Analysis tools for spectral surveys

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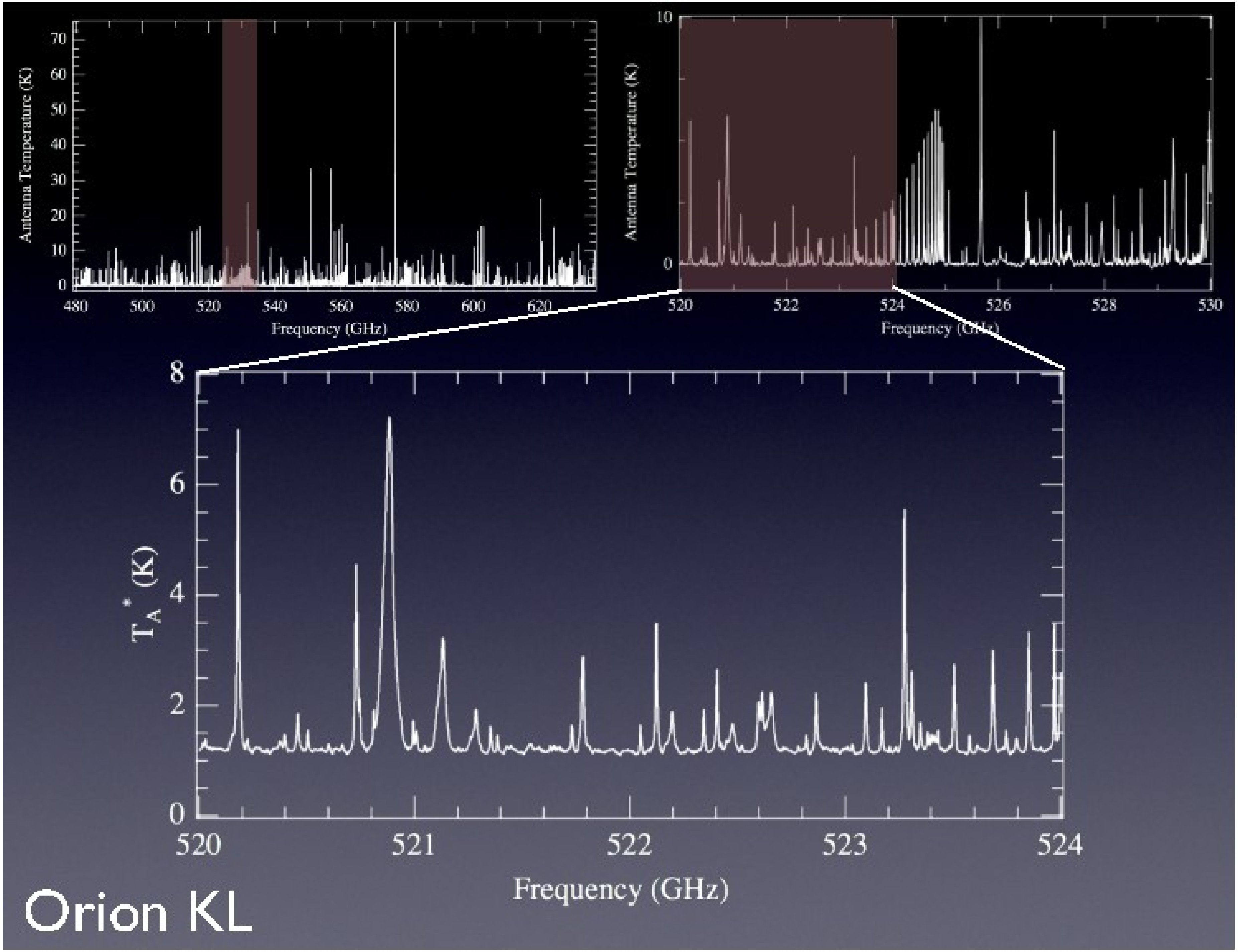
Why should you care?

- You may not want to do spectral line surveys
- You may be interested in just one line/species

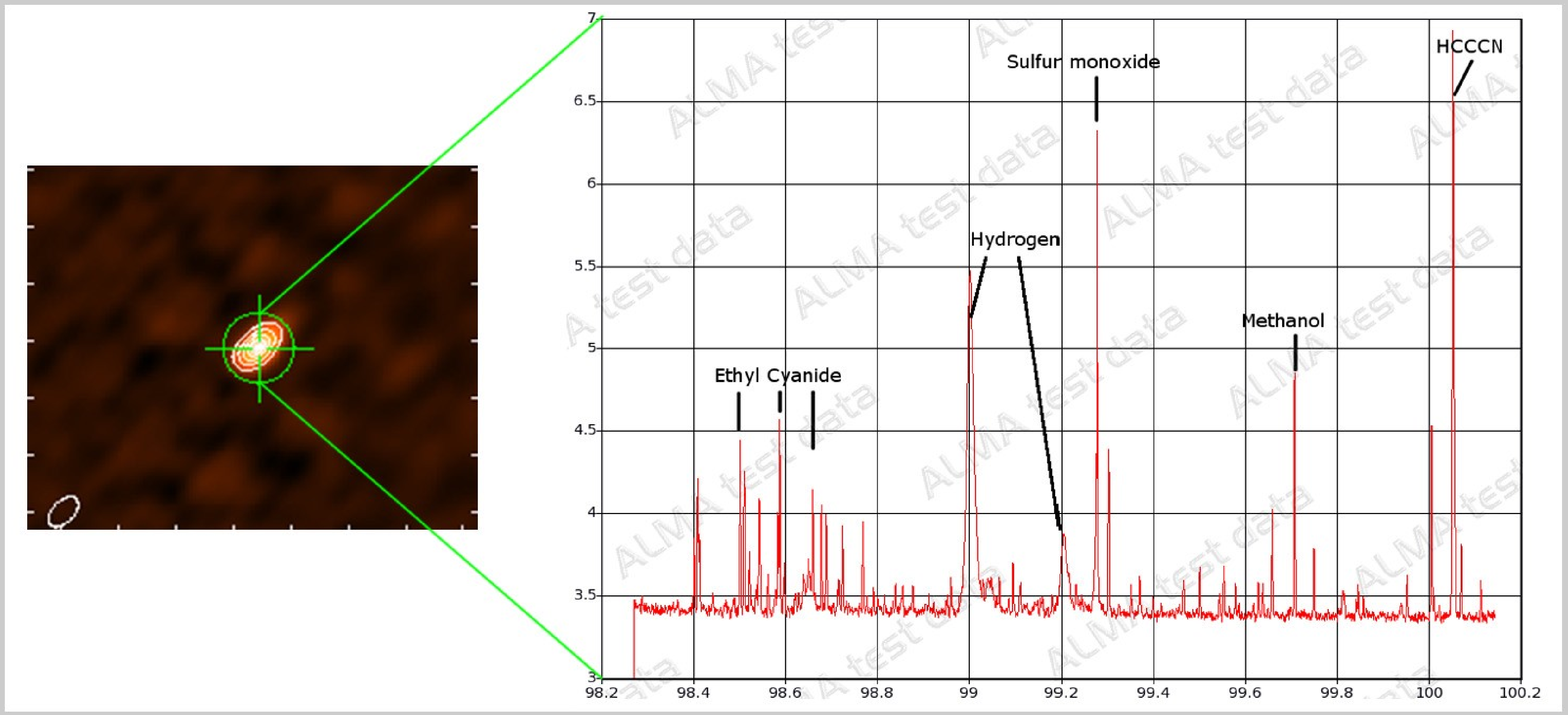
but with instruments like HIFI or ALMA

- Line surveys want you to do them
- You will (almost) always get more lines than you intended
- ...and that's a good thing!



HEXOS Orion-KL, Crockett, Bergin et al.

Typical ALMA spectrum



Fact

- With ALMA, we will see hundreds and thousands of sources with a similar line density
  - High-mass SFR
  - Low-mass SFR
  - Galactic nuclei
  - Starburst regions
- Strategy options
  - concentrate on your pet transitions and ignore 95% of the information in the spectra
    - may not be a viable option at all!
  - try to deal with it

Step back - what do we want?

- Analyze excitation of a selected set of molecules to determine source structure
- look for specific, maybe weak (new?) molecule or isomer or isotopologue
  - need weed removal, but
    - before you kill something, you have to understand it
  - or
- you want to analyze the chemistry, i.e. you want to know the abundance distributions of a lot of species

So...

- In most cases, you have to go through the sequence

Taking stock:
Line identification
→
De-weeding:
Removing of unwanted lines
→
Analysis of wanted lines

Steps forward

- Knowing what's there: Line Identification
  - Tools
    - XCLASS
      https://www.astro.uni-koeln.de/projects/schilke/XCLASS
      based on GILDAS CLASS package
    - CASSIS
      http://cassis.cesr.fr/?page=cassis
      can be used with HIPE or as standalone package
    - Weeds
      included in GILDAS package

Molecular data: catalogs

- Molecular parameters
  - Cologne Database for Molecular Spectroscopy
  - JPL database
  - Splatalogue

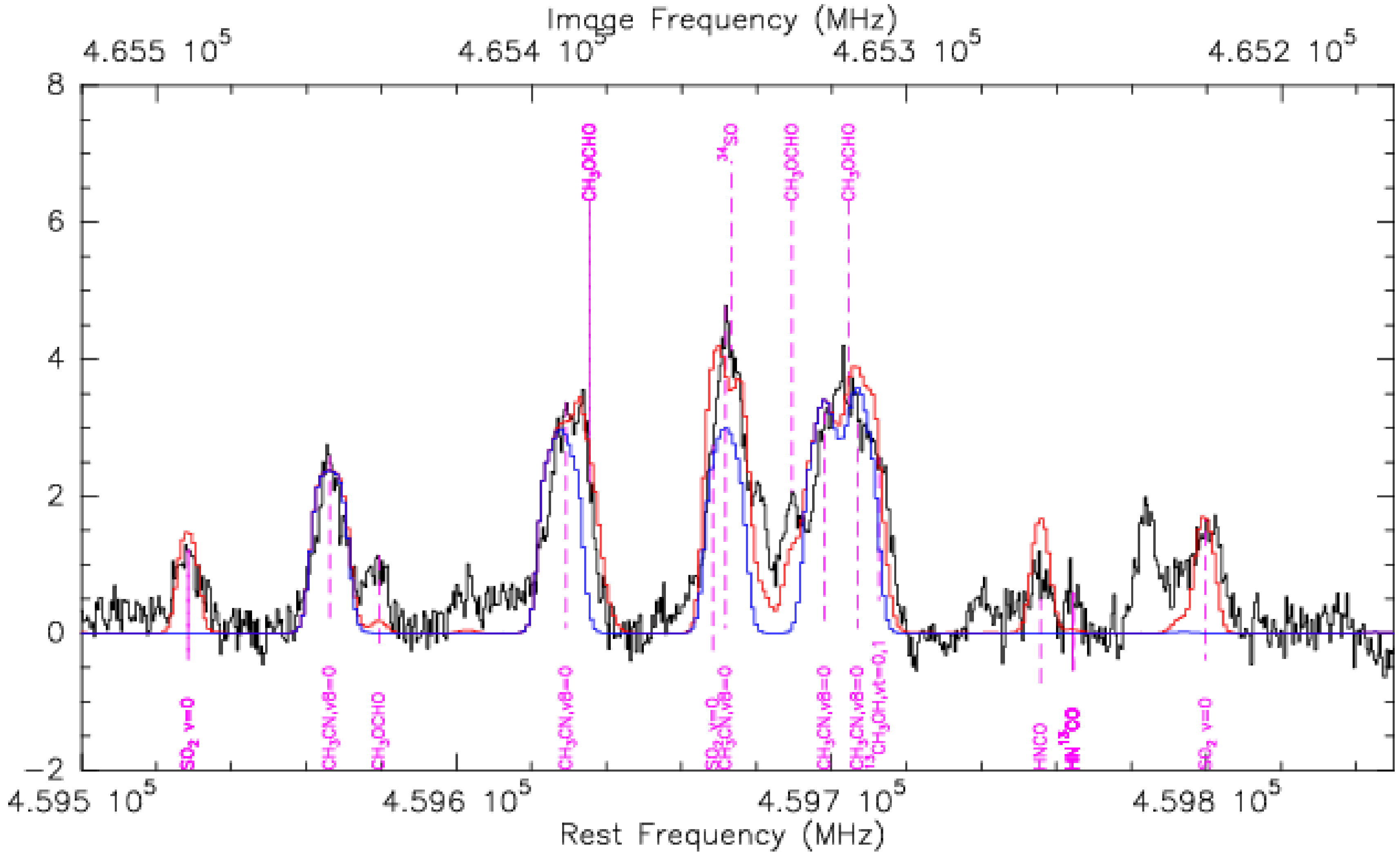
    Compilation of CDMS and JPL with a few extra entries
- Collision rates
  - BASECOL
  - LAMDA
- Chemical rates
  - KIDA, UMIST, OSU

Line Identification and Analysis

- In line rich sources, line identification of any line (except the strong, boring ones) requires a good model of the *whole* spectrum because of blending
  - it requires understanding the excitation and abundances of all species
  - only this gives an idea of how well the spectrum is known
  - including isotopologues (important to constrain optical depths)
- Holistic approach adopted by HEXOS and CHESS GT KPs for
  - Orion, SgrB2(M), SgrB2(N), NGC 6334(I)

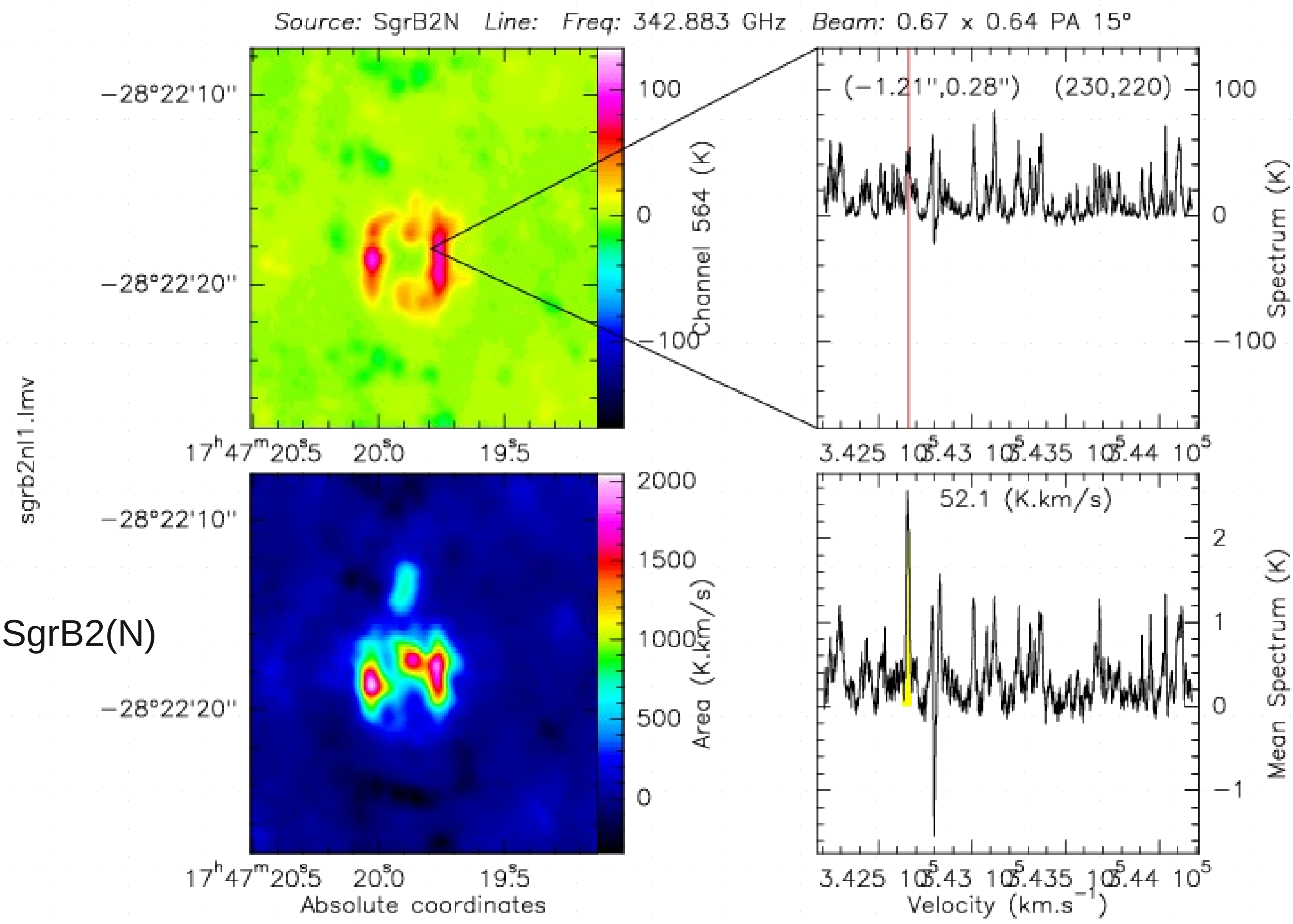
blue: CH_3CN

red: all species



Any attempt to identify any single line or species or to understand the excitation of any single species in a line rich source is ***futile***.

But ALMA will produce Data Cubes



SMA data of SgrB2(N)

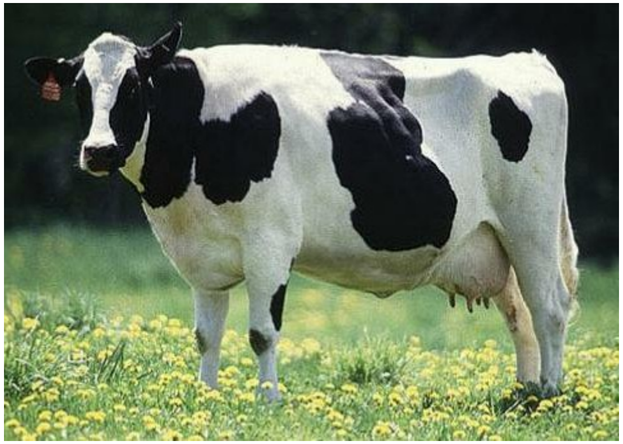
Consequences

- New instruments, particularly ALMA, will produces data in large quantities, and with high quality that demand better modeling then we are used to now
- Multi-line studies will be very common
- Need to take source structure into account
- XCLASS and friends are OK for identification, but far too primitive for any in-depth analysis
- Same is true for single-component LVG models

⇒ 3-d modeling is eventually required

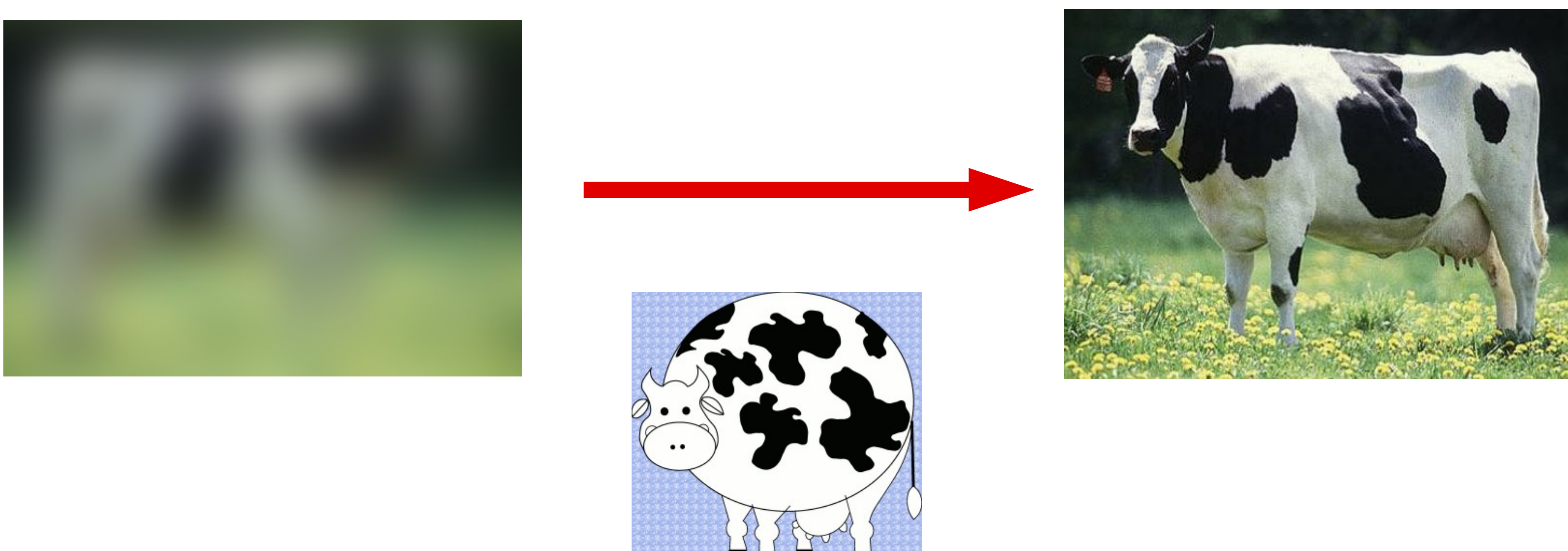
Interferometry requires

full structure modeling



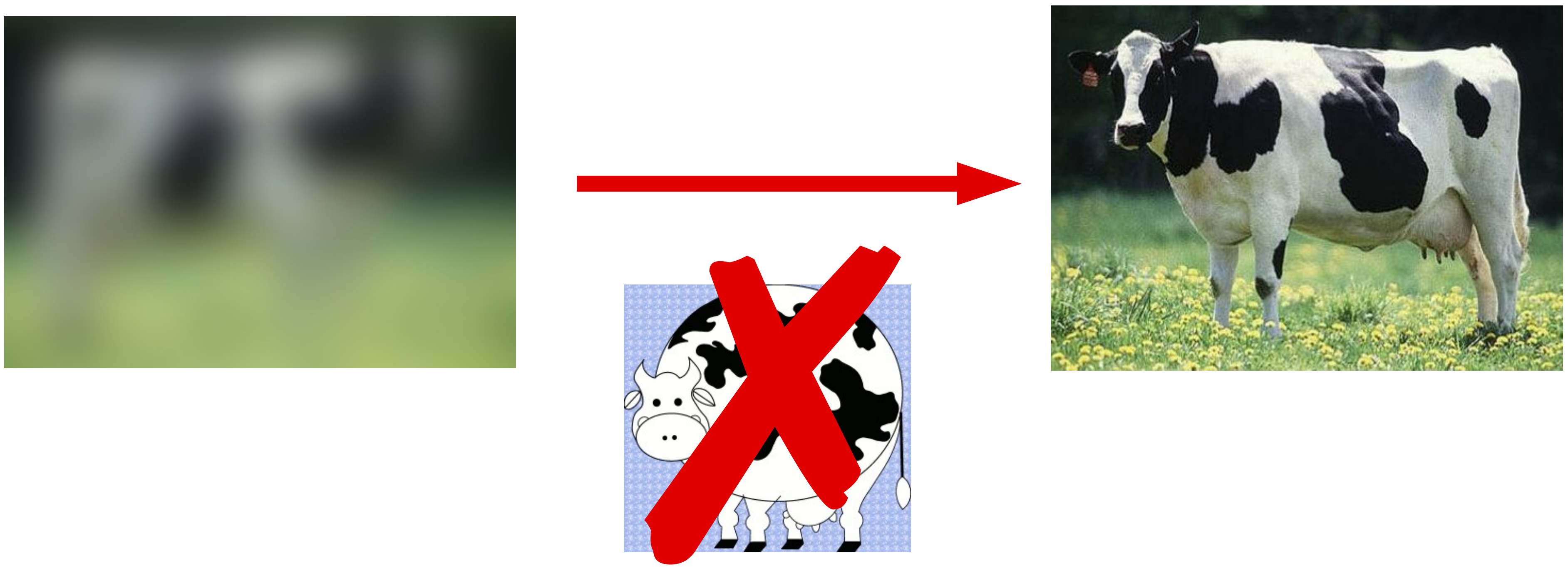
Interferometry requires

full structure modeling



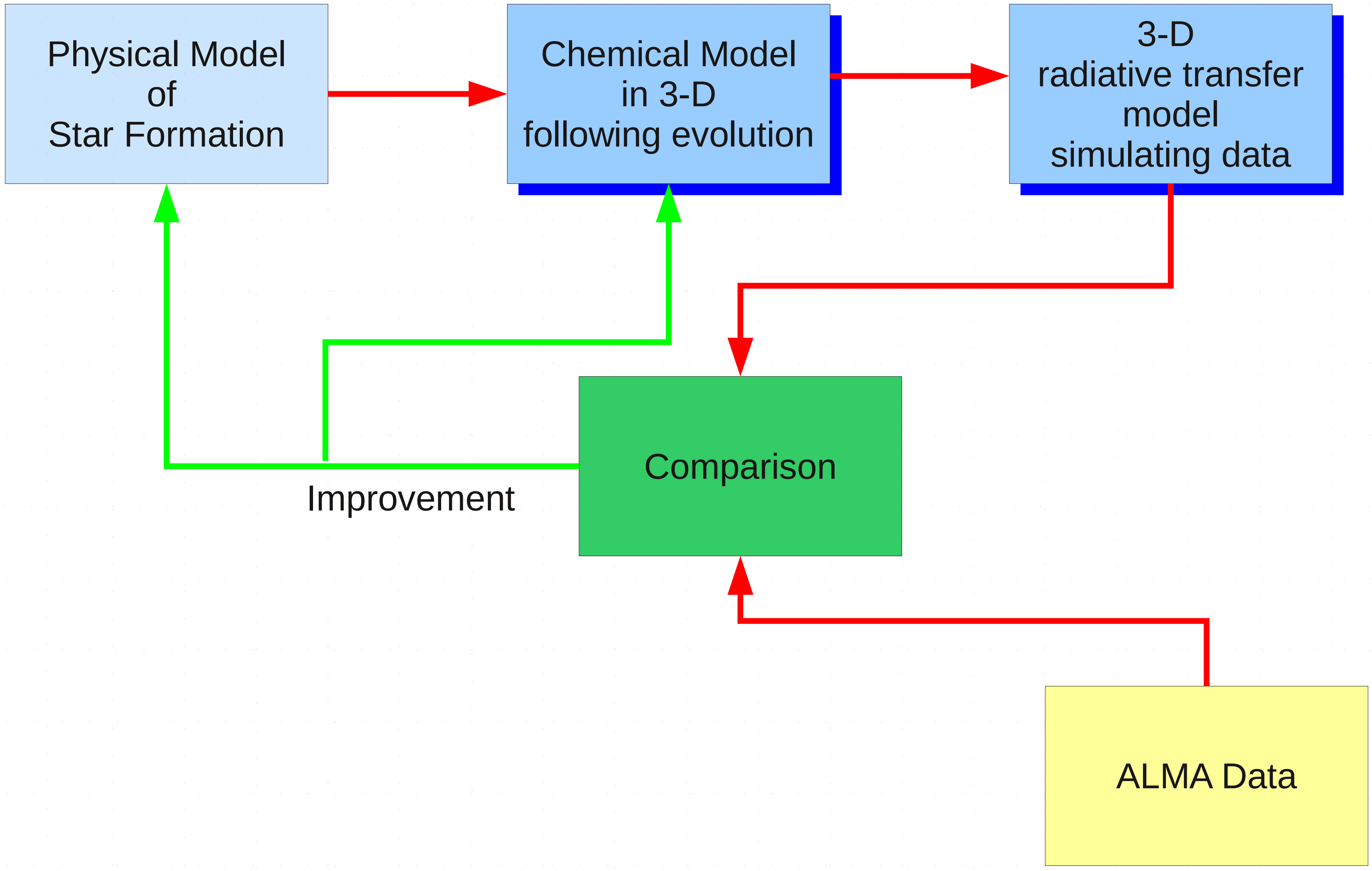
Interferometry requires

full structure modeling




Danger: drowning in the sea of free parameters

Ideally...



Physical Model of Star Formation
Chemical Model in 3-D following evolution
3-D radiative transfer model simulating data
Comparison
Improvement
ALMA Data

Method

- Has been pioneered by Leiden Group, but now we need it to be
  - Multi-molecule
  - 3-d
  - automatic,
  - with quality estimate,
  - with confidence parameters.

Components: chemical modeling

- gas phase rates including
  - interactions with photons (UV, X-ray)
  - high-temperature rates (e.g. in shocks)
- for all species, including complex organics
- dust
  - sticking coefficients
  - moveability of species
  - reaction rates on surface
  - release mechanisms

Components:
radiative transfer modeling

- Molecular Data
  - Energies
  - Frequencies
  - Line strengths
  - Collision rates
- For
  - all observable molecules, including complex organics, isotopologues
  - including transitions to and within vibrationally excited levels

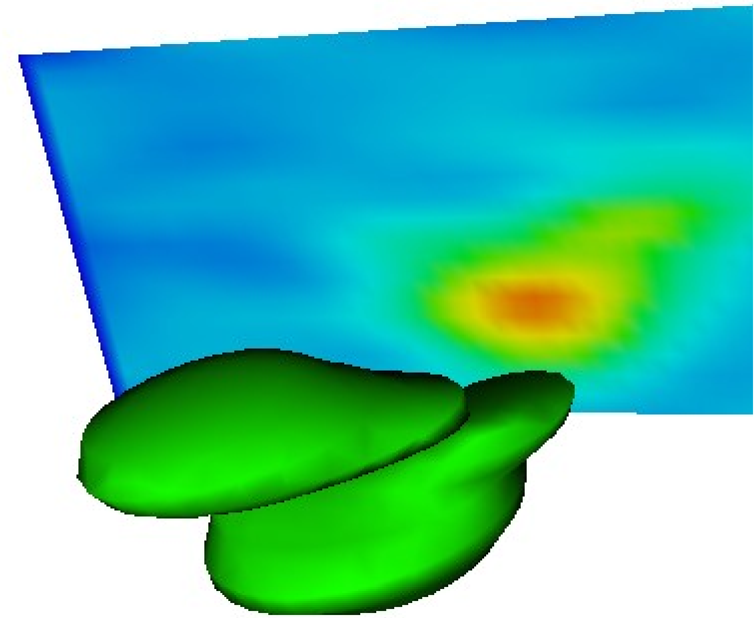
Components: radiative transfer modeling

- Dust properties
  - absorption coefficients as function of wavelength
  - for calculating thermal structure self-consistently

Components: radiative transfer modeling

- For very reactive molecules (CO^+, H_2O^+, …) chemical formation/destruction can compete with inelastic collisions
  - radiative transfer and chemistry are coupled
- Time dependent chemistry: chemistry has to follow physics (density, thermal history, radiation, shocks...)
  - chemistry and physics are coupled

Goal: solving the inverse problem

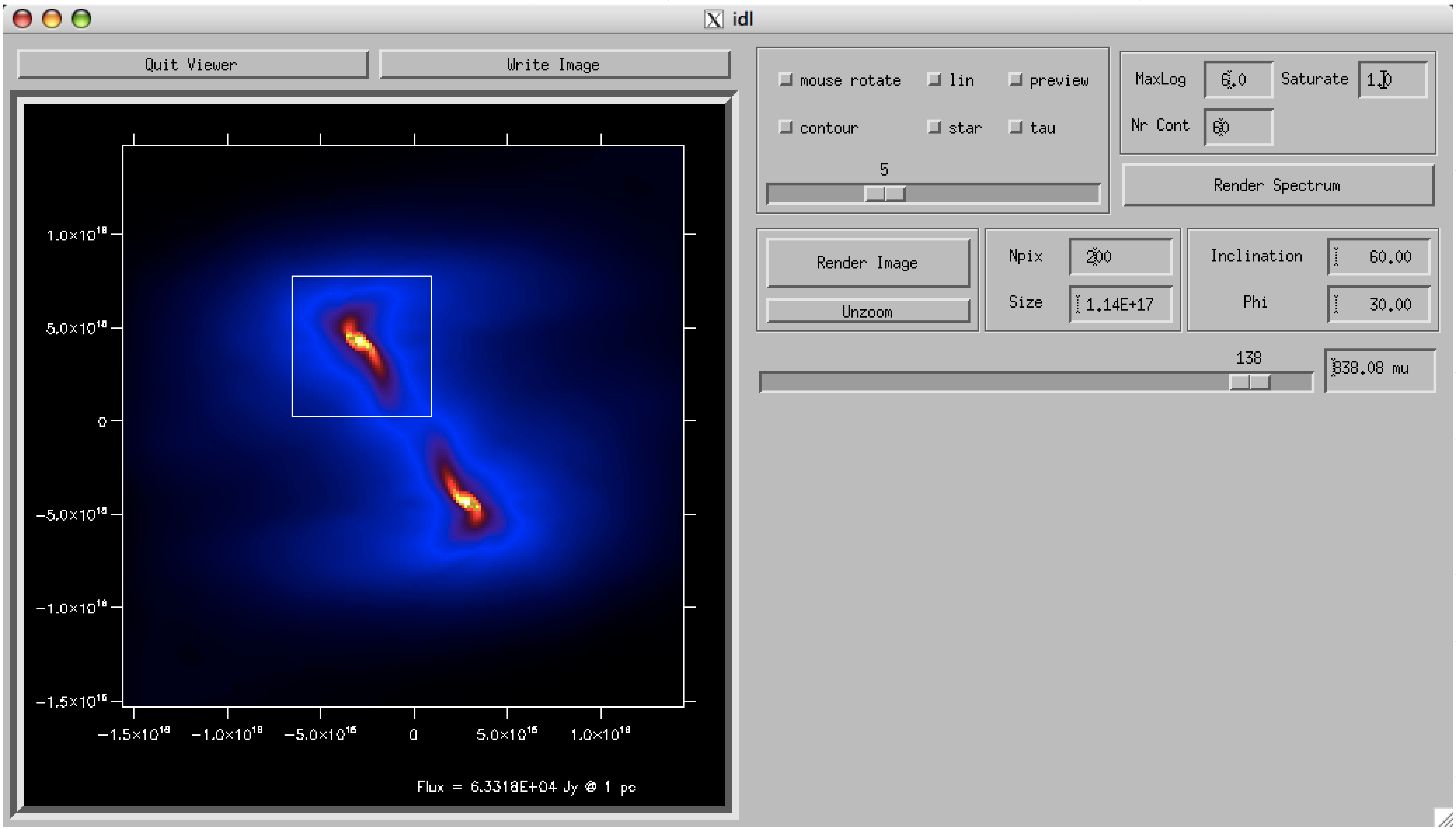


- Need to know:
  - Structure of 6-d phase space
    - 3-d spatial structure
    - Velocity vectors at each point
- Measure directly:
  - 2-d spatial structure (in continuum and lines), but integrated over line-of-sight
  - 1-d (radial) velocity (with molecular lines)
  - Velocities in the plane of the sky only in very rare cases (masers, in very small regions)

Example: radmc-3d

- Written by Kees Dullemond, Heidelberg
- Dust continuum radiative transfer
  - computation of dust temperature and scattering
- Gas line transfer
  - (ray-tracing only, i.e. LTE or user-specified populations)
  - LVG (Sobolev approximation) mode for level populations
  - Full non-LTE ALI radiative transfer [planned for 2011/2012]
- Adaptive Mesh Refinement

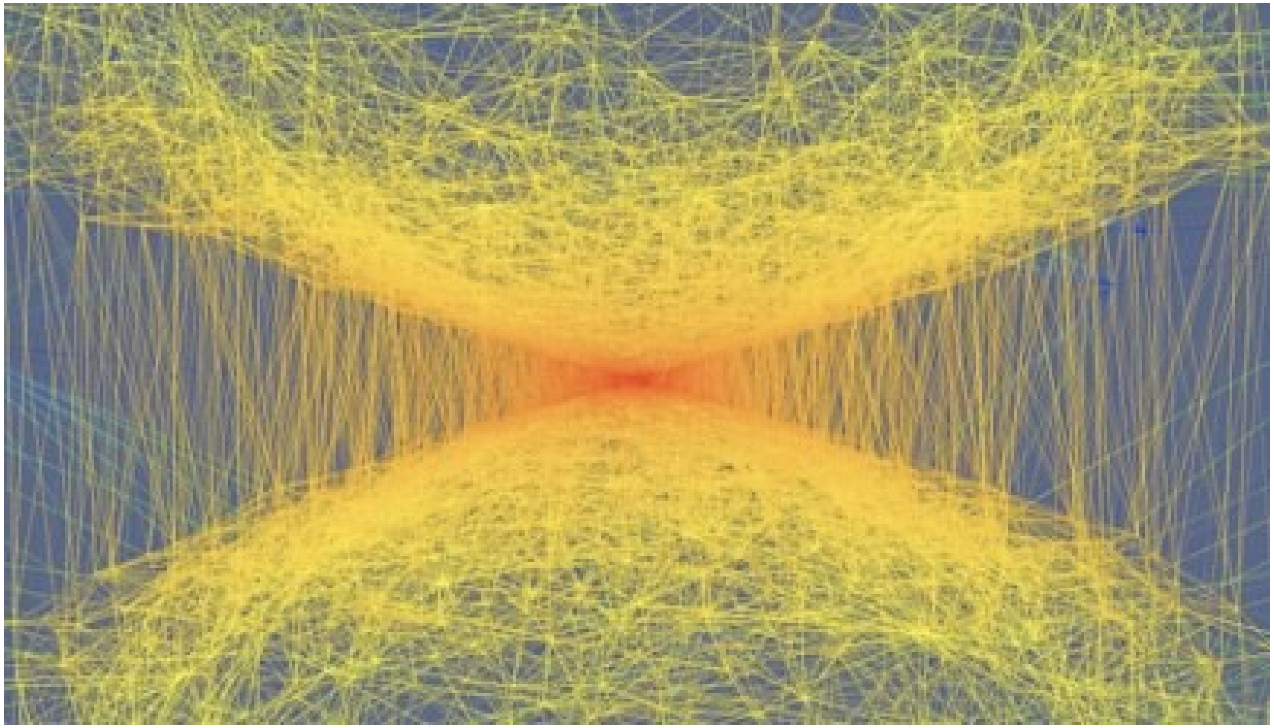
radmc-3d example

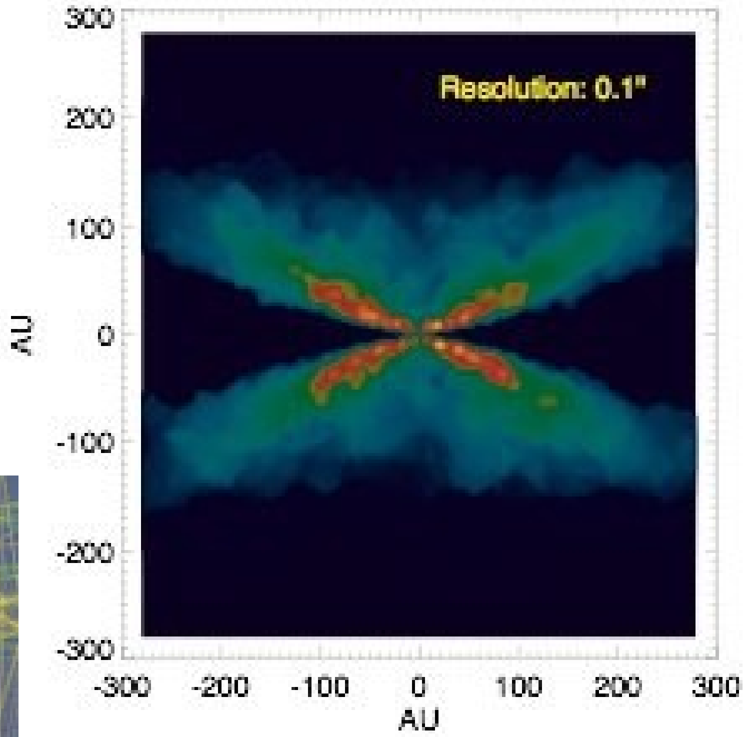


Example: LIME

- Written by Christian Brinch, Leiden
- Continuum and line radiation transfer
- Transport on unstructured Delaunay lattices
- Automatic gridding
- Full 3D model capabilities
- Proper treatments of line blending
- Multiple species
- Multi-line raytracing

LIME example



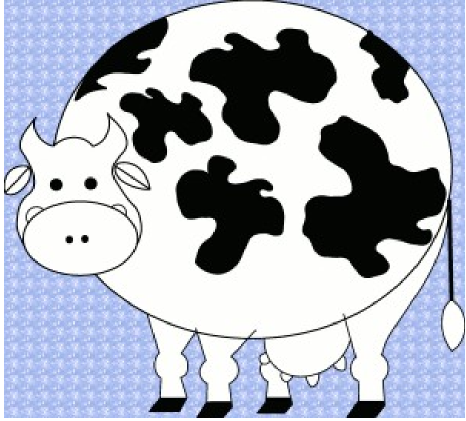


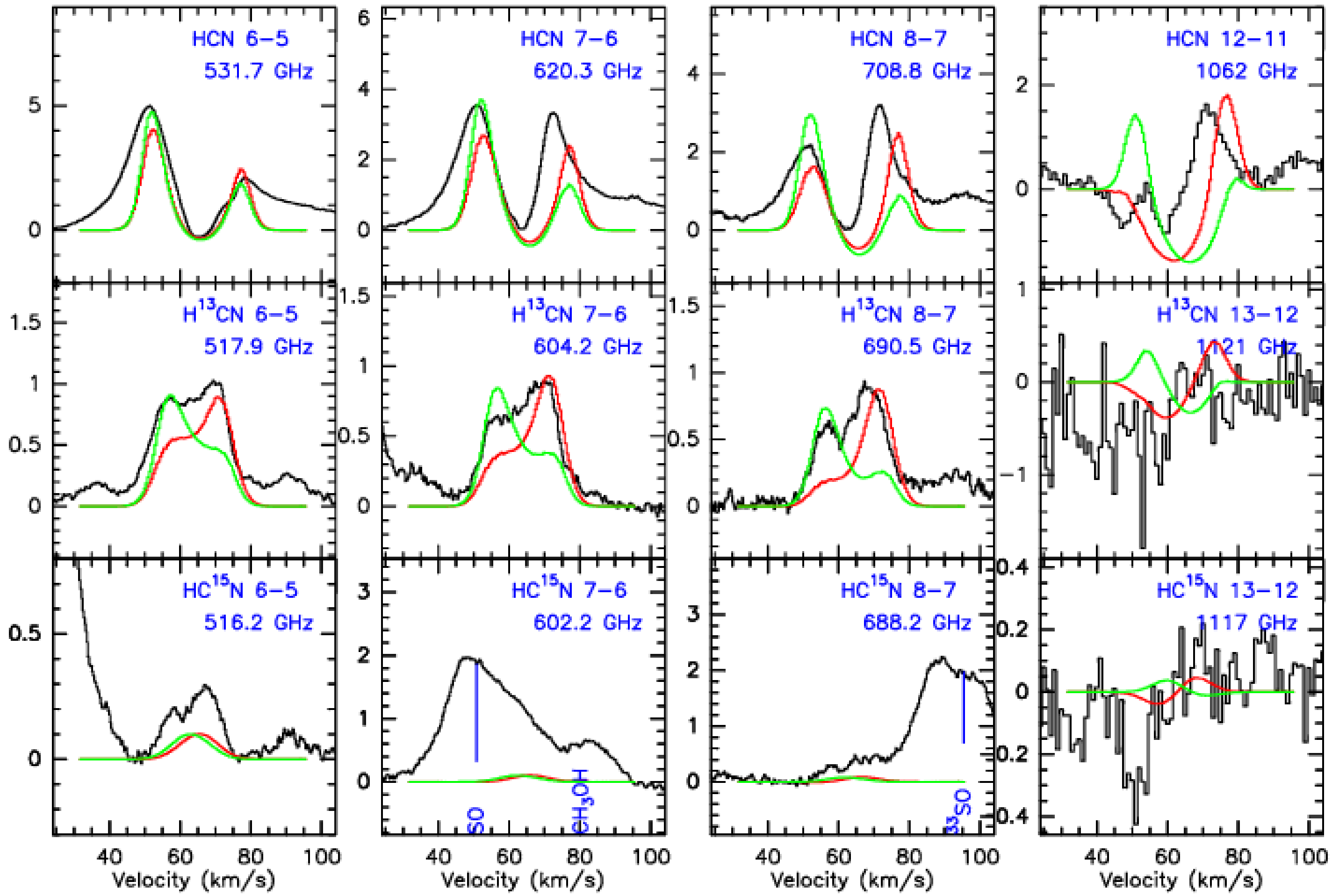
Comparison engine

- Need to find best-fit model
- Need to know confidence parameters
- MAGIX: Part of ASTRONET CATS Project
  - Preloaded models

http://www.astro.uni-koeln.de/projects/schilke/MAGIX

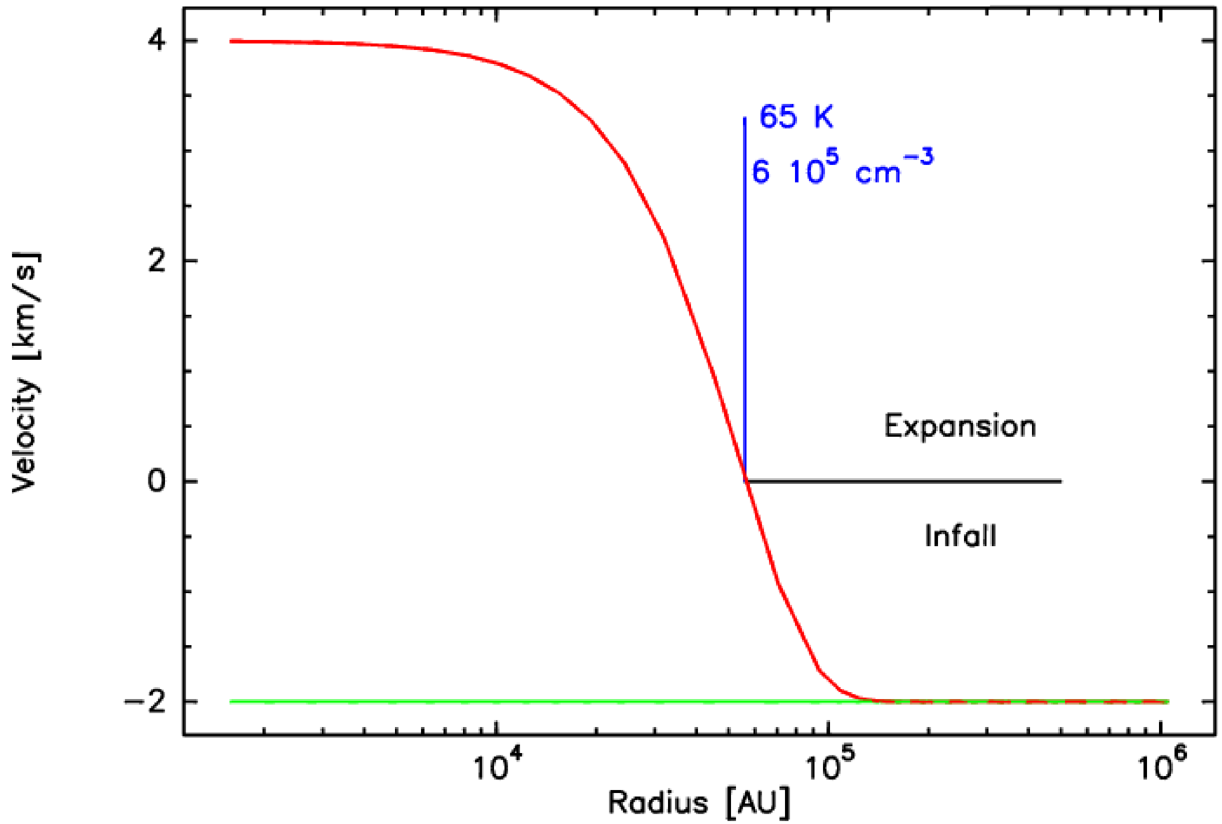
Example applications: Velocity field in SgrB2(M) from HEXOS HIFI data





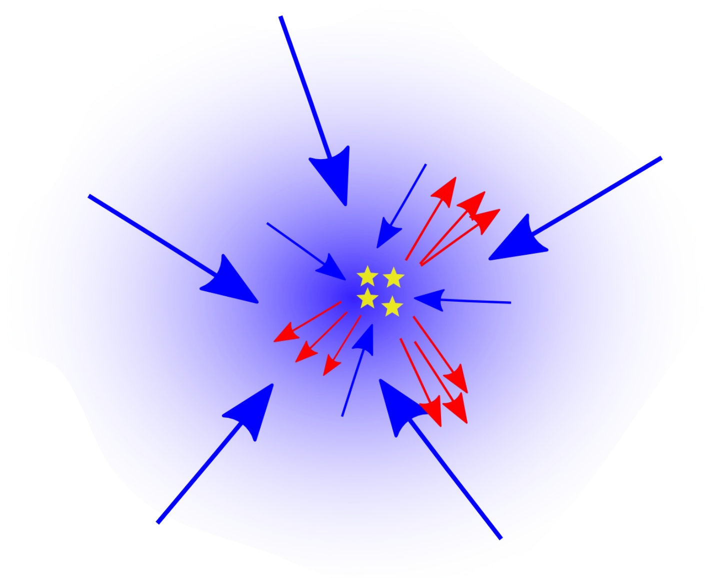
Rolffs et al. 2010, RATRAN

Example applications: Velocity field in SgrB2(M) from HEXOS HIFI data

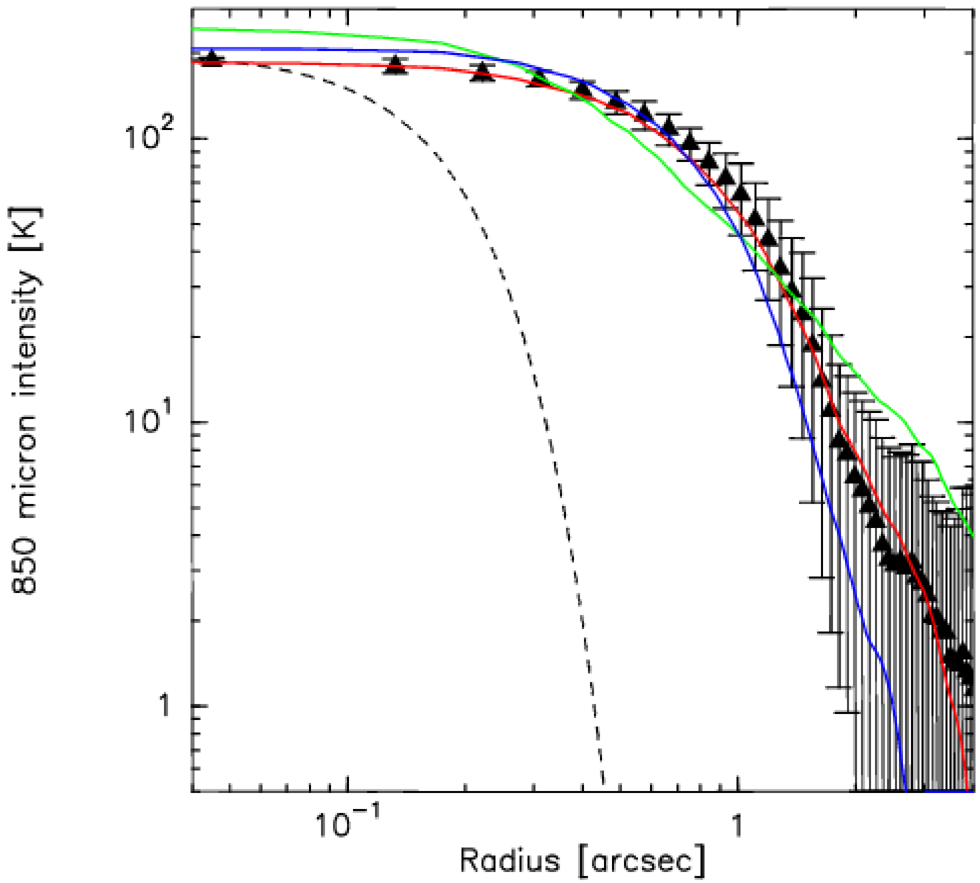


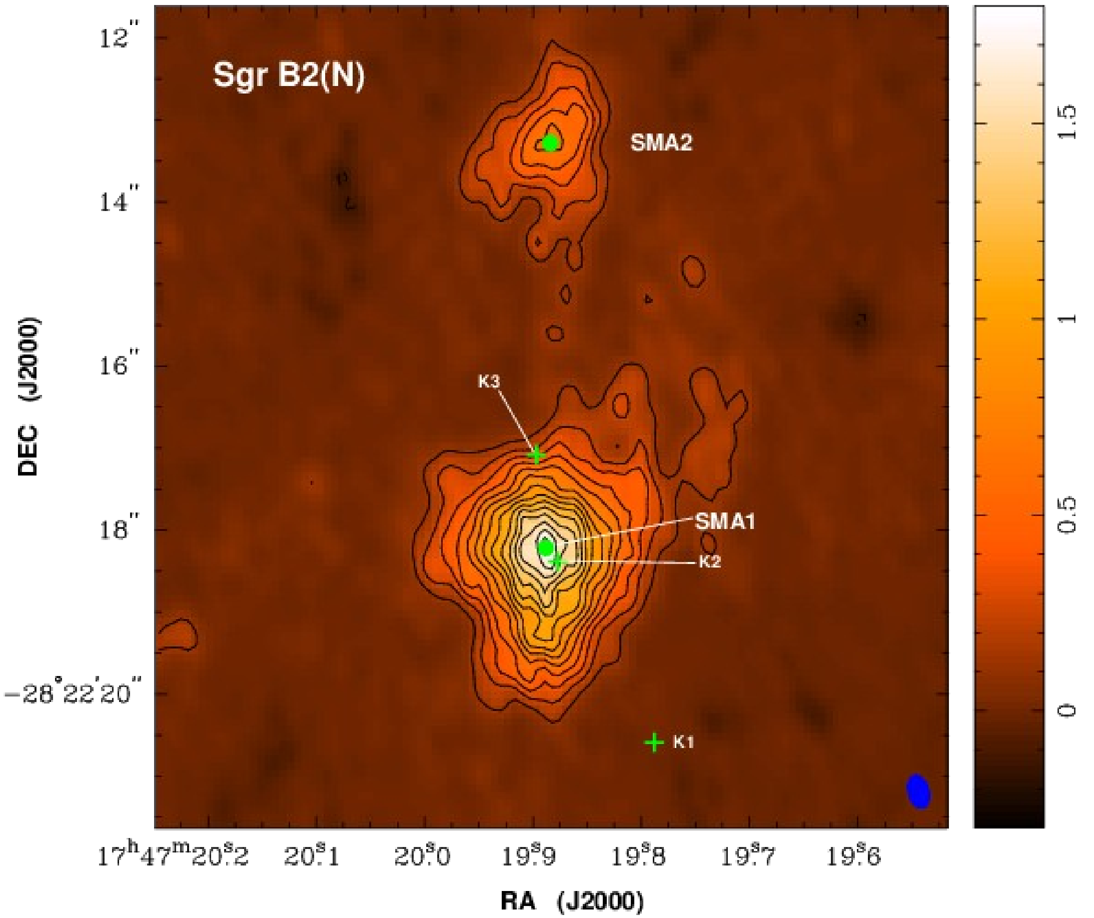
Outer infall
Inner expansion

Rolffs et al. 2010



Example application: Density profile in SgrB2(N) from SMA data

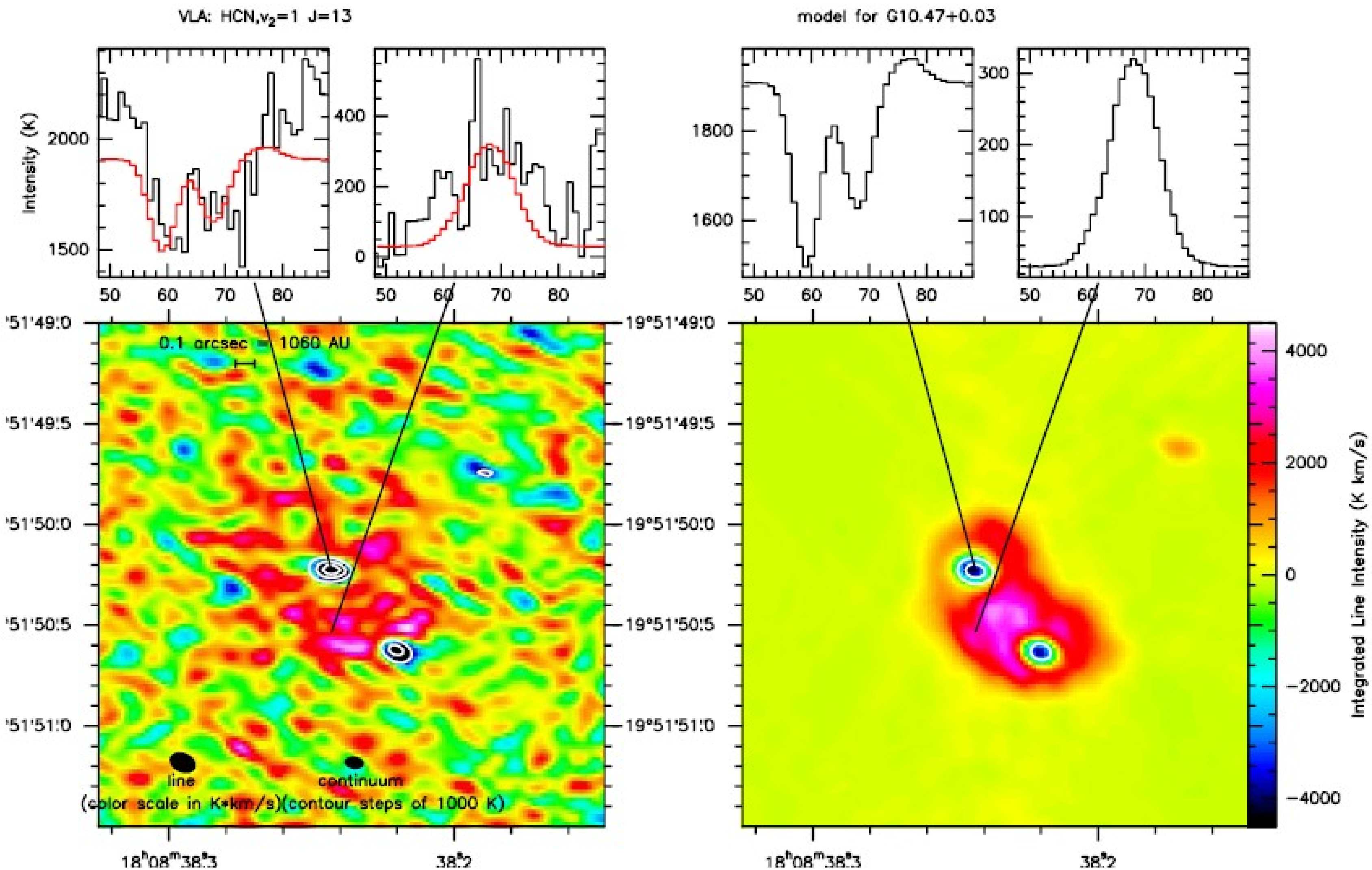




Qin et al, in press

Plummer profile, NOT r^{-2} power law

Example application: vibrationally excited HCN in G10.47



Clumpy model

Rolffs et al. submitted

Conclusions

- Modern instruments like ALMA have an enormous potential for advancing astrochemistry as diagnostics of star formation
- Sophisticated modeling is needed
- Coupling to physical and chemical models and reproducing the observations restricts the number of free parameters
- It's still a long way to go until we have established, robust procedures

We have taken only the first steps on a long road

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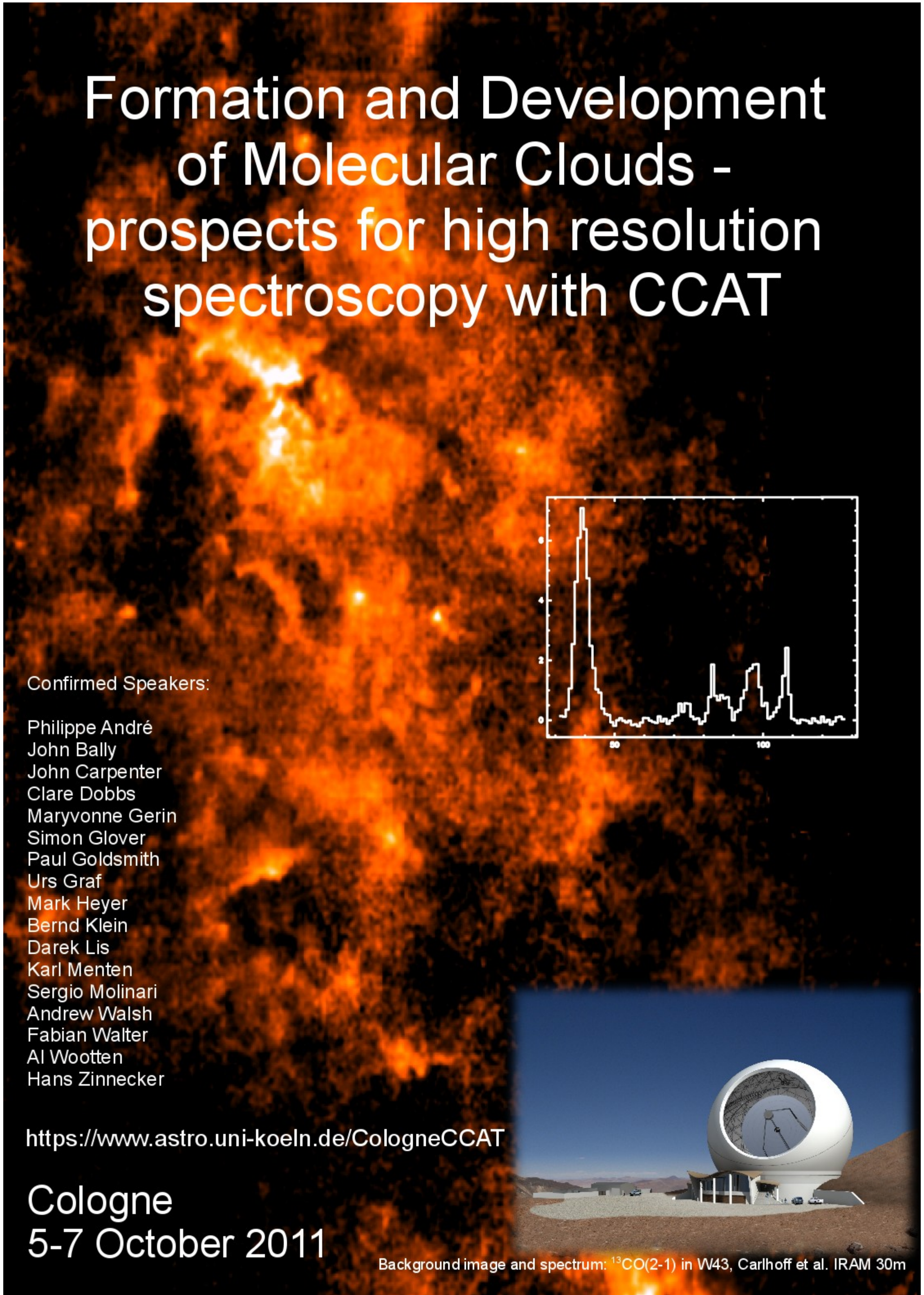
- but they are steps in the right direction!


Formation and Development of Molecular Clouds - prospects for high resolution spectroscopy with CCAT
Confirmed Speakers:
Philippe André
John Bally
John Carpenter
Clare Dobbs
Maryvonne Gerin
Simon Glover
Paul Goldsmith
Urs Graf
Mark Heyer
Bernd Klein
Darek Lis
Karl Menten
Sergio Molinari
Andrew Walsh
Fabian Walter
Al Wootten
Hans Zinnecker
https://www.astro.uni-koeln.de/CologneCCAT
Cologne
5-7 October 2011
0
2
4
6
50
100
Background image and spectrum: $^{13}CO(2-1)$ in W43, Carlhoff et al. IRAM 30m