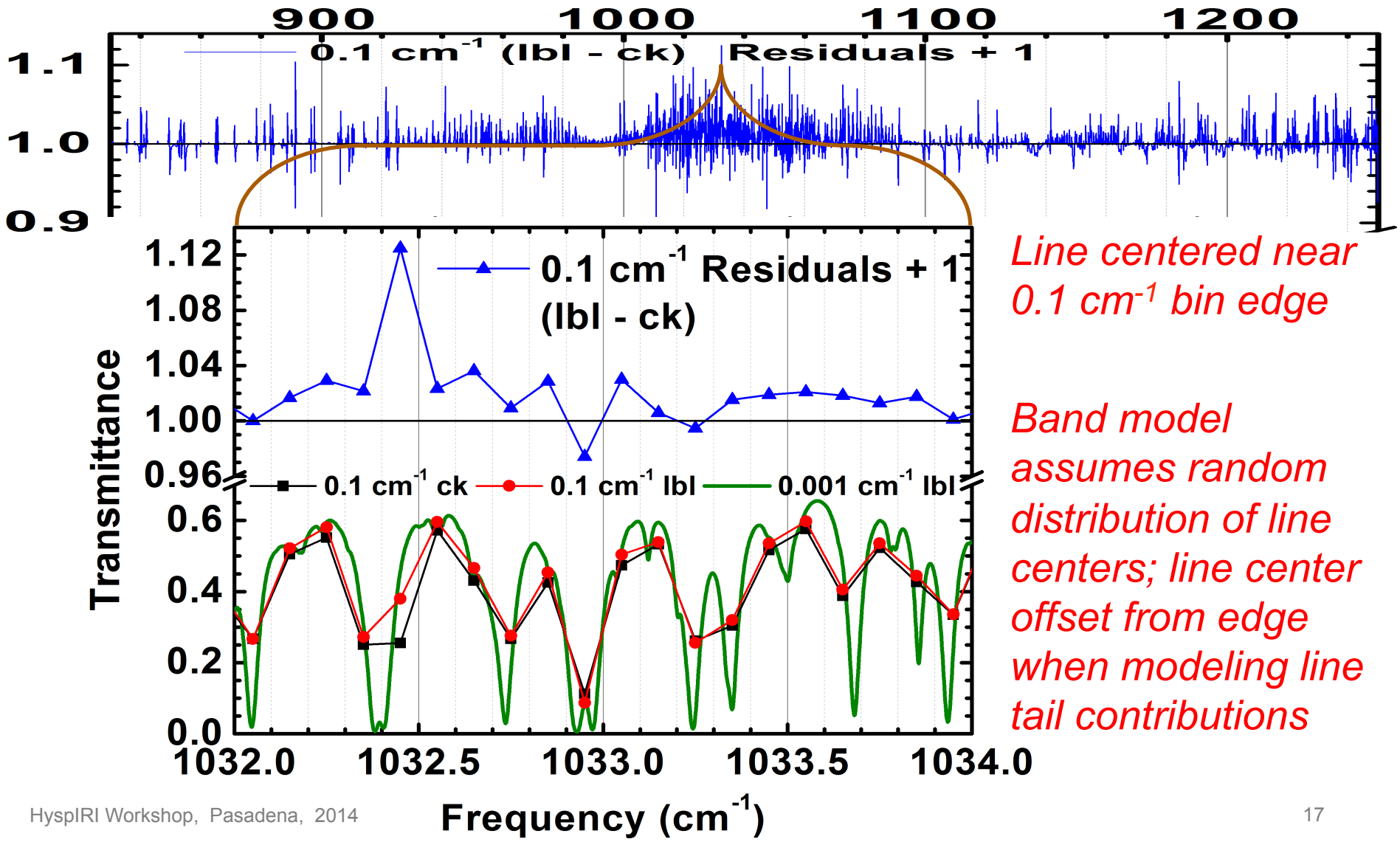
Discontinuities (offset green curves) only eliminated with physics-based pressure interpolation

MODTRAN LBL Option

Validation of Correlated-k (ck)



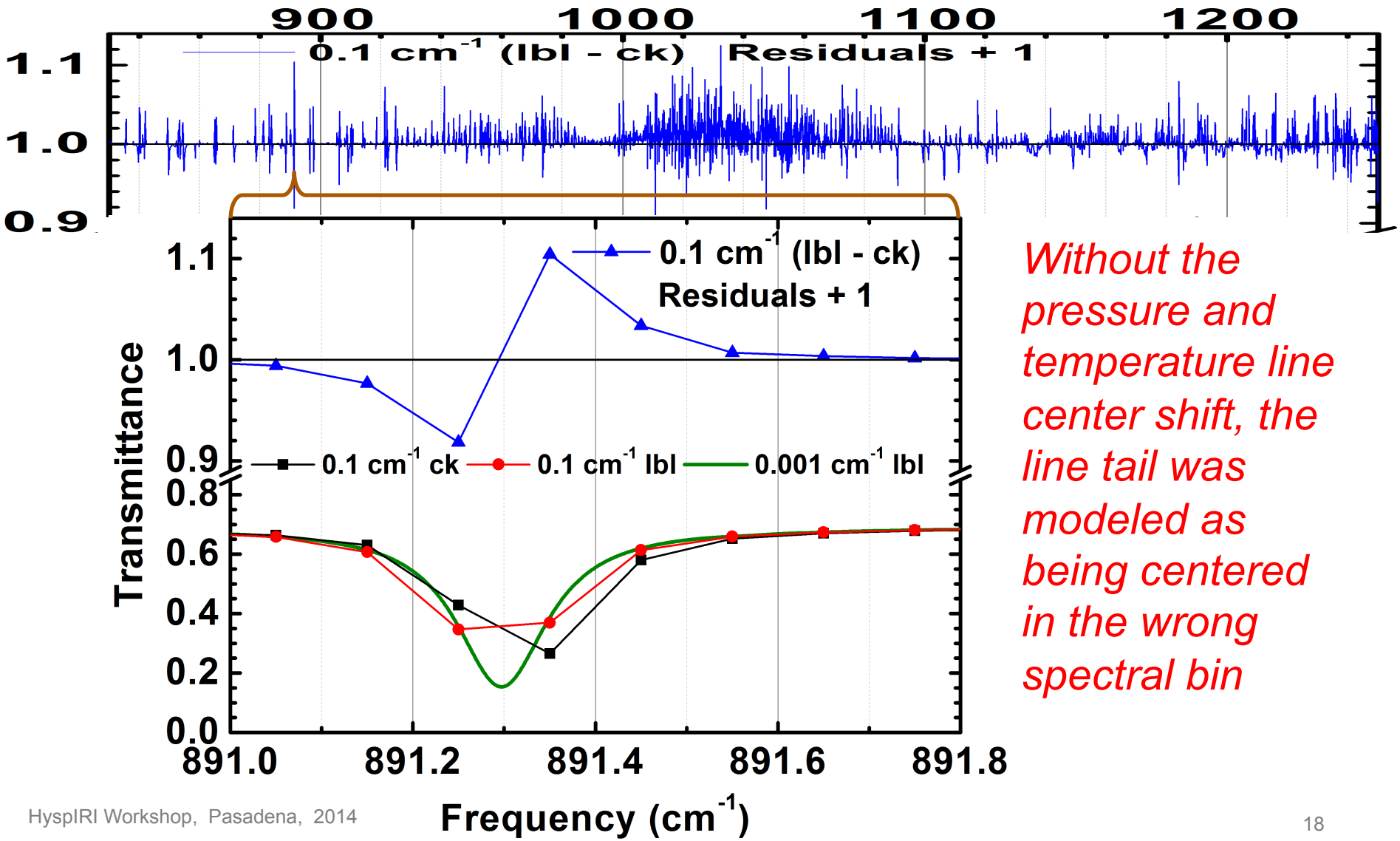
MODTRAN LBL Option
Current Implementation



Line centered near 0.1 cm^{-1} bin edge

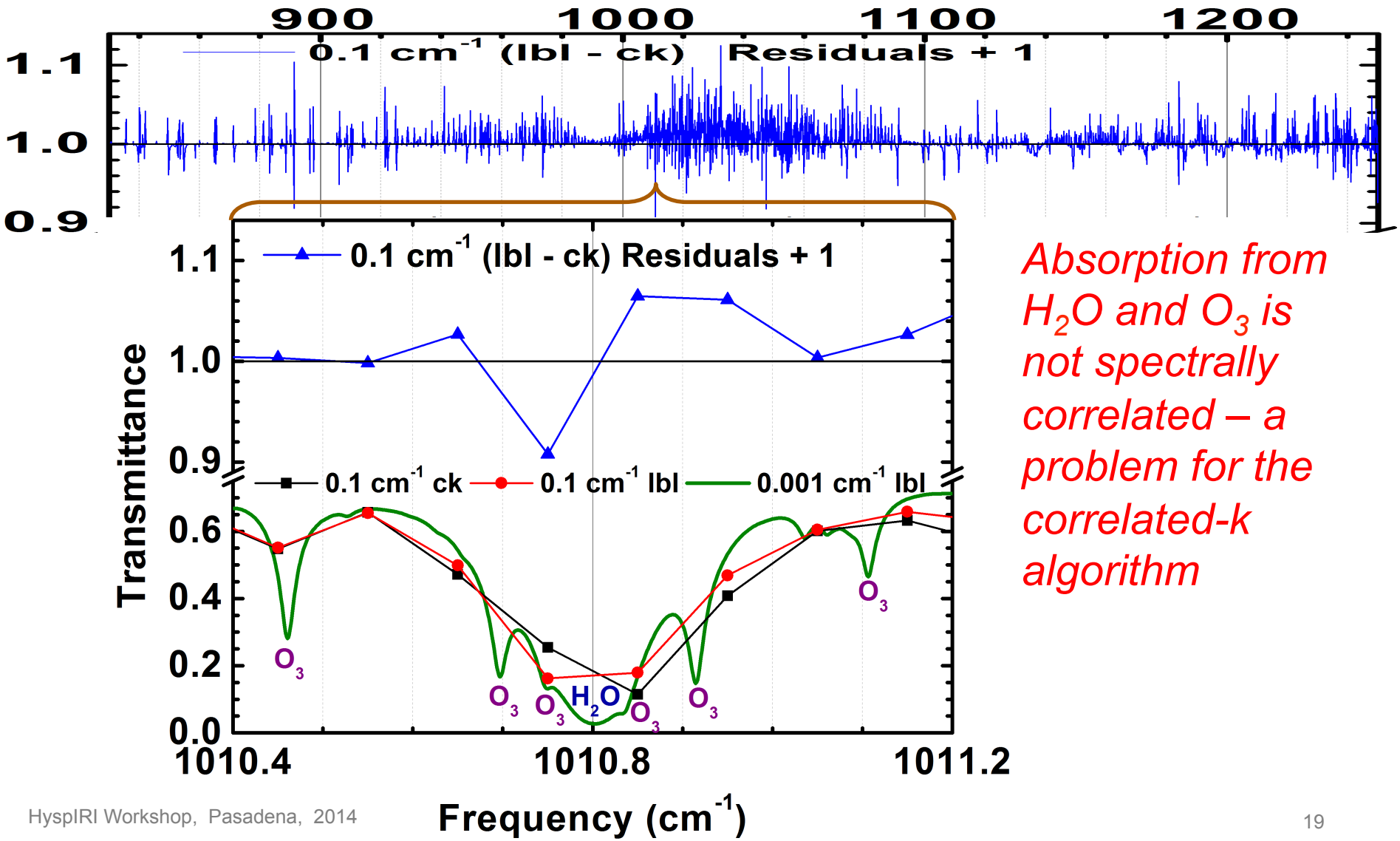
Band model assumes random distribution of line centers; line center offset from edge when modeling line tail contributions

MODTRAN LBL Option
Current Implementation



Without the pressure and temperature line center shift, the line tail was modeled as being centered in the wrong spectral bin

MODTRAN LBL Option
Current Implementation



Absorption from H_2O and O_3 is not spectrally correlated – a problem for the correlated-k algorithm

MODTRAN LBL Approach: The two-bin correction

- Problem: Padé fit of line tails not as accurate if line is centered too close to bin edge
- Solution: Explicit *line center* calculations performed over *two* 0.1 cm^{-1} bins for each molecular transition.
  - Eliminates need to off-set lines from bin edges
  - Bin pair pre-assigned to each line based on the range line center position:

$$\nu_0(P,T) = \nu_{vacuum} + \nu_{shift}\left(\frac{P}{1\,atm}\right)\frac{296K}{\max(T,180K)}$$

  - Extreme values chosen as ν_{vacuum} and $\nu_{vacuum} + \nu_{shift}\,\frac{296K}{180K}$
  - Line tails re-calculated based on two-bin model

MODTRAN LBL Approach:
Lorentz self-broadening correction

- Problem: No self-broadening in line tails calculations
- Solution: Correct for self-broadening using the effective "*Lorentzian pressure*": $P_L \equiv P + \left(\gamma_L^{self} / \gamma_L^{air} - 1\right) P_{self}$
  - For each spectral bin and molecule, line-tail strength averaged $(\gamma_L^{self} / \gamma_L^{air} - 1)'$s are included in line-tail data file
  - In practice, line tail absorption cross-sections, σ, often dominated by a single, nearly Lorentzian line, j:

$$\frac{\sigma(P,T)}{P} \approx \frac{\gamma_{L,j}^{air}}{\left(\nu - \nu_{0,j}\right)^2 + \left(\gamma_{L,j}^{air} P\right)^2} + \left(small \sum_{i \neq j} \frac{\sigma_i(P,T)}{P} \right)$$

  - The $P_k/\sigma(P_k, T)$ are interpolated as varying linearly in P^2

$$\left\{P_k^2\right\} = \left\{0.010\ \text{atm}^2, 0.505\ \text{atm}^2, 1.000\ \text{atm}^2, 1.495\ \text{atm}^2\right\}$$

Conclusions
Continuing Activities

- Fidelity of MODTRAN LBL validated against LBLRTM
  - *Successfully eliminated all bin edge discontinuities*
  - Processing will be accelerated by replacing Voigt lineshape calculation with Lorentz when appropriate
- Correlated-*k* routines will be mimicked to generate radiances
- Many model updates resulting from validation efforts
  - Integrate LBLRTM's H_2O continuum into MODTRAN
  - Provide option to use the LBLRTM lines file
  - For BAND MODEL
    - Eliminate or revise line center offsetting
    - Include line shift correction in band model line tail calculations
    - Update line tail pressure interpolation algorithm
    - Add self-broadening correction