Potential dramatic decrease of the molecfit\_model execution time

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# Introduction

So far, molecfit\_model execution time has been a major limitation to the recipe. It is dominated by the calls to the radiative transfer code, LBLRTM, which take place each time that the abundance of a molecule is changed. In fact, for each change of molecular abundance, LBLRTM is currently called (twice + once per molecule to be fitted) for each region: one to determine the new transmission spectrum, and twice to determine the derivative relative to the relative column density (once with unperturbed parameter used for each derivative, and once per molecule with perturbed parameter). An effort is already on-going to decrease the number of calls to only once per molecule to determine the derivative.

However, there is a much more efficient way which I feel ashamed not to have identified earlier: if the following is correct, it should limit the number of calls to LBLRTM to just once per molecule and per region (in absence of line coupling)!

# Using optical depths

To focus on the method, let’s assume a single atmospheric layer. The transmission spectrum, , is related to the optical depths for the molecule by the relation

, (Eq. 1)

where is the number of molecules relevant in the region being considered.

Note that a simplification here is the impact of the line coupling, which we should deal with later. The optical depth for each molecule is given by

(Eq.2)

where is the column density of molecule in the atmospheric layer, and , its wavelength-dependent cross-section. We can rewrite Eq. 2 as:

(Eq.3)

where is the column density of molecule for the chosen reference atmospheric profile, and is the relative column density. The latter is the quantity that molecfit\_model actually determines. If one now defines the optical depth for the reference atmospheric profile, then Eq. 1 can be rewritten as:

(Eq. 4)

Molecfit\_model requires the derivative of relative to , that is:

= - = - (Eq. 5)

In other words, Equation 4 and 5 mean that if one can obtain the optical depth spectrum for the reference abundance profile for each molecule separately, then one can calculate

1. the transmission spectrum for any value of the relative column density of each molecule ,
2. the derivative relative to , , for any molecular abundance.

In other words, LBLRTM would need to be called only once per molecule and per region!

# Changes to molecfit\_model

To implement this method, the following changes need to be done to molecfit\_model:

1. LBLRTM should produce optical depths instead of the transmission spectrum. This can be done by changing the 4th parameter (IEMIT) of the 1st line of TAPE5 from 1 to 0.
2. For each region, LBLRTM should be called once at the start of molecfit\_model for each selected (not necessarily to be fitted) molecule individually and the results of each molecule stored.
3. For each molecule to be fitter, mpfit should call a function which calculates following (Eq.4) and its derivatives (Eq.5) from the stored , instead of LBLRTM. Once has been calculated, the derivatives for each molecule can be calculated in parallel.

## Notes:

1. Line coupling would likely involve additional LBLRTM runs for each pair of molecules involved. I have still to work this out, but it should not be too complicated.
2. LBLRTM does not process continuum absorption in a way which is consistent with our method; this requires further changes to TAPE5 but is entirely feasible.
3. This method should work for transmission spectrum. I must make sure it also works for emission spectra, relevant for L, M, N and Q bands. Hence relevant for METIS, VISIR, ERIS, CRIRES, but not used much so far.
4. Molecfit\_calctrans is not modified. Hence, the code that creates the TAPE5 file should likely receive a flag to state if the expected output is the optical depth or the transmission spectrum.

# Suggested way forward

1. A first test that the method is worth implementing is to make sure that Equation 4 holds. Hence, one should produce the transmission spectrum and the optical depth spectrum by changing the value of the IEMIT parameter (4th parameter) in TAPE5.
2. The next step is to compare the derivatives as determined by the 2 methods, both numerically and in processing time.