Spectral Lines

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Outline

- Scientific motivation for spectral line observations
  - Examples of properties that can be derived

- What can affect your observations:
  - Instrument responses
  - Atmospheric effects
  - RFI environment

Concepts

- What to consider during observation/calibration
  - Bandpass, RFI and flagging
  - Doppler corrections
  - Spectral response
  - Continuum subtraction

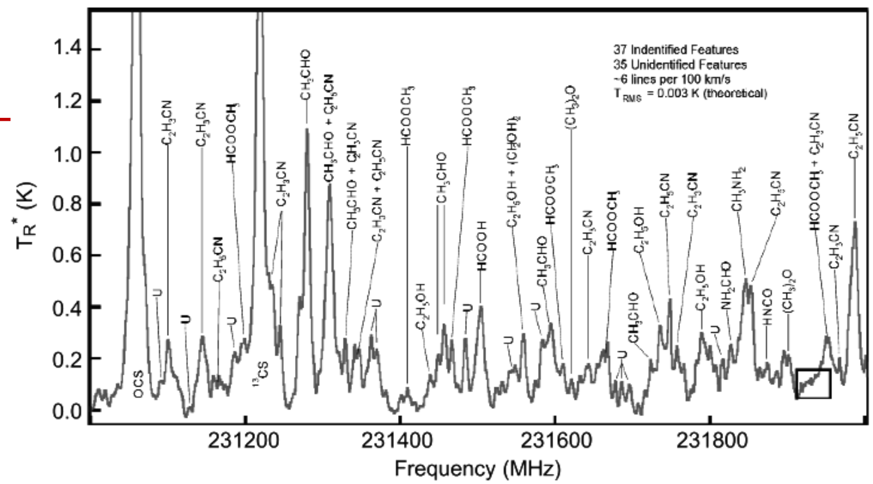
Some practical guidance

Science with spectroscopy

In the radio/mm regime we have access to a huge set of transitions from molecules and atoms. Allows us to investigate the Interstellar Medium (ISM):

- Atomic hydrogen at 21cm is tracing the neutral, cool/warm gas content of the ISM. Large reservoir of gas for future star formation.

- Molecular emission is often tracing cooler, denser regions, where star formation is likely to take place.



Ziurys et al 2006, ALMA Band 6 early observations

- We can derive properties like column density and estimate gas masses.
- We can also derive redshifts via Doppler shifts, kinematics from the velocity distribution, and velocity dispersion from the line profile.

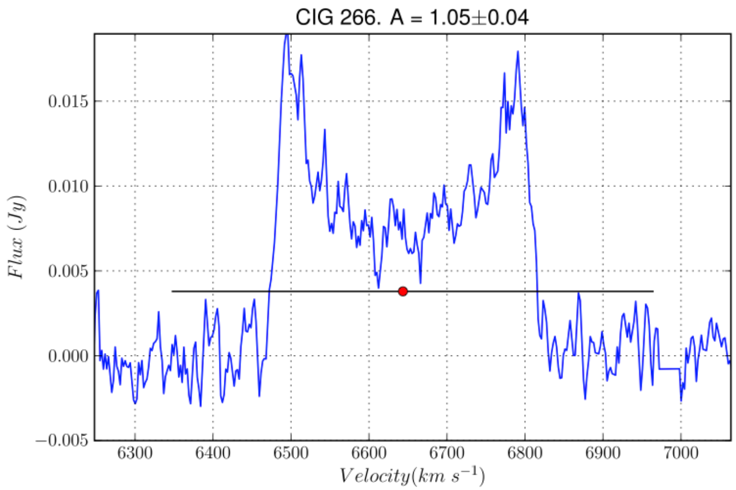
Atomic Hydrogen example

Column density

$$N_{HI} = 1.82 \times 10^{18} \int T_{\rm sp} \tau_V \, dV \quad {\rm cm}^{-2}$$

HI Mass

$$M_{HI} = 2.36 \times 10^5 \left(\frac{D}{\rm Mpc}\right)^2 \int \frac{S_V}{\rm Jy} \frac{dV}{\rm km\,s^{-1}} \quad {\rm M}_\odot$$



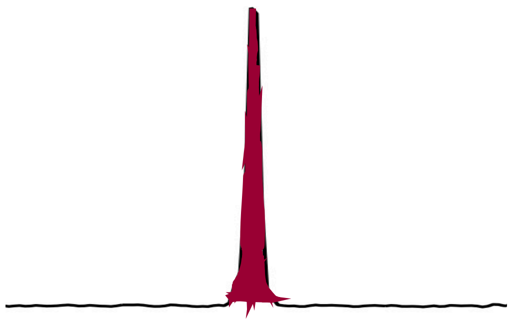
Espada et al. 2012

Moment analysis

You might want to derive parameters such as integrated line intensity, centroid velocity of components and line width - all as functions of position. Estimate the *moments* of the line profile.

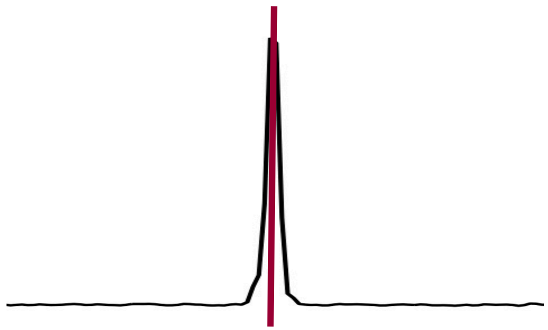
Integrated intensity:

$$\text{Moment } 0 \ = \int S_V \, dV$$



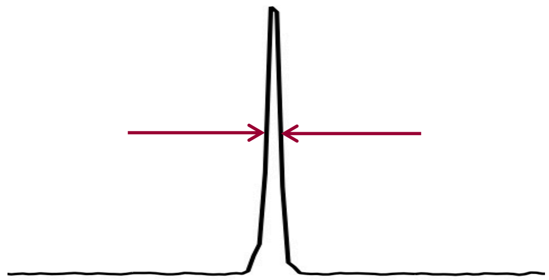
Intensity-weighted velocity:

$$\text{Moment 1} = \langle V \rangle = \frac{\int S_V V \, dV}{\int S_V \, dV}$$



Intensity-weighted velocity dispersion:

$$\text{Moment 2} = \langle V^2 \rangle^{1/2} = \sqrt{\frac{\int S_V (V - \langle V \rangle)^2 dV}{\int S_V \, dV}}$$



What determines a certain intensity?

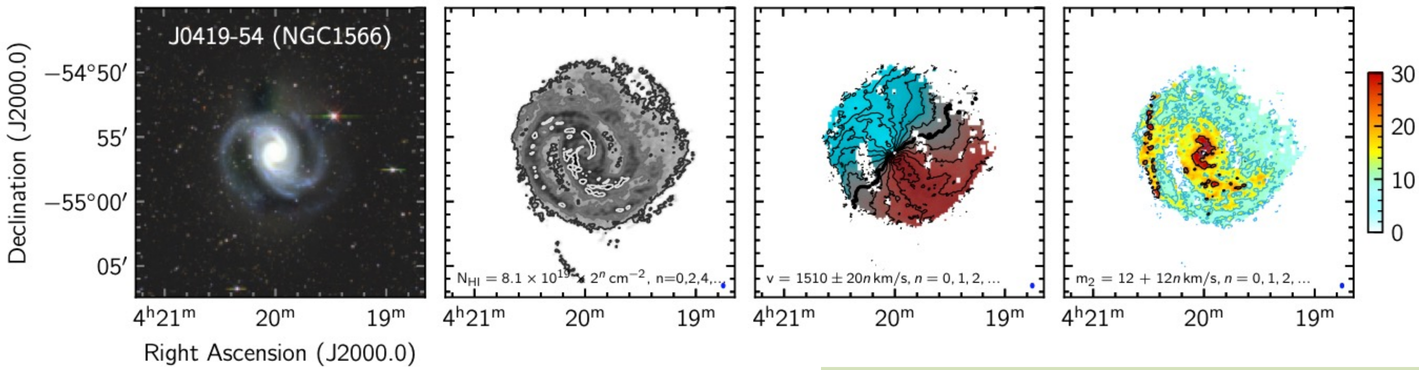
- The number of atoms/molecules responsible for the line
- The excitation stage determined by radiation and/or density

What determines a certain centroid velocity?

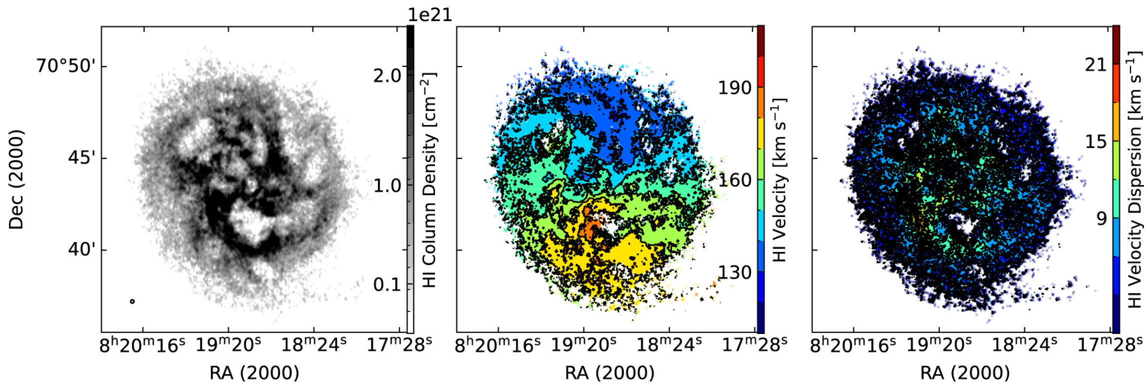
- The systemic velocity
- Additional motion wrt the systemic velocity

What determines a certain line width?

- Natural linewidth
- Thermal broadening
- Pressure broadening
- Bulk motion/system kinematics

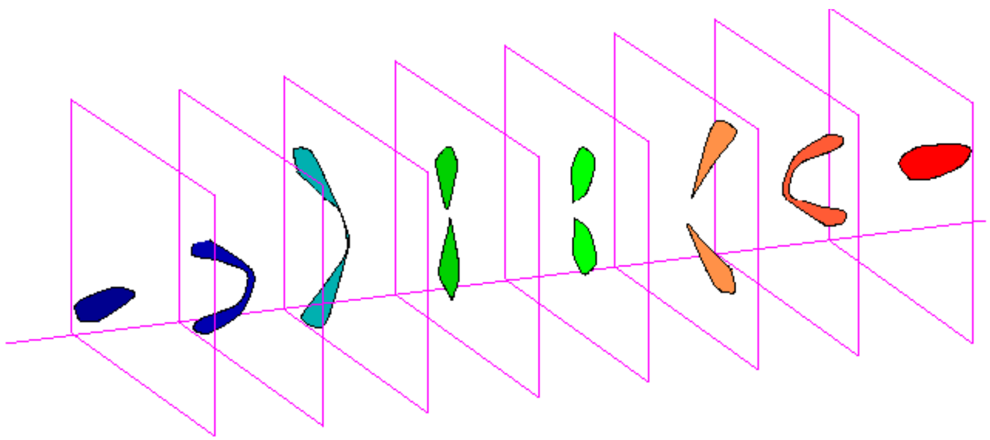


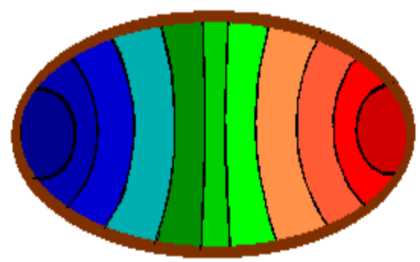
MHONGOOSE MeerKAT HI survey; de Blok et al. 2023

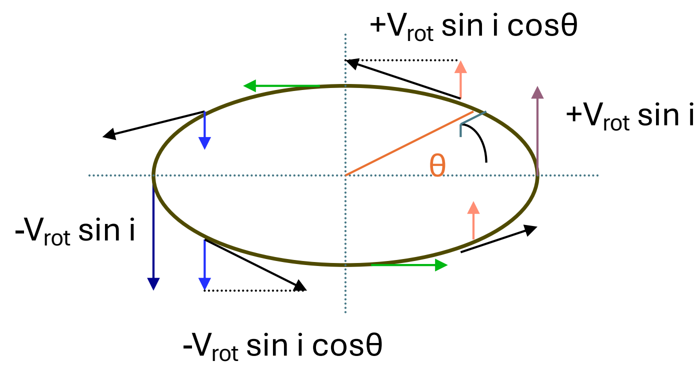


UGC 4305 VLA HI; Hunter, van Zee et al. (2023)

Velocity field: example of rotating disk model





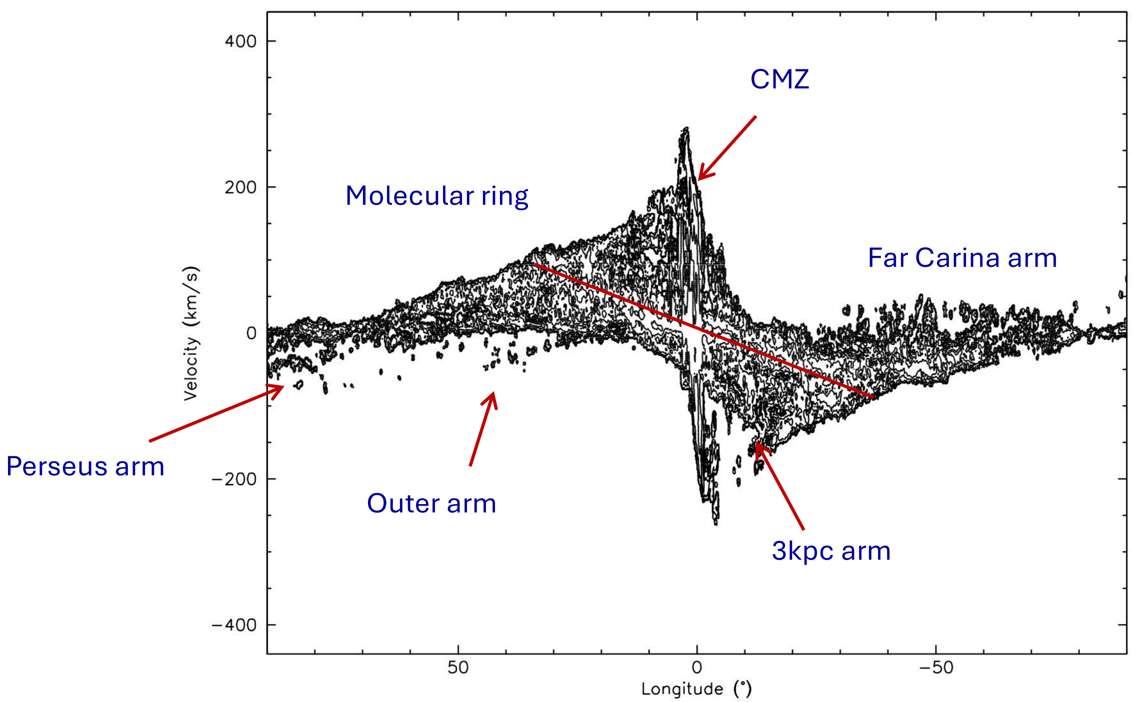


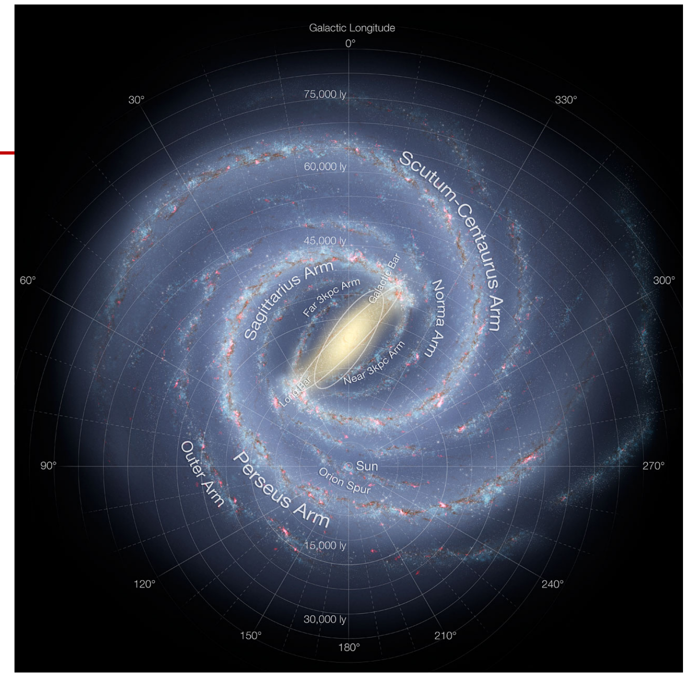
Distribution of emission within individual channels inform about the dynamics of the gas observed.

For external galaxies, HI is often displaying a velocity field comparable to that of a rotating disk.

Position-Velocity diagrams

P-V diagrams show, for example, the line derived velocities as a function of position along a selected plane (RA, Dec, Glong, Glat, radius).





CO(1-0) as a function of longitude in the Milky Way; Dame et al. (2001).

High spectral resolution

For science applications, we need high spectral resolution to resolve spectral features.

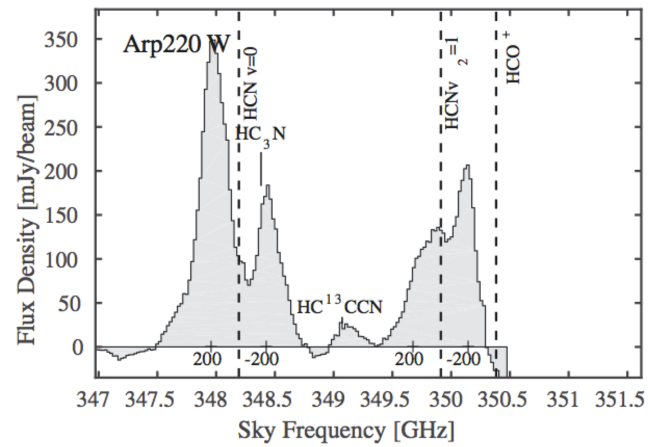
- To accurately derive properties, we need to be able to separate line from continuum.
- Sometimes necessary for detection of weak lines

Many channels across a large bandwidth allows:

- Search (and identification) of multiple transitions
- Detailed velocity distribution mapping

Source emission can change with frequency

- Spectral index, shape
- Polarized emission: Faraday rotation ∝ λ^2



ALMA observations of Arp 220W (Aalto et al. 2015).

Frequency dependent effects

For both spectral line and continuum science goals, spectral line mode is favorable to reduce at least some frequency dependent effects:

- Beam- and bandwidth smearing
- Instrumental signal transmission effects as a function of frequency
- Problems due to atmospheric changes as a function of frequency
- Unwanted, narrow-band interference.

Concepts

Beam smearing

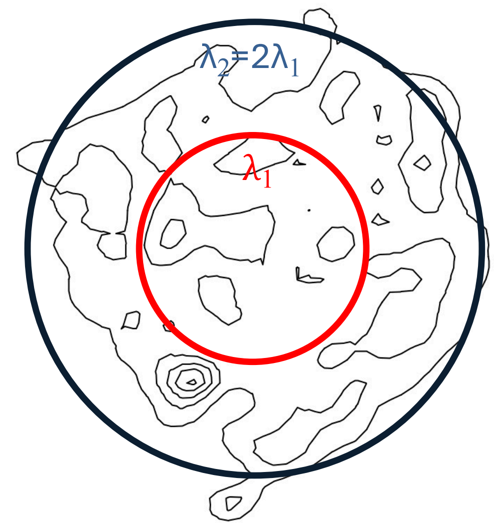
$\theta_{PB} = \lambda/D$

Band coverage λ_1-λ_2

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

More significant effect at longer wavelengths:

VLA 20cm, 1 GHz BW:	2.0
VLA 0.7cm, 2 GHz BW:	1.04
VLA 0.7cm, 8 GHz BW:	1.2
ALMA 3mm, 8 GHz BW:	1.08
ALMA 1mm, 8 GHz BW:	1.03



Bandwidth smearing: instrument response

Also called chromatic aberration.

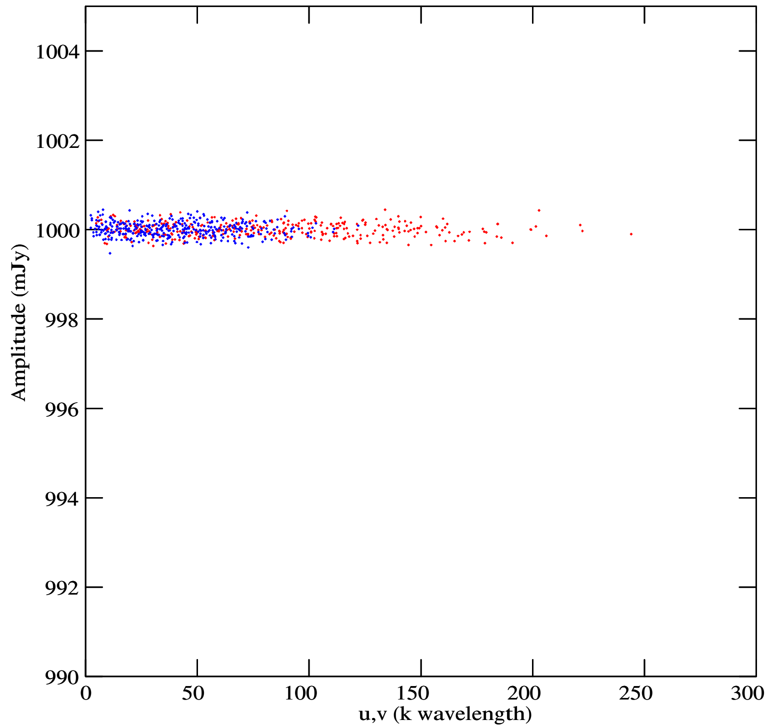
Fringe spacing = $\lambda/B = c/\nu B$

Band coverage ν_2-ν_1

- ν_1 = 1 GHz (blue)
- ν_2 = 2 GHz (red)

Frequencies sample different regions of the u-v plane.

Again, more important at longer wavelengths as fringe spacings will scale with λ_1/λ_2.



Ampl vs uv distance, VLA A-config.

Bandwidth smearing: instrument response

Band coverage ν_2-ν_1

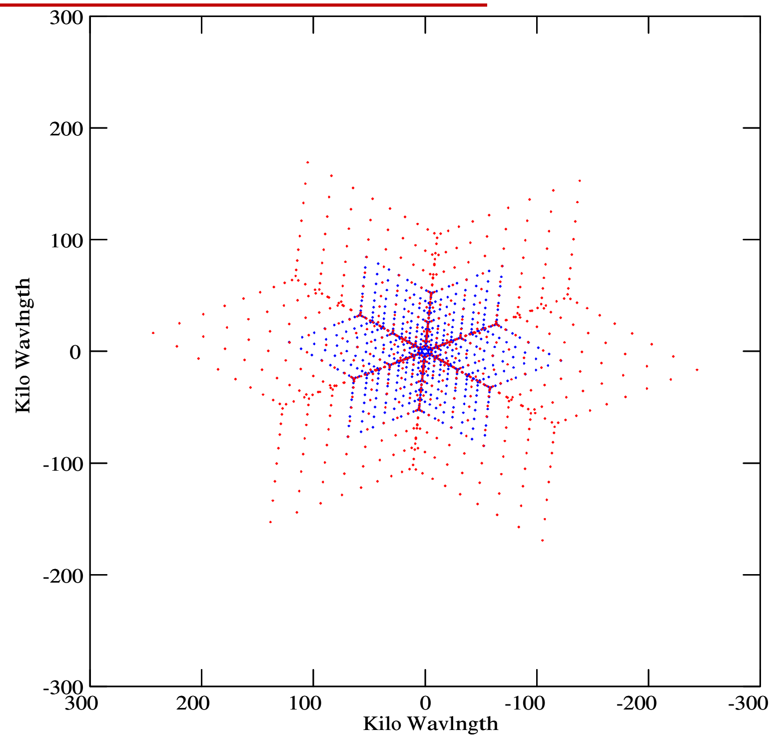
- ν_1 = 1 GHz (blue)
- ν_2 = 2 GHz (red)

Fringe spacings change by λ_1/λ_2

- u,v samples smeared radially

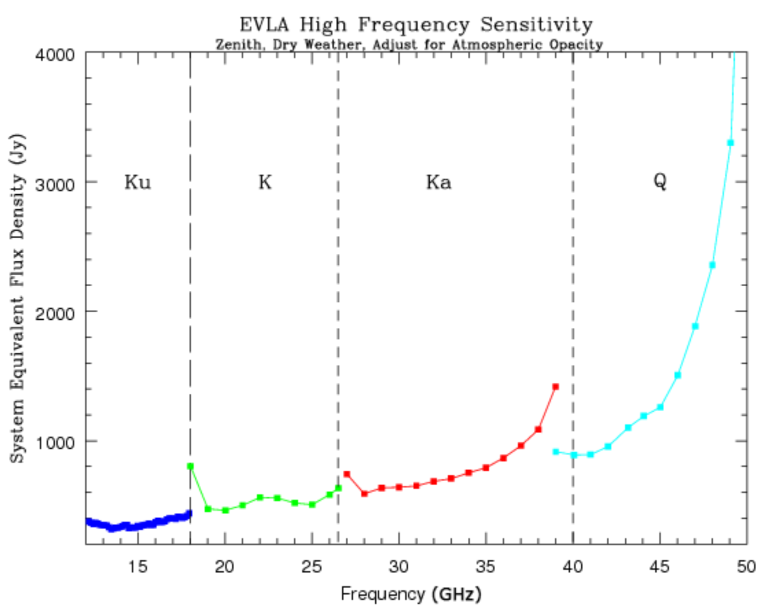
Effect more pronounced in larger configurations, and at lower frequencies.

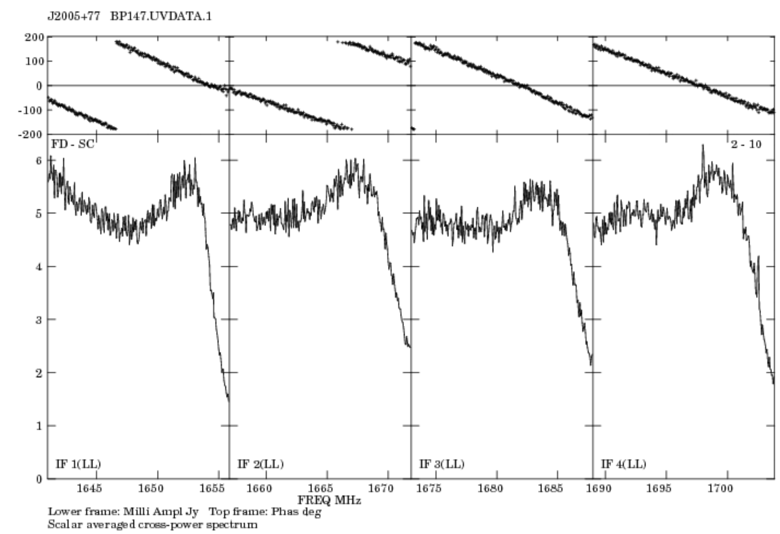
Can be utilized for multi-frequency synthesis.



Instrument frequency response

Responses of antenna receiver, feed, IF transmission lines, electronics are a function of frequency.

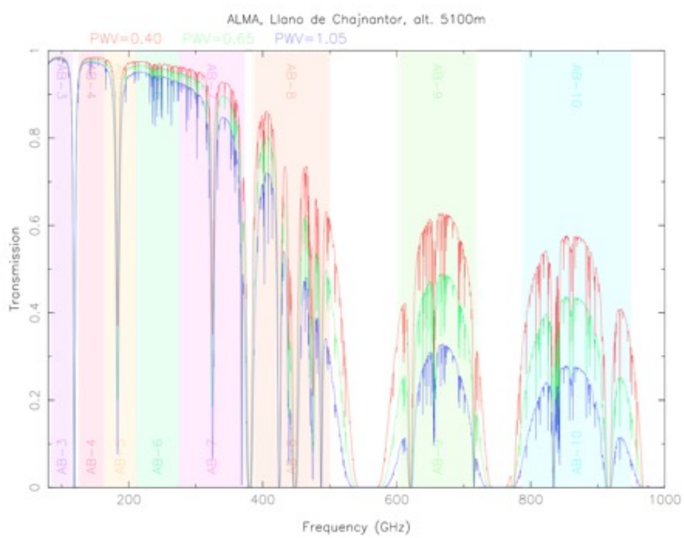


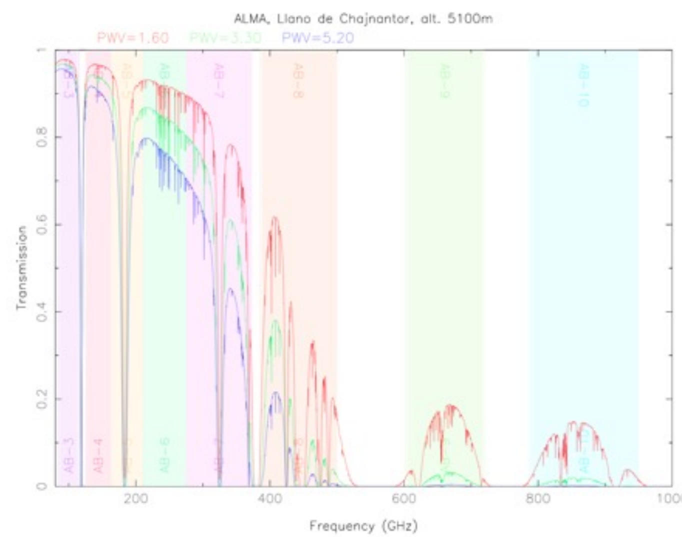


In data: phase is changing with frequency, as does the gain amplitude.

Atmospheric effects

Atmospheric opacity is a function of frequency, with largest effects over very wide bandwidths or near atmospheric lines

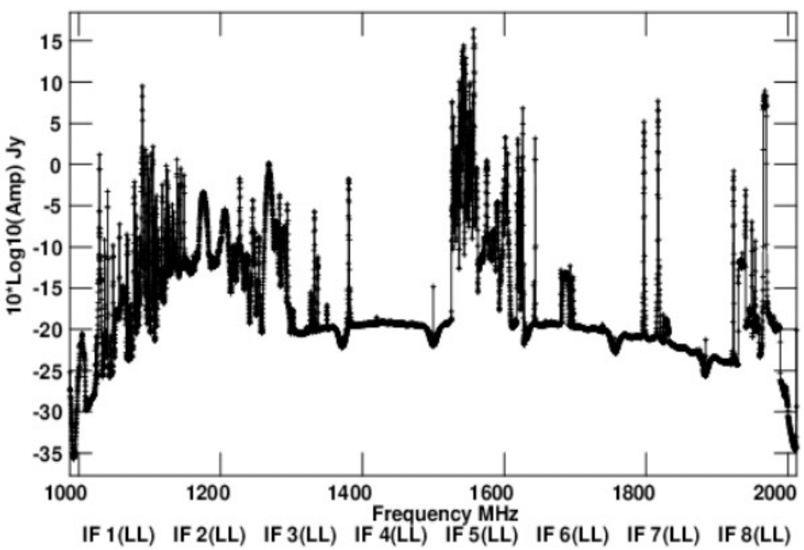




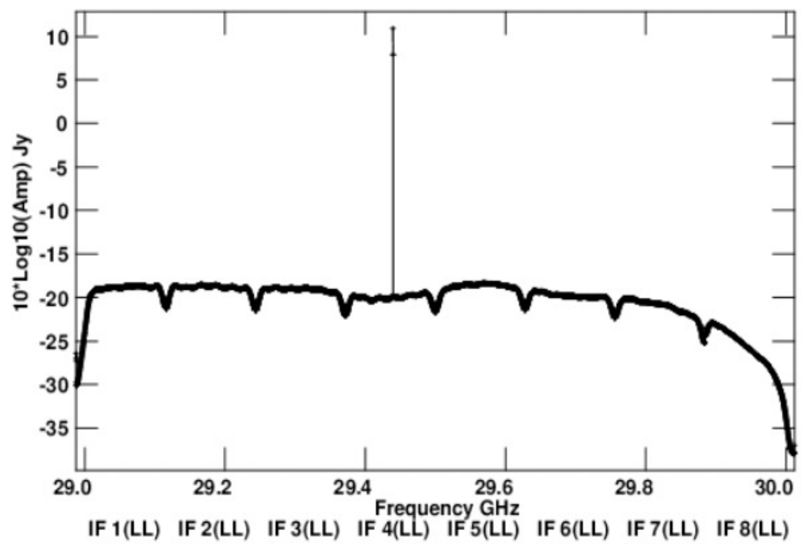
PWV: Precipitable Water Vapor
ALMA webpages

Radio Frequency Interference

Avoid known RFI if possible, e.g., by constraining your bandwidth. Use RFI plots and tables posted online for the telescope.



L-band sweep at the VLA, February 2024



Ka-band sweep at the VLA, February 2024

Calibration

Calibration concepts associated with multichannel observations:

1. Removal of RFI (data flagging)
2. Bandpass calibration
3. Correlator effects
4. Doppler corrections
5. Continuum subtraction

You also might deal with a large dataset: Averaging may be helpful to reduce size if needed, especially for the calibrators.

1. Removal of RFI

Many ways to do this, here are some examples:

Start with identifying problems affecting all channels by using an averaged data set.

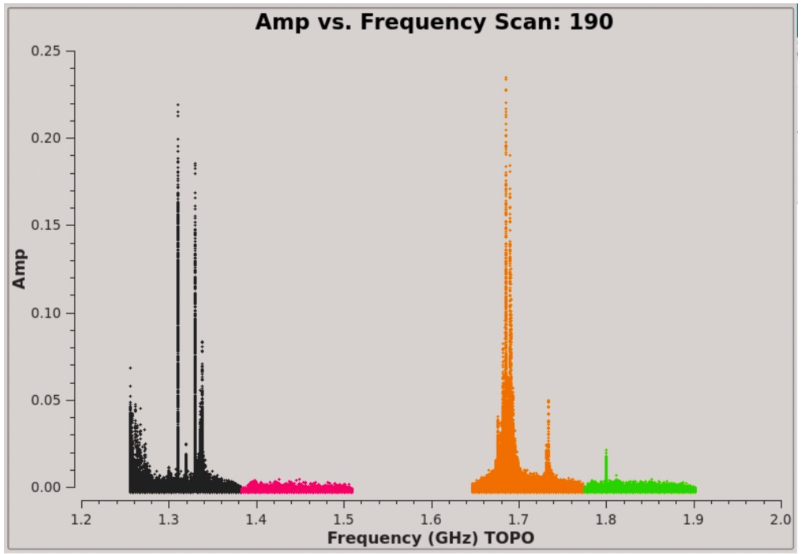
- Has better signal-to-noise ratio
- Can use calibrator data to identify specifics of RFI (telescope, time)
- Apply flag information to the full data set

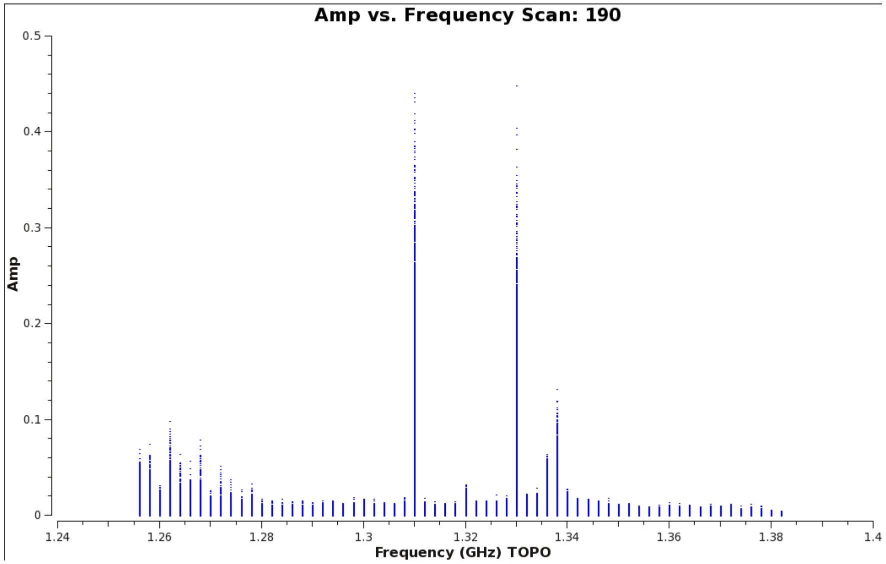
Continue with checking the line data for narrow-band, time-dependent RFI that may not show up in averaged data.

- Channel by channel is often impractical, instead identify features by using cross- and total power spectra

Example: CASA editing tutorial

Can compare to published RFI source lists, and/or RFI sweeps.

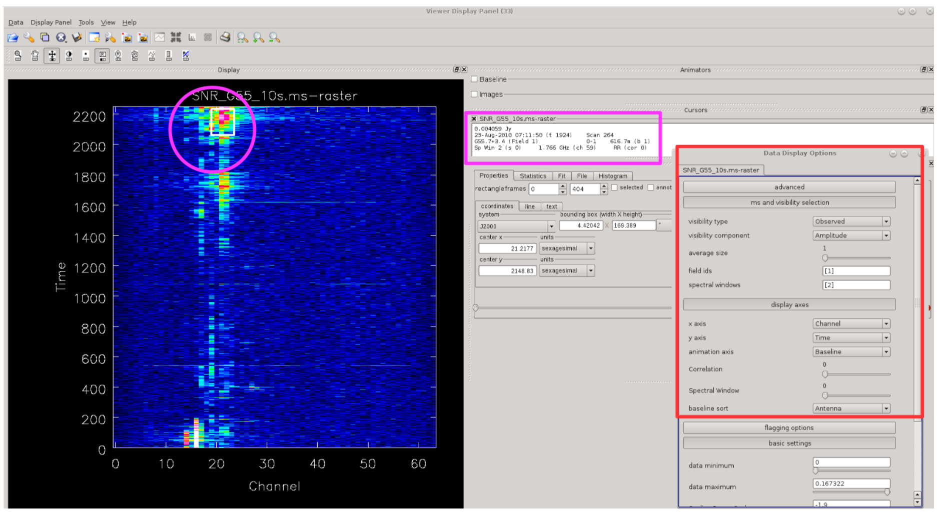




Plotms: Can do interactive flagging.

Example: CASA editing tutorial

RFI can be strongly time-variable, and looking at data as a function of time and frequency can help identifying ”clean” time ranges (*msview*).



- Be aware that changes in the uv-coverage across the band can occur if excessive frequency-dependent editing is performed
- Can also flag based on statistics: *Rflag* uses a sliding window and flags data based on statistics.

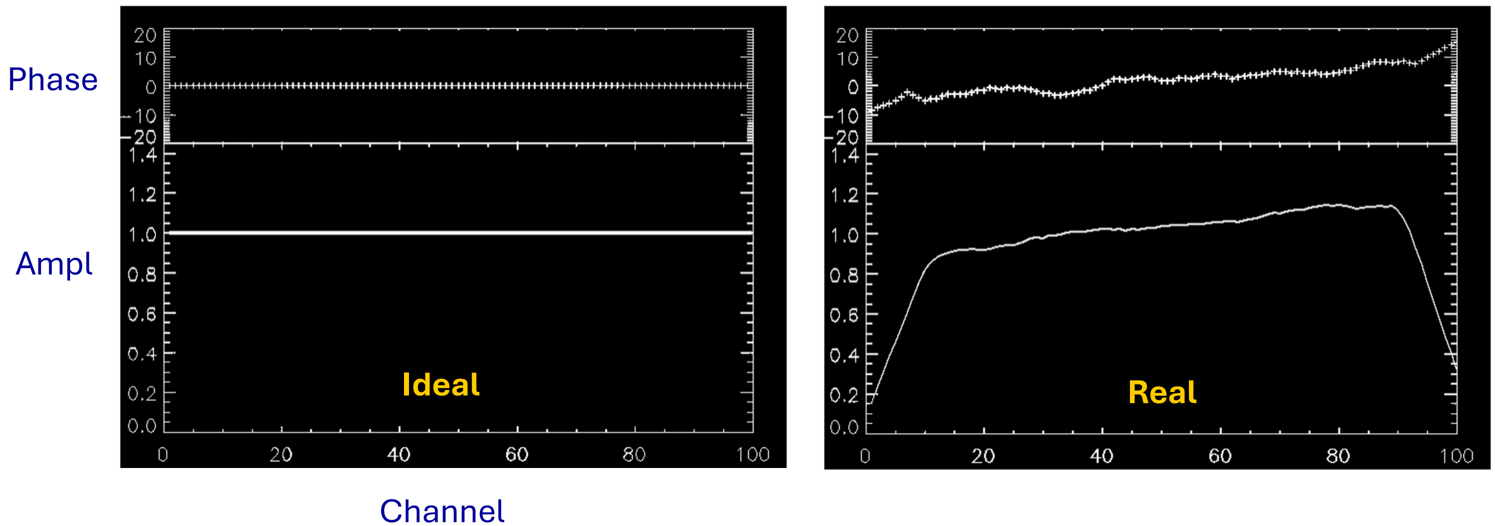
2. Bandpass calibration

Important to be able to detect and analyze spectral features:

- Frequency dependent amplitude errors limit the ability of detecting weak emission and absorption lines.
- Frequency dependent amplitude errors can imitate changes in line shapes.
- Frequency dependent phase errors can lead to spatial offsets between spectral features (imitating motions).

For continuum science, the dynamic range of final image is affected by the bandpass quality.

Ideal vs. real bandpass



The bandpass is the relative gain of an antenna/baseline as a function of frequency.

We want to correct for the *offset* of the real bandpass from the ideal one (amplitude=1, phase=0).

Bandpass calibration

The bandpass is a function of frequency and is mostly due to electronics of individual antennas.

- We need the total response of the instrument to determine the true visibilities from the observed:

$$V_{i,j}^{obs}(t,\nu) = G_{i,j}(t,\nu)V_{i,j}(t,\nu)$$

- Assume instrumental effects vary slowly with time, and break the complex gain $G_{i,j}$ into a fast-varying frequency independent part, and a slowly varying frequency dependent part:

$$G_{i,j}(t,\nu) = G'_{i,j}(t)B_{i,j}(t,\nu)$$

Different approaches can be taken. A common one is to generate complex response functions for each antenna (antenna-based):

- Least-square method applied channel-by-channel to decompose cross-power spectra: self-cal procedure

$$B_{i,j}(t,\nu) \approx B_i(t,\nu)B_j^*(t,\nu) = b_i(t,\nu)b_j(t,\nu)e^{i(\phi_i(t,\nu)\phi_j(t,\nu))}$$

Gives solutions for all antennas even if baselines are missing

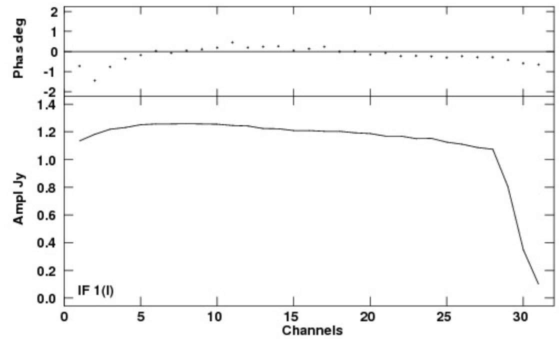
- To determine $B_{i,j}$ we usually observe a bright continuum source with flat (or known) spectrum.

The bandpass calibrator

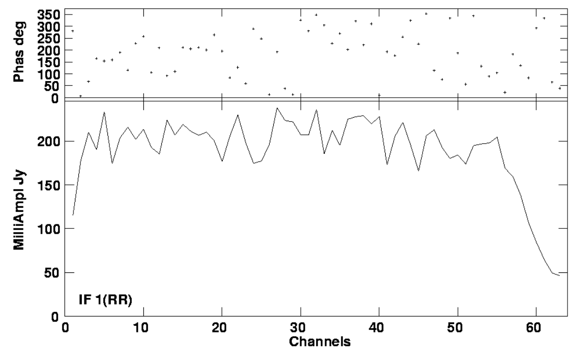
Select a continuum source with:

- High SNR in each channel
- Intrinsically flat spectrum
- No spectral lines

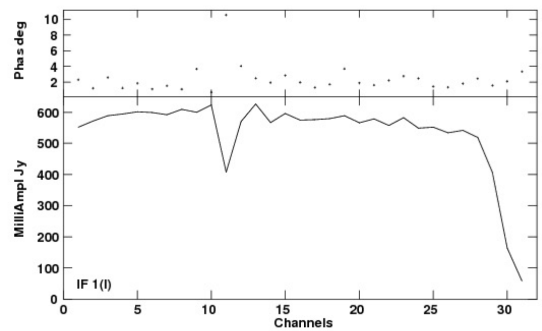
Not required to be a point source, but helpful since the SNR will be the same in the bandpass solution for all baselines.



Good calibrator



Too weak, will add noise .

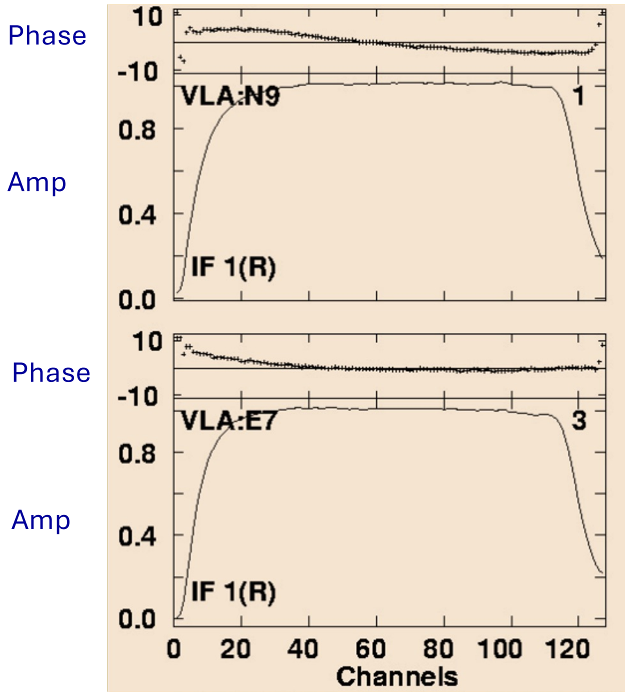


Has a line feature, which will induce a false line feature in target.

Good quality bandpass: what to look for

Examples of good-quality bandpass solutions for 2 antennas:

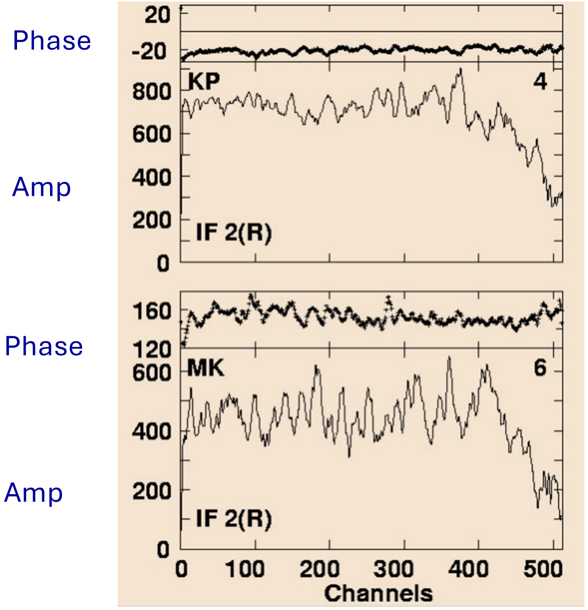
- Solutions should look comparable for all antennas
- Mean amplitude ~1 across useable portion of the band.
- No sharp variations in amplitude and phase; variations not controlled by noise



Bad quality bandpass: what to look for

Examples of poor-quality bandpass solutions for 2 antennas:

- Amplitude has different normalization for different antennas
- Noise levels are high, and are different for different antennas



Improve SNR for the bandpass

Applying the BP calibration means that every complex visibility spectrum will be divided by a complex bandpass => Noise from the bandpass will degrade all data.

A good rule of thumb to apply when preparing your observations is:

$$\mathrm{SNR}_{\mathrm{BPcal}} > 3 \times \mathrm{SNR}_{\mathrm{target}}$$

which then results in an integration time:

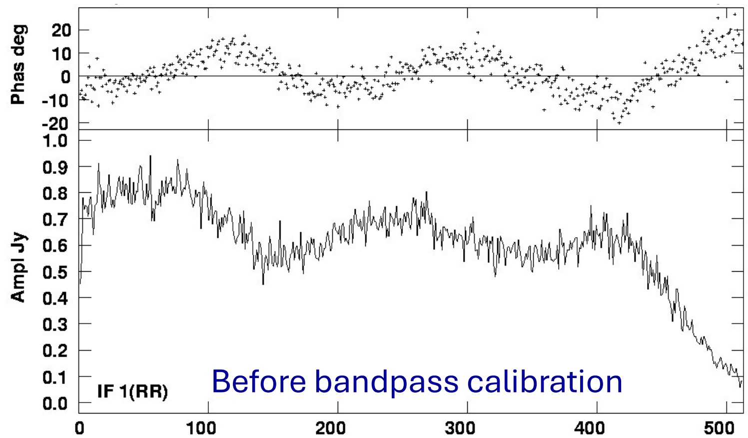
$$t_{\mathrm{BPcal}} = 9 \times \left(\frac{S_{\mathrm{target}}}{S_{\mathrm{BPcal}}}\right)^2 t_{\mathrm{target}}$$

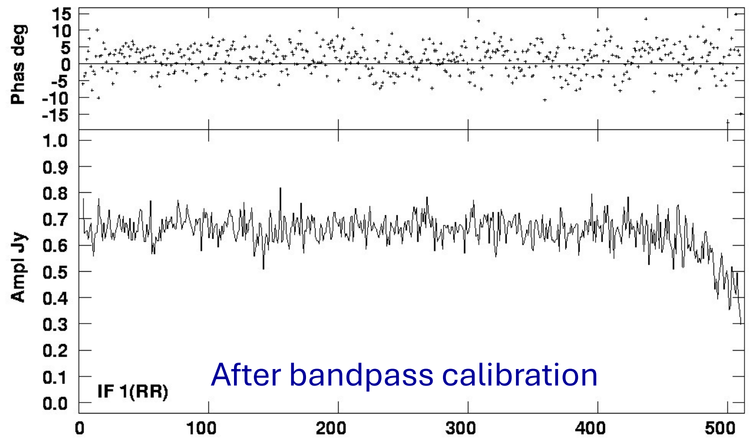
If long observations, include several scans of the BP calibrator in your experiment to account for slow time variations.

Apply to calibrator

Before applying the bandpass solutions to target, apply to a continuum source and use spectrum to check:

- Flat phases.
- Constant amplitudes.
- No increase in noise by applying the bandpass solutions.





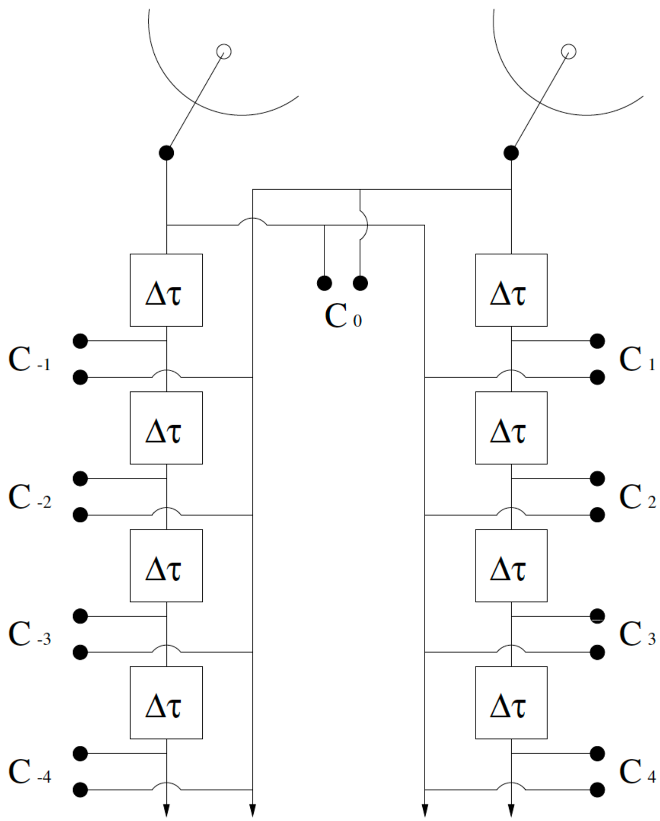
3. Correlator effects

How extract frequency information V(u,v,ν)?

If we just used filter banks, visibilities V(u,v,ν) could be formed directly. Not a versatile method.

Instead use the delay method already introduced for geometric delay & fringe stopping. This would then give V(u,v,τ).

$$V(u,v,\nu) = \int_{-\infty}^{+\infty} V(u,v,\tau) e^{-i2\pi\nu\tau} d\tau$$



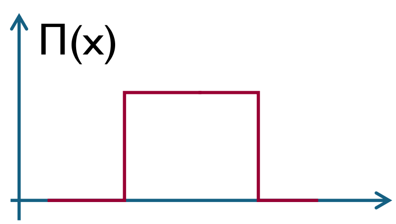
Spectral response of XF correlator

For spectroscopy in an XF correlator “lags” $\Delta\tau$ are introduced.

- Correlation function is measured for as many lags as possible
- FT gives the spectrum.

We don’t have an infinitely large correlator (number of lags) and infinite amount of time, so we don't measure an infinite number of Fourier components.

- A finite number or lags means a *truncated* lag spectrum.
- Corresponds to multiplying the true spectrum by a boxcar function, Π(x).



The spectral response is the FT of Π(x), which is a sinc(x) function with nulls spaced by the channel separation: 22% sidelobes.

Spectral response of FX correlator

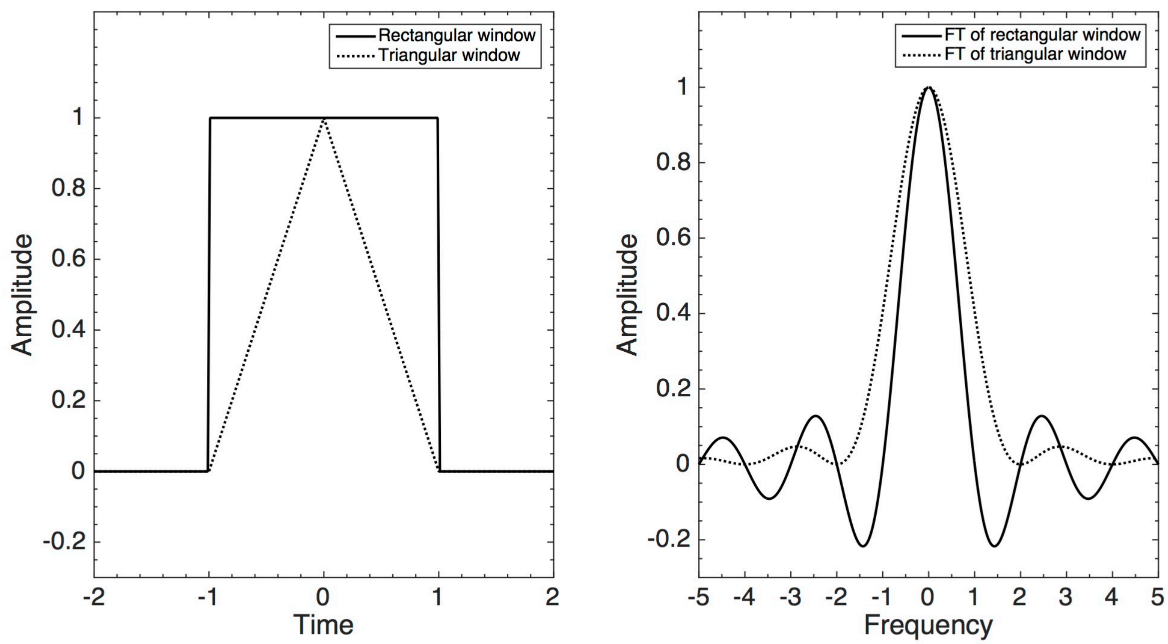
Example FX correlators: ALMA, VLBA, EVN SFXC

For FX correlators:

- Time sequence of voltages FT into a spectrum
- Spectra from pairs of telescopes cross-multiplied

Since the spectrum at each antenna formed from sample with limited time extent, this will also represent a truncated signal

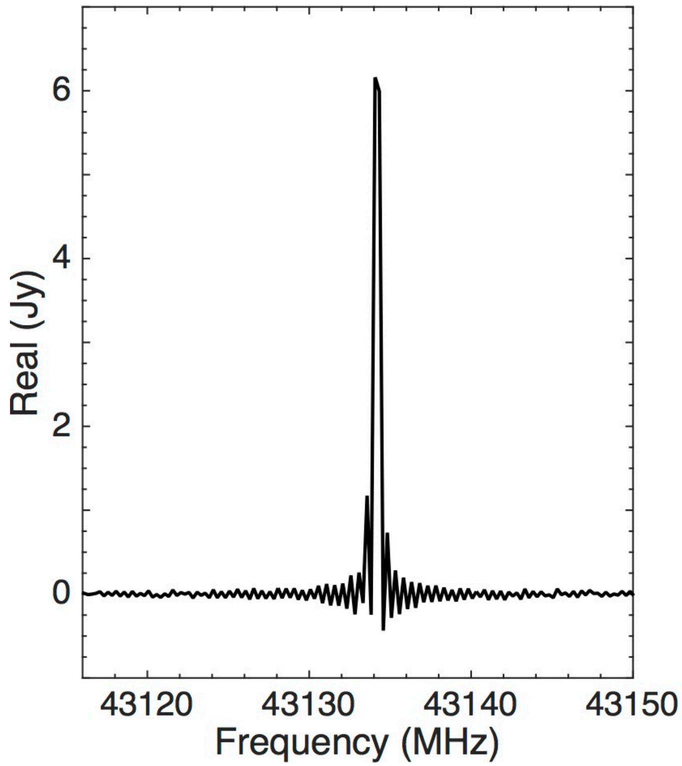
=> Total response $\text{sinc}^2(x)$ with 5% sidelobes



Example spectral responses for a rectangular and triangular window ("truncation").

Gibbs ringing

- We care about this since this response introduces unwanted spectral features
- Produces a "ringing" in frequency called the Gibbs phenomenon.
- Occurs at sharp transitions:
  - Narrow banded spectral lines (masers, RFI)
  - Band edges



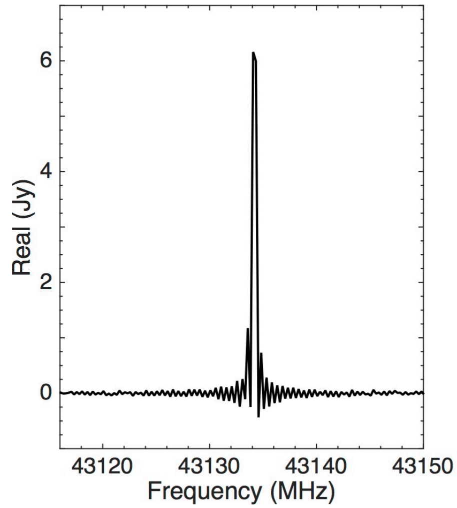
Gibbs ringing example.

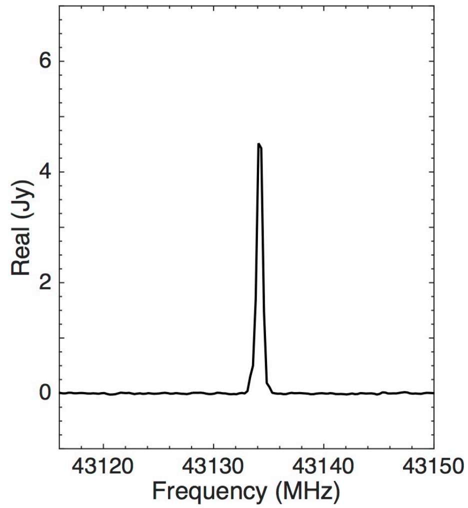
Gibbs ringing

To reduce effects, window functions can be applied in the correlator.

- Reduces sidelobes at the expense of main peak resolution.
- Can also smooth in post-processing: often a Hanning window is applied.

$$S_h(\nu_i) = \frac{S(\nu_{i-1}) + 2S(\nu_i) + S(\nu_{i+1})}{4}$$

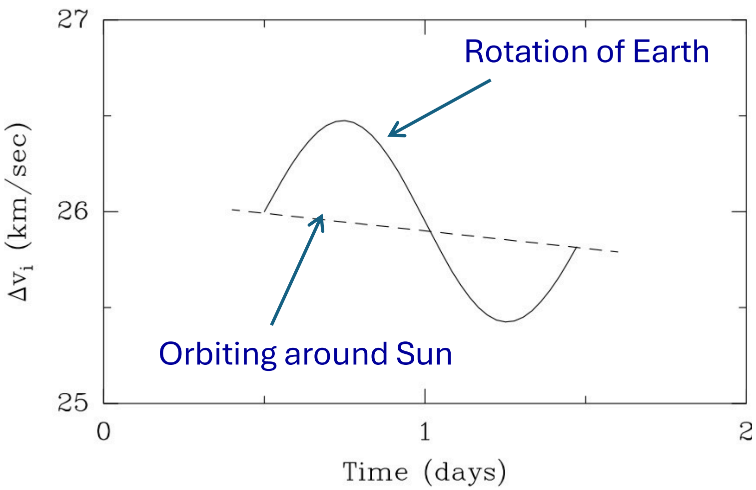




After Hanning smoothing.

4. Doppler corrections

- Observing from the surface of the Earth, our velocity with respect to astronomical sources is not constant in time or direction.
- Caused by rotation of the Earth and its orbit around the Sun



- If not corrected, will cause spectral line to slowly drift through spectrum

Velocity 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
Sun/planets barycenter	< 0.012 km/s	Solar system Barycentric
Sun peculiar motion	< 20 km/s	Local Standard of Rest
Galactic rotation	< 300 km/s	Galactocentric
Galactic motion	< 100 km/s	Local Group
Local Group motion	< 300 km/s	Virgocentric
Local Supercluster motion	< 600 km/s	CMB

Start with the topocentric frame, then successively transform to other frames. Transformations standardized by IAU.

Velocity definitions

Doppler tracking could be applied in real time to track a spectral line in a given reference frame, and for a given velocity definition:

$$\frac{V_{\rm radio}}{c} = \frac{\nu_{\rm rest} - \nu_{\rm obs}}{\nu_{\rm rest}}$$

$$\frac{V_{\rm optical}}{c} = \frac{\nu_{\rm rest} - \nu_{\rm obs}}{\nu_{\rm obs}}$$

Make sure the correct velocity frame and definition is used when planning your observations.

Note that the bandpass shape is a function of frequency, not velocity!

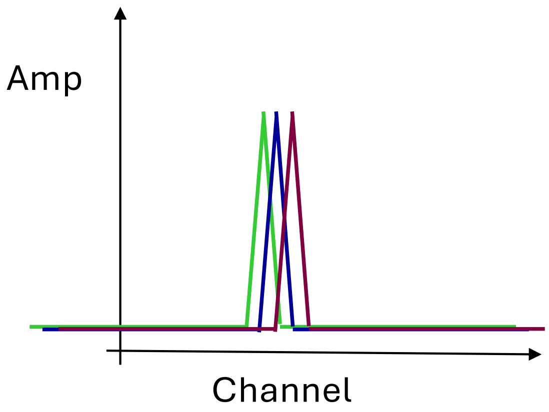
- Applying Doppler tracking will introduce a time-dependent and position-dependent frequency shift.

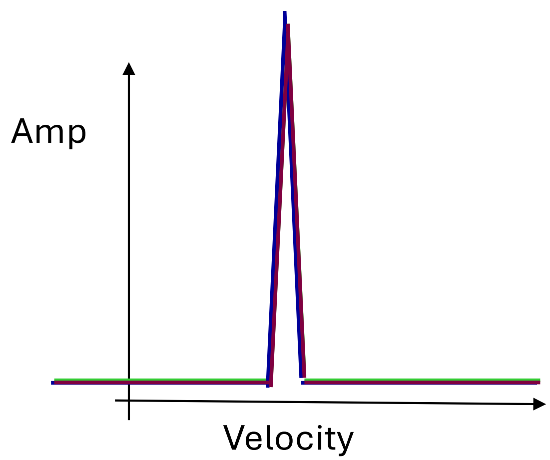
- If you Doppler track/set your BP calibrator to the same velocity as your target, it will be observed at a different sky frequency!
  - Apply Doppler setting to the source position.

Most times, a Doppler setting is applied at the beginning of the observation, and then additional corrections can be applied during post-processing.

Doppler corrections

Post-observing doppler corrections can also be done through software. The sky frequency for a selected channel can be calculated depending on target position, velocity frame and definition, and the rest frequency of the transition.





Before and after Doppler correction

5. Continuum subtraction

- We have edited the data and performed band pass calibration.
- We have also done Doppler corrections if necessary.

NB: CASA can do this on-the-fly in the imaging process.

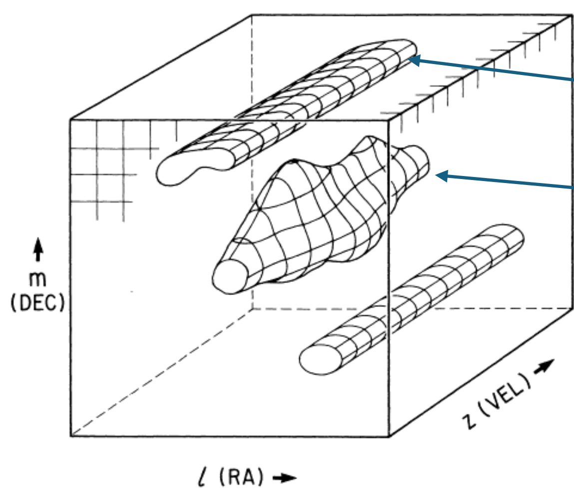
Before imaging a few things can be done to improve the quality of your resulting spectral line data:

- Image the continuum in the source and perform a self-calibration. Apply to the line data, which provides good positions of line features relative to continuum
    - Can also use a bright spectral feature, like a maser

- Remove the continuum emission, to separate out the line: continuum subtraction process.

5. Continuum subtraction

- Spectral line data often contains continuum emission, either from the target or from nearby sources in the field of view.
- This emission complicates the detection and analysis of line data



Spectral line cube with two separate continuum sources (structure independent of frequency) and one spectral line source.

Roelfsma 1989

Benefits

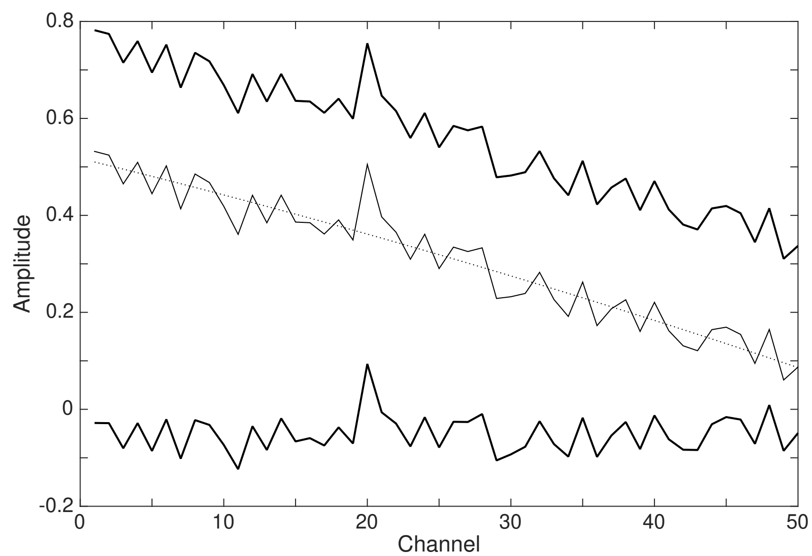
- Spectral lines easier to see, especially weak ones in a varying continuum field.

  Statistically, and by-eye.

- Easier to compare the line emission between channels.

- Faster to clean as most channels will be empty if continuum is removed

- If continuum sources exists far from the phase center, we do not need to deconvolve a large field of view to properly account for their sidelobes.



To remove the continuum, different methods are available: visibility based, image based, or a combination thereof.

Visibility-based

- A low order polynomial (0th, or often 1st) is fit to a group of line free channels in each visibility spectrum, the polynomial is then subtracted from whole spectrum.

- Advantages:
  - Fast, easy, robust
  - Corrects for spectral index slopes across spectrum
  - Can implement with automatic flagging (based on residuals on baselines)
  - Can produce a continuum data set

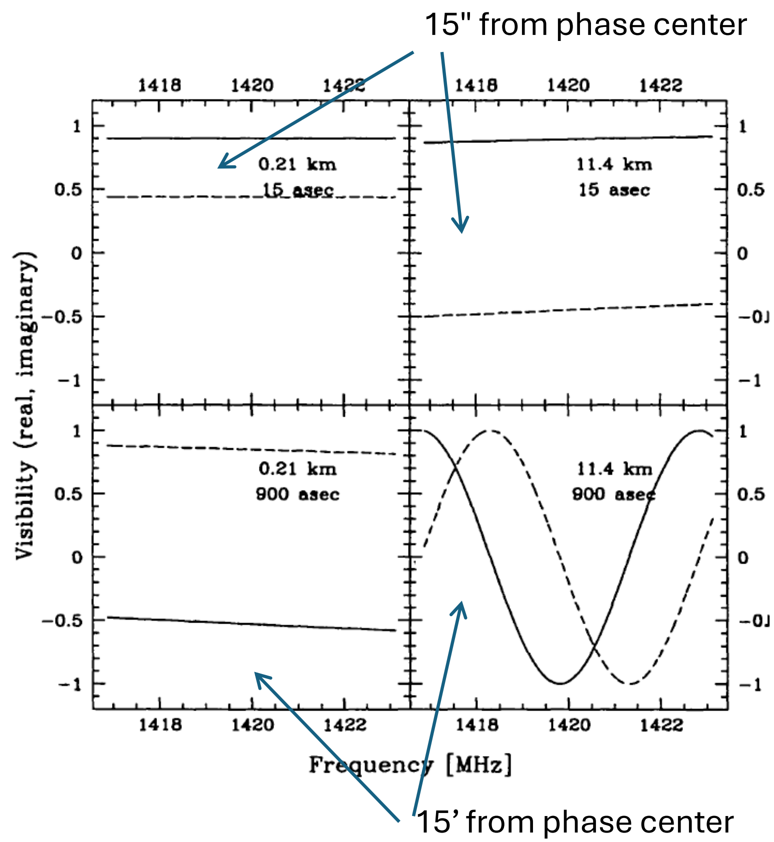
- Restrictions:
  - Channels used in fitting must be line free (visibilities contains emission from all spatial scales)
  - Only works well over small field of view $\theta \ll \theta_B \frac{\nu}{\Delta\nu_{\mathrm{tot}}}$

Small FOV restriction

- A consequence of the visibility of a source being a sinusoidal function
- For a source at distance *l* from phase center observed on baseline *b*:

$$V = \cos(\frac{2\pi\nu bl}{c}) + i\sin(\frac{2\pi\nu bl}{c})$$

- This is linear only over a small range of frequencies and for small *b* and *l*.



Rupen 1999

Image-based

- Fit and subtract a low order polynomial fit to the line free part of the spectrum measured at each spatial pixel in cube.

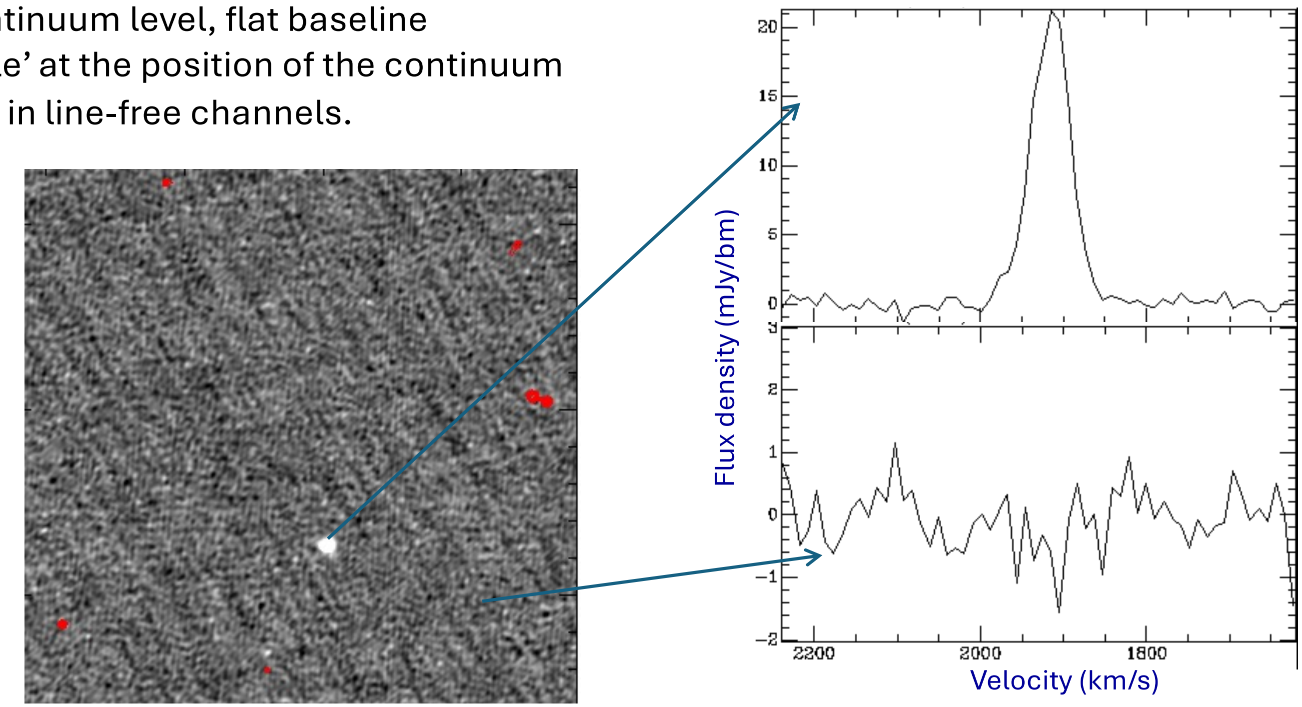
- Advantages:
  - Fast, easy, robust to spectral index variations
  - Better at removing point sources far away from phase center (Cornwell, Uson and Haddad 1992).
  - Can be used with few line free channels.

- Restrictions:
  - Can't flag data since it works in the image plane.
  - Line and continuum must be simultaneously deconvolved.

Check subtraction after imaging

Look at spectra on/off source position:

- No continuum level, flat baseline
- No 'hole' at the position of the continuum source in line-free channels.

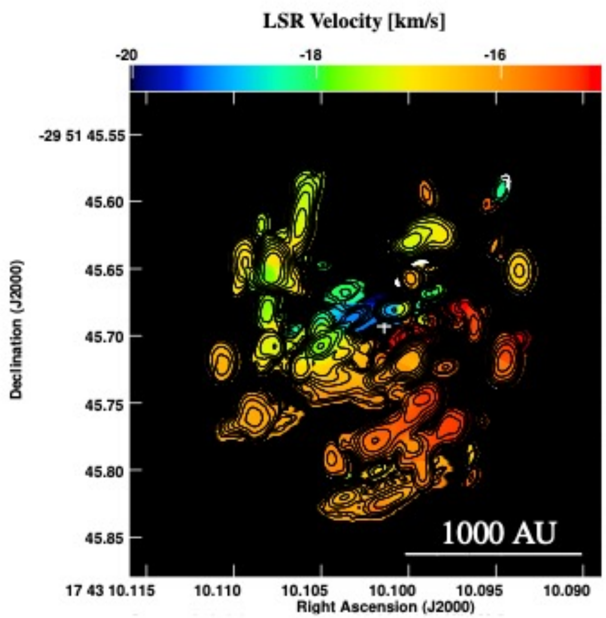


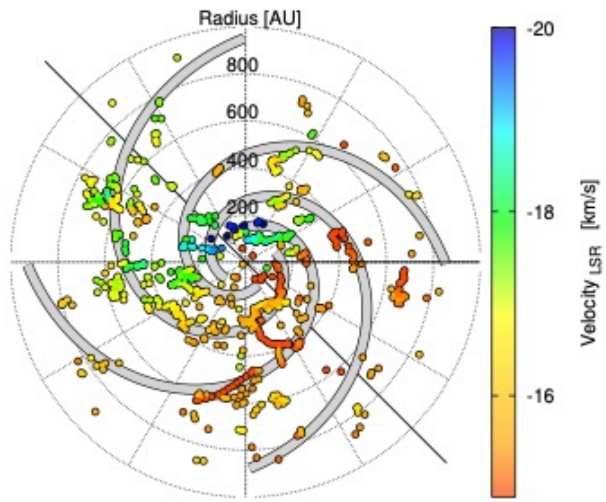
Useful spectral-line catalogs

Online databases with spectral line information:

- Splatalogue (VLA/ALMA/GBT): http://www.cv.nrao.edu/php/splat/
- NIST Recommended Rest Frequencies 'Lovas Catalogue': http://physics.nist.gov/cgi-bin/micro/table5/start.pl
- JPL/NASA molecular database: http://spec.jpl.nasa.gov/
- Cologne database for molecular spectroscopy: http://www.astro.uni-koeln.de/cdms/

Spectral line science examples

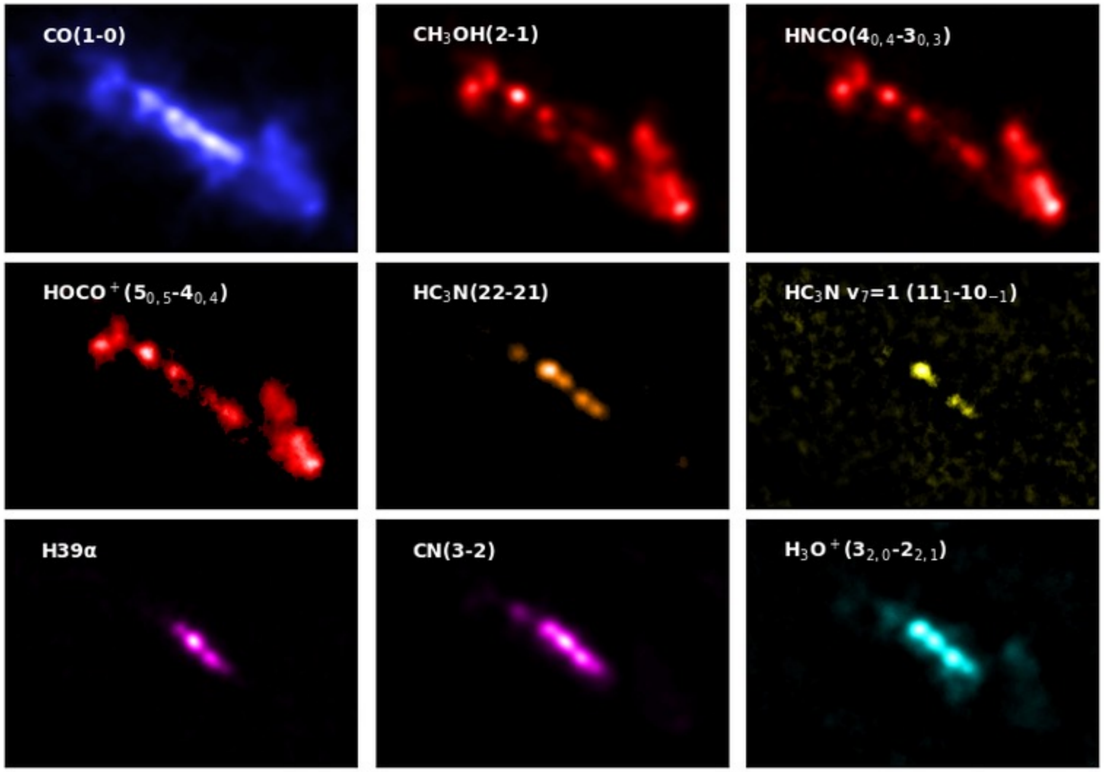




Multi-epoch VLBI 6.7 GHz methanol maser observations in YSO G358-MM1.

Shows spiral arm instabilities associated with accretion event.

Burns et al. (2023)

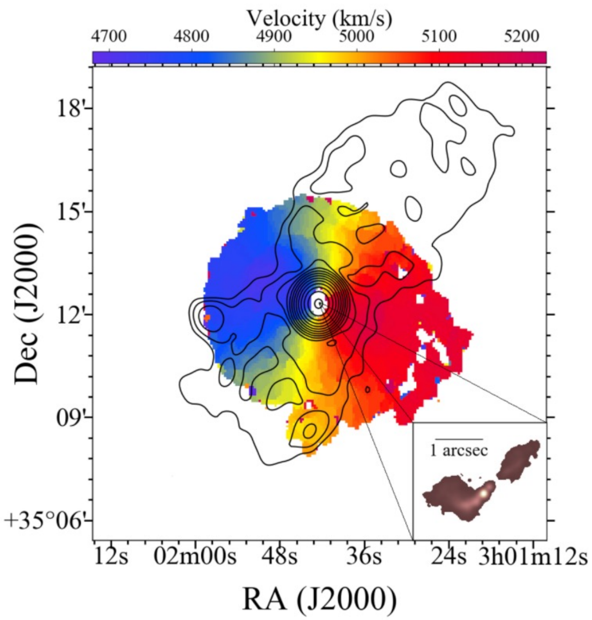


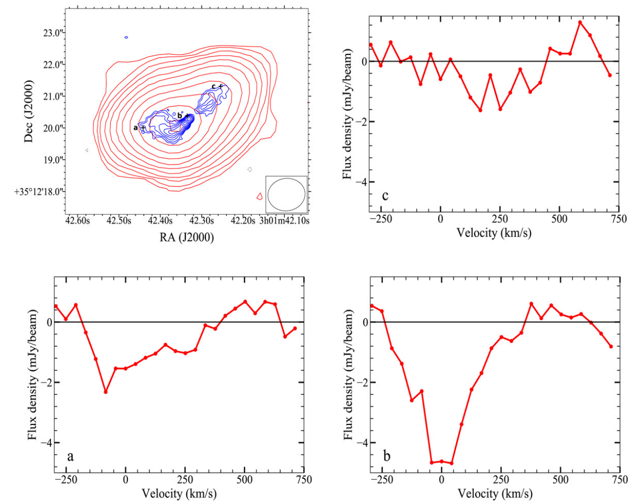
ALMA Comprehensive High-resolution Extragalactic Molecular Inventory, ALCHEMI:

Nearby galaxy NGC 253, showing the central molecular zone.

Depending on what species and transitions are observed, regions can be classified as, e.g., young starbursts, cloud-collision shocks, or outflows.

Martín et al. (2024)

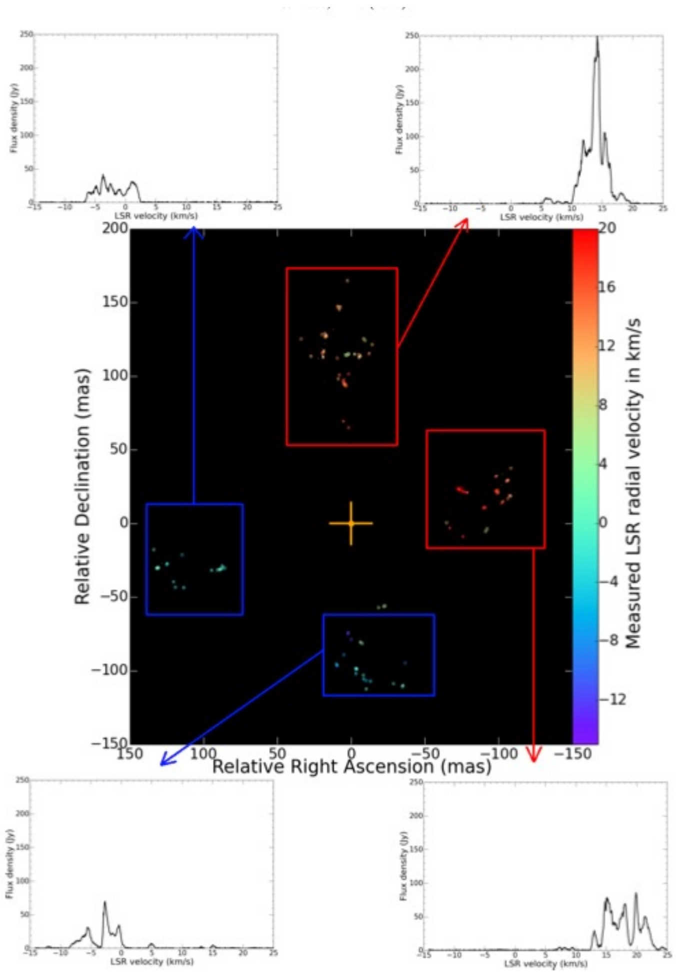




A young radio source embedded within the galaxy NGC 1167.

A large-scale HI disk is seen in emission, but VLA and VLBI HI absorption data shows gas different from the large disk. Affected by the radio jets causing turbulence.

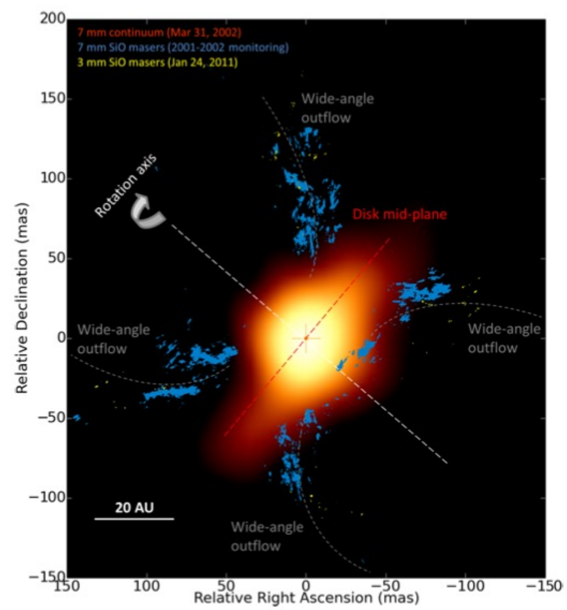
Muthy et al. (2019)



Issaoun et al. (2017)

VLBA mapping of SiO masers in the YSO Orion Source I.

Complex emission structure, which can be understood by interpreting the velocity field. Masers are part of a wide-angled outflow, arising from a disk rotating around the central source.



Summarizing remarks

- Multi-channel observations are standard, although calibration needs might be different depending on science goals.

  => Make sure goal is defined before preparing observations

- Spectral line science is rich and addresses chemistry, dynamics, gas reservoir sizes, star formation, gas dynamics in external galaxies and AGNs, and much more.

Happy observing!