Spectral Lines

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Outline

- Motivation for spectral line observations
  - Advantages also for continuum experiments

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

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

Introduction

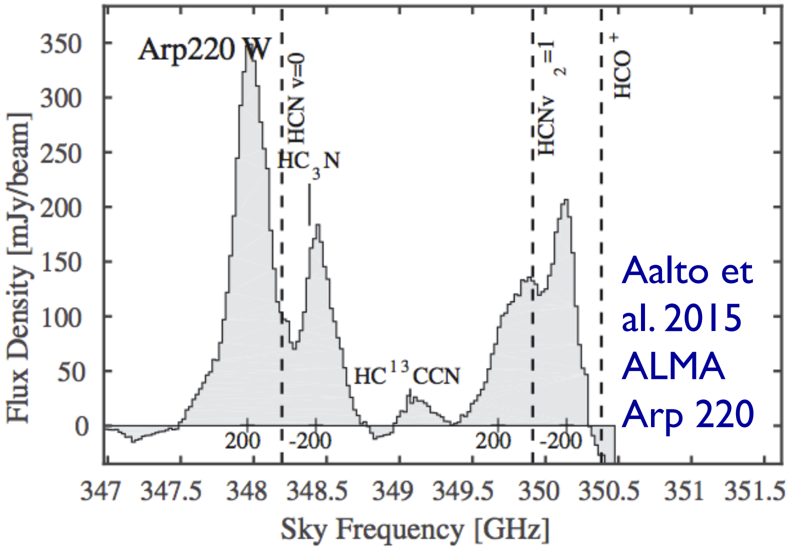
Multi-channel observations utilize *n* channels of width $\Delta\nu$, over a total bandwidth $BW = n\Delta\nu$. Why?

- **Science-driven**: science depends on frequency (spectroscopy)
  - Emission and absorption lines, and their Doppler shifts (HI, OH, H_2O, SiO, CH_3OH, etc.)
  - Slope across continuum bandwidth (spectral index)
- **Technically driven**: science does not depend on frequency
  - Science quality improved using multiple channels (pseudo-continuum)

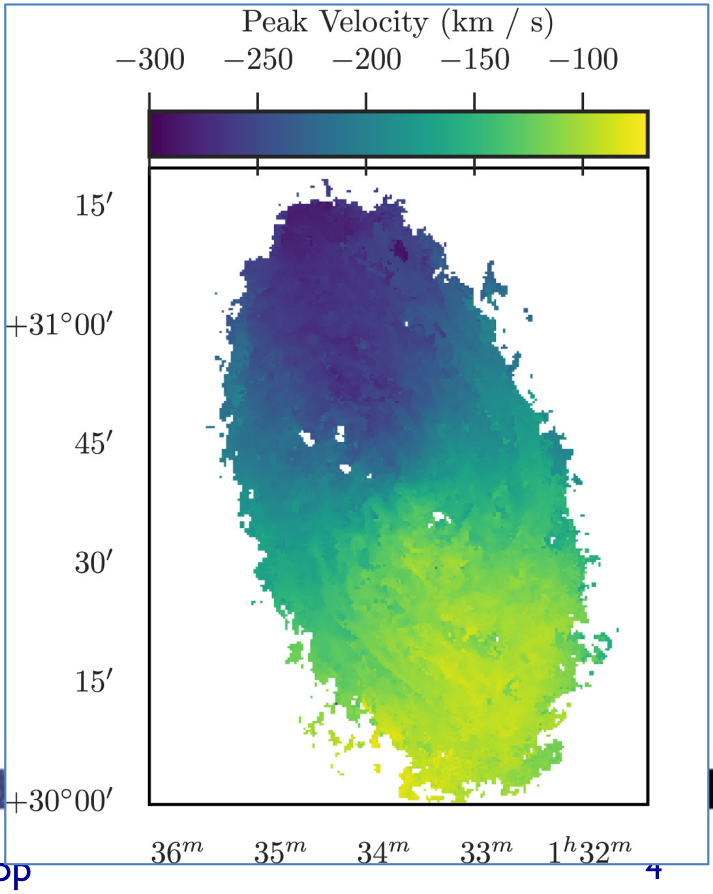
Most instruments today observe in multi-channel mode.

Spectroscopy

- Need high spectral resolution to resolve spectral feature(s)
- Many channels across a large bandwidth allows
  - Doppler shift determinations
  - Search for many transitions
- Detection of spectral line: need to separate the line from the continuum



Aalto et al. 2015
ALMA
Arp 220



Koch et al. 2018
M33 HI

Pseudo-continuum

Science does not depend on frequency, but using spectral line mode is favorable to reduce at least some frequency dependent effects:

- Bandwidth smearing
- Problems due to atmospheric changes as a function of frequency
- Instrumental signal transmission effects as a function of frequency
- Editing for unwanted, narrow-band interference.

Bandwidth smearing: instrument response

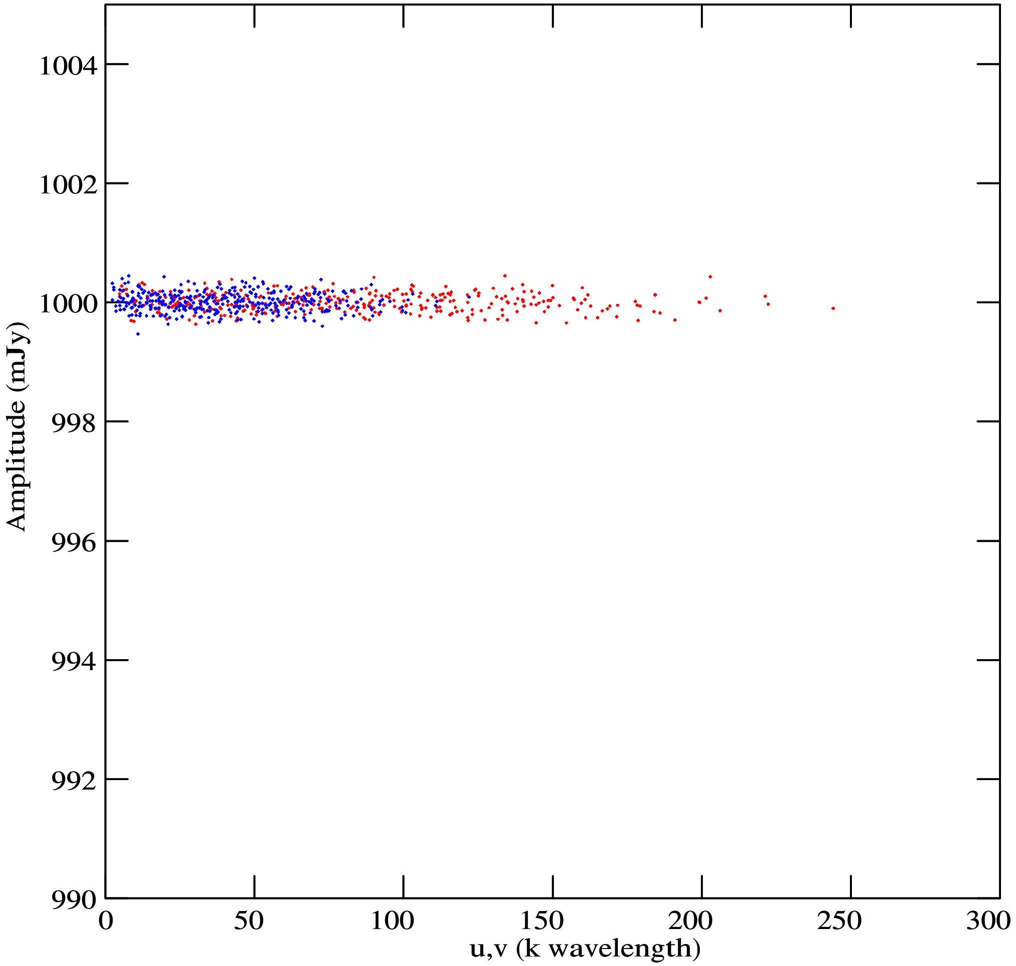
Also called chromatic aberration.

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

Band coverage $\nu_2 - \nu_1$

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

Frequencies sample different regions of the u-v plane.



Ampl vs uv distance, VLA A-config.

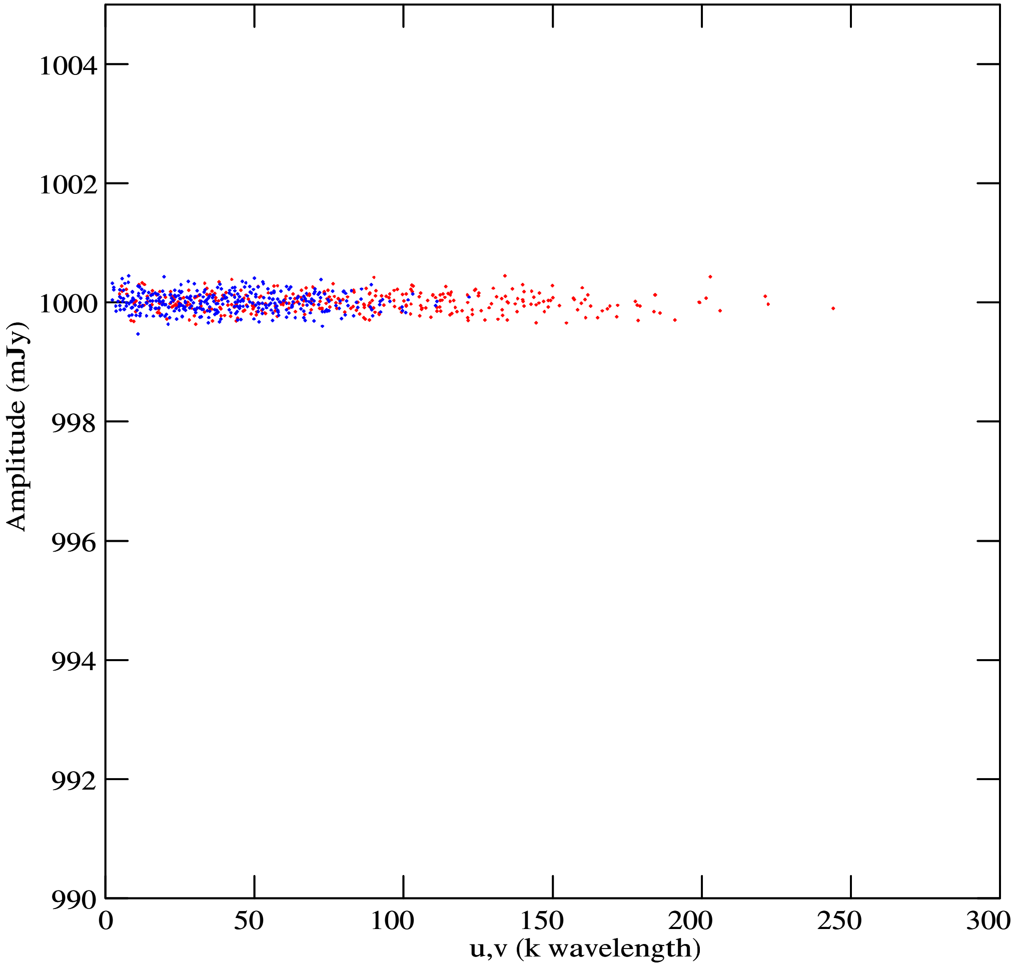
Bandwidth smearing: instrument response

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

Frequencies sample different regions of the u-v plane.

More important at longer wavelengths as it scales with λ_1/λ_2 :

- 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



Ampl vs uv distance, VLA A-config.

Bandwidth smearing: instrument response

Band coverage $\nu_2 - \nu_1$

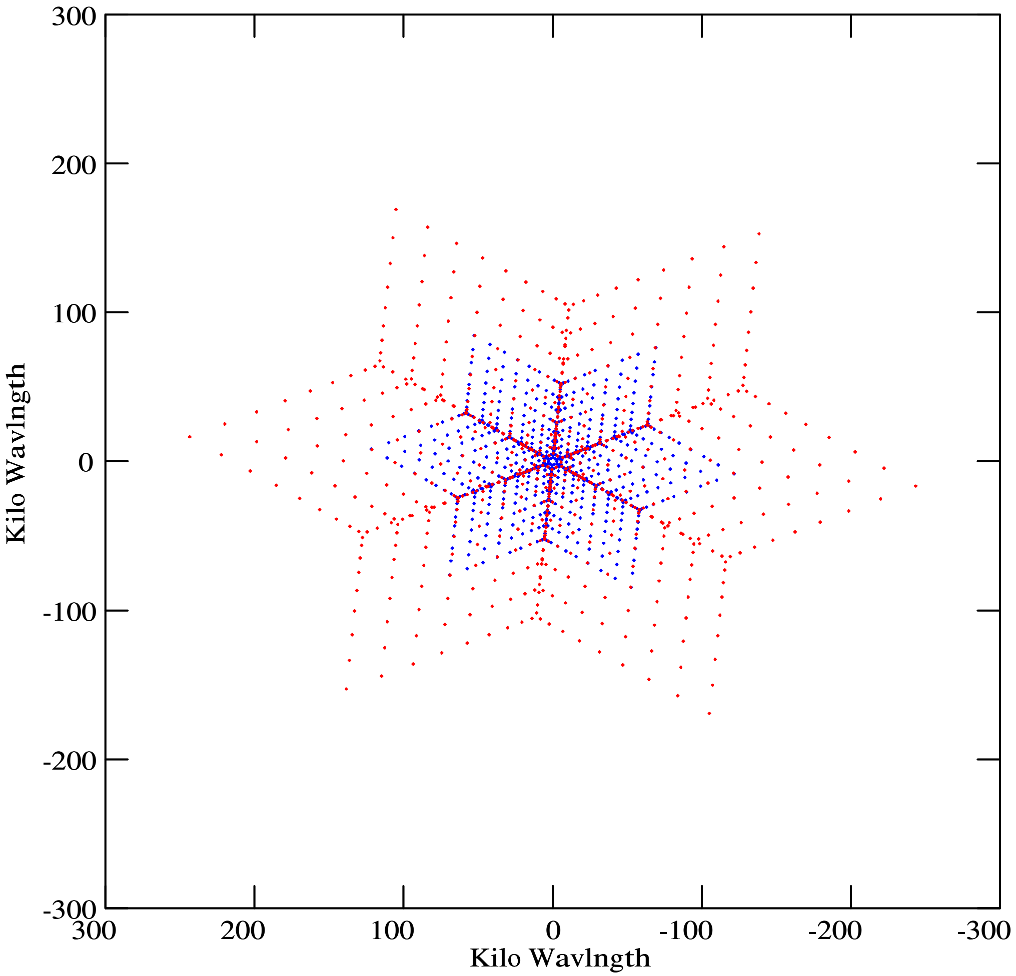
- ν_1 = 1 GHz (blue)
- ν_2 = 2 GHz (red)

Fringe spacings change by λ_1/λ_2

- *u,v* samples smeared radially

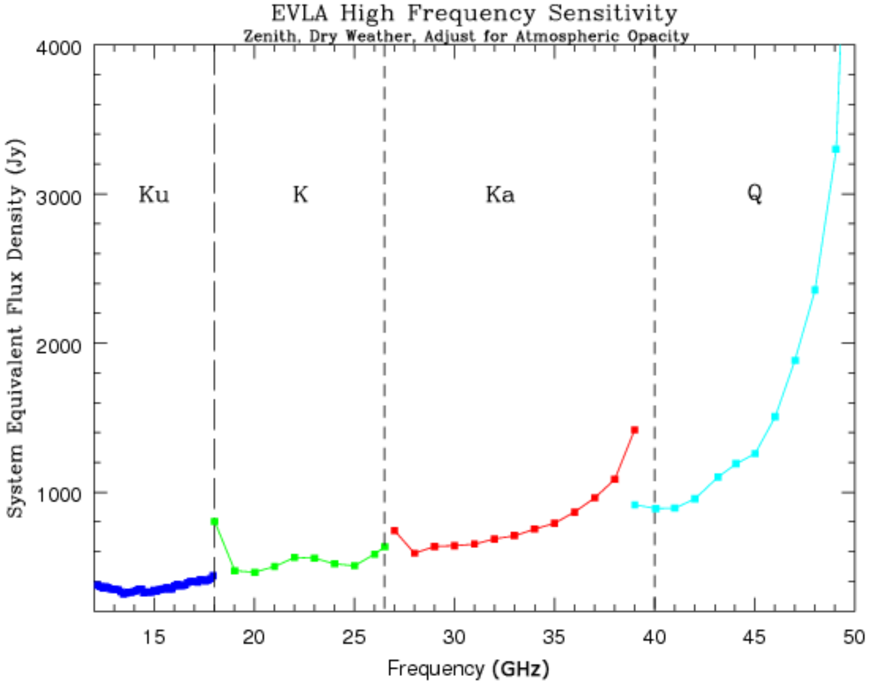
Effect more pronounced in larger configurations, and at lower frequencies.

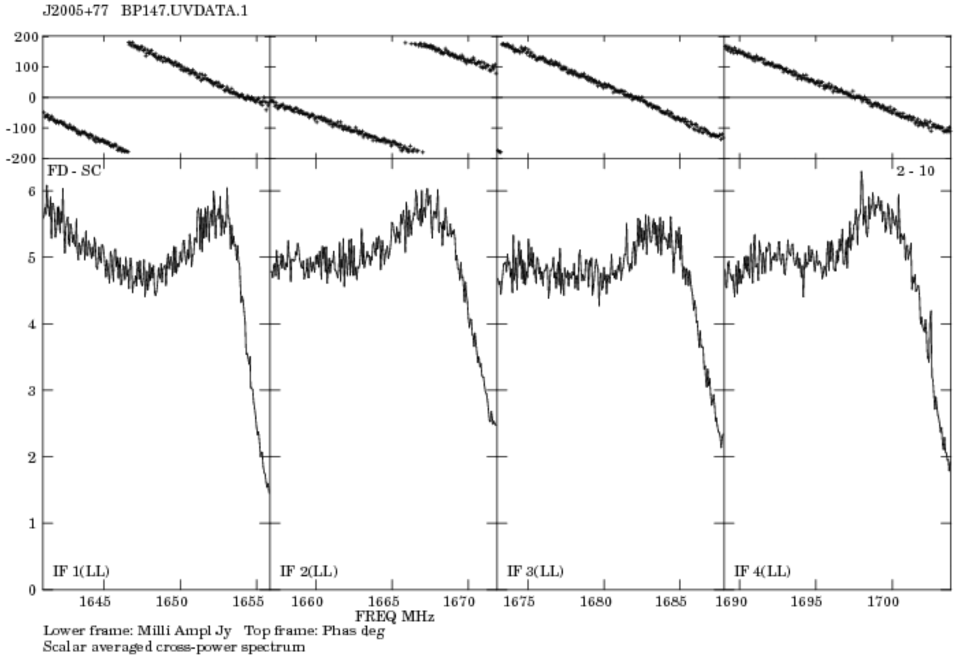
Can be utilized for multi-frequency synthesis!



Instrument frequency response

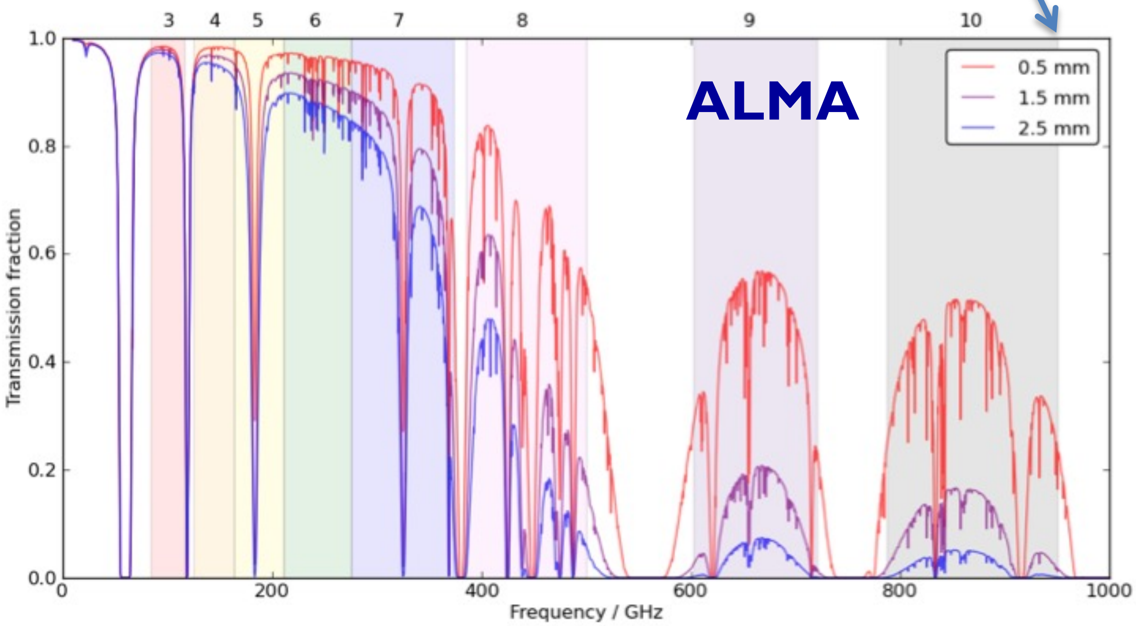
Responses of antenna receiver, feed, IF transmission lines, electronics are a function of frequency.





Atmospheric effects

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

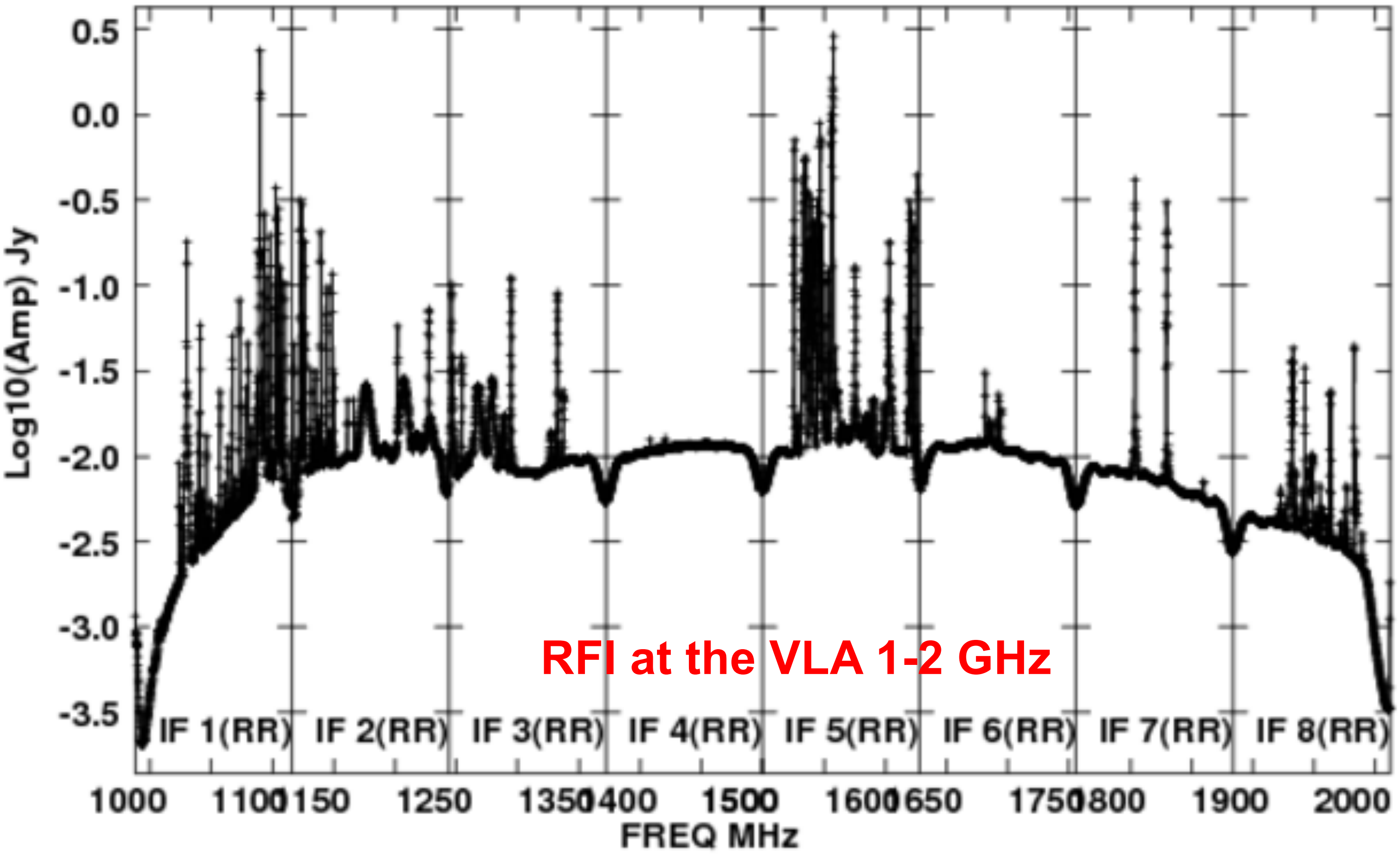


PWV=Precipitable Water Vapor

- Source emission can change with frequency too:
  - Spectral index, shape
  - Polarized emission: Faraday rotation $\propto \lambda^2$

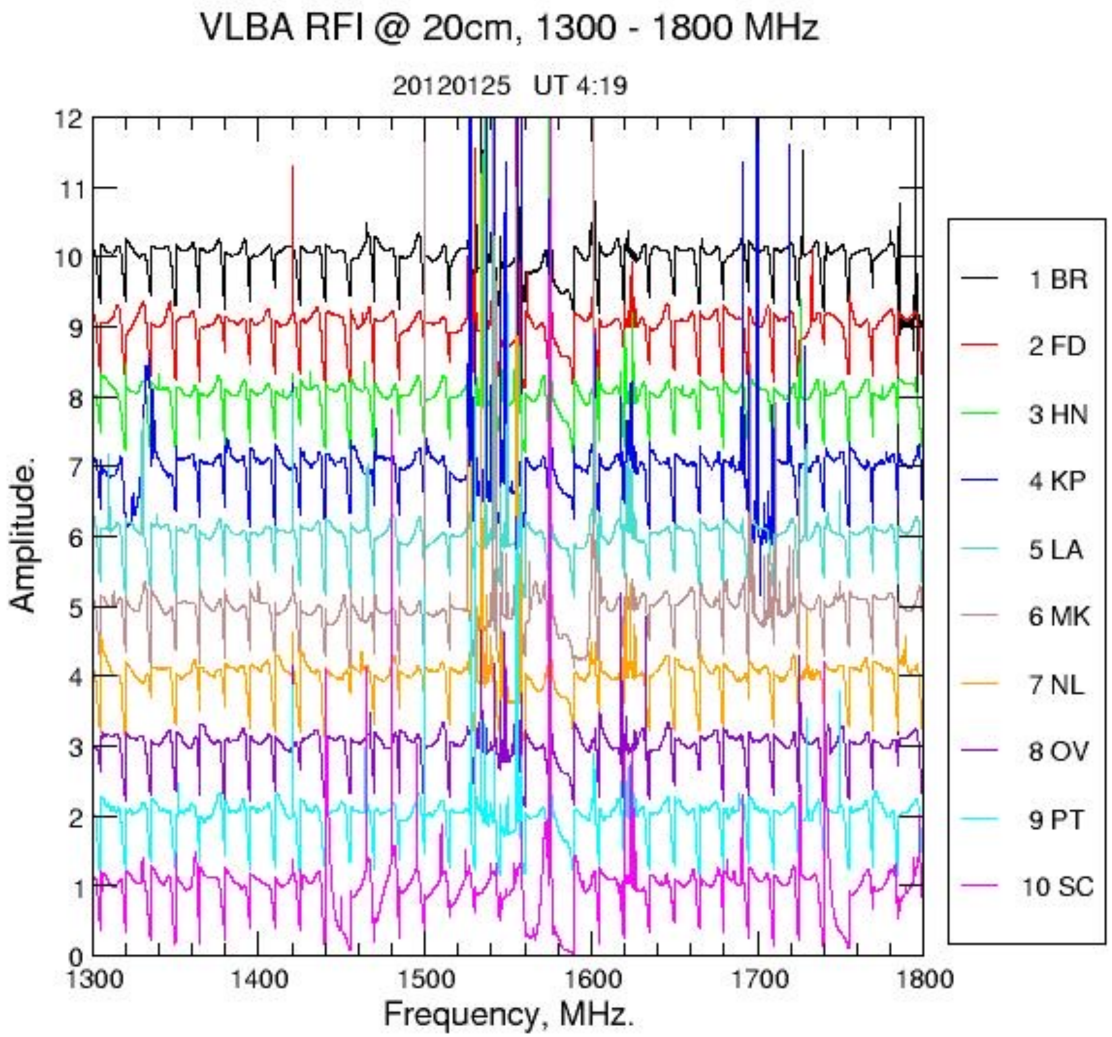
Radio Frequency Interference (RFI)

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



RFI at the VLA 1-2 GHz

Example VLBA



Calibration

- Data editing and calibration is not fundamentally different from continuum observations, but a few additional items to consider:
  - Presence of RFI (data flagging)
  - Bandpass calibration
  - Correlator effects
  - Doppler corrections

- You also might deal with a large dataset
  - Averaging (time) may be helpful to reduce size if needed
  - Flagging edges of your band

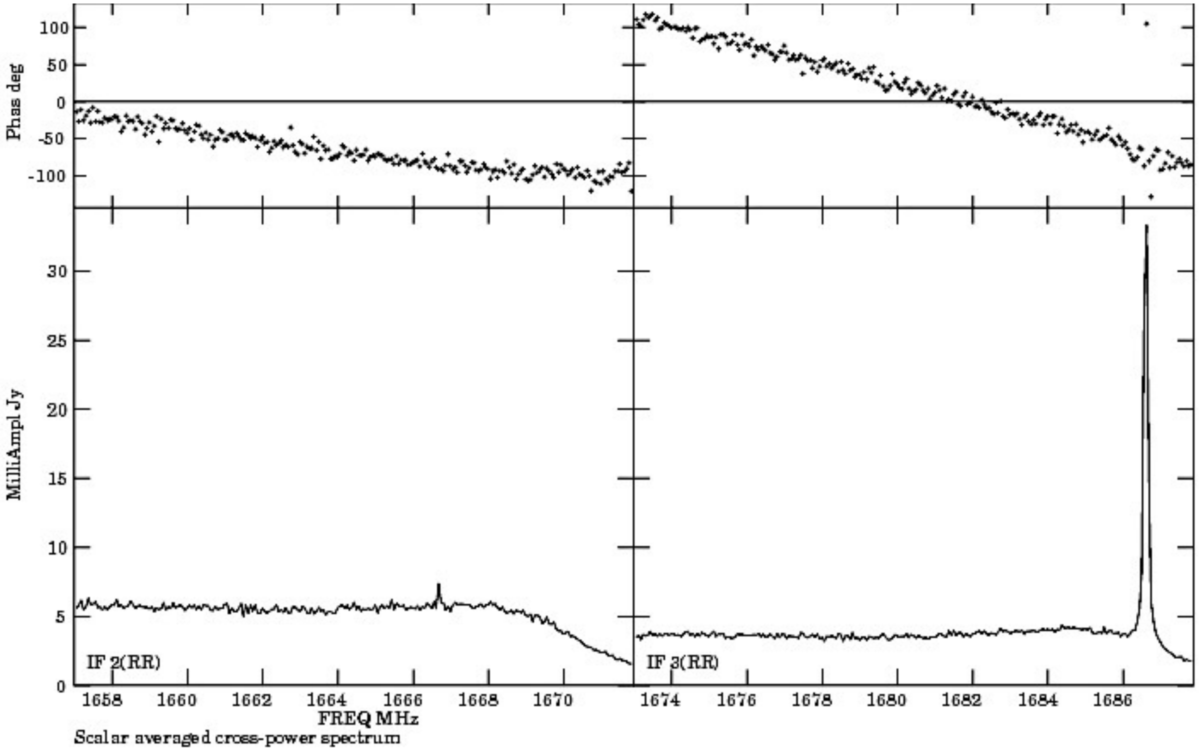
Preparation: Editing your data

Many ways to do this, here 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
  - 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 impractical, instead identify features by using cross- and total power spectra (**POSSM** in AIPS, **plotms** in CASA)

Example VLBA spectra

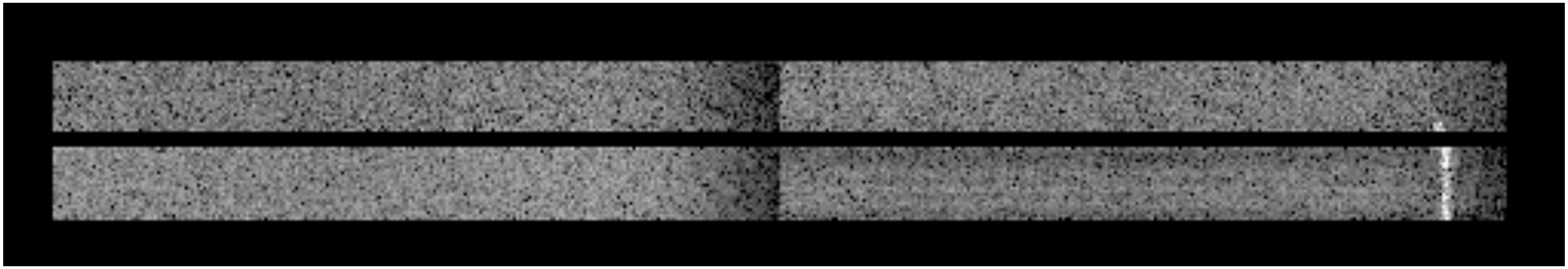


Scalar averaging helps to identify RFI features

- Is it limited in time? Limited to specific telescopes?
- Plot the RFI affected channels as a function of time can be useful to identify bad time ranges and antennas (**VPLOT/plotms)**

Spectral flagging

- Flag based on the feature
- SPFLG/Viewer/plotms
- Try avoiding excessive frequency dependent editing, since this introduces changes in the *uv* - coverage across the band.



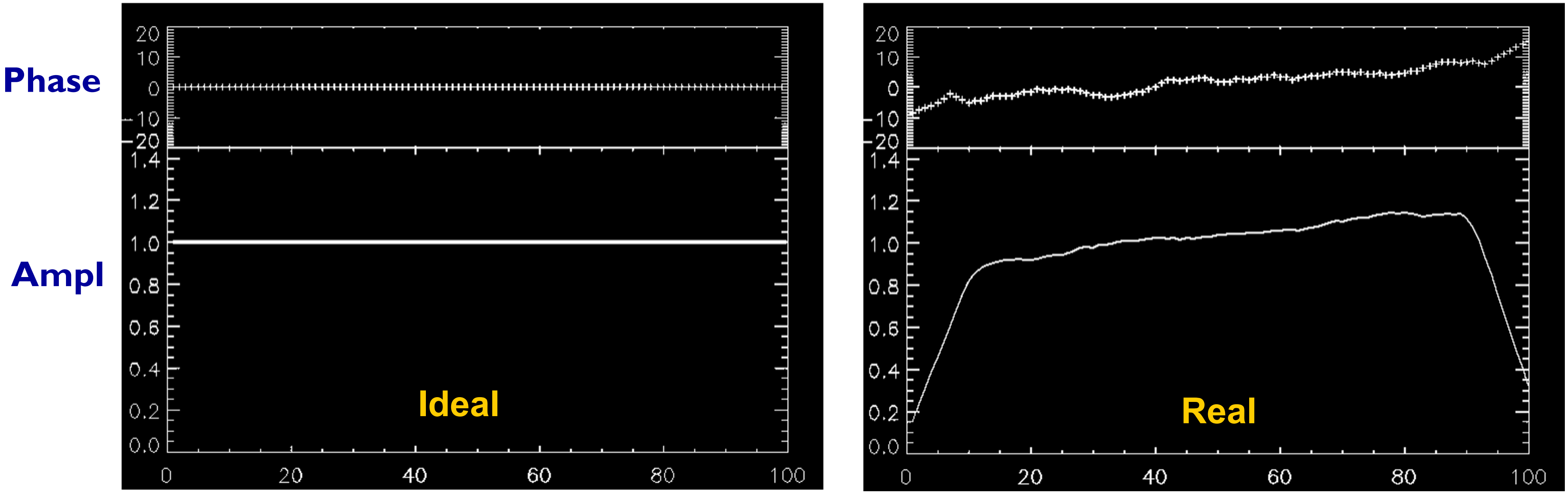
Bandpass calibration: Why?

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 pseudo-continuum, the dynamic range of final image is affected by the bandpass quality.

Example ideal and real bandpass



- Want to correct for the offset of the real bandpass from the ideal one (amplitude=1, phase=0).
- The bandpass is the relative gain of an antenna/baseline as a function of frequency.

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
  - Break the complex gain G_{ij} into a fast-varying frequency independent part, and a slowly varying frequency dependent part:

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

Bandpass calibration

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

The BP calibrator

- 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 is to use

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

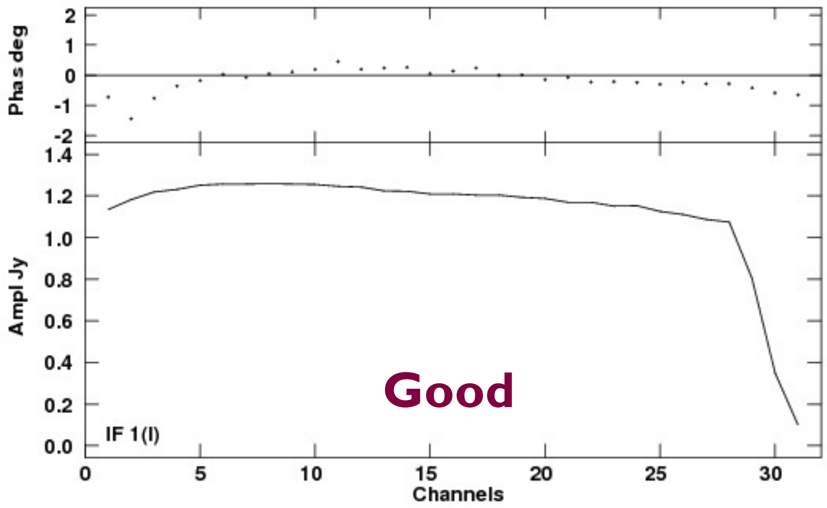
which then results in an integration time:

$$t_{\mathrm{BPcal}} = 9 \times (S_{\mathrm{target}} / S_{\mathrm{BPcal}})^2 \, t_{\mathrm{target}}$$

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

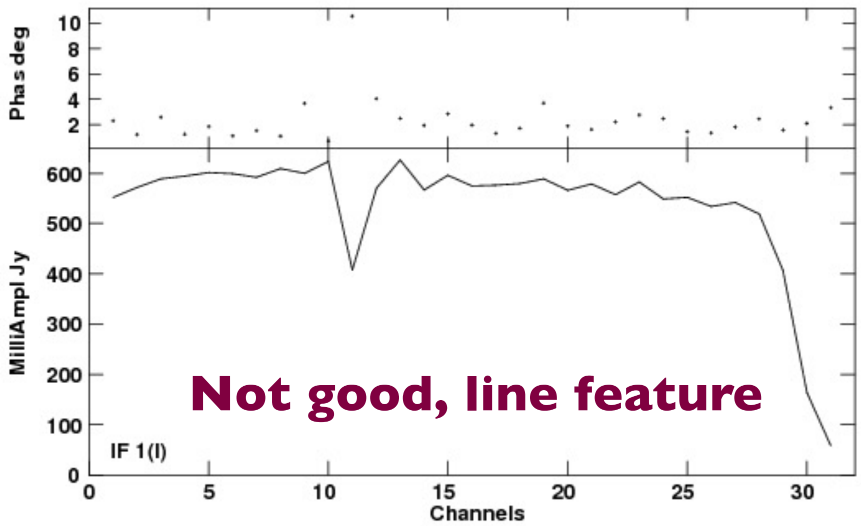
The BP calibrator

- Select a continuum source with:
  - High SNR in each channel
  - Intrinsically flat spectrum
  - No spectral lines

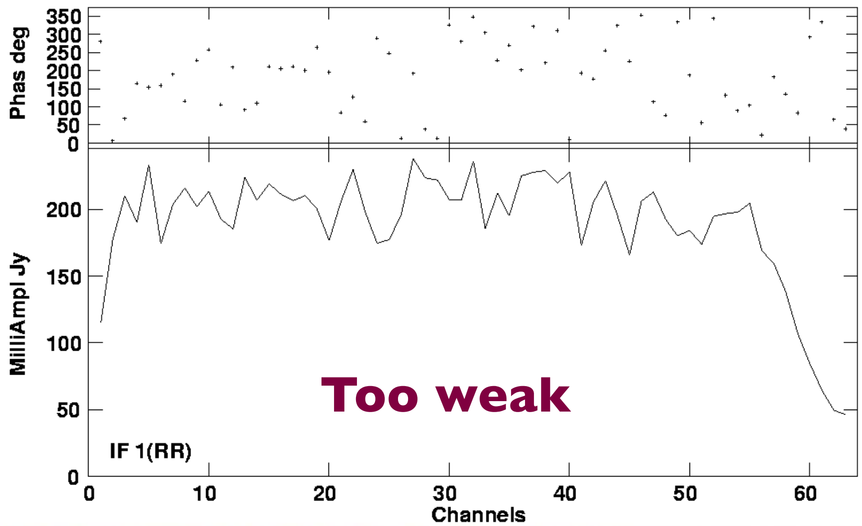


Good

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



Not good, line feature

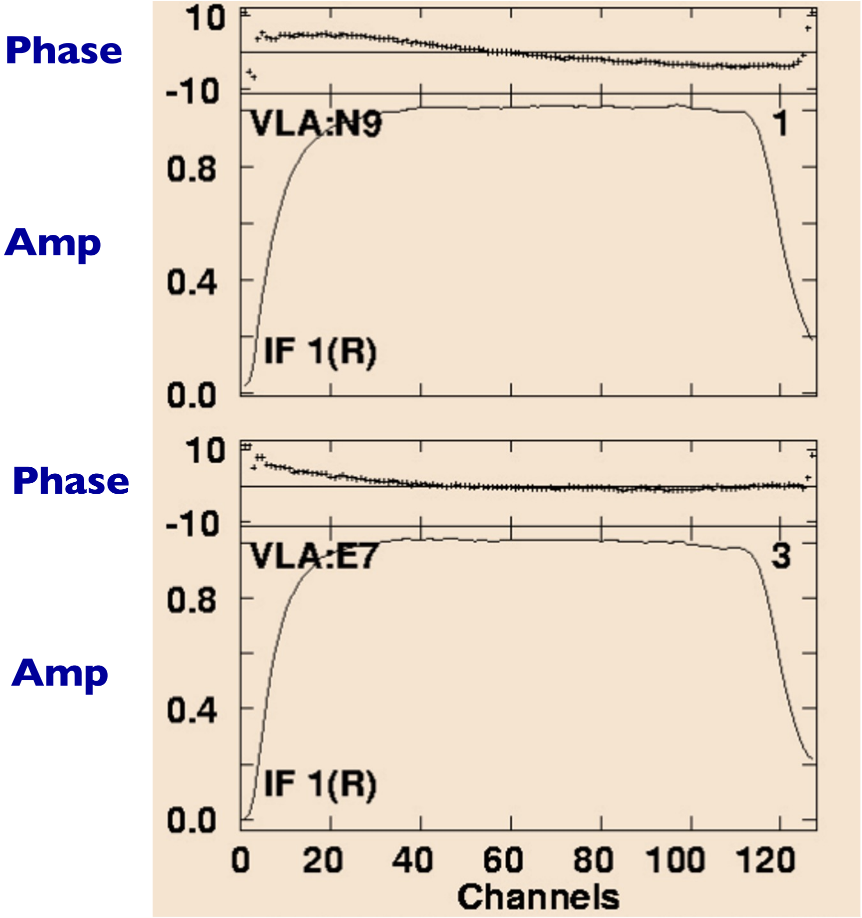


Too weak

Good quality bandpass calibration

Examples of good-quality bandpass solutions for 2 antennas:

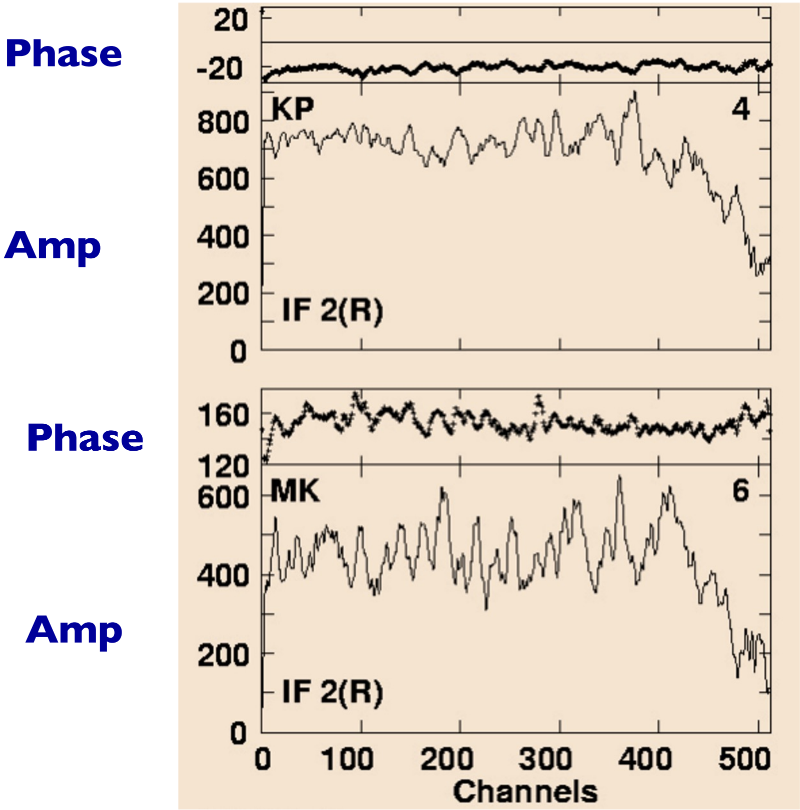
- Solutions should look comparable for all antennas
- Mean amplitude ~1 across useable portion of the band.
- No sharp variations in amplitude and phase; variations not controlled by noise



Bad quality bandpass calibration

Examples of bad-quality bandpass solutions for 2 antennas:

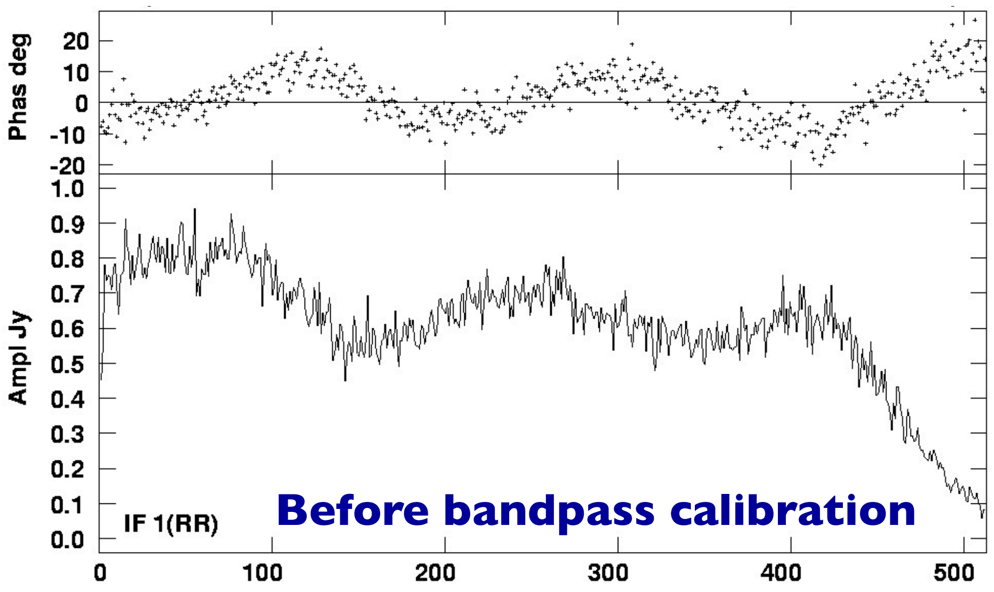
- Amplitude has different normalization for different antennas
- Noise levels are high, and are different for different antennas

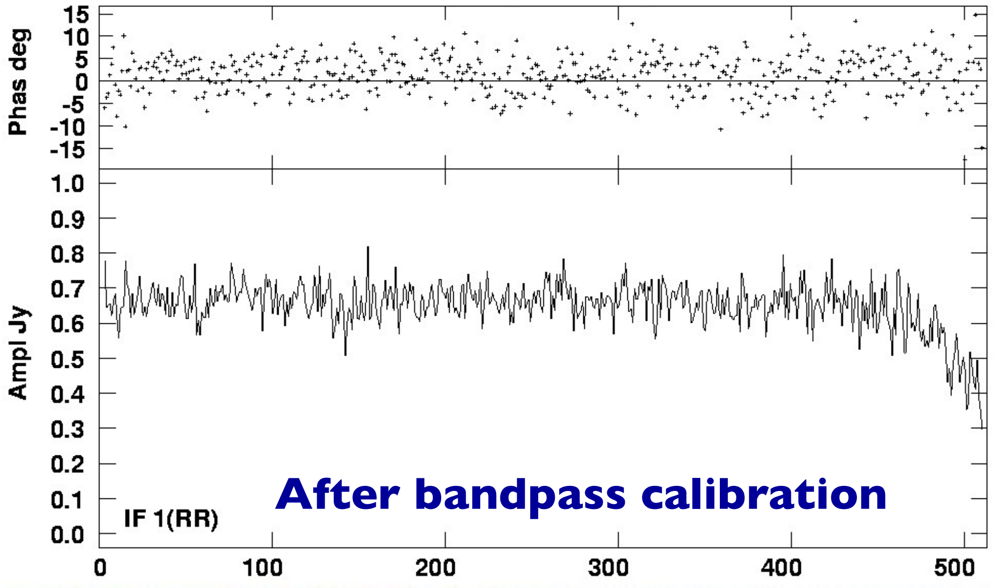


Test: Apply to continuum source

Before accepting the BP solutions, apply to a continuum source and use cross-correlation spectrum to check:

- Flat phases
- Constant amplitudes
- No increase in noise by applying the BP





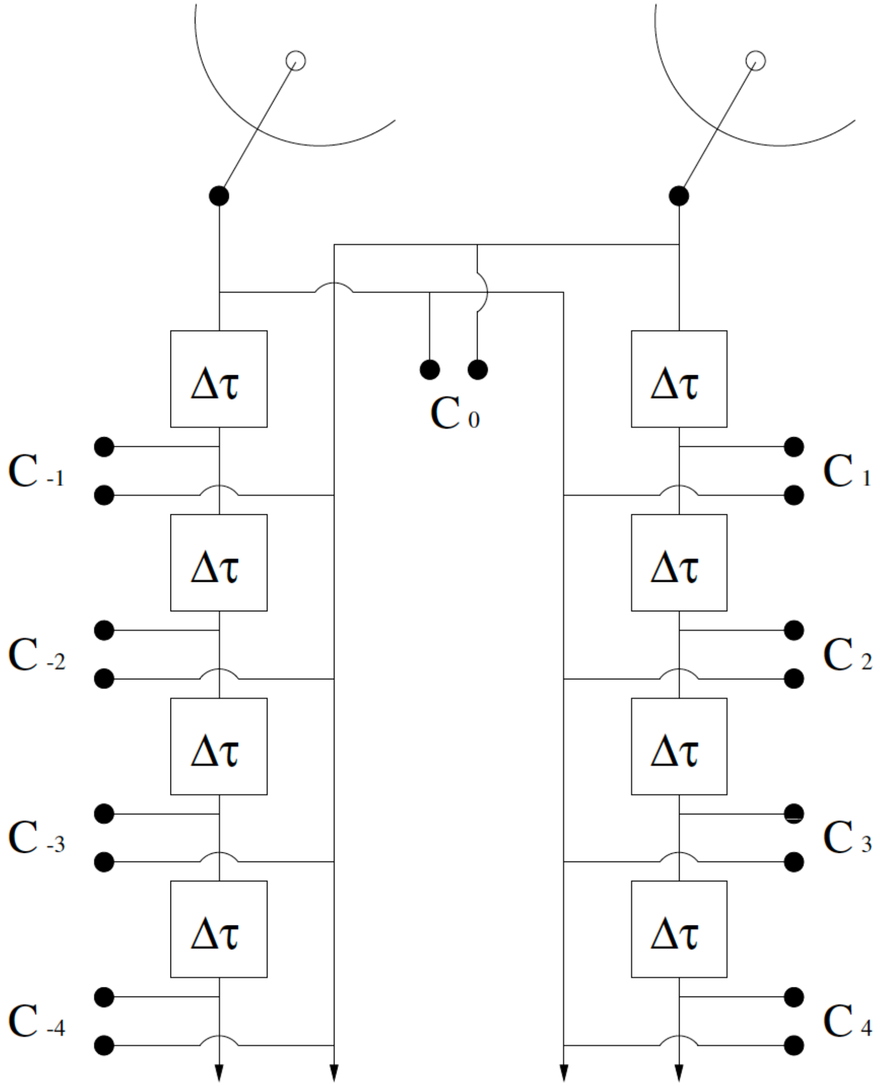
Spectral response correlator

How extract frequency information $V(u,v,\nu)$? If we just used filter banks, visibilities $V(u,v,\nu)$ could be formed directly. Not a versatile method.

Instead use the delay method already introduced for geometric delay & fringe stopping.

This would then give $V(u,v,\tau)$.

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



Spectral response: XF correlator

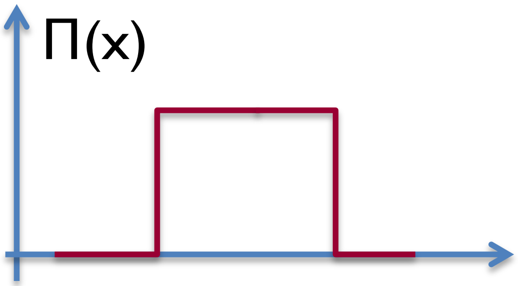
For spectroscopy in an XF correlator "lags" $\Delta\tau$ are introduced

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



Spectral response: FX correlator

Example FX correlators: ALMA, VLBA, EVN SFXC

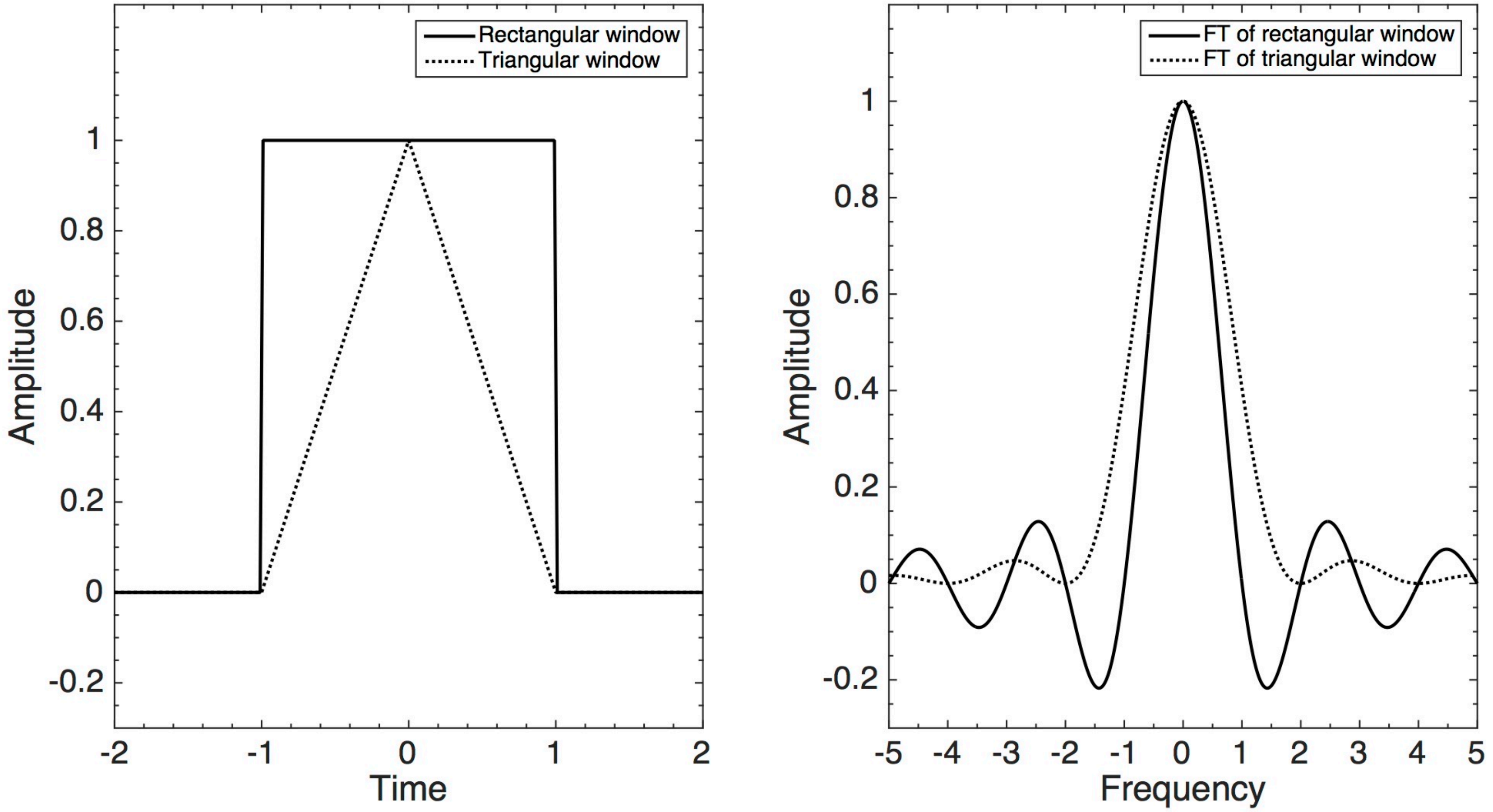
For FX correlators:

- 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, hence also a truncated signal

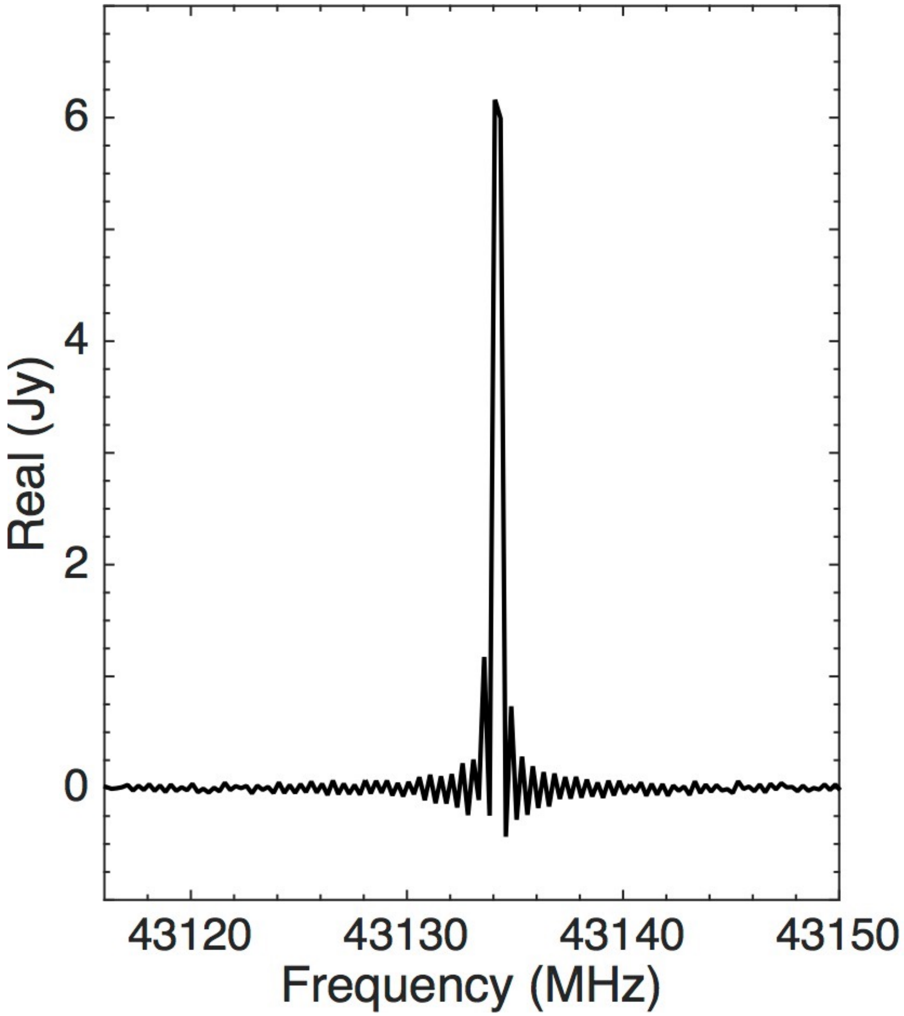
=> Total response $\mathrm{sinc}^2(x)$ with 5% sidelobes

Spectral response example



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



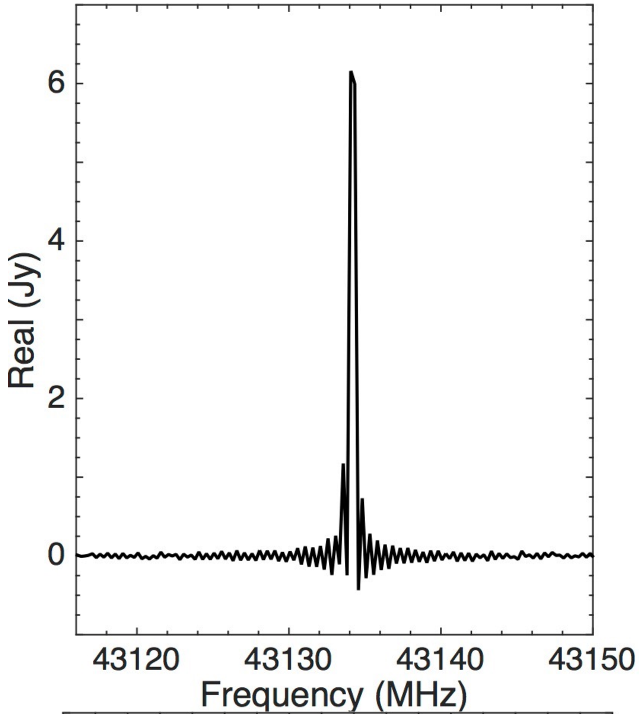
Gibbs ringing

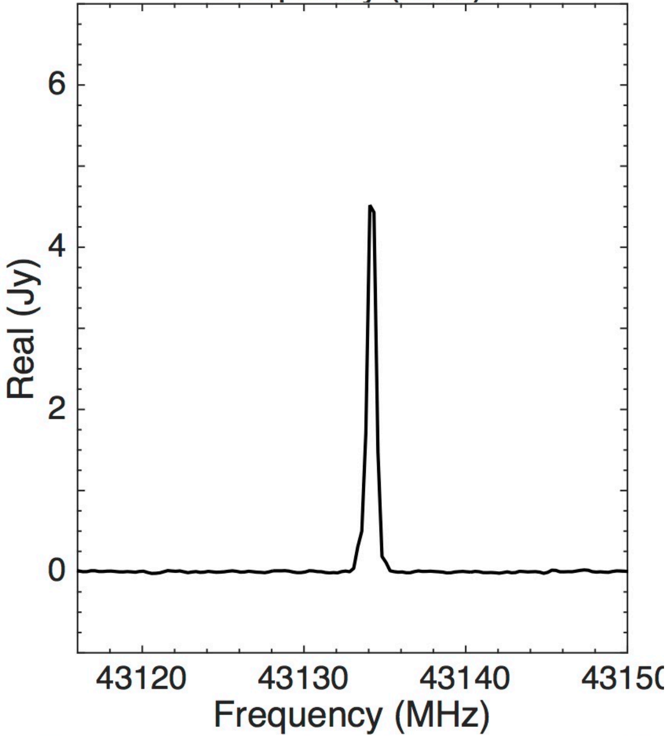
To reduce effects, window functions can be applied in the correlator

- Reduces sidelobes at the expense of main peak resolution

- Can also smooth in post-processing (often Hanning window applied)

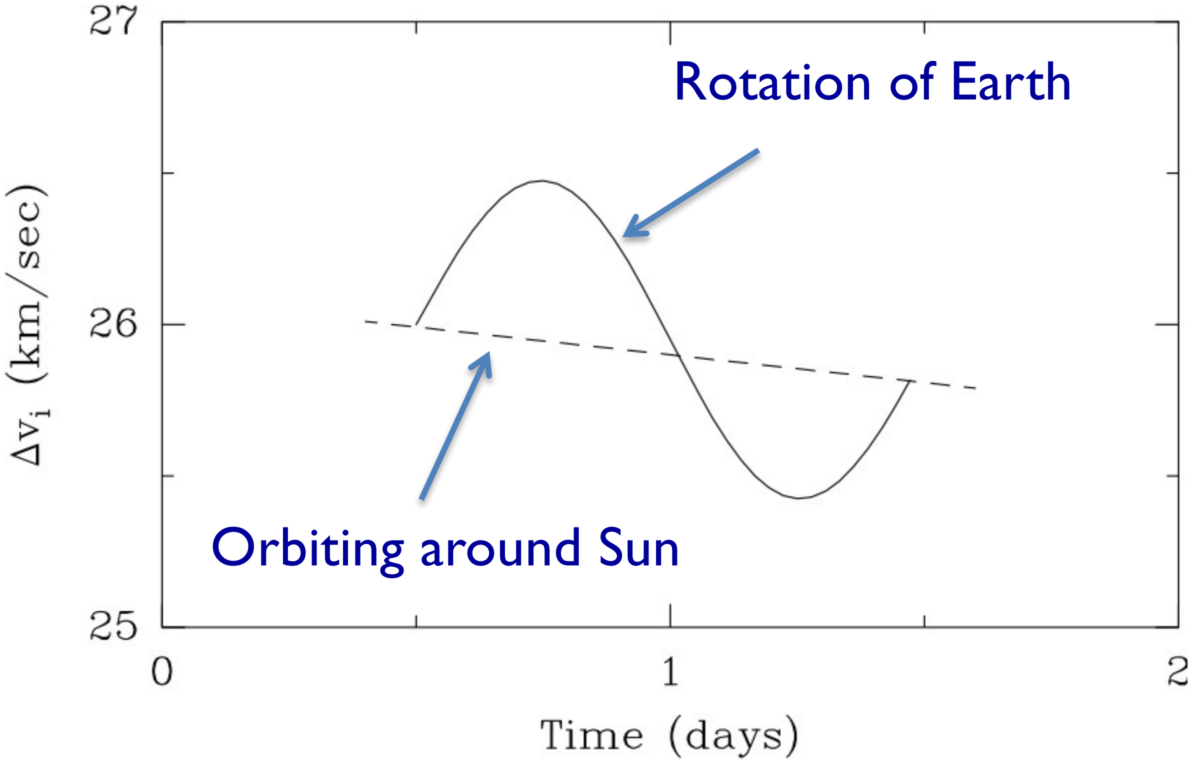
$$S_h(\nu_i) = \frac{S(\nu_{i-1}) + 2S(\nu_i) + S(\nu_{i+1})}{4}$$





Doppler tracking/setting

- 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.

- Doppler tracking used to 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 you have determined the correct velocity frame and definition when planning your observations.

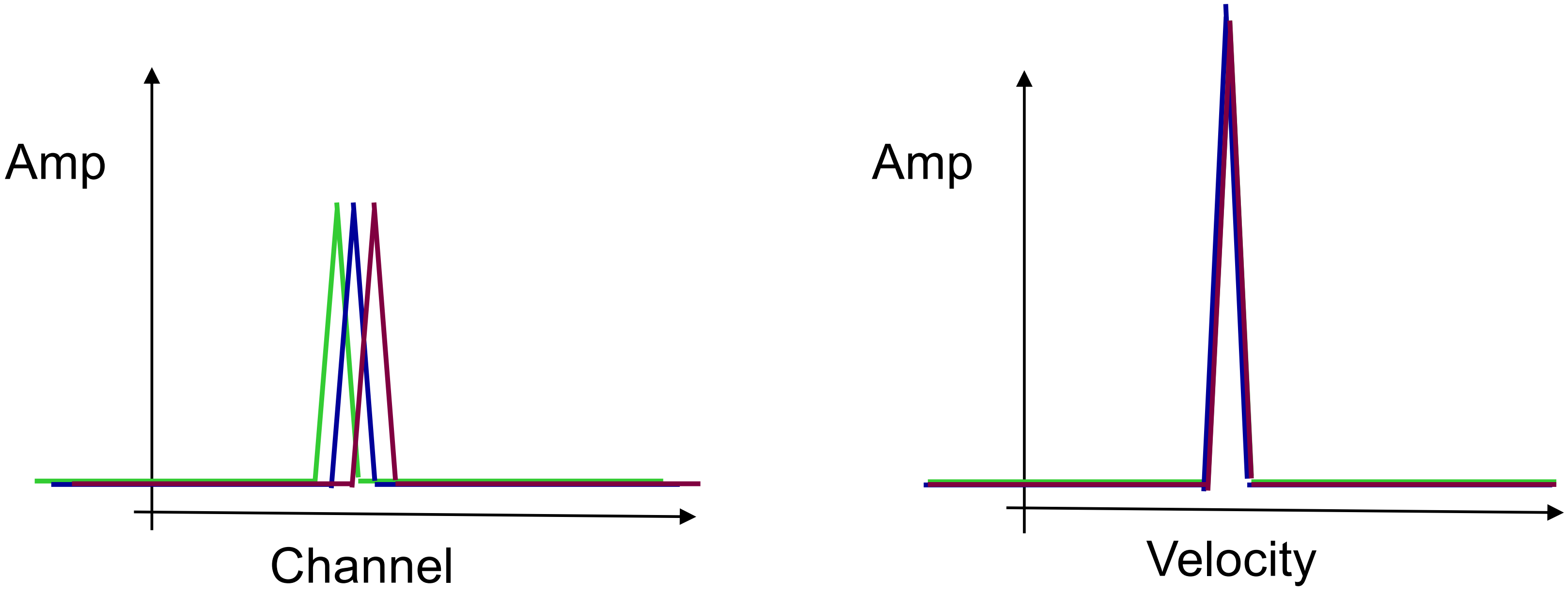
Note that the bandpass shape is a function of *frequency*, not velocity!

- 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 source, it will be observed at a different sky frequency!
  - Apply Doppler setting to the source position

Most times, we apply a Doppler *setting* at the beginning of the observation, and then apply additional corrections during post-processing.

Doppler corrections in post-processing

- Calculate the sky frequency for, e.g., the center channel of your target source depending on RA, Dec, rest frequency, velocity frame and definition, and time of observations (VLA has an online Dopset Tool)
  - Shift using **cvel/cvel**



Before and after Doppler correction

Before imaging

We have edited the data and performed band pass calibration. Also, we have done Doppler corrections if necessary.

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

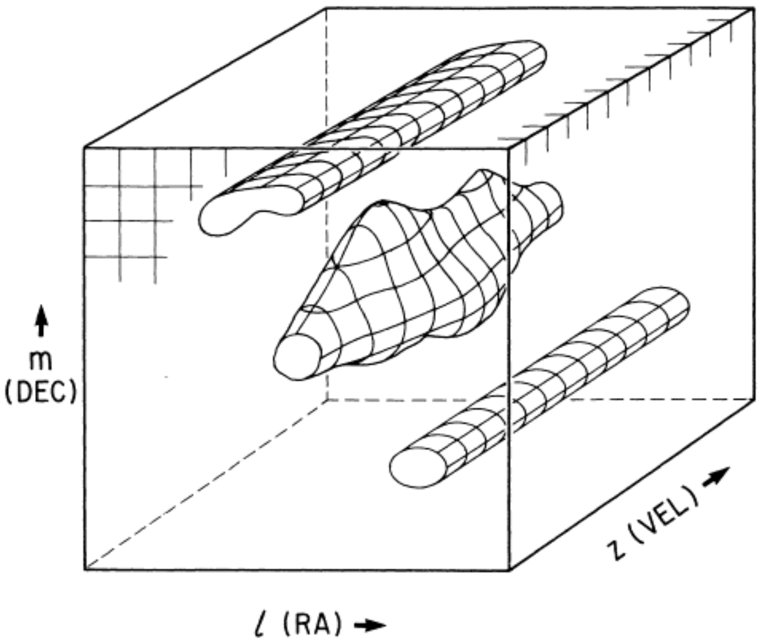
Before imaging a few things can be done to improve the quality of your spectral line data:

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

- For line analysis we want to remove the continuum, to separate out the line: continuum subtraction

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

Why continuum subtraction?

- Spectral lines easier to see, especially weak ones in a varying continuum field.
- 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 don't 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 (0^{th}, or often 1^{st}) 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 $\theta \ll \theta_B \, \nu/\Delta\nu_{tot}$

UVLIN/uvcontsub

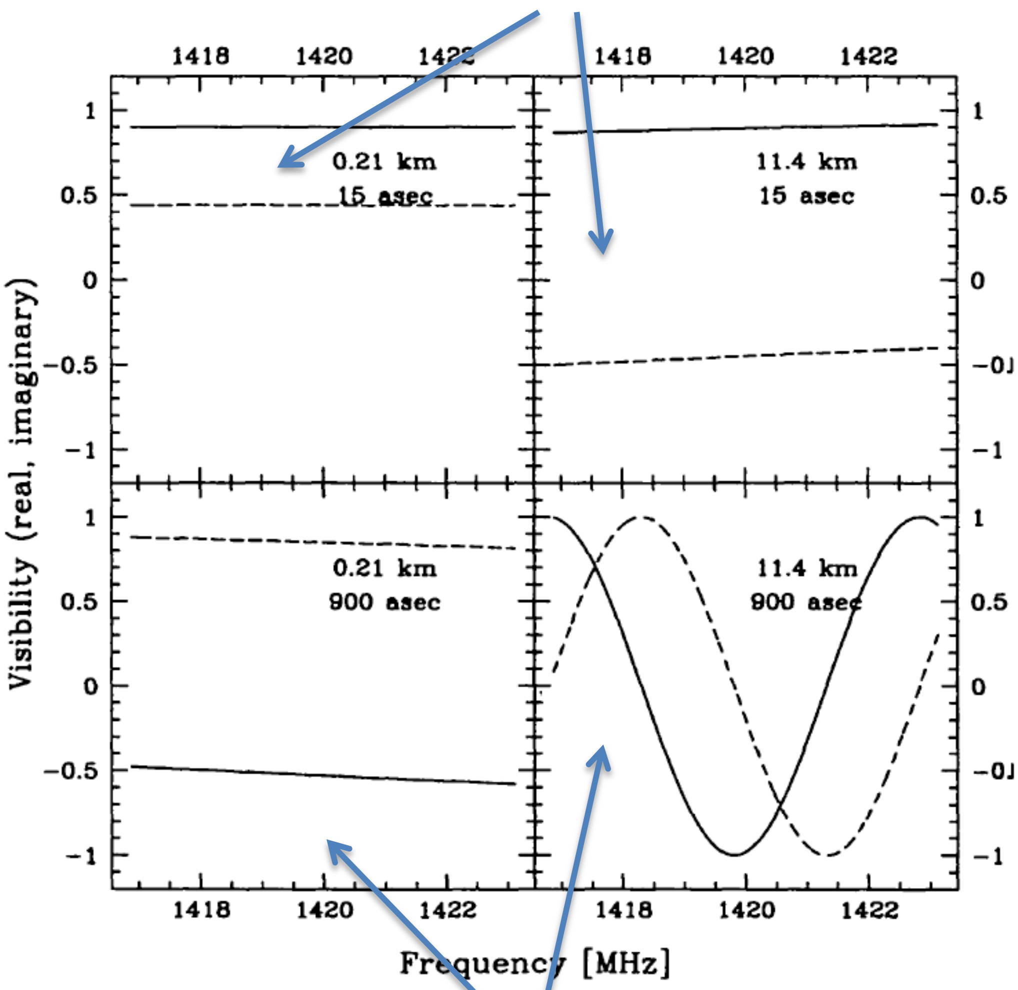
Restriction: small FOV

- 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.*



15” from phase center

15’ from phase center

Imaged based

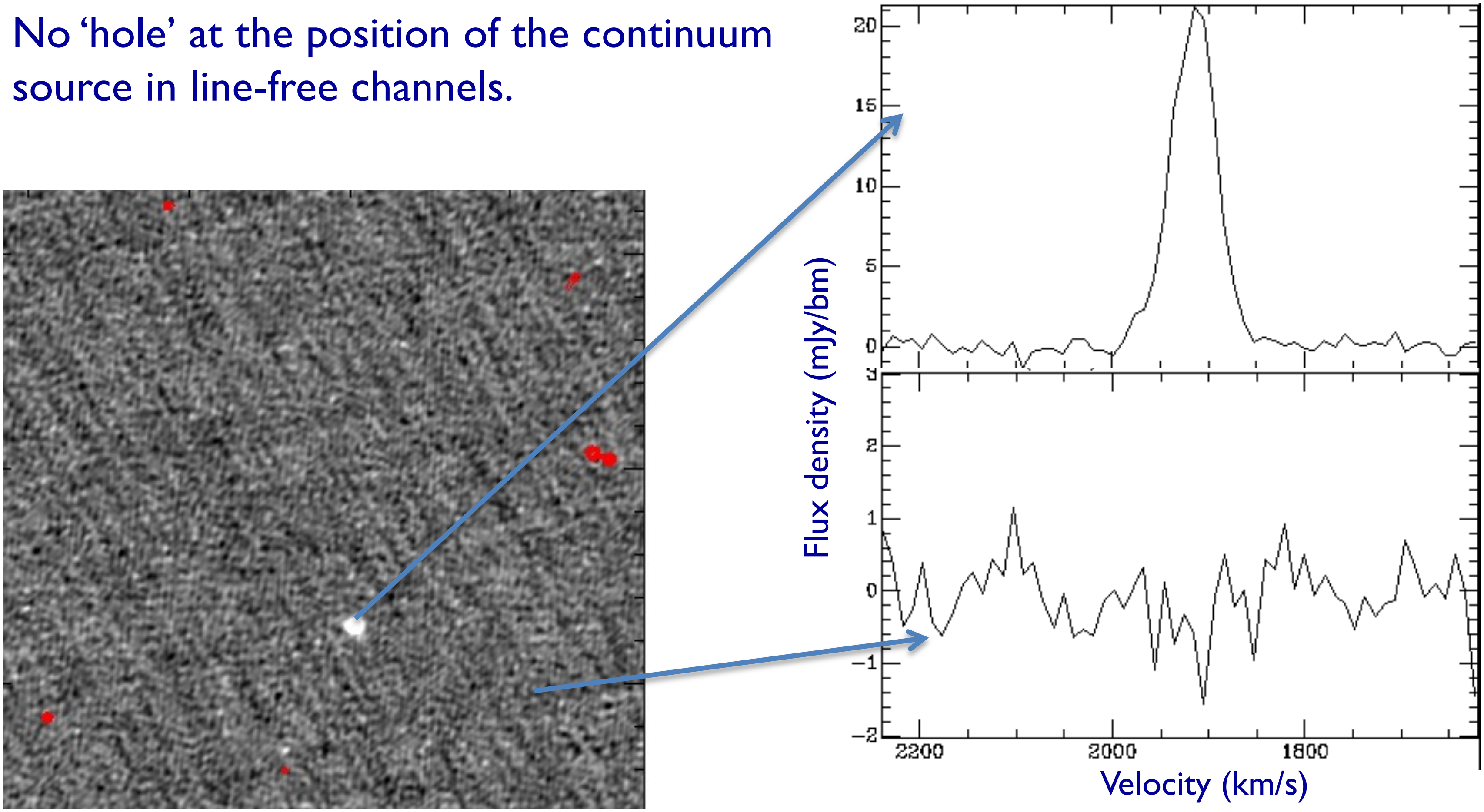
- Fit and subtract a low order polynomial fit to the line free part of the spectrum measured at each spatial pixel in cube.

- 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 your 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.



Imaging spectral line data

Deconvolution (CLEANing) will image the data and in the process it will:

- Remove sidelobes that could obscure faint emission
- Interpolate to zero spacing to estimate flux

Challenges include:

- Emission structure that changes from channel to channel
  - Try to keep deconvolution as similar as possible for all channels (same restoring beam, clean to same depth)
- Large data volumes (computationally expensive)

Want both:

- Sensitivity for faint features and full extent of emission
- High spectral & spatial resolution for kinematics
  - Averaging channels will improve sensitivity but may limit spectral resolution
  - Choice of weighting function will affect sensitivity and spatial resolution, Robust weighting is often a good compromise

Smoothing

Smoothing your data in x, y, or z (spatial or spectral), can be done either when mapping or in the analysis stage.

Spatial smoothing

- Can help emphasizing large-scale structures
- Useful if you want to compare observations made with different beam sizes
- Can be done by uv 'tapering', or in the image domain by convolution

Spectral smoothing

- Can help emphasizing low SNR lines
- Can reduce your data size
- Be careful with noise propagation, adjacent channels will be correlated

Visualizing

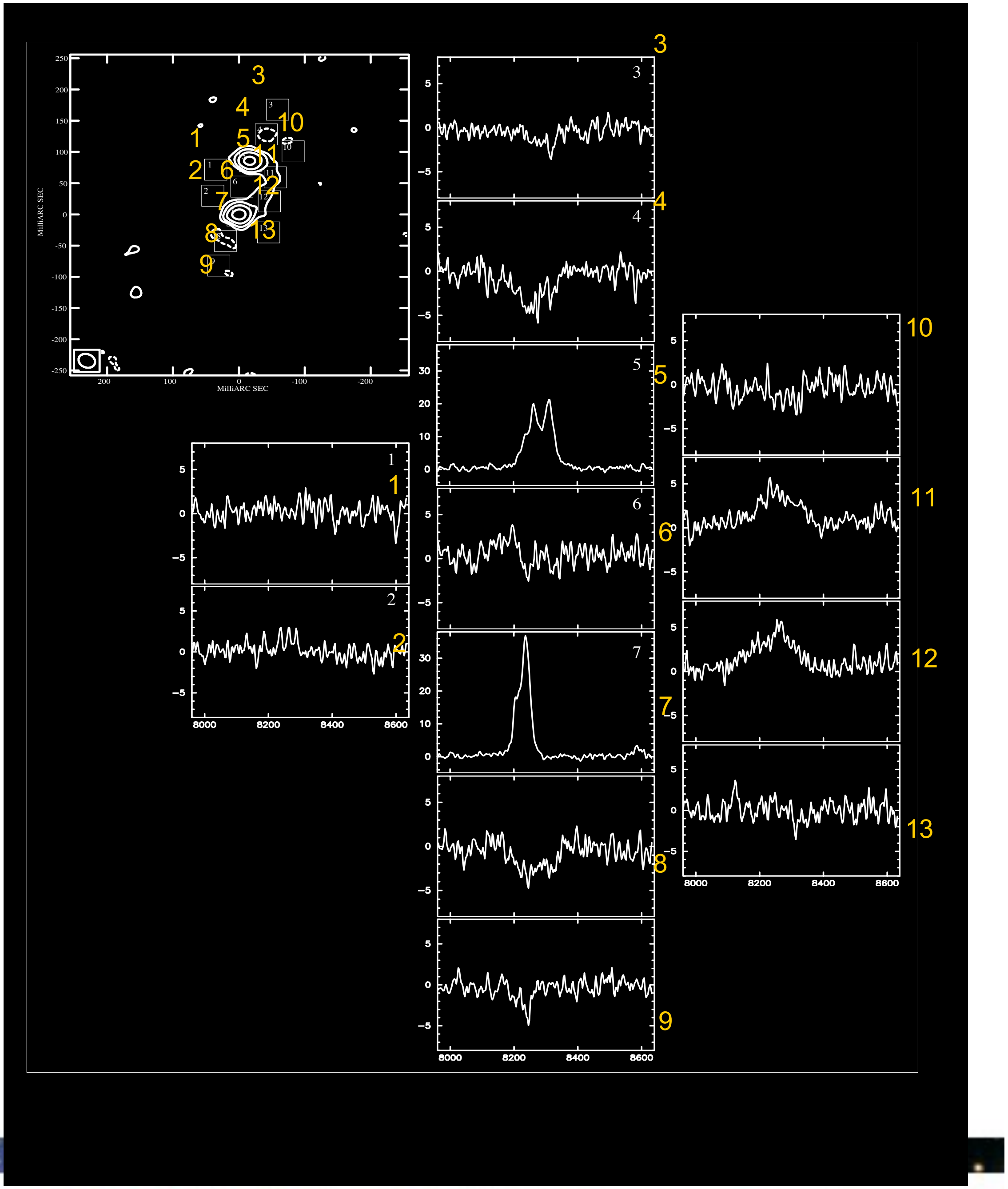
- Imaging will create a spectral line *cube,* which is 3-dimensional: RA, Dec and Velocity (frequency).

- 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)
    - ‘Movies’ can be formed from the channel maps
  - Moment maps (integration along the velocity axis)
  - Position-velocity plots (slices along spatial dimension)

- 3-D rendering programs also exist: CARTA

1-D line profiles

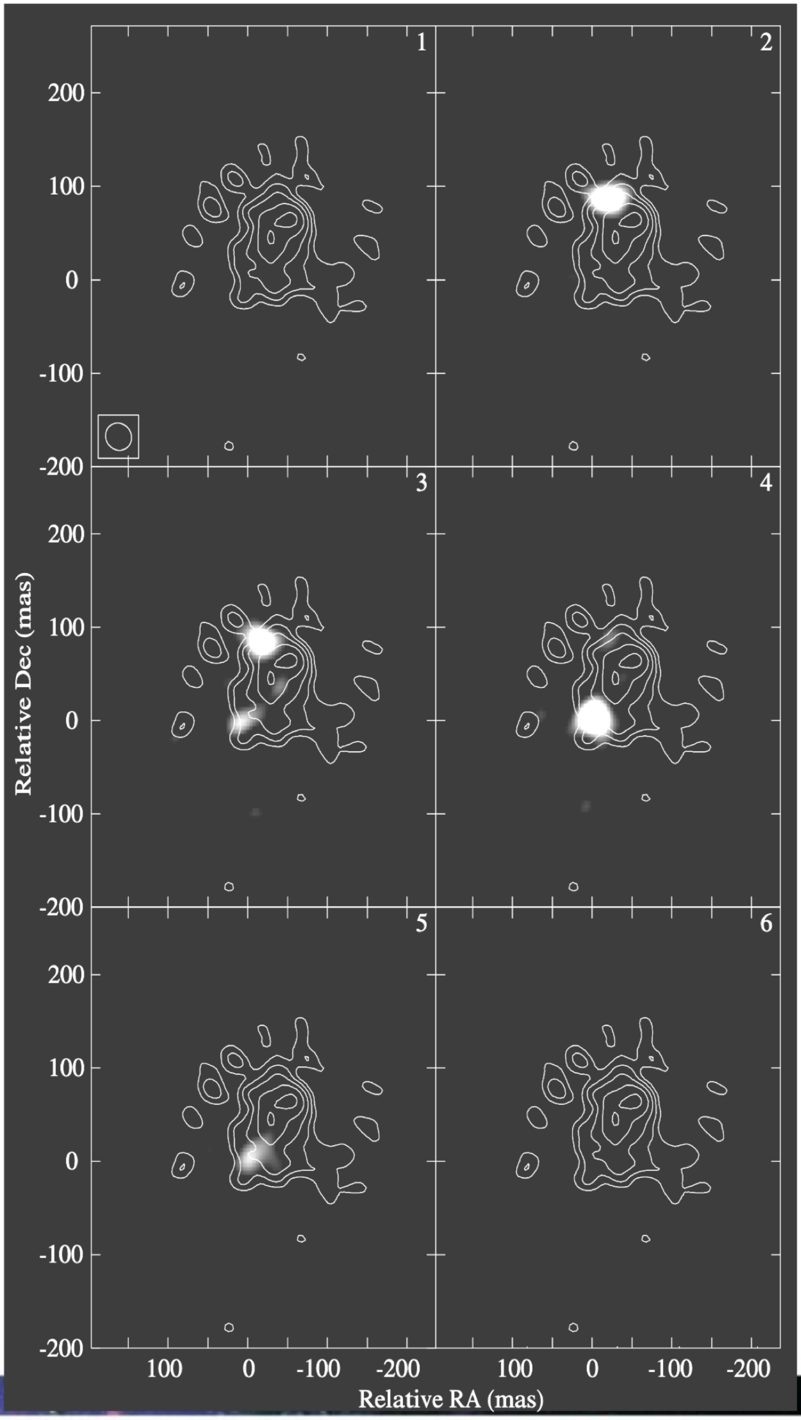
- Line profiles show changes in line shape, width and depth as a function of position.
- Can give information of relative position of features (absorption in front)
- Velocity width



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

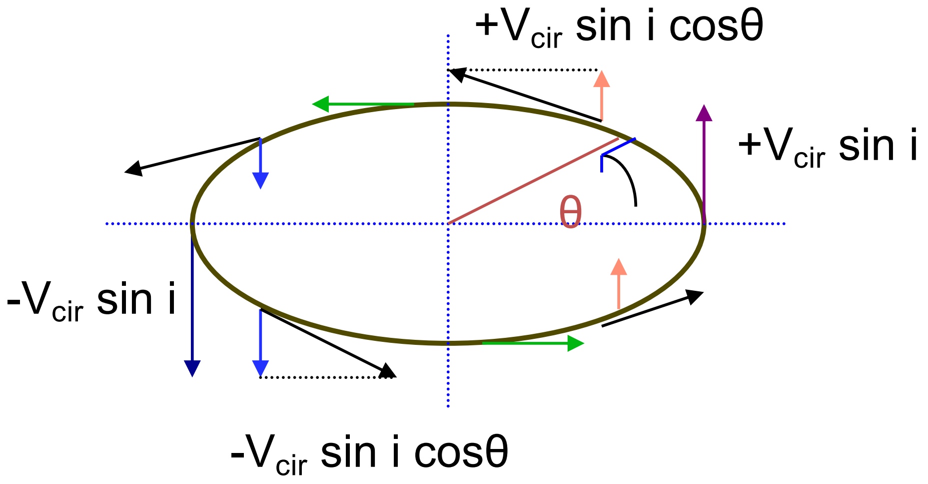
2-D channel maps

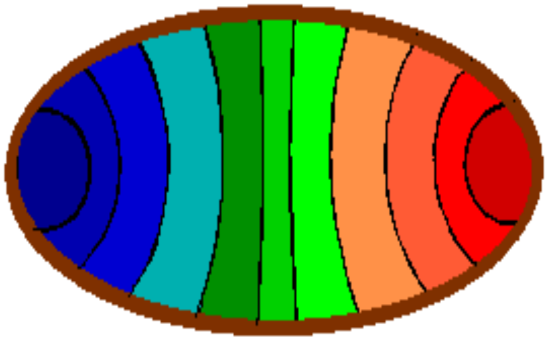
- Channel maps show how the spatial distribution of the line feature changes with frequency/velocity.
- Information about kinematics.



Contours continuum emission, grey scale 1667 MHz OH line emission in IIIZw35.

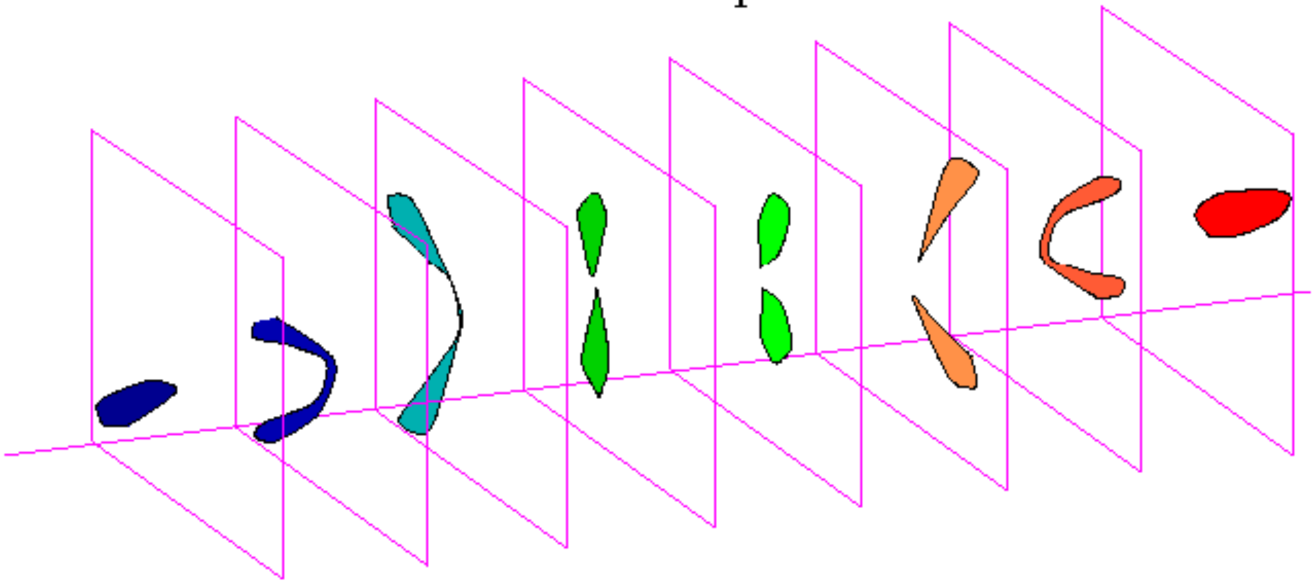
Rotating disk model





Mean Velocity Field

Channel Maps

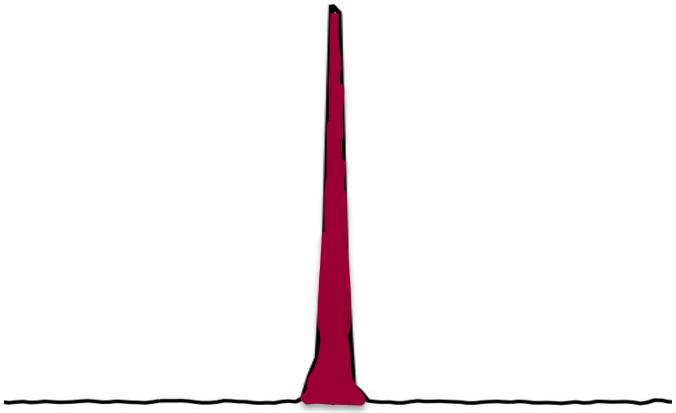


Moment analysis

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

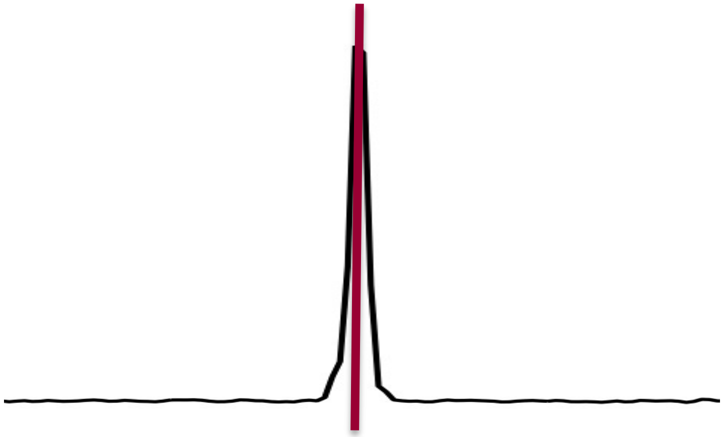
- Integrated intensity

$$\text{Moment } 0 = \int S_v dv$$



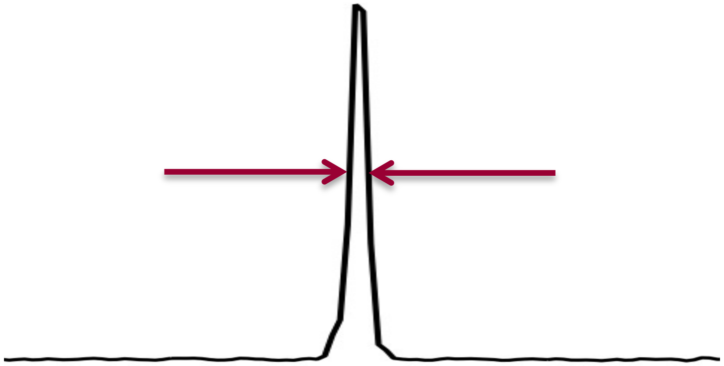
- Intensity weighted velocity

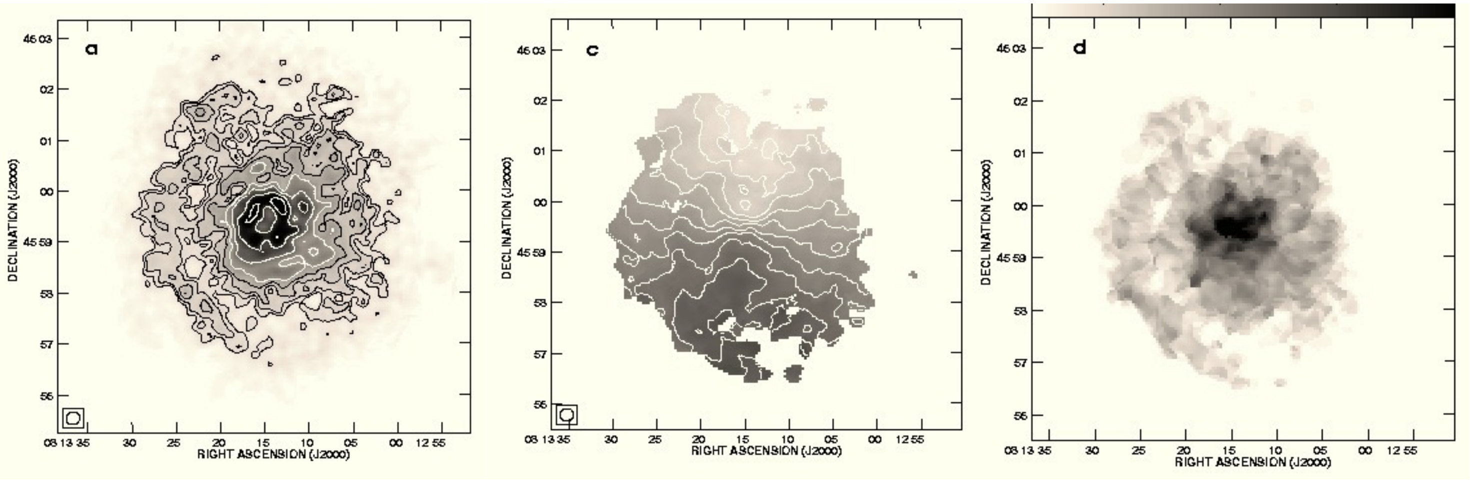
$$\text{Moment 1} \;= \langle V \rangle = \frac{\int S_v v dv}{\int S_v dv}$$



- Intensity weighted velocity dispersion

$$\text{Moment 2} \;= \langle V^2 \rangle^{1/2} = \sqrt{\frac{\int S_v (v - \langle V \rangle)^2 dv}{\int S_v dv}}$$





Moment 0

Total intensity

Moment 1

Velocity field

Moment 2

Velocity dispersion

- Moments sensitive to noise so clipping is required
- Higher order moments depend on lower ones so progressively noisier.

XMOM, MOMNT/immoments

Moment map challenges

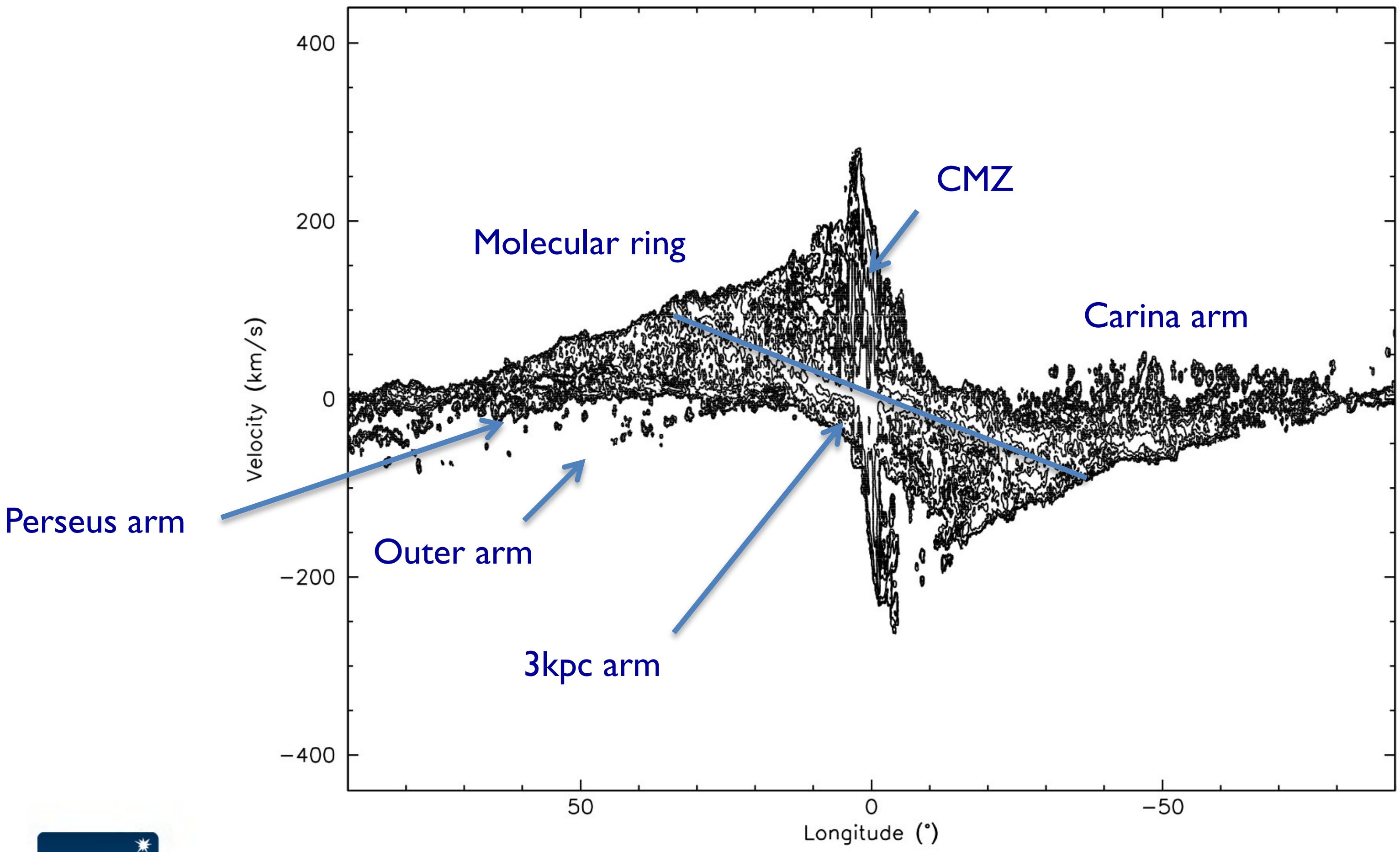
- Can be demanding to interpret correctly:
  - Both emission and absorption may be present
  - Velocity patterns can create misleading moment maps
  - Biased towards regions of high intensity
  - Complicated error estimates: number or channels with real emission used in moment computation will greatly change across the image.

- Use as guide for investigating features, or to compare with other ν.

- Alternatives…?
  - Gaussian fitting for simple line profiles (CASA viewer/CARTA)
  - "Maxmaps" show emission distribution (finding the max in each x,y pixel through the cube: **SQASH**)

Position-Velocity diagrams

PV-diagrams show, for example, the line emission velocity as a function of position (RA, Dec, longitude, latitude, radius).



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

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/

Summarizing remarks

Most instruments observe in high resolution, multi-channel mode meaning

- Large bandwidths implying bandwidth smearing effects
- RFI effects: preparation of observations and removal in data
- Correction for atmospheric and instrumental gain variations

Better, it also implies:

- Ability to reveal details of kinematics of line emission
- Line searches: multiple transitions can be used to derive temperature and density in a region.

The End