Radiative transfer modeling on AU-Scales of Infrared Molecular Lines from Protoplanetary Disks

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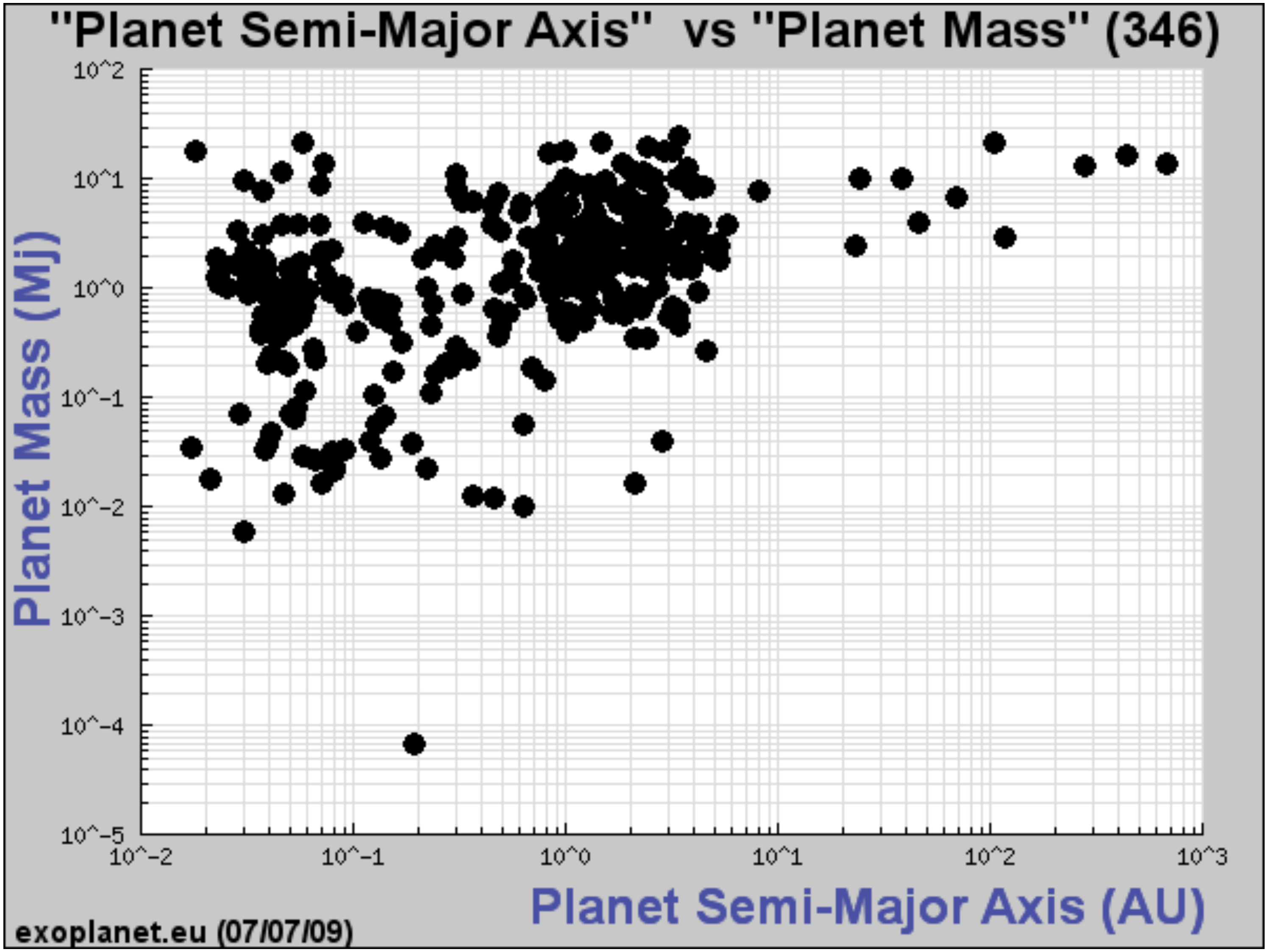
Collaborators for this work

- **Klaus Pontoppidan (Caltech)**
- Geoffrey Blake (Caltech)
- Dieter Poelman (St. Andrews)
- Cornelis Dullemond (MPIA)
- Input from many others…

Planets form at radii R~1-10 AU

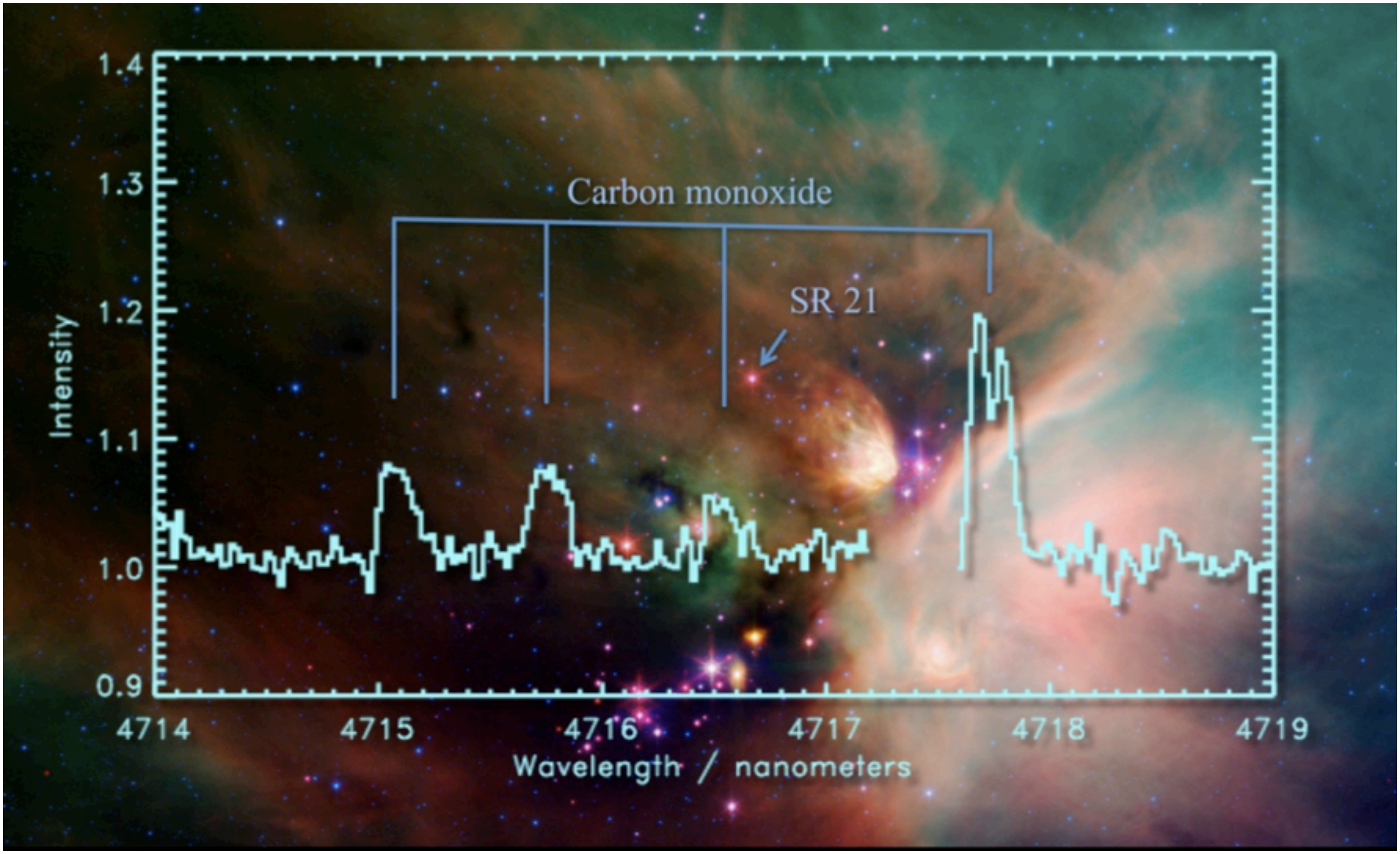


How can the Planet-Forming Region be observed?

- 1-10 AU: 7 – 70 milli-arcsecs @ Taurus
- Spatially resolved tracers: gas or dust
  - Scattered light – Visible/NIR (e.g., Roberge et al. 2005)
    - 100 mas
  - Thermal dust emission – NIR/MIR interferometry (e.g., Van Boekel et al. 2004)
    - 10 mas
  - Gas continuum emission – NIR interferometry (e.g., Akeson et al. 2005, Eisner et al. 2008, Tannirkulam et al. 2008)
    - 1 mas
  - Atomic lines – OI – visible (Acke & Ancker 2006)
    - 10 mas
  - Molecular lines – IR/submm/mm (Goto et al. 2006)
    - 150 mas
- Spectro-astrometry of CO < 1 mas imaging of lines with kinematic information (Pontoppidan et al. 2008)

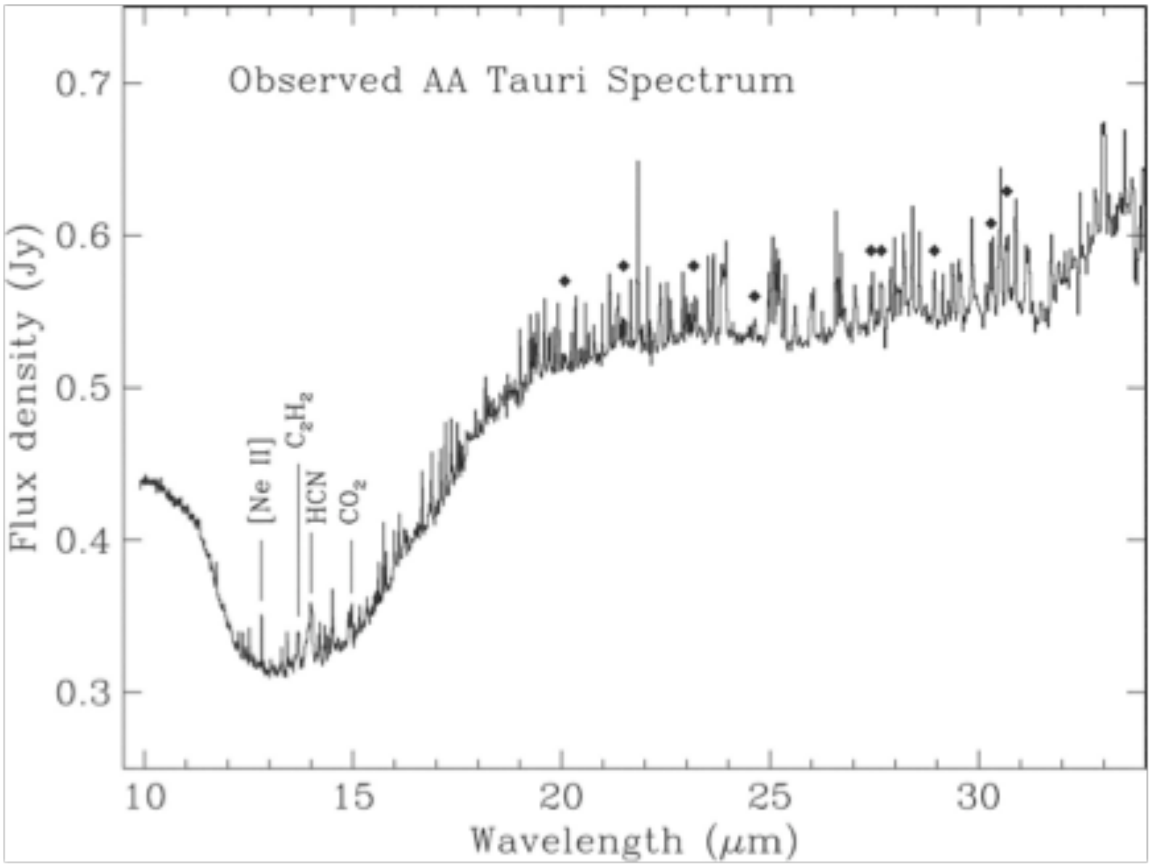
Note: ALMA will likely not break the 10-15 AU barrier for line emission, but plays a highly complementary role.

Infrared lines as tracers of inner disks



Molecules in the inner regions of regions of protoplanetary disks

In addition to H2, OH, CO, and H2O observed in the NIR, Spitzer detected molecules in the MIR (Carr & Najita 2008, Salyk et al. 2008)



Most lines are H2O. OH lines are marked by ◆. Some line of C2H2, HCN, and CO are marked.

Preliminary analysis indicates that lines arise from warm gas (500-1000 K) inside 2 AU.

More complex molecules are expected to be found in this regions associated with planetformation.

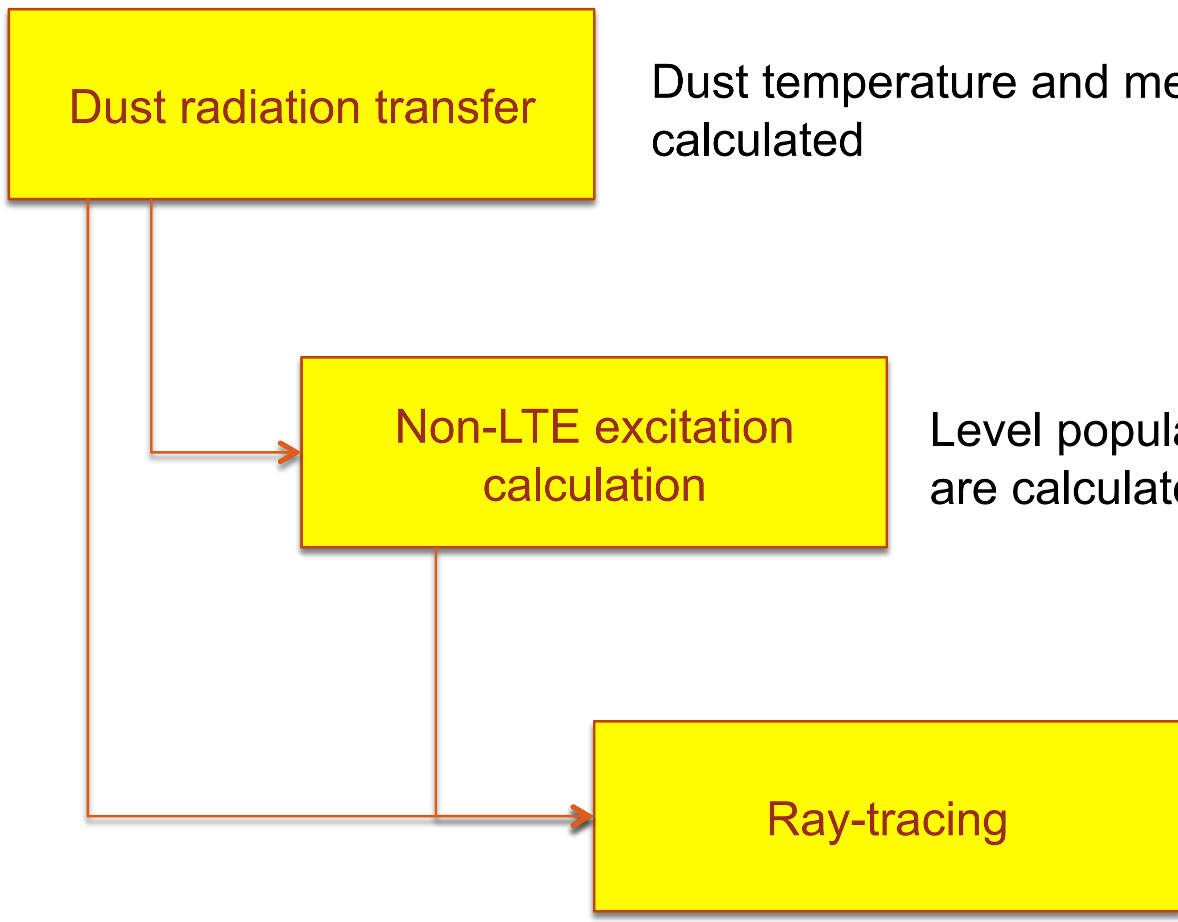
Radiative transfer

- To interpret data one needs radiative transfer:
  - Extract physical parameters as density, temperature, abundance, geometry, irradiation, dynamics
  - Thermal/Chemical/Dynamical balance depends on radiative transfer (MJ or EOS, t_{ad})
- Excitation involves:
  - Collisions (H,H2), radiation (dust continuum, line trapping), chemical formation.

Modeling of molecular emission in MIR

- 2D Dust radiative transfer (RADMC)
  - Dullemond & Turolla (1998)
- Images and spectra rendered in 3D (RADLite)
  - Pontoppidan, Meijerink et al. 2009, ApJ, 704
- 1+1D non-LTE detailed balance (beta3D)
  - Meijerink, Pontoppidan et al. 2009, ApJ, 704
- In preparation for Herschel/JWST/E-ELT

Flow chart of the codes

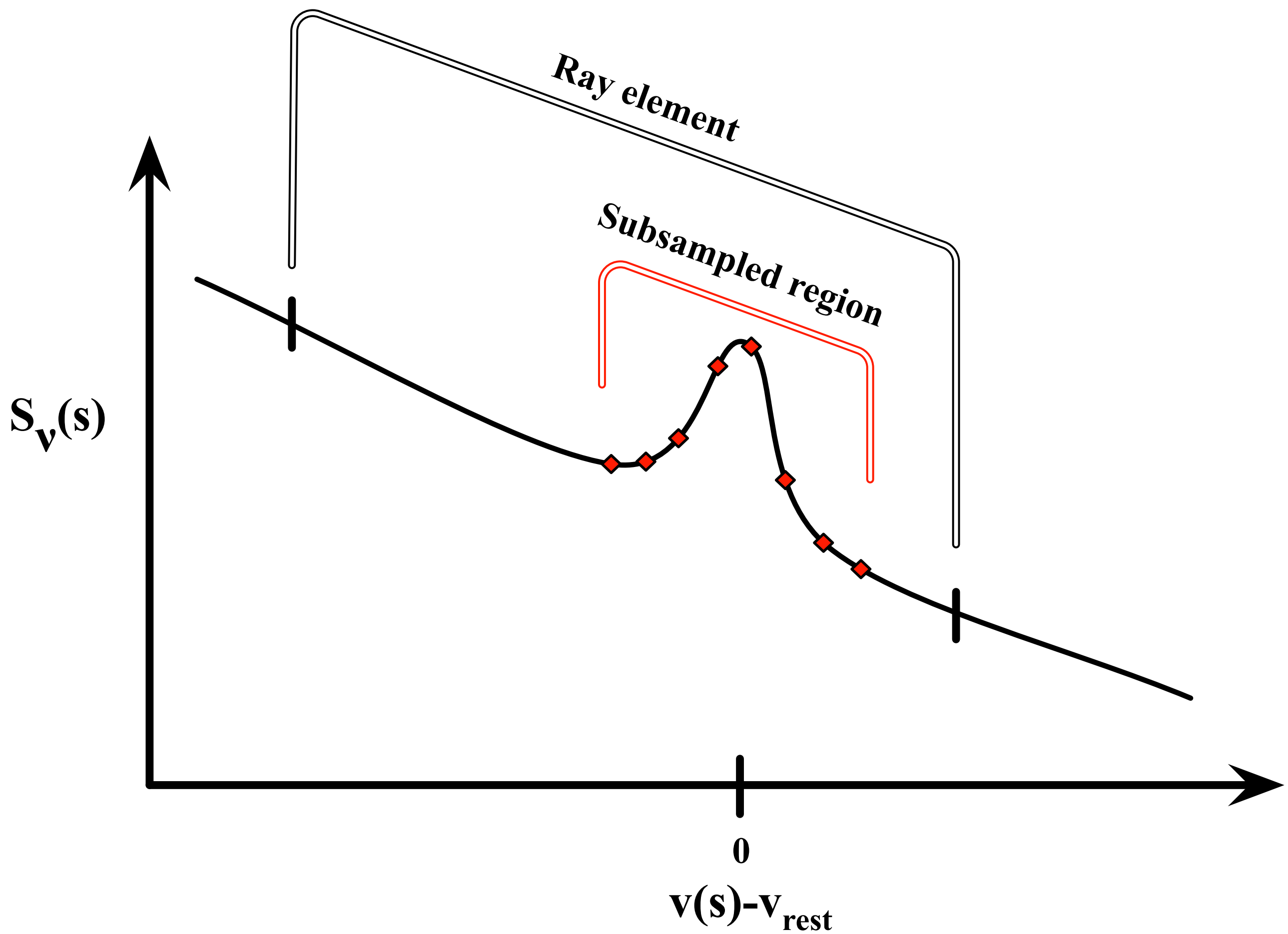


Dust temperature and mean intensity is calculated

Level populations of molecule are calculated

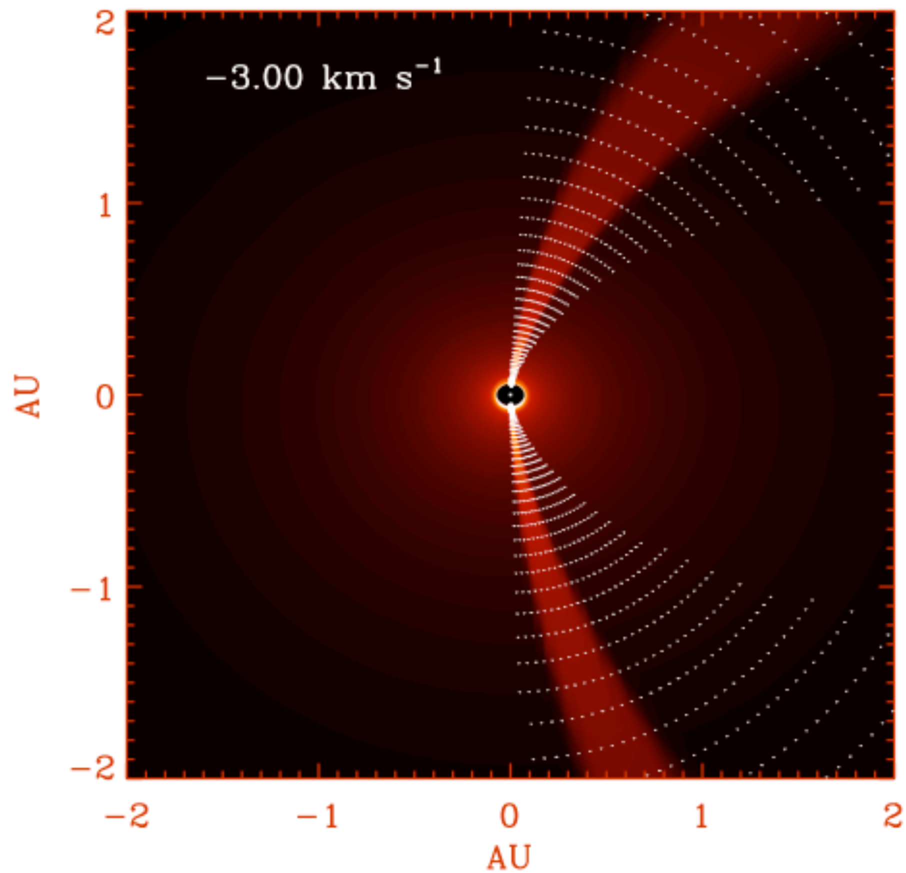
Spectrum or image of object is rendered

RADLite



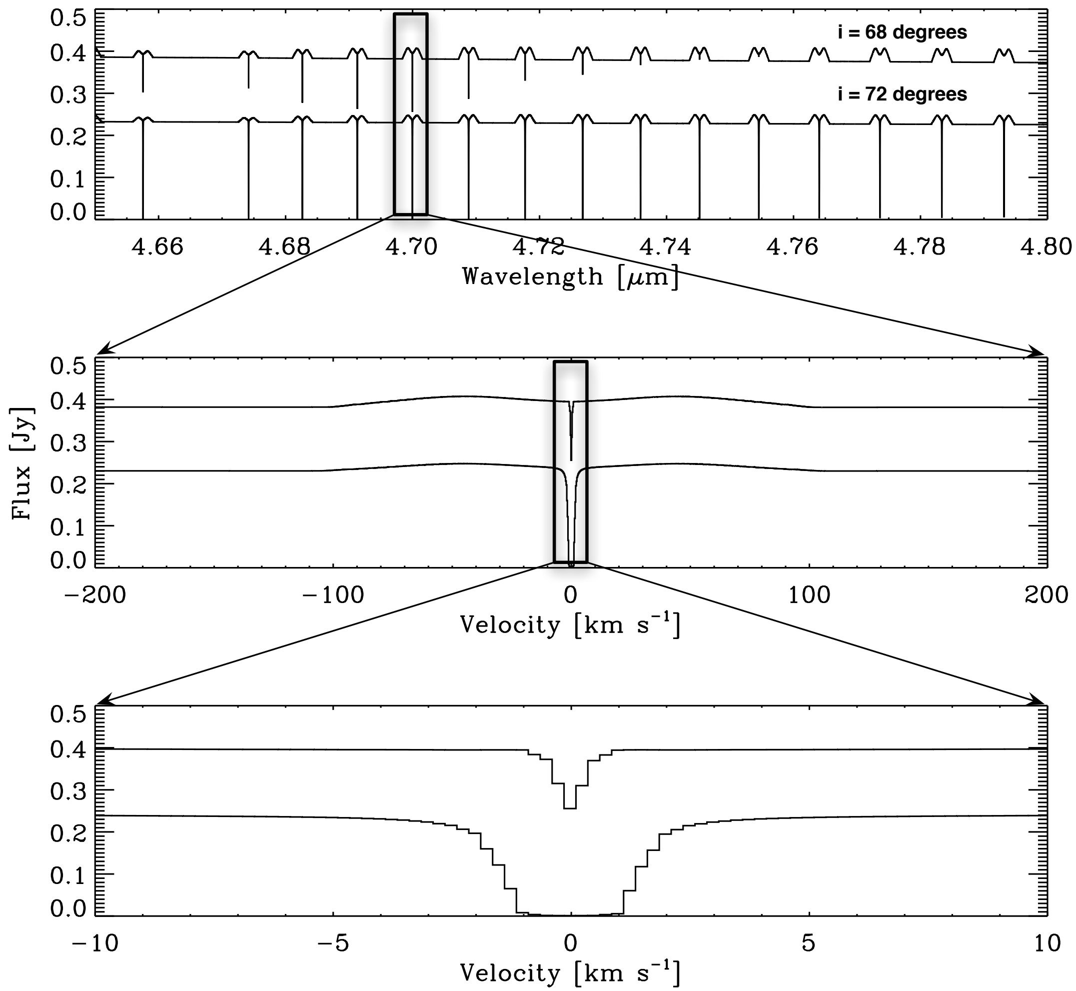
- Small intrinsic linewidths combined with large velocity gradients are present in the inner regions of protoplanetary disks.
- Common codes integrate from boundary to boundary, but lines with narrow local broadening may be missed.
- RADLite subsamples in each gridcell with a sufficient number of points across the line.

Optimization of the code



- If the image is not sufficiently resolved, the thin isovelocity band may be missed.
- Code should be also be able to render thousands of lines efficiently.
- A large number of closely spaced rays are defined.
- Rays that interact with the lines are integrated.
- ‘Continuum rays’ are integrated only once.
- A spectrum and image velocity cube of a line at 3 km/s resolution is rendered in 15-30 seconds on a single 3 Ghz Intel Xeon processor

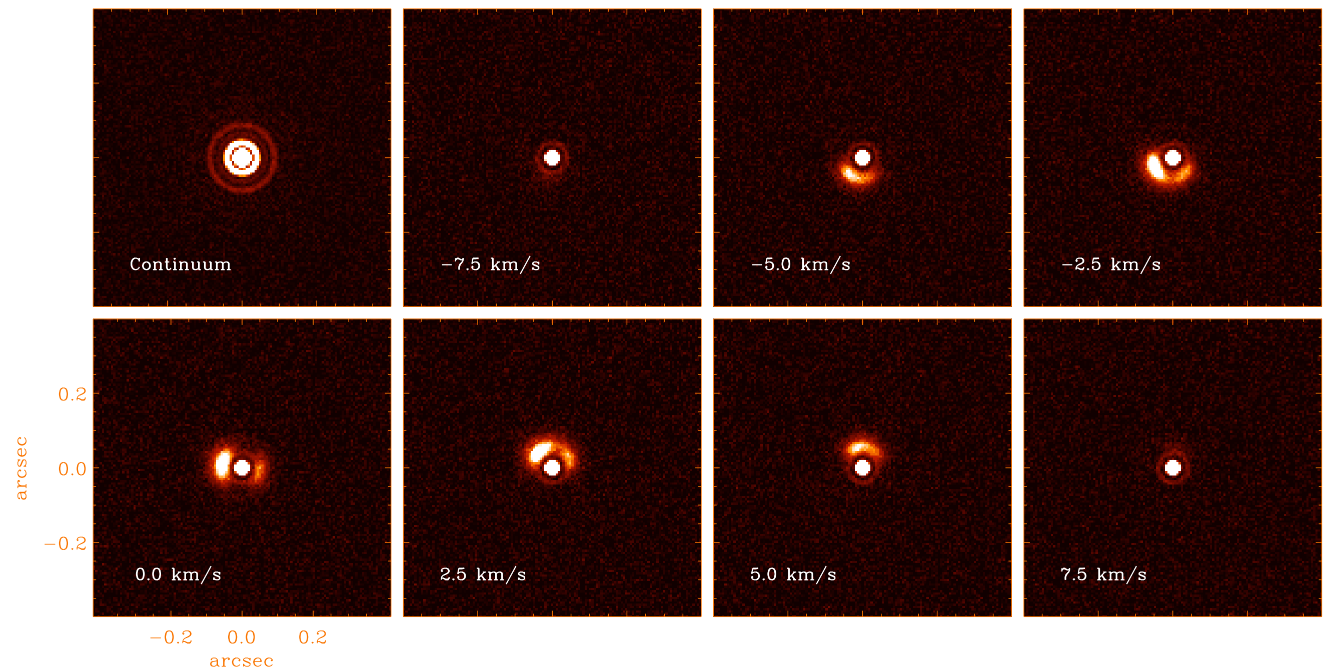
CO ro-vibrational band



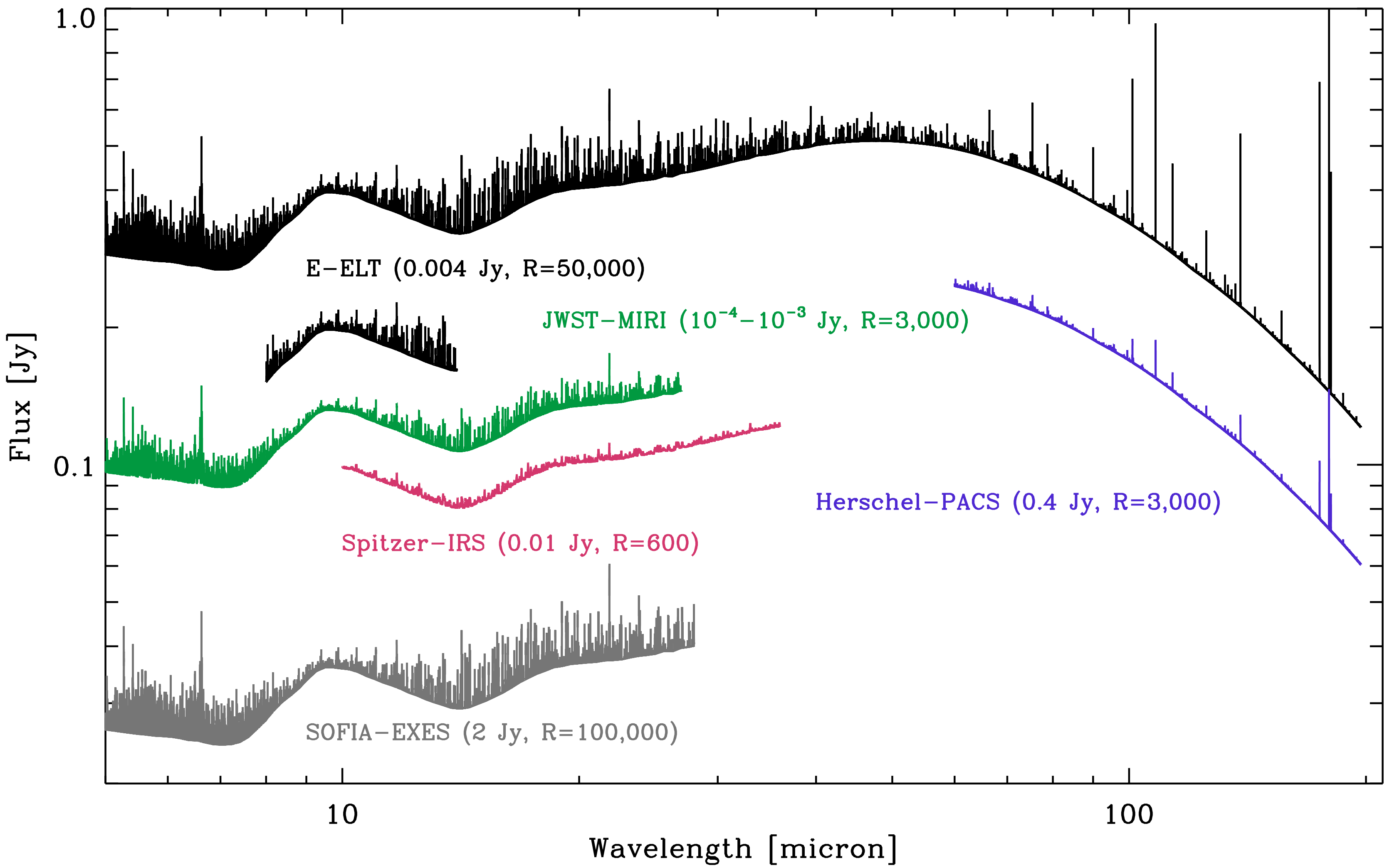
- Spectrum at inclination angles of 68 and 72 degrees, as rendered by RADLite.
- Both absorption and emission components are shown.
- RADLite can deal with spacial scales < 0.1 to > 100 AU as well as spectral scales ranging from < 0.1 km/s to the entire spectrum in one instance.
- Example shows that dynamic ranges of 4 – 5 orders of magnitude can be treated simultaneously.

Image cube of a CO line for SR21

• Simulated E-ELT integral field unit (IFU) observation of the v = 1 – 0 P (8) CO line at 4.736μm for SR21 at a distance of 125 pc.
• CO emission would be imaged across at least 50 spaxels (spectrally dispersed pixel in an IFU).
• It will be possible to look for kinematic structures in the disk, directly related to star formation.



Full range infrared water spectrum from a typical protoplanetary disk



Summary (Part 1)

- RADLite is a code that can rapidly render large number of lines for full axisymmetric spectra of, e.g., CO and H2O.
- A water spectrum (~1000 lines) in the infrared (2-200 μm) can be rendered with a velocity resolution of 1 km/s in 1-2 hours on a single workstation.
- The code has applications to chemical and excitation models as well as observations from infrared spectrometers on 8 – 10 m class ground based telescoped, Spitzer-IRS, Herschel-PACS, and future telescopes as JWST, SOFIA, E-ELT, TMT and the Giant Magellan Telescope (GMT).
- We find that the primary reason that infrared spectroscopy of disks in the N-band has not received much attention is due to a sensitivity deficit of roughly an order of magnitude, which will be remedied by the ELT generation and JWST.

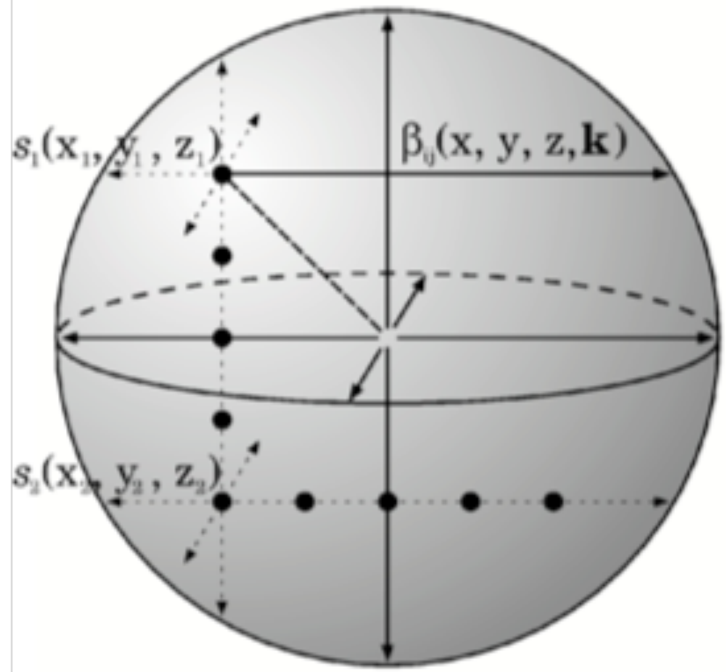
LTE slab versus Non-LTE 2D models

- Good matches have obtained to H2O line observations in the MIR Spitzer IRS band, using single temperature, single column density LTE models (Salyk et al. 2008, Carr & Najita 2008), but a good fit does not imply that model is correct.
- Slab models ignore: complex geometries, densities ranging from $n < 10^3$ to 10^{16} cm^{-3}, and temperature $T \sim 100 – 5000$ K.
- Upper level energies range from $E < 500$ to > 5000 cm^{-1}, and transitions are highly scattered throughout spectrum.
- LTE only holds when collisions dominate level populations.

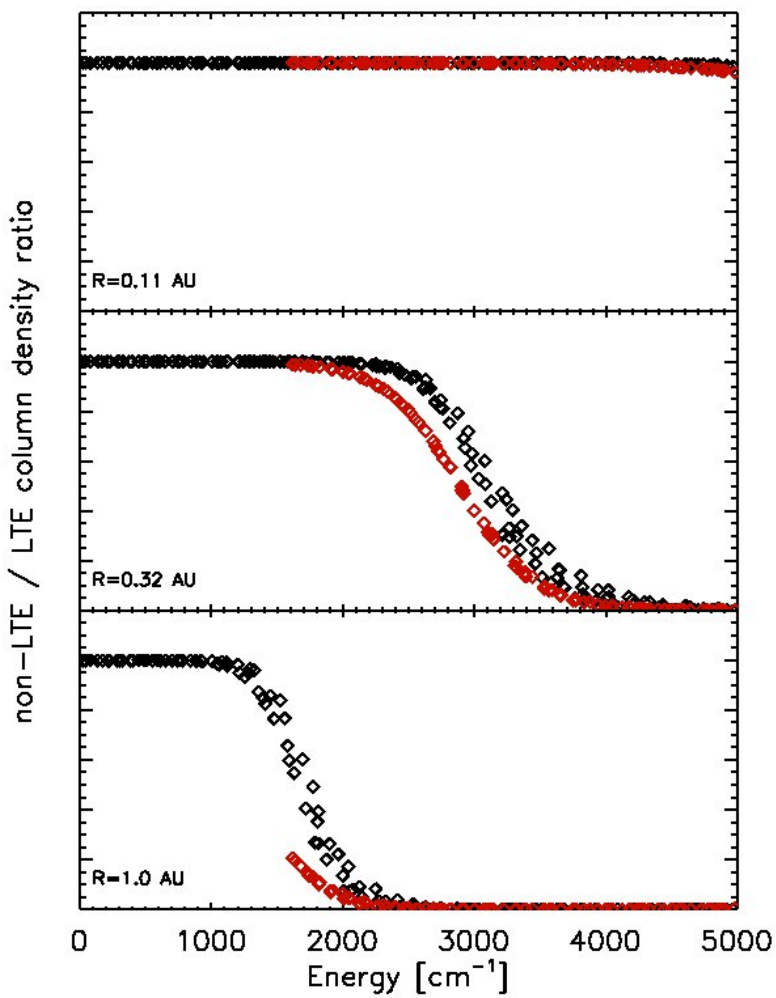
Beta3D

$$\beta_{ul}(x, y, z, \boldsymbol{k}) = \frac{1 - \exp(-\tau_{ul}(x, y, z, \boldsymbol{k}))}{\tau_{ul}(x, y, z, \boldsymbol{k})}$$

- Gridcells interact with each other (Poelman & Spaans 2005, 2006).
- Suitable for arbitrary geometries.
- Suitable for any atom & molecule.
- 10/100 times fast than existing MC/ALI codes especially at high optical depths.

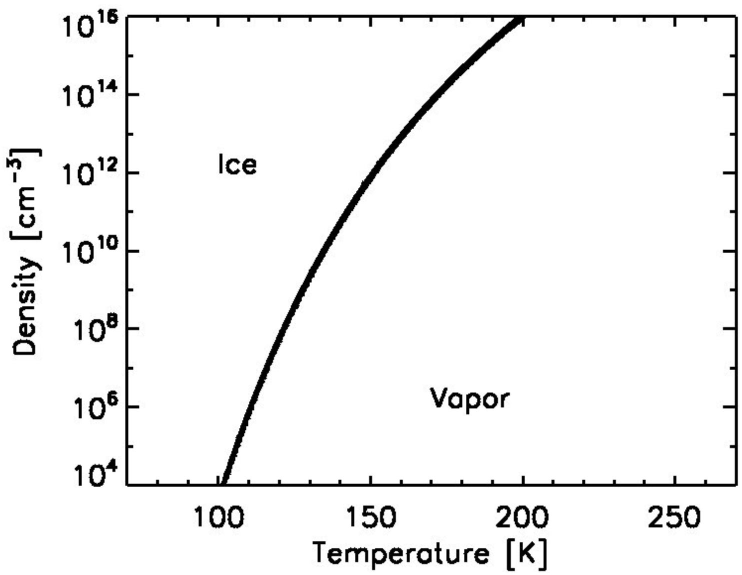


Non-LTE/LTE column density ratios



- LTE approximation is only valid at small radii.
- The subthermal decrease in column density is larger for levels with a higher excitation energy.
- Radiative excitation counteracts lower excitation rates, but does not result in a significant flux increase.

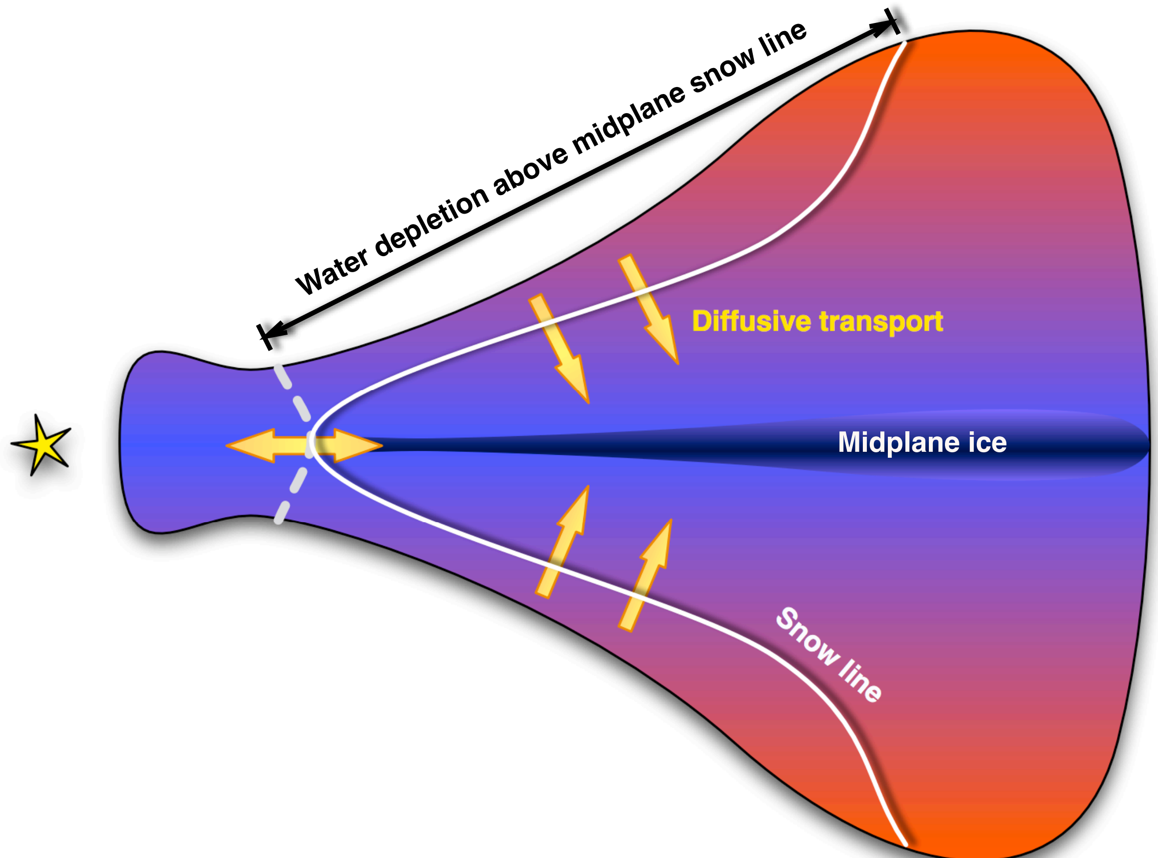
Toward a fiducial model

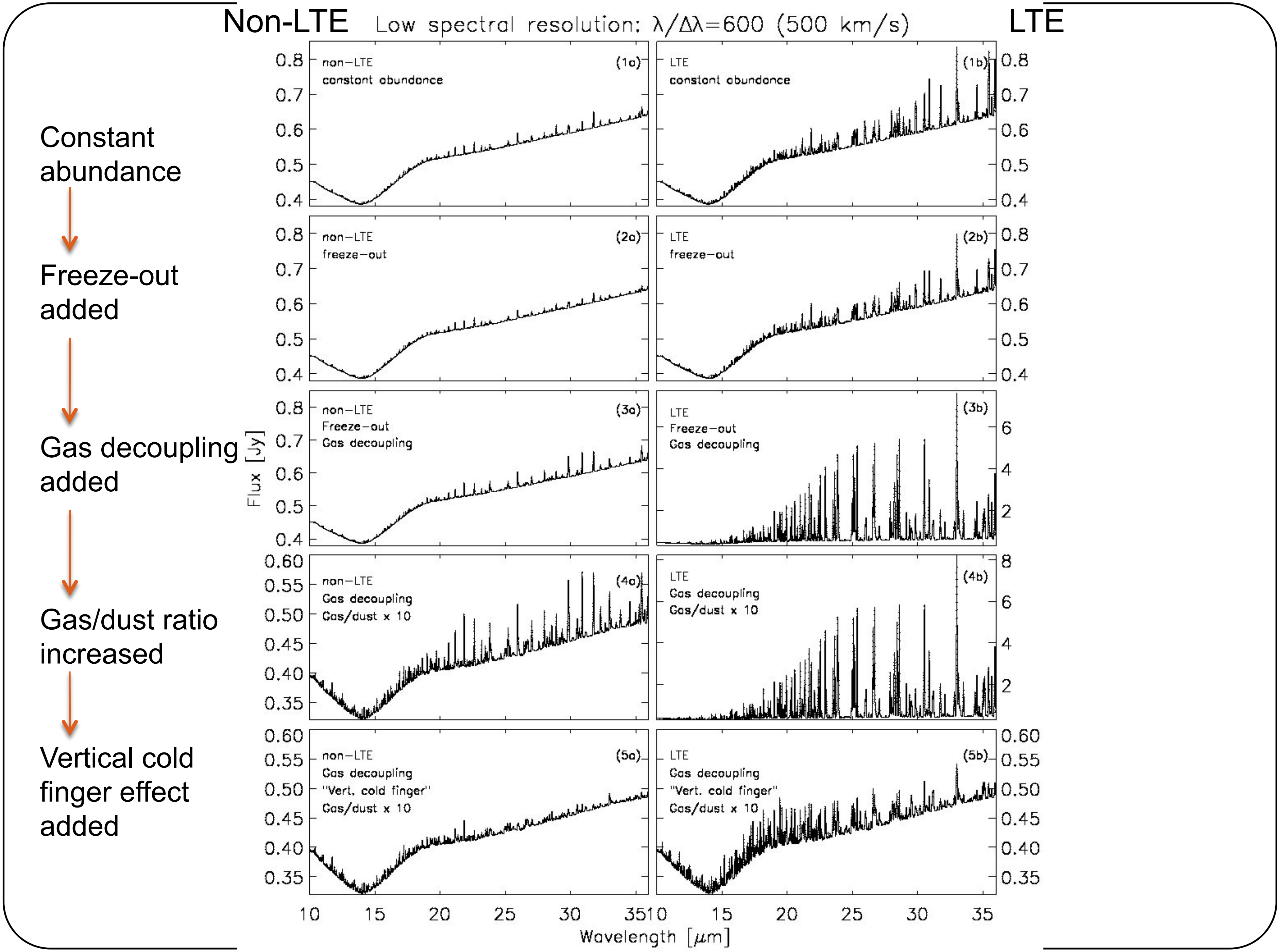


- Freeze-out onto grains can significantly reduce the amount of water in the gas phase.
- The gas temperature in the disk surface is decoupled from dust. Due to heating by FUV, X-rays or both.
- The gas to dust ratio is larger than the canonical ISM value due to dust settling.

Vertical cold finger effect

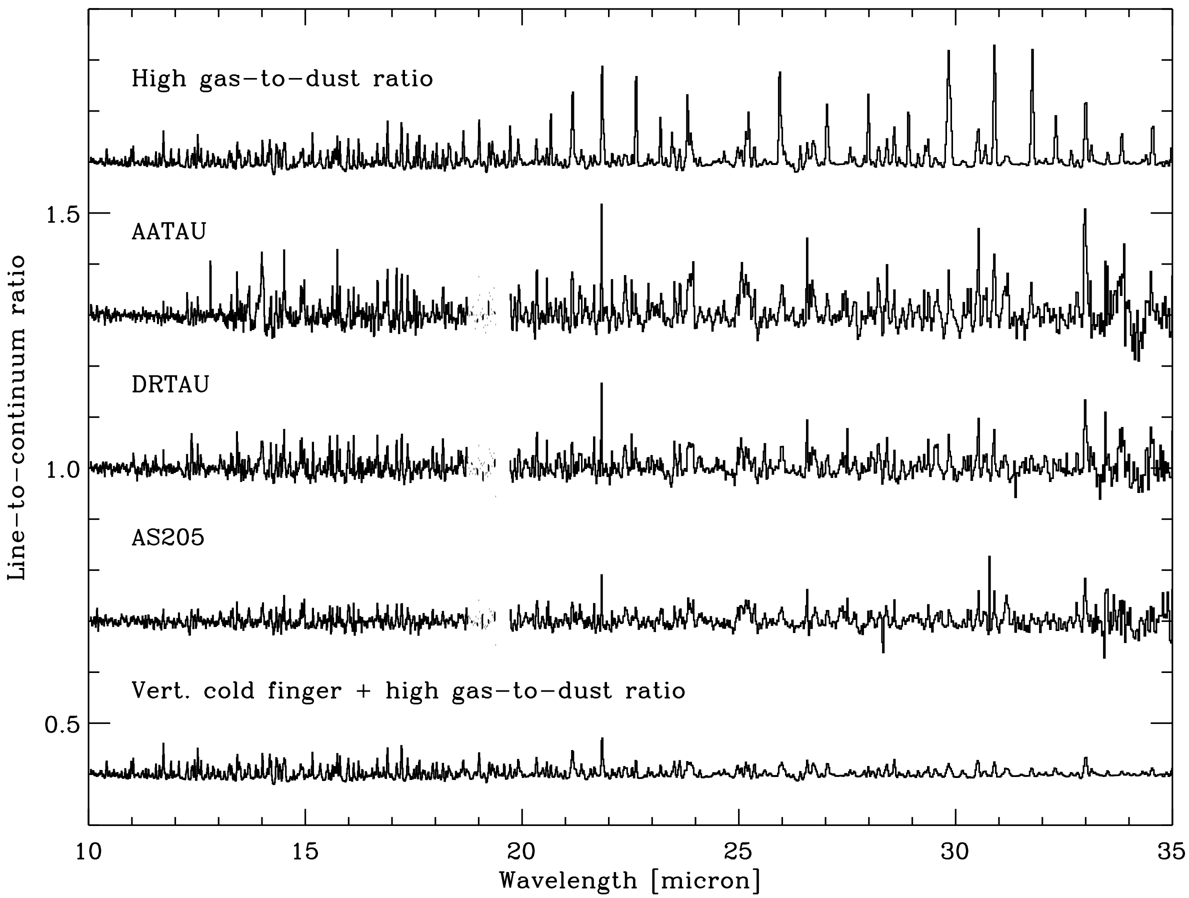
- Static chemical models predict a lowered water abundance below T~300 K
- Higher depletions are necessary, due to high optical depths.
- Proposal: Water is transported below snow-line and freezes out, and will take part in settling to mid-plane (variation of Stevenson & Lunine 1988 radial cold finger effect)





Non-LTE
Low spectral resolution: λ/Δλ=600 (500 km/s)
LTE
Constant abundance
Freeze-out added
Gas decoupling added
Gas/dust ratio increased
Vertical cold finger effect added
non−LTE constant abundance (1a)
LTE constant abundance (1b)
non−LTE freeze−out (2a)
LTE freeze−out (2b)
non−LTE Freeze−out Gas decoupling (3a)
LTE Freeze−out Gas decoupling (3b)
non−LTE Gas decoupling Gas/dust x 10 (4a)
LTE Gas decoupling Gas/dust x 10 (4b)
non−LTE Gas decoupling "Vert. cold finger" Gas/dust x 10 (5a)
LTE Gas decoupling "Vert. cold finger" Gas/dust x 10 (5b)
Flux [Jy]
Wavelength [μm]

Comparison of models to observations



- Comparison to observations of AA Tau, DR Tau, and AS 205 (Carr & Najita 2008, Salyk et al. 2008).
- No attempt is made (yet!) to make a match to observations, just the ability to bracket parameter space is shown.
- A full parameter study is in preparation (Meijerink et al.)

Summary (part 2)

- A non-thermal treatment is essential in determining the water distribution given an observed spectrum.
- In order to boost the high excitation lines, we introduced a steep gas temperature gradient, which is motivated by both observations and models.
- Essential is the increase of the gas-to-dust ratio from the canonical value of ~ 100 – 200 in order to approach the observed line strengths and line-to-continuum ratios.
- The predicted lower limit to the water abundance in cold regions, still produces too much emission. A vertical cold finger effect is proposed to lower the abundance even more.
- Current study is only qualitative.

Current investigations include:

- Intrinsic line width: This is currently dominated by thermal broadening. Additional broadening from MRI driven turbulence would be able to double this.
- Stellar properties: The central start in the observed Spitzer sample have masses ranging from M(star) = 0.3 to 3.0 M(Solar)
- Inner holes: The maximum dust density will decrease when the inner rim is located at larger radii.
- The model setup can easily be extended to other molecular species, such as CO, HCN, C2H2, OH, etc.