Surviving the flood – data analysis of maps and spectra toward line rich sources

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Goals/Context

Multi-line observations of molecular emission are an important tool for understanding the structure of star forming regions. While it has been known since a long time that many high mass star-forming regions possess very rich spectra in the millimeter/submillimeter regime (in hot cores), the discovery that also low-mass cores can have a similar number of lines (in hot corinos) is fairly recent. At the same time, new, sensitive telescopes have appeared (APEX, SMA) to be surpassed within a few years by even more powerful ones (Herschel/HIFI, eVLA and above all ALMA), so that more and more complex spectra are observed, either by design, or inadvertently.

What so far has been a somewhat eccentric hobby of a few astrochemists, line surveys, is now becoming an unavoidable byproduct of star formation research with modern instruments. With the new instruments, particularly ALMA, we will observe hundreds and thousands of hot cores and hot corinos throughout the Galaxy, with hundreds and thousands of lines each. Hundreds and thousands of maps each, if the data come from interferometers. That's a lot of information which – potentially! - tells us a lot about the source structure: temperature, density, velocity field and chemical structure. Fitting the maps and spectra – if we can do it – should constrain the free parameters of physical and chemical candidate models significantly. However, with present day tools, we only scratch on the surface. In this poster, we argue that

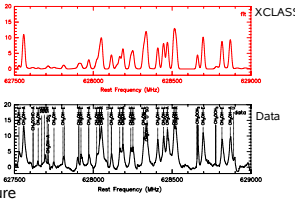
- it is a bad use of modern, sophisticated telescopes to exploit only a few percent of the information content of the data
- we can make significant progress with todays resources

Bottlenecks for analysis of line-rich spectra

- Line identification
  - Line databases incomplete
  - Lots of interstellar weed lines missing (vibrationally excited C_2H_5CN etc.)
    - this interstellar weed obscures interesting lines, so we need to remove it
- Existing Modeling tools
  - Some 1-D and few 2-D models for single molecules
  - Few 1-D LTE models for multi-molecule modeling
  - Nothing more sophisticated for multi-molecule modeling
    - Transfer: LVG, ALI, MC, CEP
    - Collision rates for many molecules not available
  - Need to be automatized to deal with large data volumes that even today are being produced
  - Close interaction with theorists
    - Star formation processes
    - Chemical processes

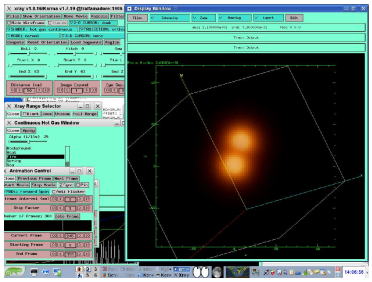
Example for 1-D multi-molecule fits: XCLASS

- Good:
  - Models all lines from catalog with LTE
  - Opacities taken into account
  - Blending taken into account
- Bad:
  - Simplistic source model:
    - Different components added in intensity
    - Very high optical depths are not well modeled
- Adequate for line identification purposes
  - Holistic approach: need to model whole spectrum
- Not good enough for modeling source structure
- Obviously completely inadequate for interferometric surveys

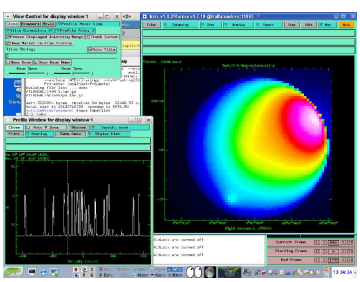


XCLASS in 3-D: myCloud

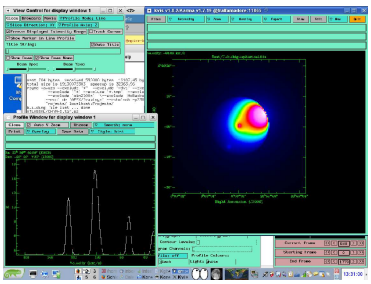
The shortcomings of `XCLASS` motivated us to build a 3-D version of it: `myCloud`. This program, like `XCLASS`, models ALL transitions of ALL molecules in a given frequency range, in the LTE approximation, but unlike `XCLASS`, it uses a source structure (temperature, density field, infall, rotation velocity field), and then does a proper radiative transfer to produce data cubes. While in principle arbitrary source structures are possible, currently we restrict ourselves to multiple spheres or disk-like structures. Comparison with the data involves folding with the instrumental response, in the case of interferometers that means using the same sampling in the *uv* plane as the data, and the same data processing. In the following, we show some screen-shots of the output products of some models.



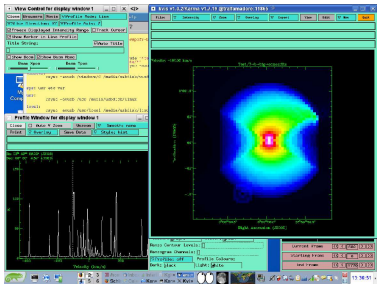
More realistic source structure. Here: temperature structure of twin cores. Visualization of the true 3-D structure is an important aspect. Here, it has been achieved with the `xray` and `kvis` programs from the `karma` suite.



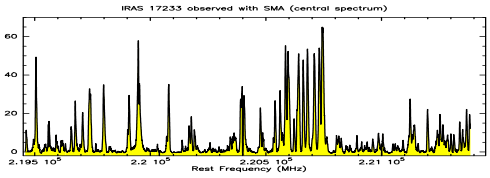
Output line data cube: spectra and channel maps of a structured source. Many molecular lines from many species have been modeled here.



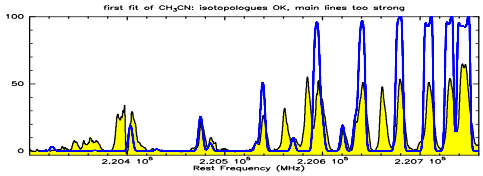
Zoom into the lines: the line shape becomes visible.



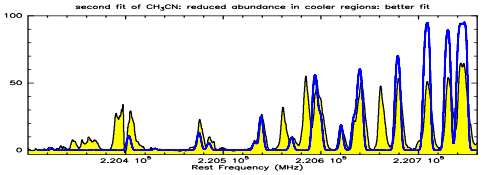
More complicated source structures like disks can be modeled.



Illustrative example with real data: SMA spectrum of IRAS 17233 (courtesy S. Leurini). ALMA will see thousands of sources like this.



First attempt at modeling CH_3CN with `myCloud`: constant abundance. While the fit of the isotopologues is not bad, it is not a good fit of low energy lines. Note: no other molecules have been modeled.



Next iteration: lower CH_3CN abundance where the temperature drops below 100 K: better, but not yet perfect fit. Further iterations are necessary, which also need to fit the spatial structures. In this particular model, the synthetic data have not been "observed" with the instrument, as they should

Where to go from here?

For many molecules it is obvious that LTE is not a good approximation. We plan to add more choices to calculation of molecular excitation: LVG, which should be adequate for optically thin lines, and CEP (coupled escape probability), which should be exact, but also more computing intensive. Since collision rates for many molecules do not exist or are not adequate (do not provide rates for all the levels we observe), modeling spectral ranges will have to employ a mixture of these methods.

Another important step is close interaction with theoreticians, to embed physical and chemical parameters into current structure models of star forming regions. This should limit the parameter space, which is too vast to be explored in a purely empirical fashion.

Outlook

- The Good:
  - New instruments are bringing, and will bring, lots of new data, which potentially can constrain models of star formation and early stellar evolution, and evolution of AGB stars, and galaxy evolution, and…
- The Bad:
  - We are lacking the tools to fully exploit these data.
- The Ugly:
  - It's a lot of work, and we haven't really started to tackle the Problem.