Some Topics in Spectral Line Observing and Data Analysis

Jim Braatz (NRAO)

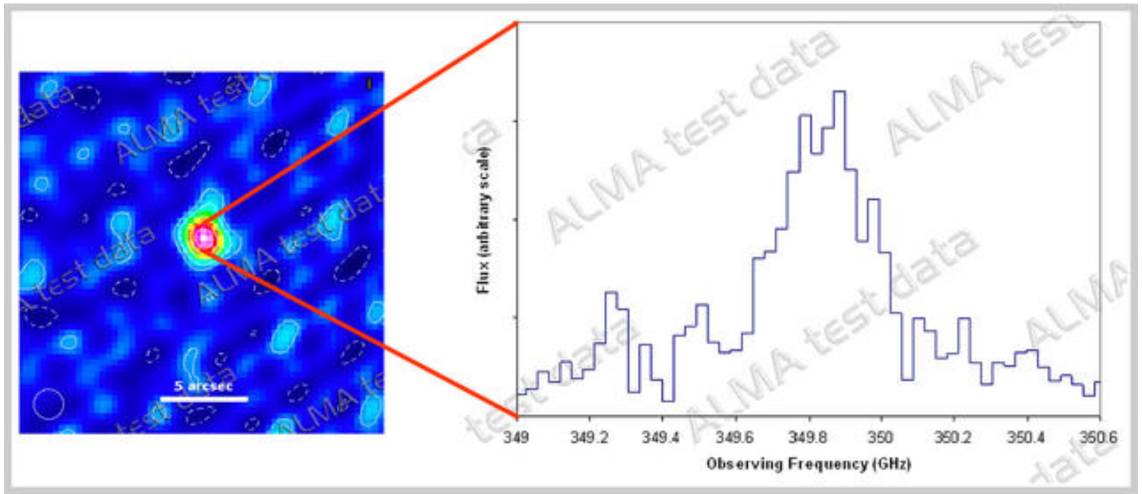
Thanks to Mark Lacy, Dave Meier.

Atacama Large Millimeter/submillimeter Array
Expanded Very Large Array
Robert C. Byrd Green Bank Telescope
Very Long Baseline Array

Outline

- Why spectroscopy?
- What do we observe?
- Some observational considerations
- Analyzing spectral line data

Why Spectroscopy?



- Probe physical conditions
  - Density – different transitions have different critical densities, also specific tracers of dense gas (optically thinner than CO) like HCN, CS, NH_3
  - Temperature – observe different energy transitions of the same species (e.g. Ammonia)
- Chemistry
- Dynamics

“Continuum”

- Even continuum observations are taken in spectroscopic correlator modes to reduce bandwidth smearing.

- Modern electronics allows for wide-band continuum observing

- Science does not depend sensitively on frequency, but using spectral line mode is favorable to correct for some frequency dependent issues:
  - Limitations of bandwidth smearing
  - Limitations of beam smearing
  - Problems due to atmospheric changes as a function of frequency
  - Problems due to signal transmission effects as a function of frequency
  - Opportunity to flag RFI

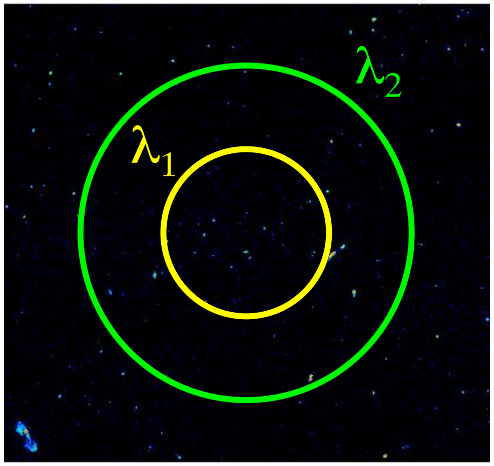
- Using a spectral line mode also allows editing for unwanted, narrow-band interference.

Effects of Broad Bandwidth:

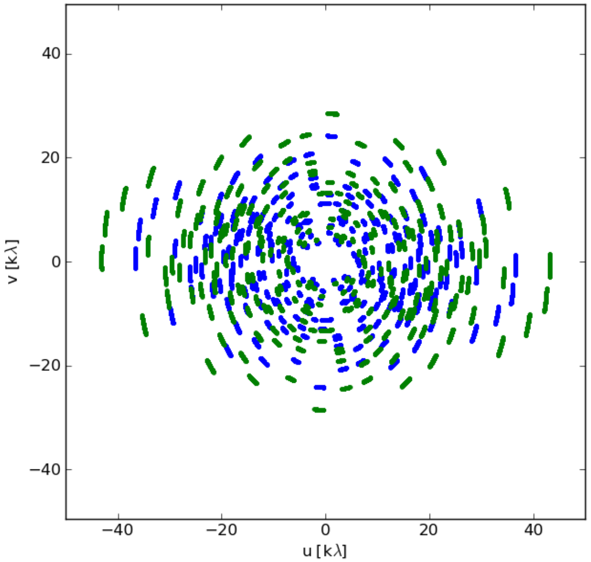
- Consider an observation covering the bandwidth (λ_1, λ_2)
- Changing Primary Beam ($\theta_{PB} = \lambda/D$)

  $\Rightarrow$ θ_{PB} changes by λ_1/λ_2

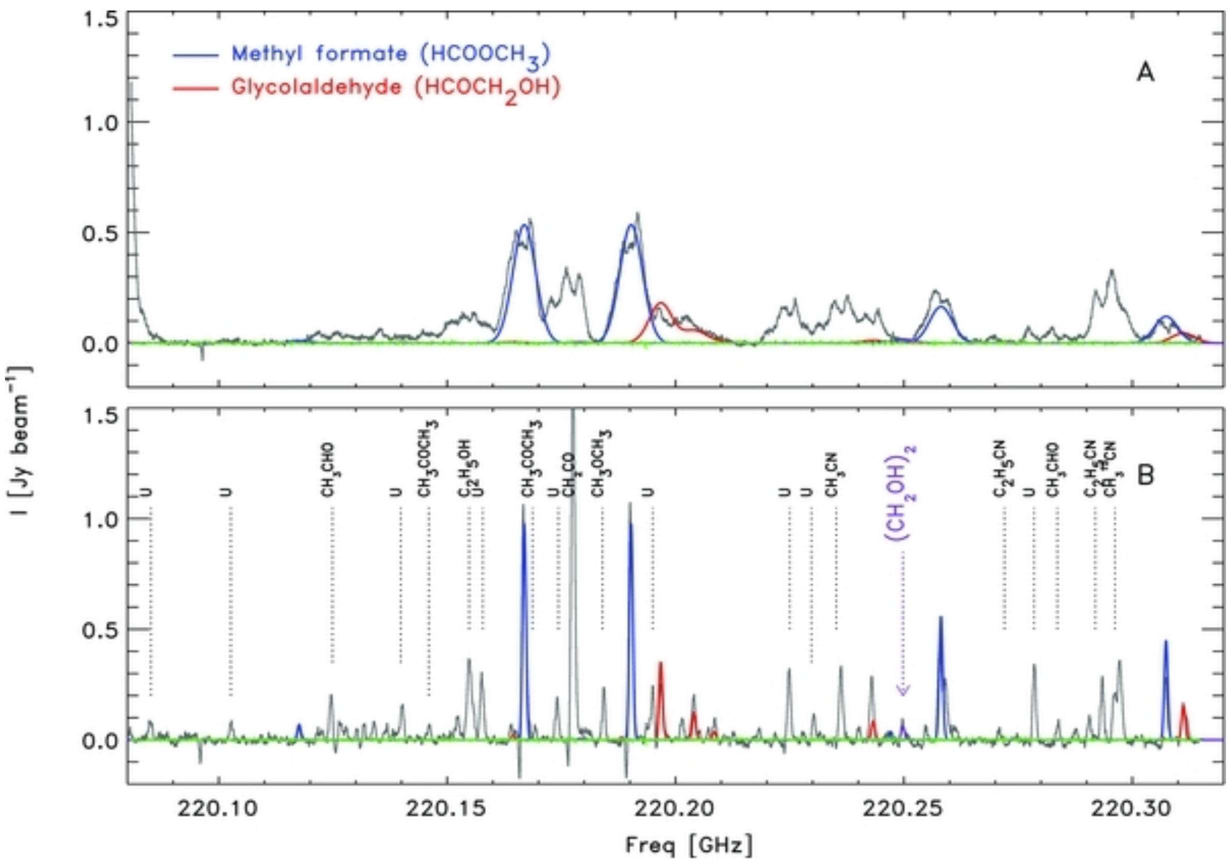
- Dependent on fractional bandwidth observed, so more important at lower frequencies



- Bandwidth Smearing (chromatic aberration)
- Fringe spacing = λ/B
  - Fringe spacings change by λ_1/λ_2
  - *u,v* samples smeared radially
  - More important in larger configurations, and for lower frequencies
- Huge effects for VLA
- Multi-frequency synthesis



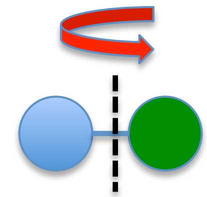
Example: complex molecules in protostars

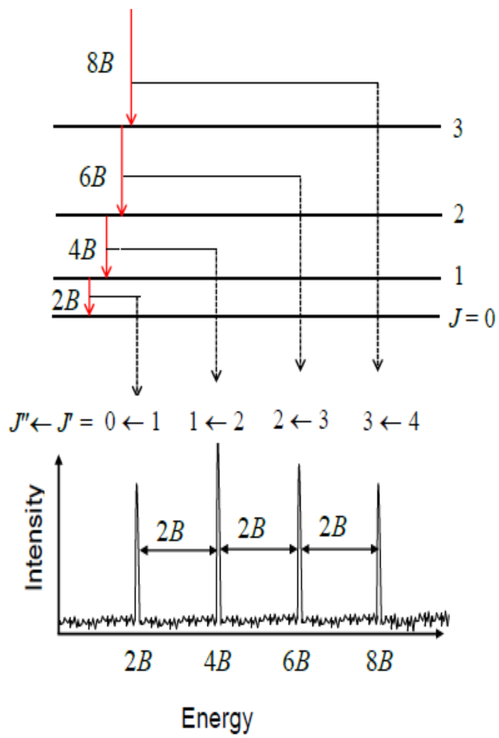


Detection of the Simplest Sugar, Glycolaldehyde, in a Solar-type Protostar with ALMA
Jørgensen et al. 2012

Molecular spectroscopy: linear molecules

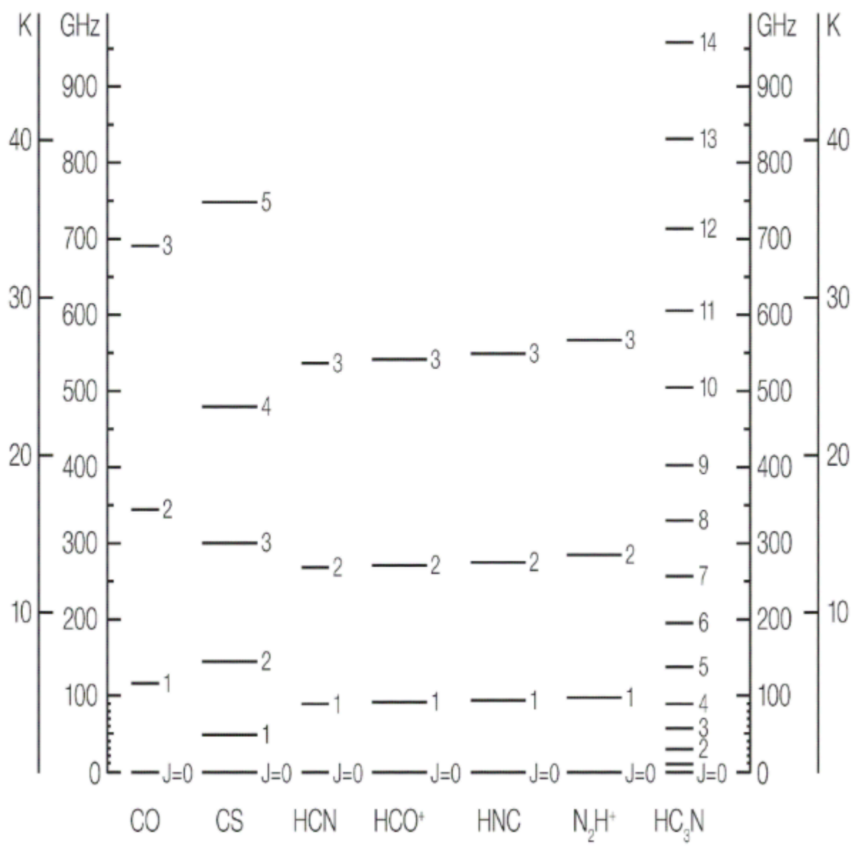
- The richness of a given molecule's spectrum depends on its shape.
- Molecules can have one, two or three rotation axes with dipoles.
- Linear molecules like CO have just one rotation axis, making a simple and evenly-spaced energy ladder
- Line intensity depends on, e.g., temperature and abundance of gas, optical thickness





CO: a Simple rigid rotor

Linear molecules: a rotation ladder



- States uniquely defined by total angular momentum quantum level J

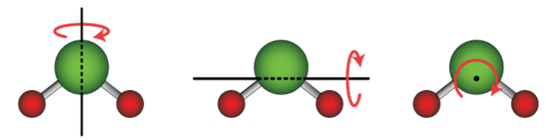
- Selection rules: $\Delta J = \pm 1$

- Successive transitions are evenly spaced, e.g.

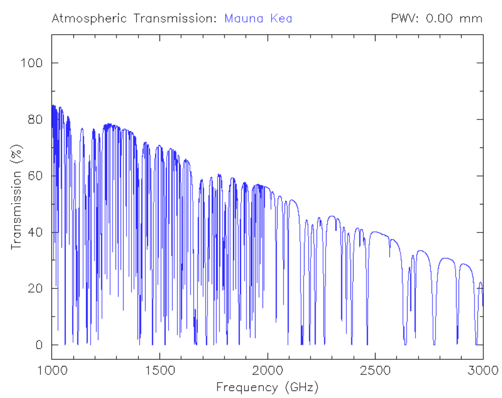
CO (1-0) at 115 GHz
CO (2-1) at 230 GHz
CO (3-2) at 345 GHz
Etc.

Molecular spectroscopy: More complex shapes

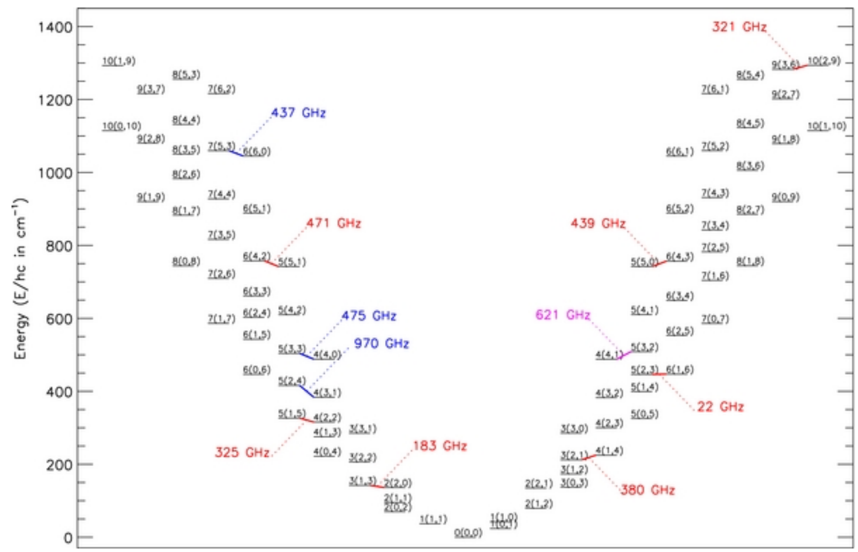
- Most molecules have more than one axis, and much more complex spectra.



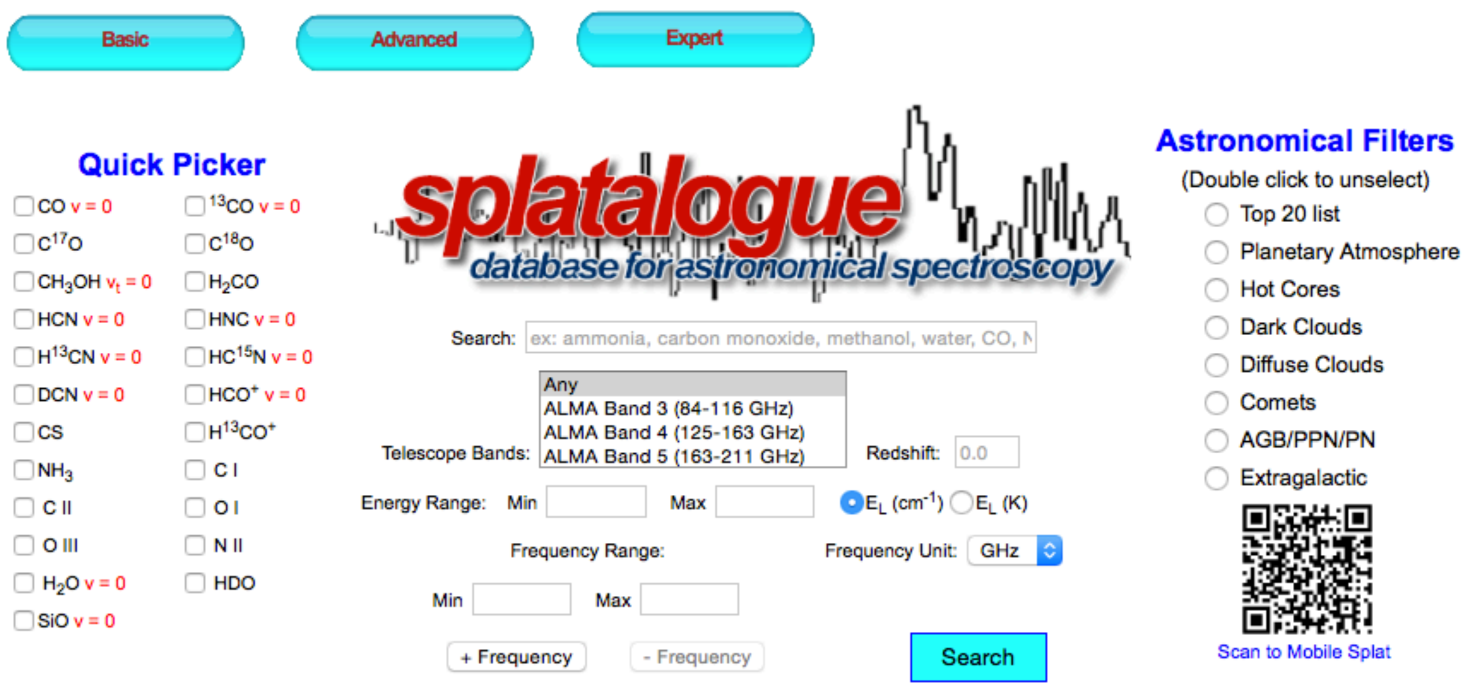
H_2O is an asymmetric top



Water (in absorption)



Splatalogue



Splatalogue

	Species	Chemical Name	Ordered Freq (GHz) (rest frame, redshifted)	Resolved QNs
1	CO v = 0	Carbon Monoxide	115.27120, 115.27120	1- 0
2	CO v = 0	Carbon Monoxide	230.53800, 230.53800	2- 1
3	CO v = 0	Carbon Monoxide	345.79599, 345.79599	3- 2
4	CO v = 0	Carbon Monoxide	461.04077, 461.04077	4- 3
5	CO v = 0	Carbon Monoxide	576.26793, 576.26793	5- 4
6	CO v = 0	Carbon Monoxide	691.47308, 691.47308	6- 5
7	CO v = 0	Carbon Monoxide	806.65180, 806.65180	7- 6
8	CO v = 0	Carbon Monoxide	921.79970, 921.79970	8- 7
9	CO v = 0	Carbon Monoxide	1036.91239, 1036.91239	9- 8

	Species	Chemical Name	Ordered Freq (GHz) (rest frame, redshifted)	Resolved QNs
1	SiO v = 0	Silicon Monoxide	43.42376, 43.42376	1- 0
2	SiO v = 0	Silicon Monoxide	86.84696, 86.84696	2- 1
3	SiO v = 0	Silicon Monoxide	130.26861, 130.26861	3- 2
4	SiO v = 0	Silicon Monoxide	173.68831, 173.68831	4- 3
5	SiO v = 0	Silicon Monoxide	217.10498, 217.10498	5- 4
6	SiO v = 0	Silicon Monoxide	260.51802, 260.51802	6- 5
7	SiO v = 0	Silicon Monoxide	303.92681, 303.92681	7- 6
8	SiO v = 0	Silicon Monoxide	347.33058, 347.33058	8- 7
9	SiO v = 0	Silicon Monoxide	390.72861, 390.72861	9- 8
10	SiO v = 0	Silicon Monoxide	434.12018, 434.12018	10- 9

	Species	Chemical Name	Ordered Freq (GHz) (rest frame, redshifted)	Resolved QNs
1	H_2O v=0	Water	22.23508, 22.23508	6(1, 6)- 5(2, 3)
2	H_2O v=0	Water	183.31009, 183.31009	3(1, 3)- 2(2, 0)
3	H_2O v=0	Water	321.22568, 321.22568	10(2, 9)- 9(3, 6)
4	H_2O v=0	Water	325.15290, 325.15290	5(1, 5)- 4(2, 2)
5	H_2O v=0	Water	380.19736, 380.19736	4(1, 4)- 3(2, 1)
6	H_2O v=0	Water	437.34666, 437.34666	7(5, 3)- 6(6, 0)
7	H_2O v=0	Water	439.15079, 439.15079	6(4, 3)- 5(5, 0)

Sensitivity

$$\sigma_{\mathrm{S}} = \frac{2\,k\,T_{\mathrm{sys}}}{\eta_{\mathrm{q}}\eta_{\mathrm{c}}A_{\mathrm{eff}}\sqrt{N(N-1)\,n_{\mathrm{p}}\,\Delta\nu\,t_{\mathrm{int}}}}.$$

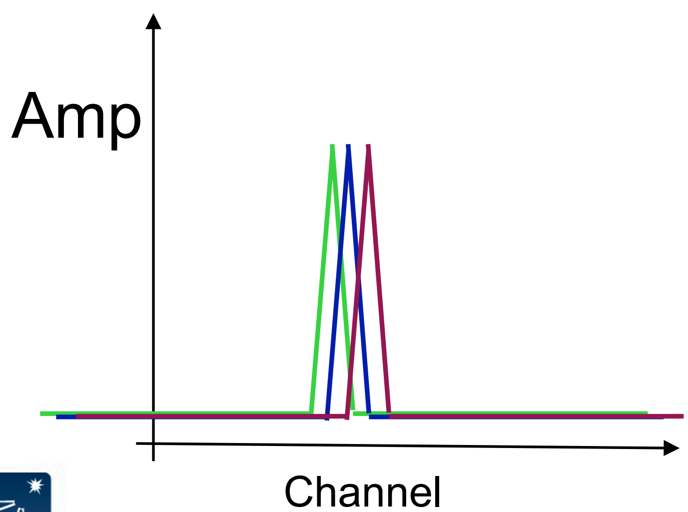
Spectral line sensitivity is *not* improved with broader bandwidth. It requires:

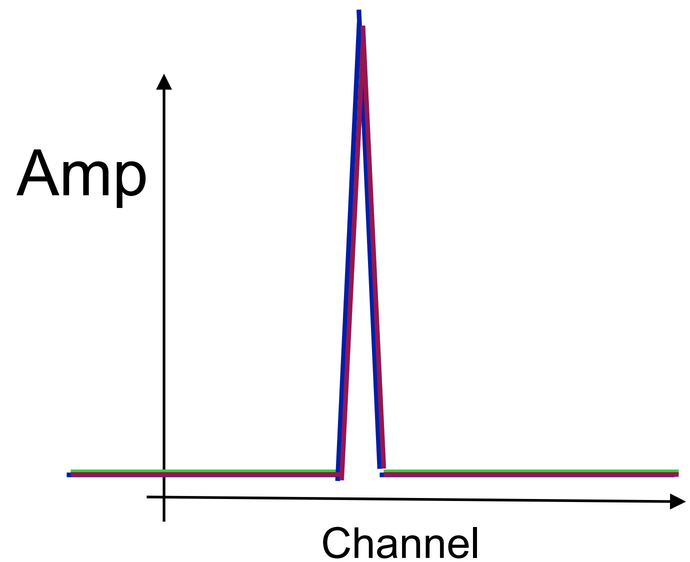
– Adding antennas/collecting area
– Improving collecting efficiency
– Observing in better weather
– Long integrations

Some Observing considerations

Doppler Tracking

- Observing from the surface of the Earth, our velocity with respect to astronomical sources is not constant in time or direction.
- Note that the bandpass shape is really a function of *frequency*, not velocity!
  - Applying Doppler tracking will introduce a time-dependent and position dependent frequency shift.
  - If differences are large, apply corrections during post-processing instead.
  - With the wider bandwidths now common, online Doppler setting is done but not tracking.
- Doppler tracking is done in post-processing (AIPS: CVEL; CASA: CLEAN)





Velocity conventions

- $V_{rad} = c\ \Delta\nu/\nu_0$
- $V_{opt} = c\ \Delta\lambda/\lambda_0 = cz$

- Differences become large as redshift increases
- For the V_{opt} definition, constant frequency increment channels do not correspond to constant velocities increment channels

Velocity Reference Frames:

Correct for	Amplitude	Rest frame
Nothing	0 km/s	Topocentric
Earth rotation	< 0.5 km/s	Geocentric
Earth-Moon barycenter	< 0.013 km/s	E/M Barycentric
Earth around Sun	< 30 km/s	Heliocentric
Solar System barycenter	< 0.012 km/s	SS Barycentric (~Heliocentric)
Sun peculiar motion	< 20 km/s	Local Standard of Rest
Galactic rotation	< 300 km/s	Galactocentric

Transformations standardized by IAU.

See Frank Ghigo's Doppler Tracking web page for great details:

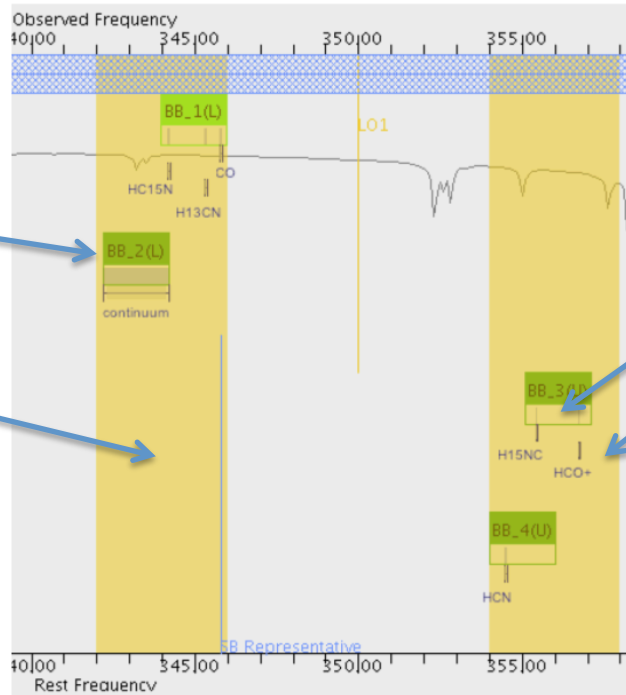
http://www.gb.nrao.edu/~fghigo/gbtdoc/doppler.html

Example ALMA spectroscopic setup

Atmospheric transparency

Basebands in Green

IF ranges in yellow



Individual spws

- For ALMA, basebands up to 2 GHz wide must be tuned within 4 GHz sidebands that are separated by 8 GHz
- Tune to avoid atmospheric absorption lines, when possible!

Spectroscopy with ALMA

- FDM : Frequency Division Mode
  - Used for high-res spectroscopy
  - Up to 32 Spectral Windows (spws) per baseband, each spw can be 60MHz-1875MHz wide.
  - Within a baseband, the total number of channels is fixed at $7680/N_{pol}$, and are distributed amongst the assigned spws. (N_{pol}=2 usually)
  - Highest resolution is 15kHz (Hanning smoothed, single polarization).

- TDM : Time Division Mode
  - Used for continuum, service observations (pointing), low-res spectroscopy

Data rates

- Modern correlators can produce more data than the storage and processing facilities can deal with.
- Data rates important for both VLA and ALMA.
- ~ 1 TB per day
- What to do?
  - Match spectral resolution to science.
  - Time average if possible (but beware of time smearing in wide fields).

- For the VLA, data rate, R:

$$R = 160\mathrm{GB/hr}\frac{N_{chan}N_{pol}}{16384}\frac{N_{ant}(N_{ant}-1)}{26\times 27}\frac{1\mathrm{s}}{\Delta t}$$

- ~32 bits/visibility
- Proportional to ~N_{ant}^2
- ALMA in full resolution mode is similar (but more antennas; calculation is done for you in the ALMA Observing Tool).
- Because of high data volumes, nothing comes "for free"

The ALMA correlator – world's highest supercomputer

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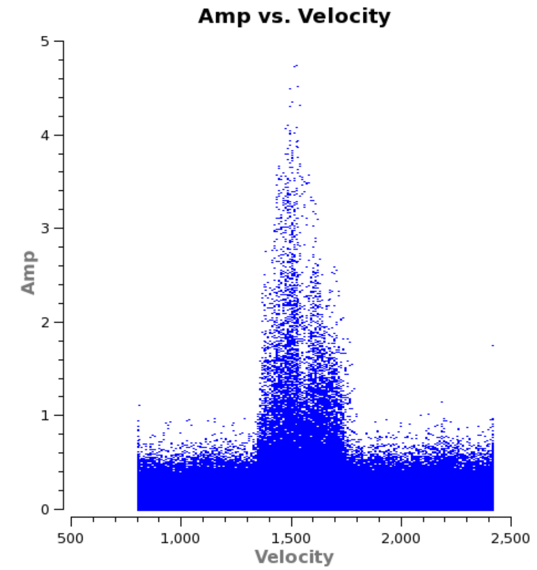
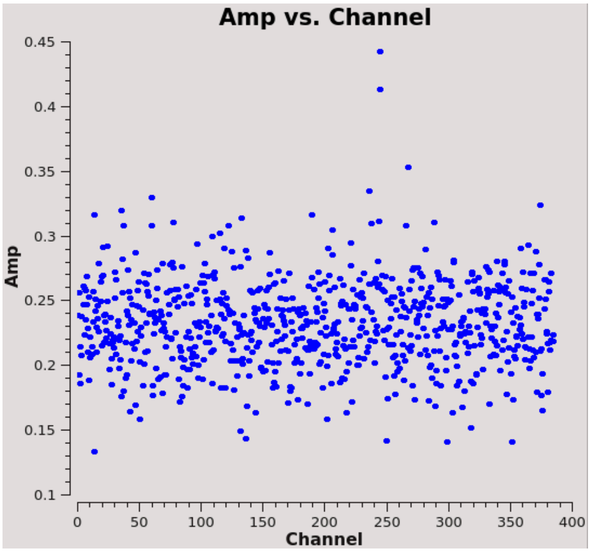
Continuum Subtraction:

- Spectral line data often contains continuum emission from the target.
  - This emission complicates the detection and analysis of lines
  - Easier to analyze line emission with continuum removed.
- Use channels with no line features to model the continuum; low-order polynomial fit
  - Subtract this continuum model from all channels
- Always bandpass calibrate before continuum subtracting
- Can be done before imaging (uvcontsub) or after imaging (imcontsub)
- Check results carefully!





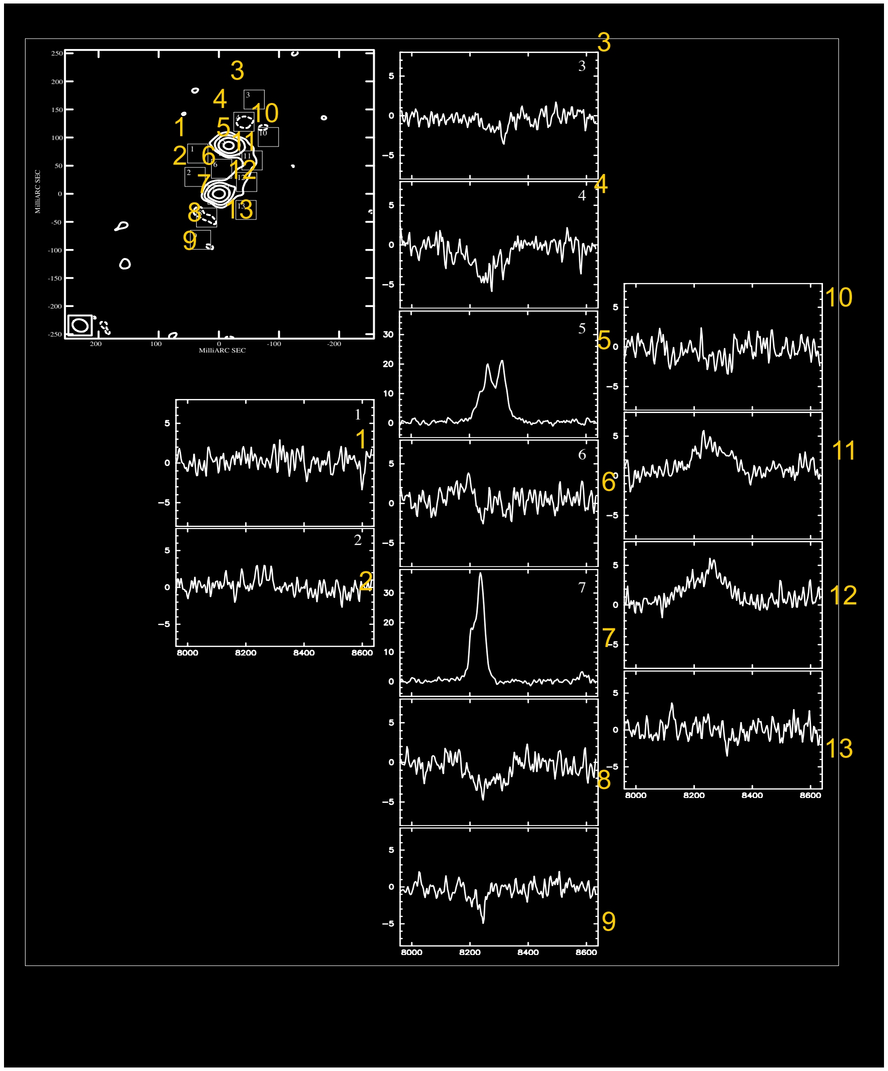
Visualizing and analyzing spectral line data

- Imaging will create a spectral line *cube*, which is 3-dimensional: RA, Dec and Velocity.

- With the cube, we usually visualize the information by making 1-D or 2-D projections:
  - Line profiles (1-D slices along velocity axis)
  - Channel maps (2-D slices along velocity axis)
  - Position-velocity plots (slices along spatial dimension)
  - Moment maps (integration along the velocity axis)

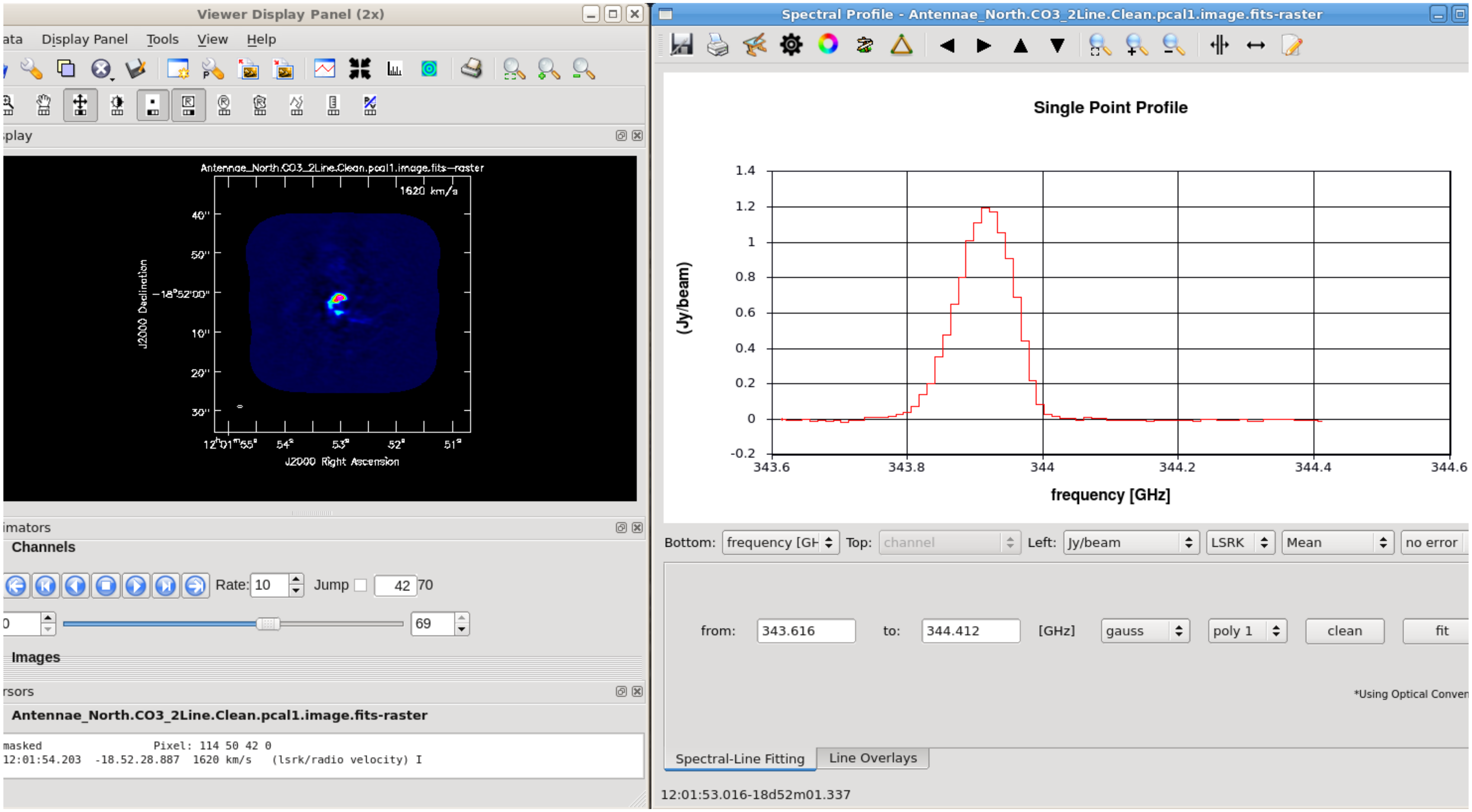
Example: line profiles

- Line profiles show changes in line shape, width and depth as a function of position.



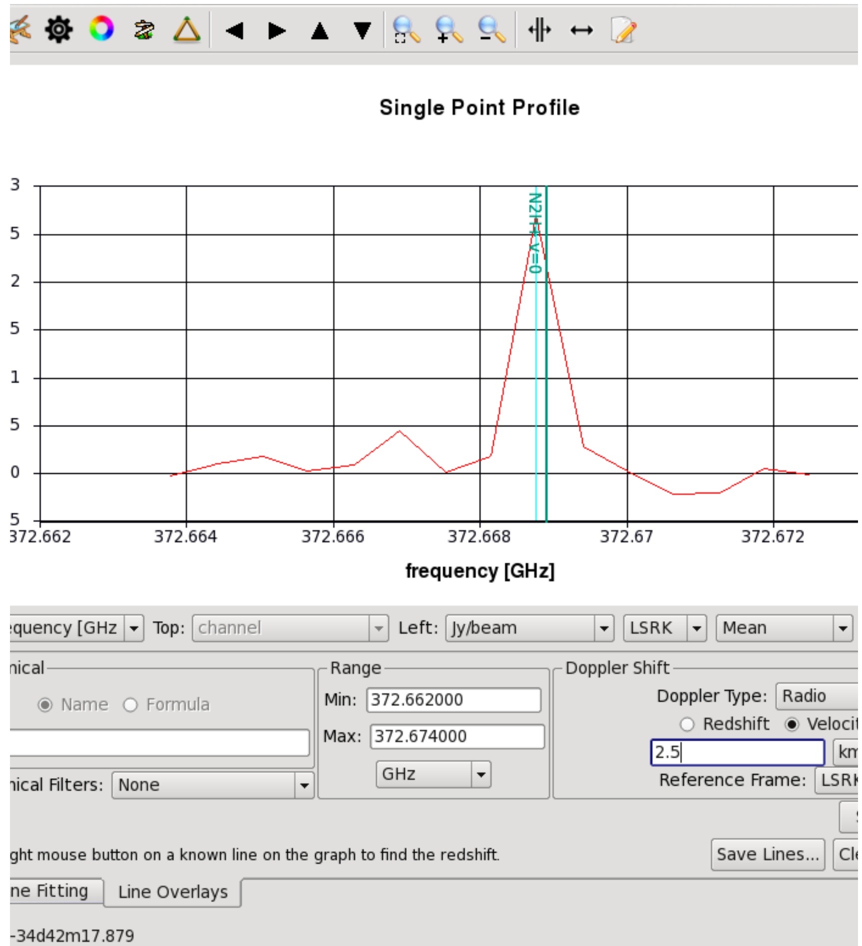
EVN+MERLIN 1667 MHz OH maser emission and absorption spectra in a luminous infrared galaxy (IIIZw35).

Spectral Profiles in CASA



Spectral extraction and line identification

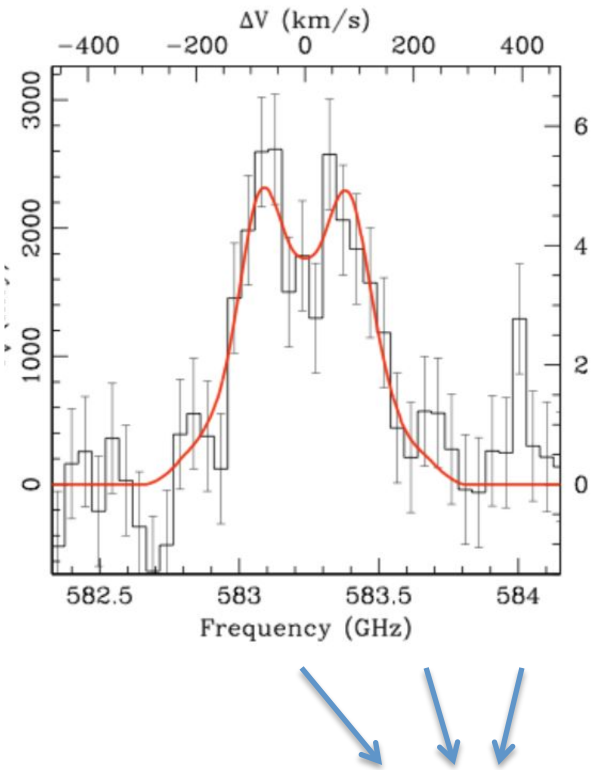
- Can use e.g. the CASA Viewer for line identification with the aid of Splatalogue.
- Can filter by species or common astrophysical lines to avoid getting too many results.
- Often, transitions of interest are in the ground vibrational state (v=0). E.g. CO (1-0) v=0 is the usual 115 GHz line.



Spectral profile example

- These profiles are commonly seen in extragalactic radio spectra, revealing inclined, disk-dominated galaxy

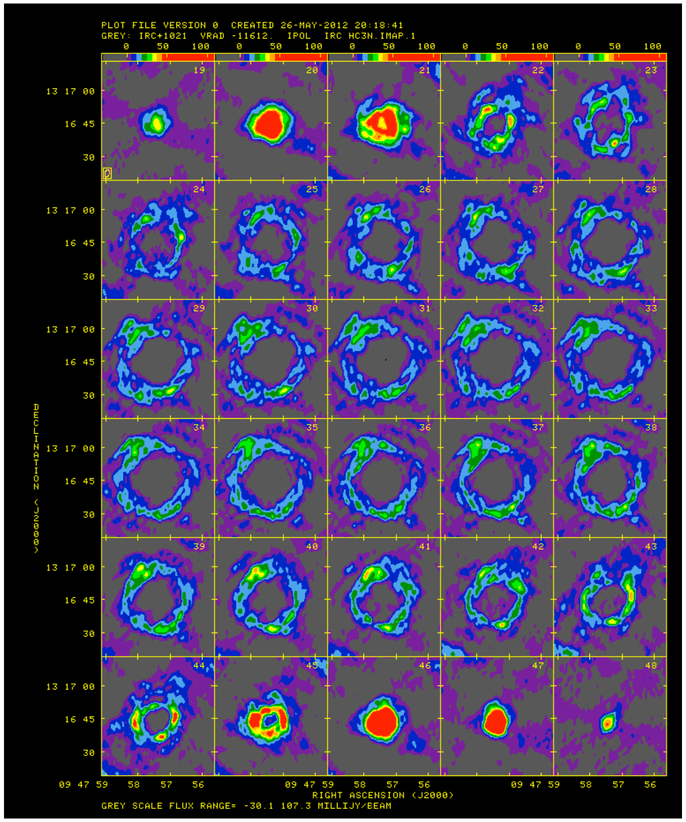
- But beware, there are other possibilities, e.g. merging galaxies



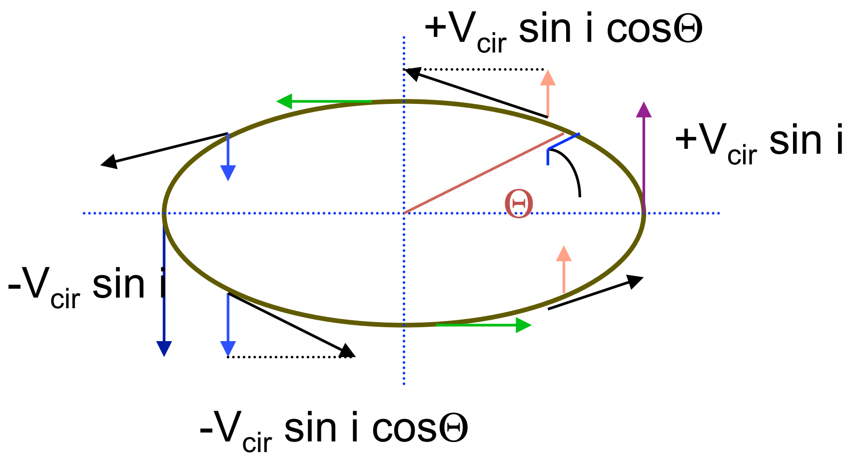
Channel maps give dynamical information

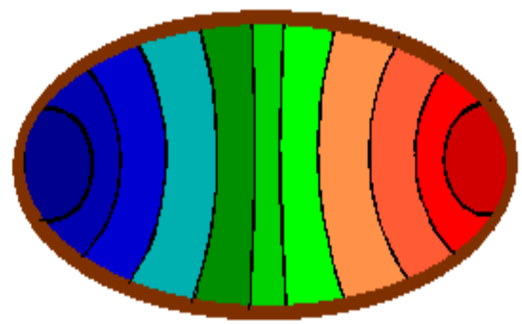
- IRC 10216 is a 16th mag AGB star but brightest star at 5 µm
- Expanding shell is clearly delineated in channel maps showing emission from the linear molecule HC_3N

HC_3N – IRC 10216



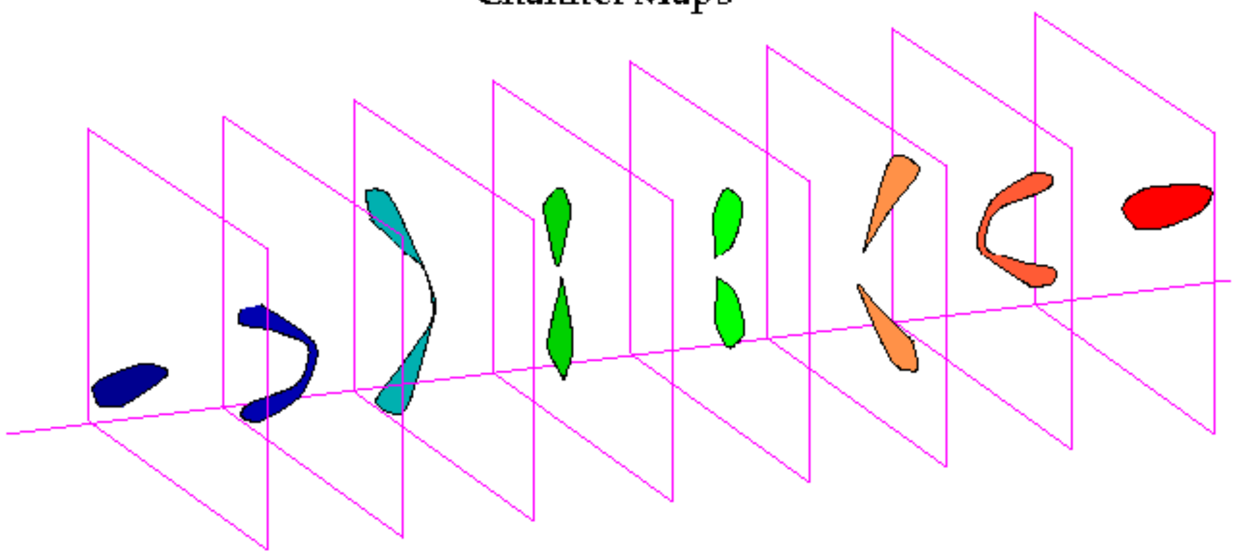
Example: A thin, tilted rotating disk





Mean Velocity Field

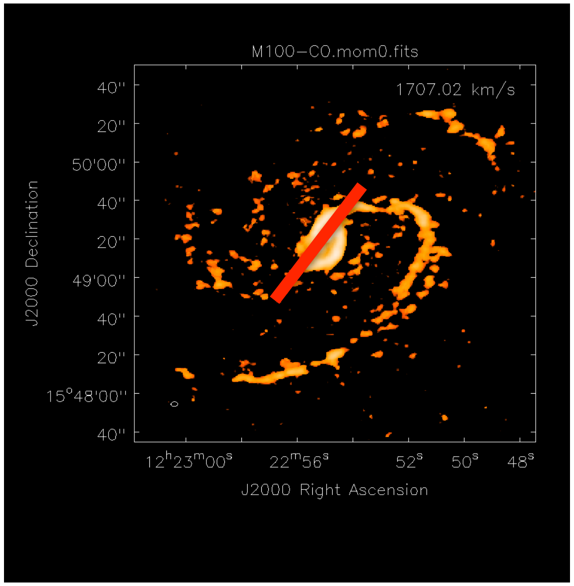
Channel Maps

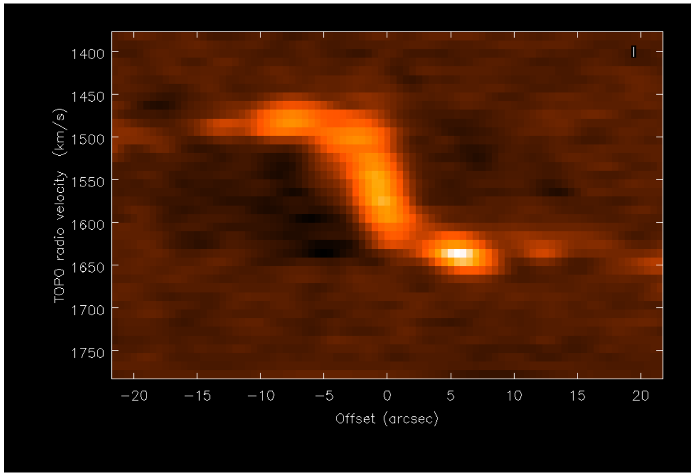


Position-velocity diagrams

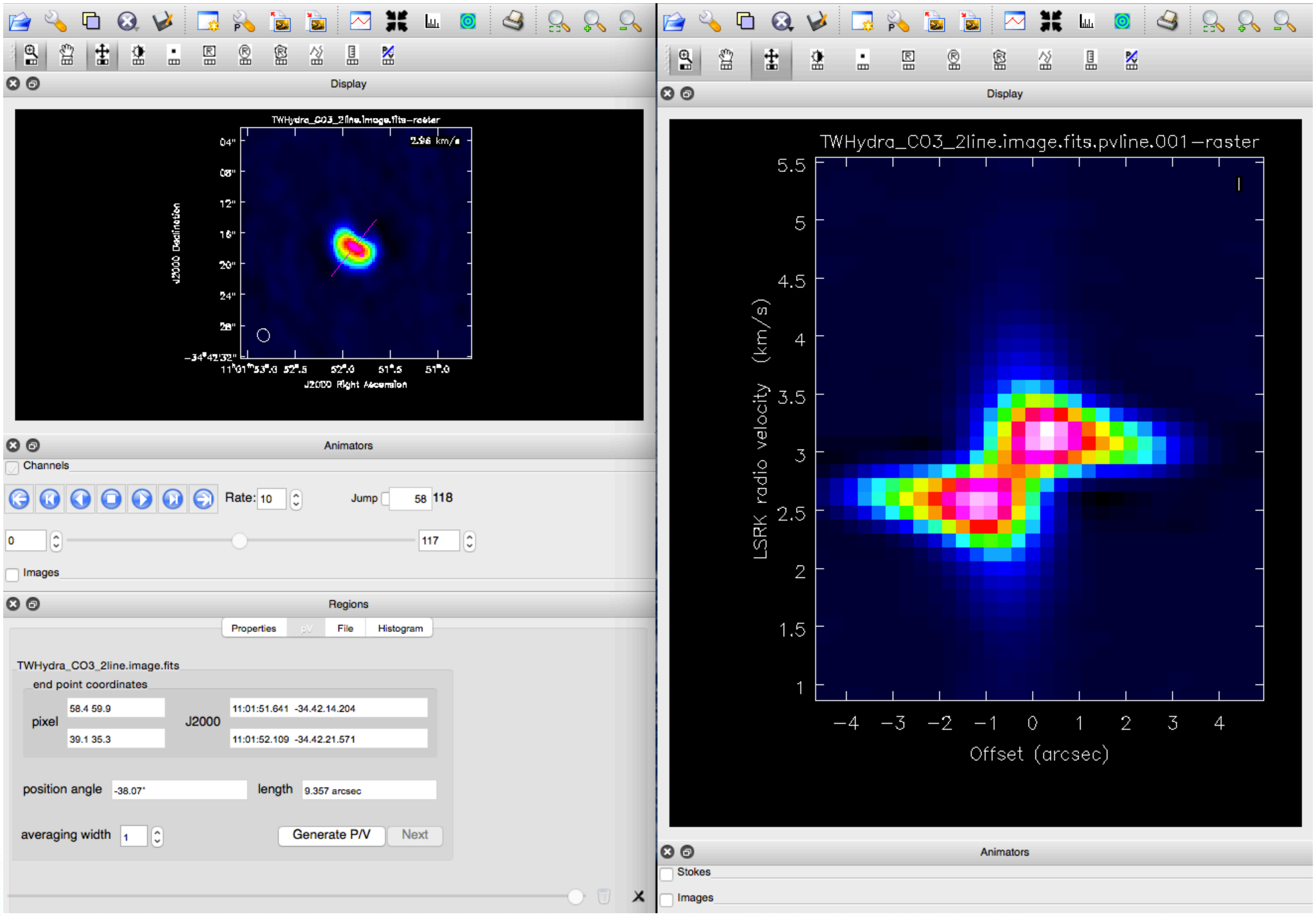
- PV-diagrams show, for example, the line emission velocity as a function of radius.
  - Here along a line through the dynamical center of the galaxy

- CASA task impv, or use the viewer





PV diagrams with the CASA viewer



3D (volume-rendered) visualization

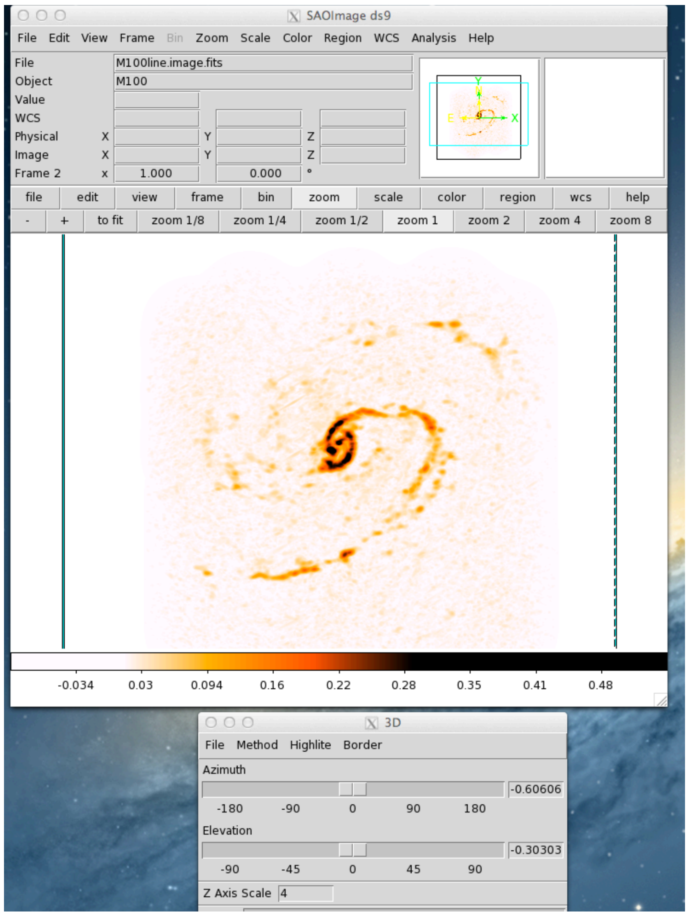
- Some software allows 3D visualization of image cubes.
- Can be useful for inspection of cube, and to find features that conventional moment analyses would miss.
- Can be hard to interpret though – velocity/frequency axis is not a spatial axis.

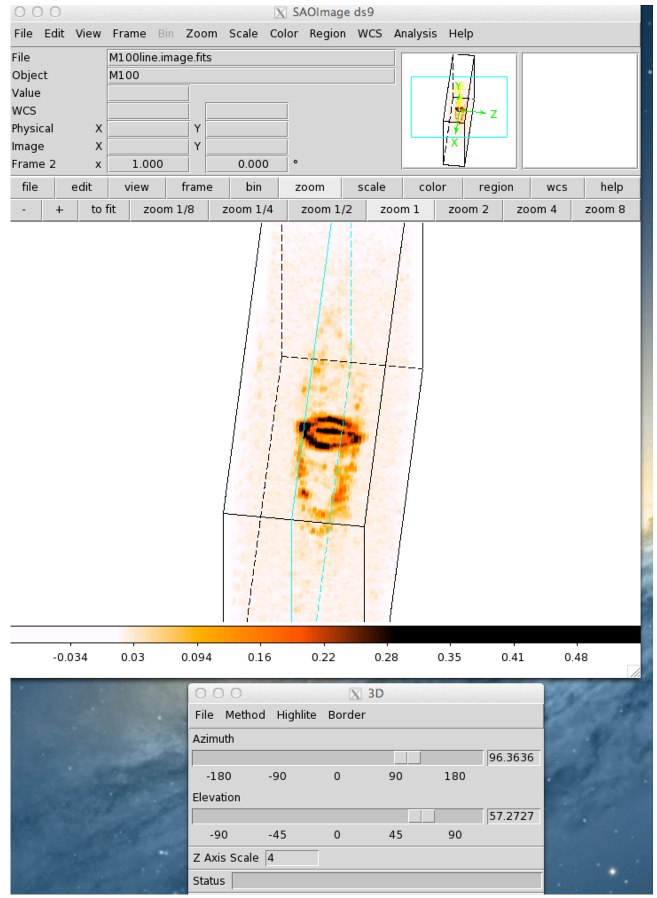
3D display software

- SAOimage ds9 is available from http://ds9.si.edu
- GAIA is available from star-www.dur.ac.uk/~pdraper/gaia/gaia.html (long-term support unclear)
- Karma kvis is available (though no longer updated) from http://www.atnf.csiro.au/computing/software/karma/
- Other, not observational astronomy specific 3D rendering packages are also available (ParaView, VisIt, yt….). Drawback is lack of understanding of astronomical coordinate systems.

SAOimage ds9 renderings of M100

ds9 -3d my_image_cube.fits





Moment maps

- A popular way of reducing a 3D line to 2D
- Moment 0 : line map
- Moment 1 : velocity map
- Moment 2 : velocity dispersion

- Each higher moment requires better S/N; mask the low S/N
- Higher order moments (skew, kurtosis…) are also defined, but not usually useful

- Moment 0 (integration of flux density *S* is carried out over the full width of the line profile):

$$\int S\mathrm{d}v$$

- Moment 1 = <v>:

$$\frac{\int vS\mathrm{d}v}{\int S\mathrm{d}v}$$

- Moment 2:

$$\frac{\int (v - <v>)^2 S\mathrm{d}v}{\int S\mathrm{d}v}$$

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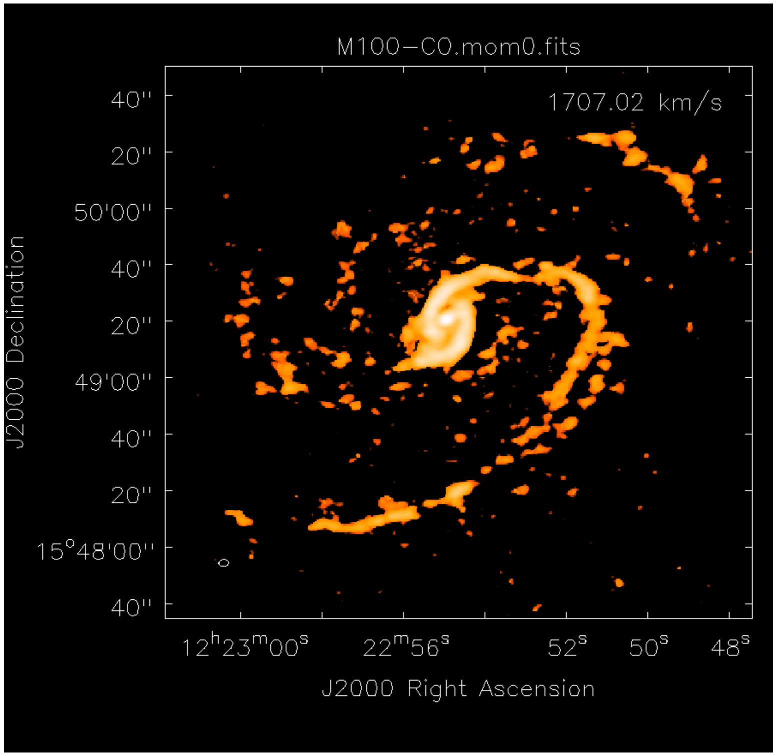
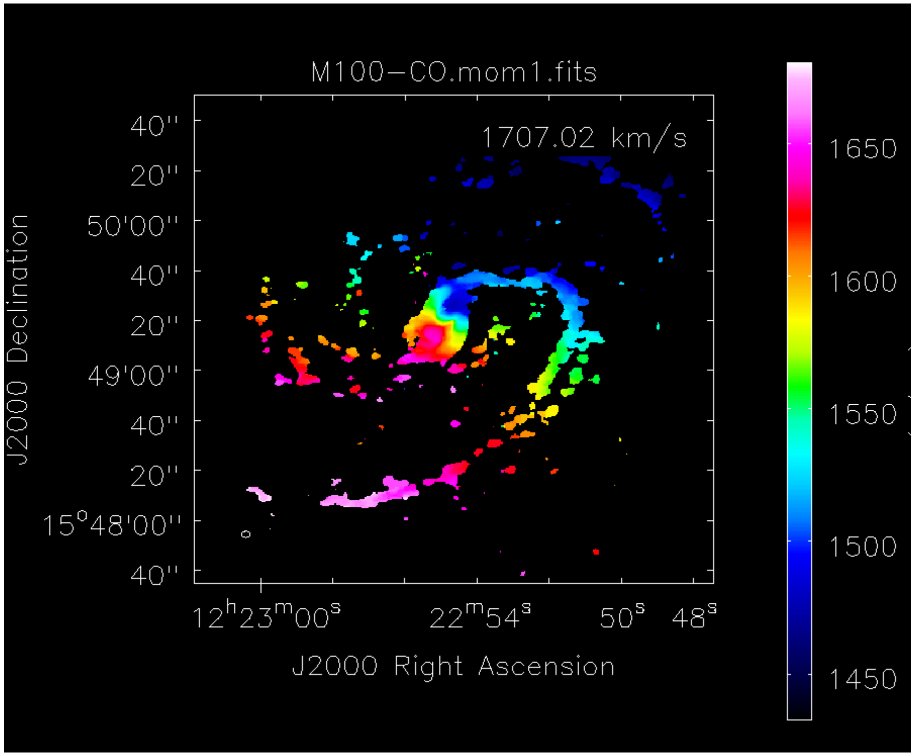
Example moment maps (CO in M100)

Moment 0



Moment 1



Moment maps: caution

- Moment maps should be just one component to an analysis strategy. Use them as a guide for investigating spectral features, or comparing with other λ.

- Moments sensitive to noise so clipping is required
  - Higher order moments depend on lower ones so progressively noisier.
- Hard to interpret correctly:
  - Both emission and absorption may be present, emission may be double peaked.
  - Biased towards regions of high intensity.
  - Complicated error estimates: number or channels with real emission used in moment computation will greatly change across the image.

The End