Non-LTE, line mixing, and related improvements of ARTS

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List of features added

- Non-Local Thermodynamic Equilibrium
- Line Mixing
- Lineshape beyond Voigt
- Other stuff

Introducing NLTE in ARTS

- NLTE in ARTS means that the radiative transfer can be computed when the state distribution of a molecule is in a known state away from from LTE
  - No computations of this state in ARTS
  - Only supports vibrational NLTE (at this time)
- Formalism change:
  - Old single layer clear-sky transfer: $\vec{I}_1 = \bar{\mathbf{T}}\vec{I}_0 + (\mathbf{1} - \bar{\mathbf{T}})\vec{\bar{B}}$
  - New single layer clear-sky transfer: $\vec{I}_1 = \bar{\mathbf{T}}\vec{I}_0 + (\mathbf{1} - \bar{\mathbf{T}})\left(\vec{\bar{B}} + \bar{\mathbf{K}}^{-1}\vec{\bar{S}}\right)$

    (We are trying to unify clear-sky and scattering-sky calculations in Hybrid to use similar formalism. This could lead to updates in other iy-methods)

Using NLTE in ARTS

- Provide vibrational temperature profiles (array of same data-type as the temperature field)
- Match those profiles to energy levels (vector of vibrational state energies, and array of matching vibrational state identifiers)

Introducing Line-Mixing in ARTS

- Line mixing in ARTS means that the mixing of state distributions within a single band can be accounted for, provided necessary data is available (or derivable)
- There are 3 separate line mixing implementations in ARTS
  1. Old-and-tested: Full model computations
  2. Well-tested: input should consist of the first- or second-order perturbation parameters on line-by-line basis
  3. Experimental: input pure HITRAN data and ARTS will attempt to compute the line mixing of the matched bands
- Formalism change:
  - Old way: $\mathbf{K} = \sum_j S_j F_j(f) \mathbf{P}_j$
  - New way 1: $\mathbf{K} = \sum_j (1 - i \cdot y_j \cdot p + g_j \cdot p^2) S_j F_j(f, \delta f_j \cdot p^2) \mathbf{P}_j$
  - New way 2: $\mathbf{K} = \sum_j \mathtt{Tr} \left(\mathbf{S}_j \left[\mathbf{1} f - \mathbf{f}_{0,j} - i \cdot p \cdot \mathbf{W}_j \right]^{-1} \right) \mathbf{P}_j$

    (Second method is the one that is reduced to first using perturbation theory)

Using Line-Mixing in ARTS 1

- The line mixing parameters must be available in the input line parameter catalog. Supported formats are
  - The ARTS line catalog with appropriate LM-tag (ARTSCAT-5)
  - The AER/LBLRTM line catalog
- If you do not want to dig into details here but need line-mixing, I recommend using the AER/LBLRTM catalog for easiest approach
  - Advice will change once Alex test is done
  - Use strict altitude limits with AER/LBLRTM
  - ARTS cutoff implementation is incompatible for line mixing
  - If you update any line parameters, recompute the line mixing

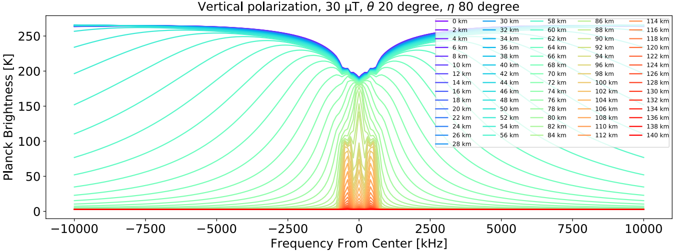
Using Line-Mixing in ARTS 2

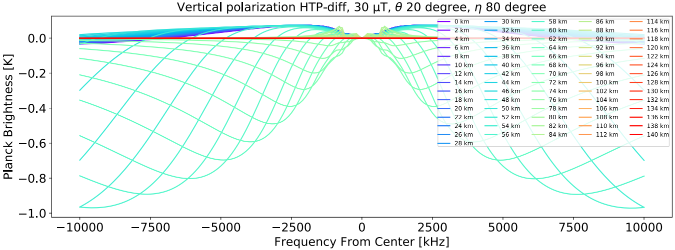
- Relaxation matrix computation software developed by T. Mendaza is included in ARTSas experimental feature
- The software takes pure HITRAN data and computes the sudden collision error-correction relaxation matrix (based on work by Niro etal 2004, and on her own theoretical work)
- Its advantage over the precomputed parameters is that it will adapt to changes in other catalog parameters
- Its disadvantage is that the standalone computations are very very slow
- Still work in progress, but hopefully ready soon

Introducing Hartmann-Tran Line Shape in ARTS

- HTP in ARTS means that lineshapes beyond Voigt and its predecessors are available
- There is only experimental support for HTP
- Formalism change:
  - Voigt: $F(\nu) = f(\Gamma_0, \delta f_0, \Gamma_D) = w(z)/\sqrt{pi}\Gamma_D$
  - HTP: $w(z)/\sqrt{pi}\Gamma_D; F(\nu) = f(\Gamma_0, \Gamma_2, \delta f_0, \delta f_2, \eta, f_{VC}, \Gamma_D) = ...$ (Too long an expression for a simple overview formulation)

Example (continua missing)





Using HTP in ARTS

- You cannot...
- Support is available in the theory by applying the HTP line shape and inputting the data into your ARTSCAT-5 line catalog file

Introducing other things in ARTS

- Partition functions can now be added manually rather than presumed from inbuilt Errors of few degrees experienced just in the test files. No attempts made to find extremes
- Deep analytical Jacobian makes line parameter partial derivatives accessible to user
- We have a new PropagationMatrix class in ARTS that solves matrix exponent 30x times faster (and its partial derivatives equally much faster). Credit to Philippe Baron for this
- ARTSCAT-5 line catalog format allows for easy feature testing/adding

Future problems

- Pressure retrievals
- Isotopologue ratio profiles
- Getting the untested things verified
- (Breaking more control-files)
- Subsurface water retrievals with RADAR (in ARTS if possible once done — little work done so directions appreciated)

Questions?

Talk to me if you are interested in any of these features/bugs!