Spectral Line Data Analysis

Ylva Pihlström, UNM

Sixteenth Synthesis Imaging Workshop

16-23 May 2018

Outline

- Motivation for spectral line observations
  - Advantages also for continuum experiments
- What can affect your observations:
  - Know instrument responses
  - Know standard RFI environment
- What to consider during calibration
  - Bandpass, RFI and flagging, Doppler corrections
  - Spectral response, subtracting continuum emission
- Visualizing spectral line data
  - Common types of visualizations

Introduction

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

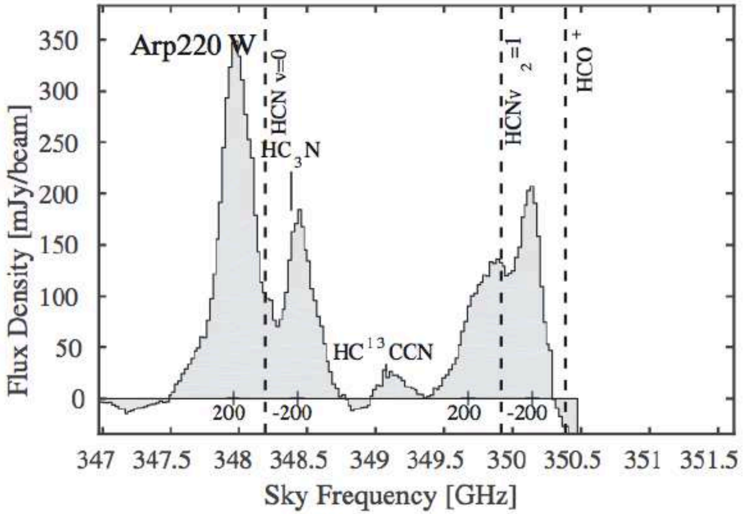
- **Science driven**: science depends on frequency (spectroscopy)
  - Emission and absorption lines, and their Doppler shifts
  - Slope across continuum bandwidth (spectral index)

- **Technically driven**: science does not depend on frequency
  - Science quality improved using multiple channels (pseudo-continuum)

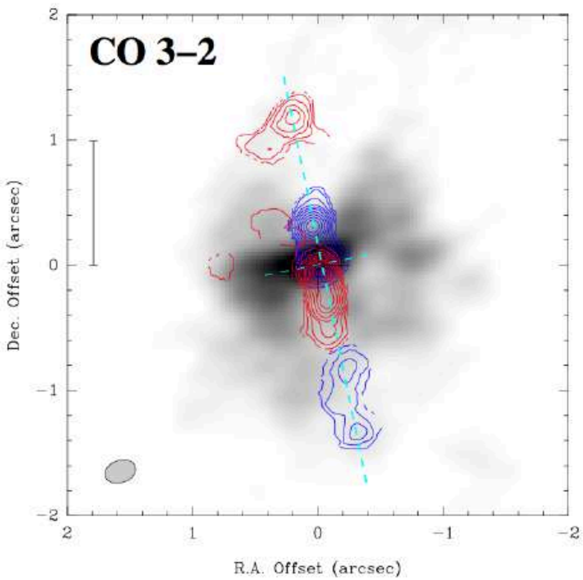
Most instruments today observe in multi-channel mode.

Spectroscopy

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



Aalto et al. 2015: ALMA Arp220 spectrum



Aalto et al. 2015: NGC1377 molecular jet

Pseudo-continuum

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

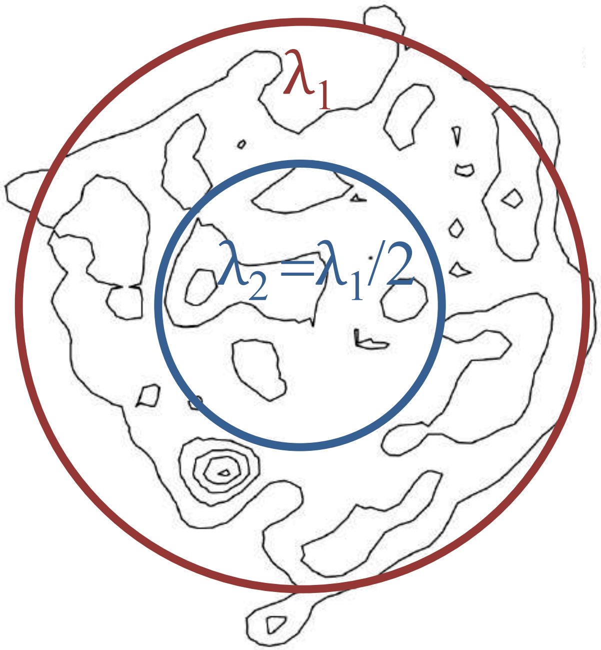
- Beam smearing
- Bandwidth smearing
- Problems due to atmospheric changes as a function of frequency
- Instrumental signal transmission effects as a function of frequency

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

Beam smearing: instrument response

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

- Band coverage $\lambda_1 - \lambda_2$
  $\Rightarrow$ θ_{PB} changes by λ_1/λ_2



More important 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

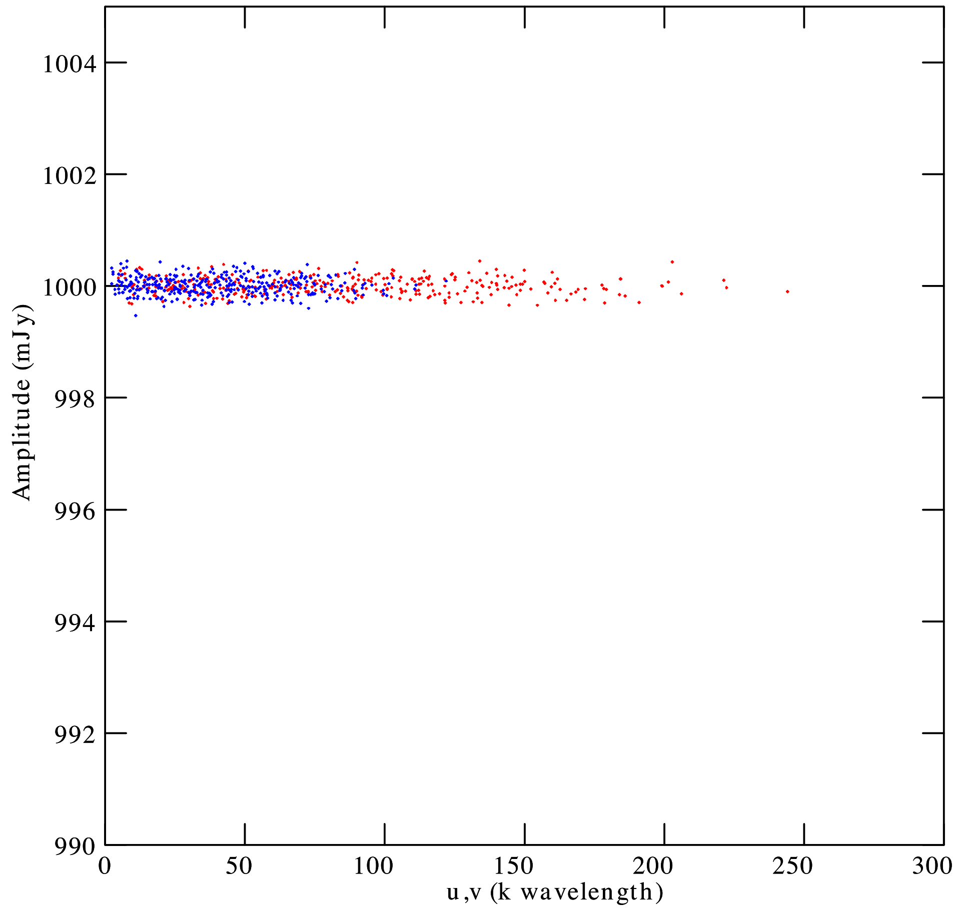
Also called chromatic aberration.

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

Band coverage $\nu_2 - \nu_1$

- 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

Band coverage $\nu_2 - \nu_1$

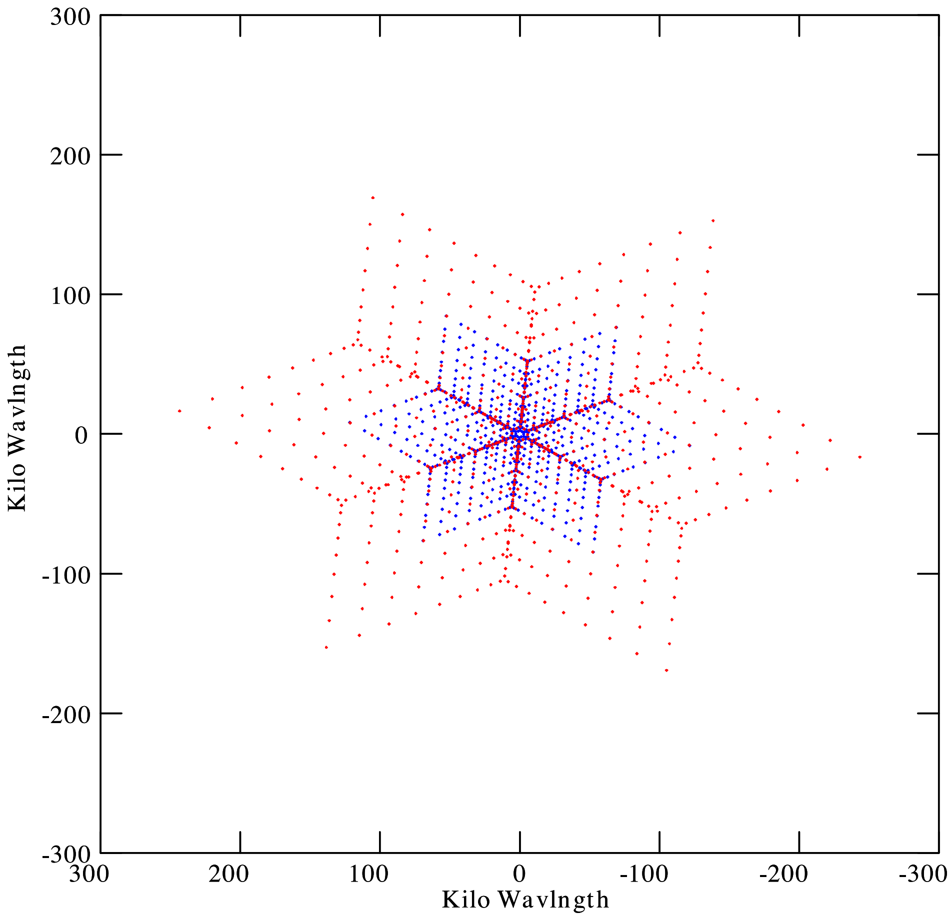
- ν_1 = 1 GHz (blue)
- ν_2 = 2 GHz (red)

Fringe spacings change by λ_1/λ_2

- *u,v* samples smeared radially

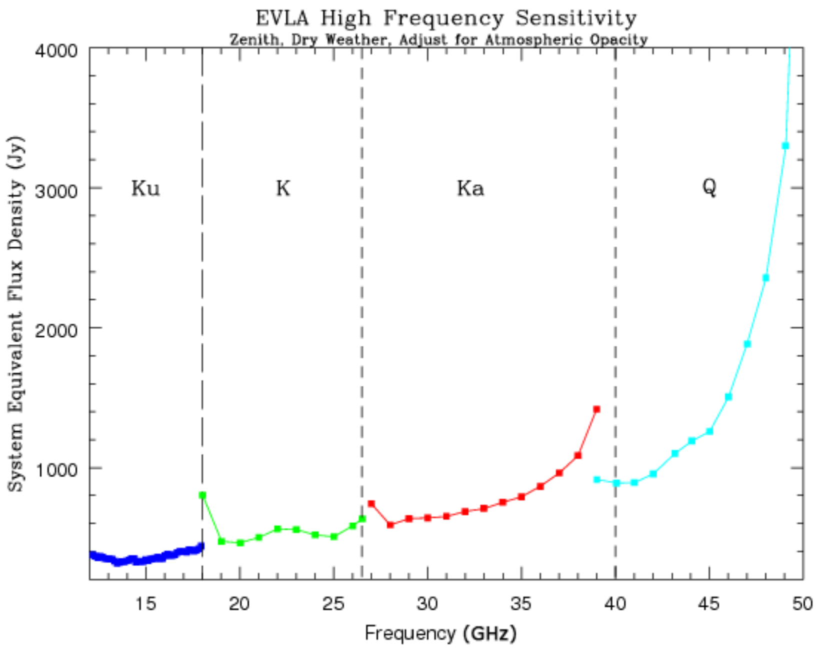
More important in larger configurations, and for lower frequencies

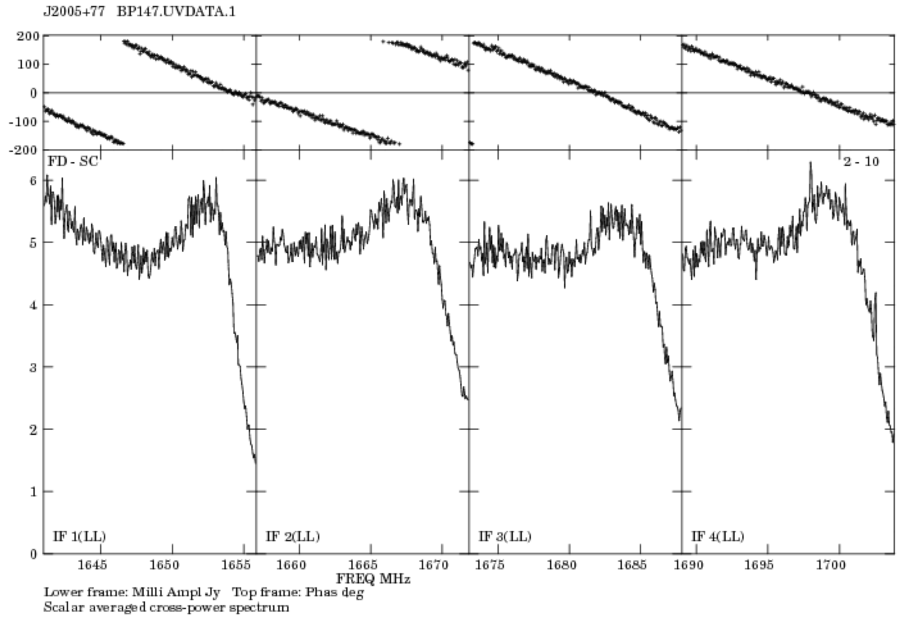
Pseudo-continuum uses smaller ranges to be combined later.



Instrument frequency response

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



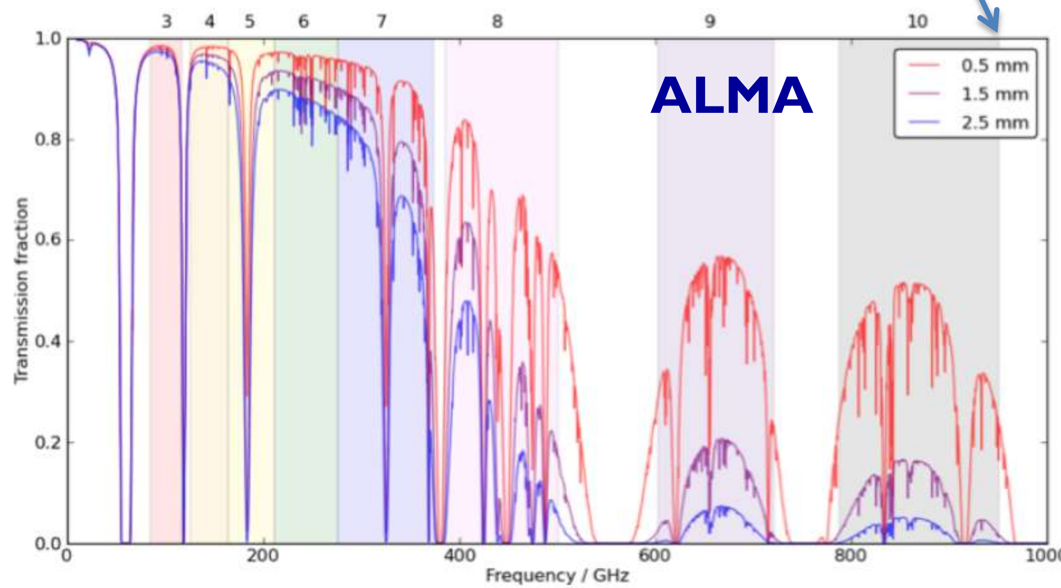


Phase slopes can be introduced by incorrect clocks or positions.

Atmospheric effects

PWV=Precipitable Water Vapor

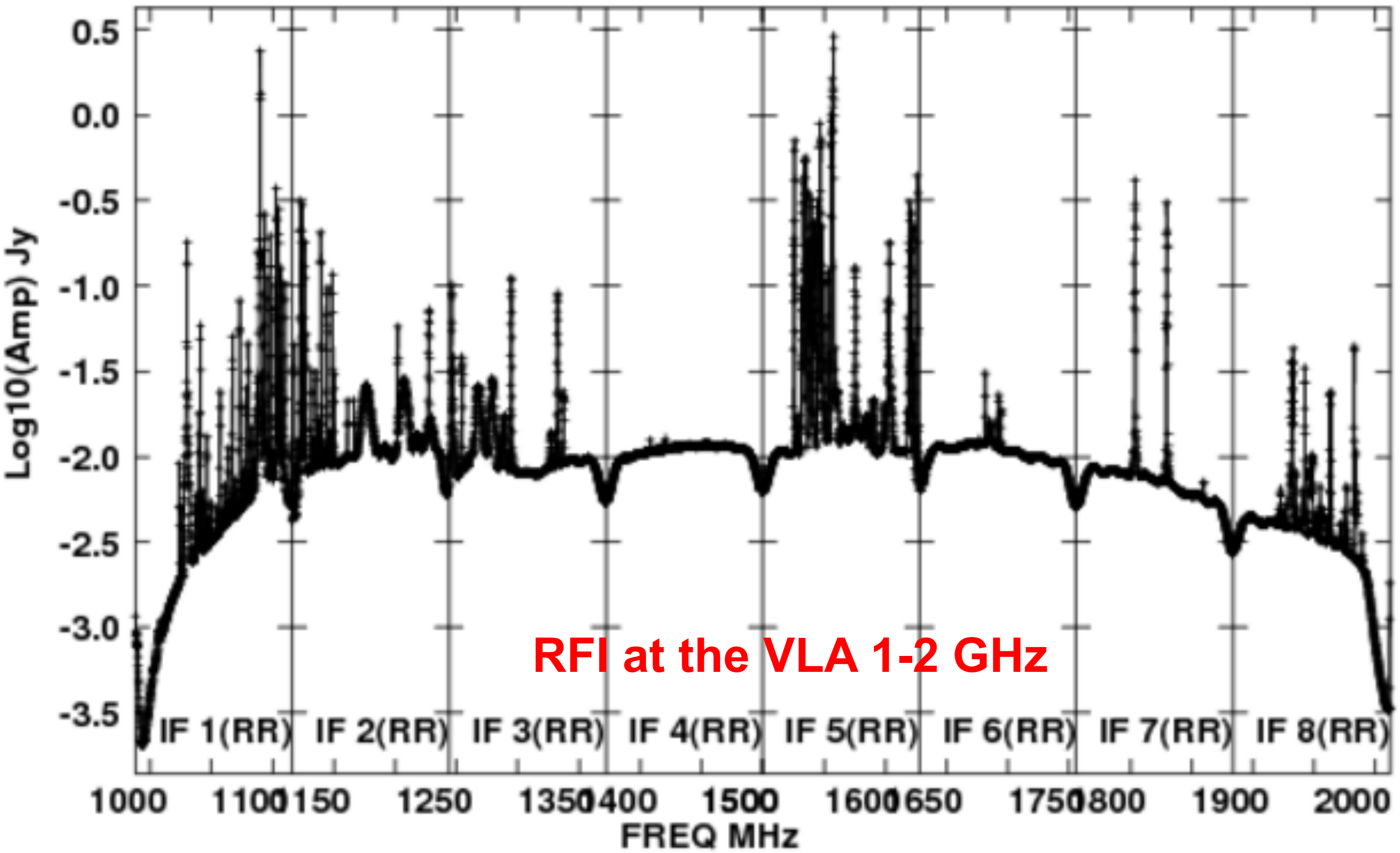
- Atmospheric opacity is a function of frequency, generally only important over very wide bandwidths or near atmospheric lines



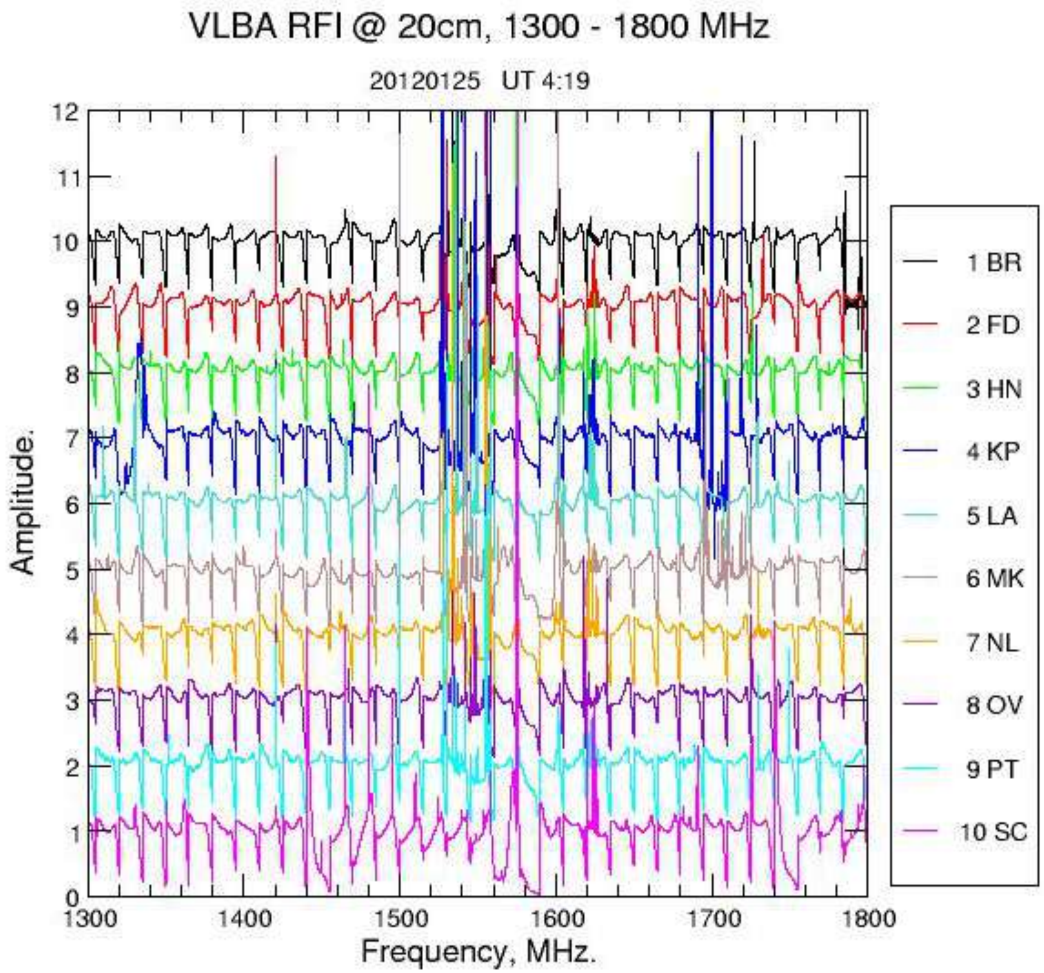
- Source emission can change with frequency too:
  - Spectral index, shape
  - Polarized emission; Faraday rotation $\propto \lambda^2$

Radio Frequency Interference (RFI)

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



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
  - Doppler corrections
  - Correlator effects
- You probably also have to deal with a large dataset
  - Averaging may be helpful to reduce size if needed

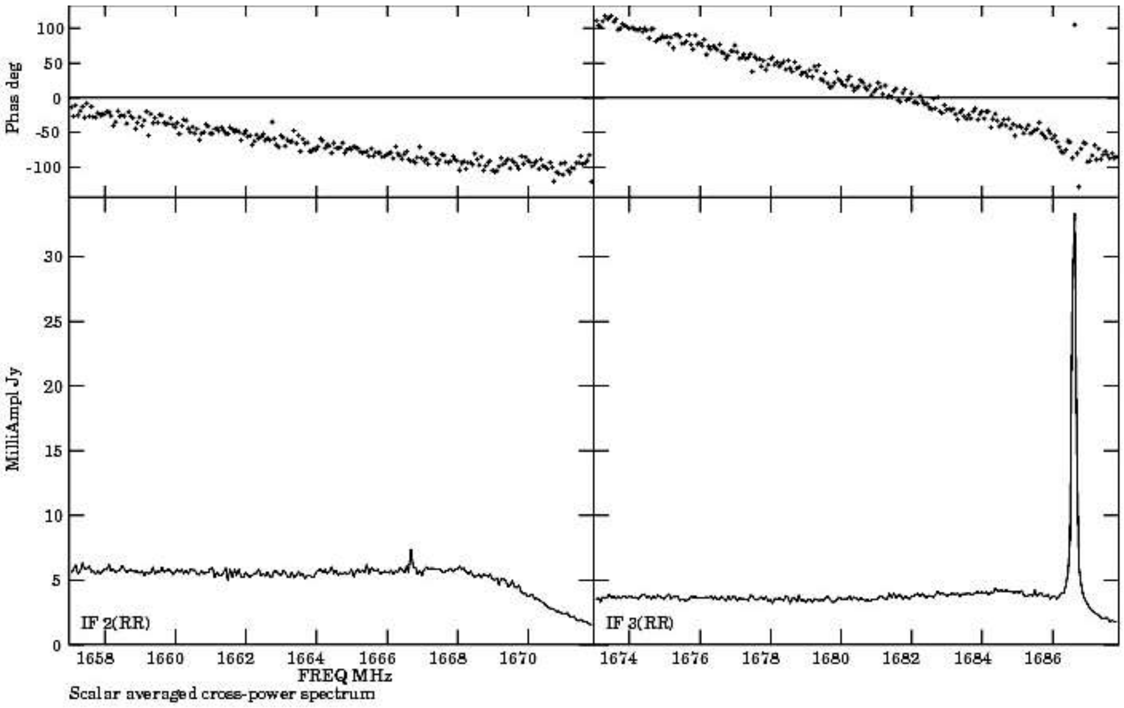
Preparation: Editing your data

Many ways to do this, here example:

- Start with identifying problems affecting all channels, but using a frequency averaged 'channel 0' data set.
  - Has better signal-to-noise ratio
  - Copy flag table to the line data

- Continue with checking the line data for narrow-band RFI that may not show up in averaged data.
  - Channel by channel is very impractical, instead identify features by using cross- and total power spectra (**POSSM** in AIPS, **plotms** in CASA)

Example VLBA spectra

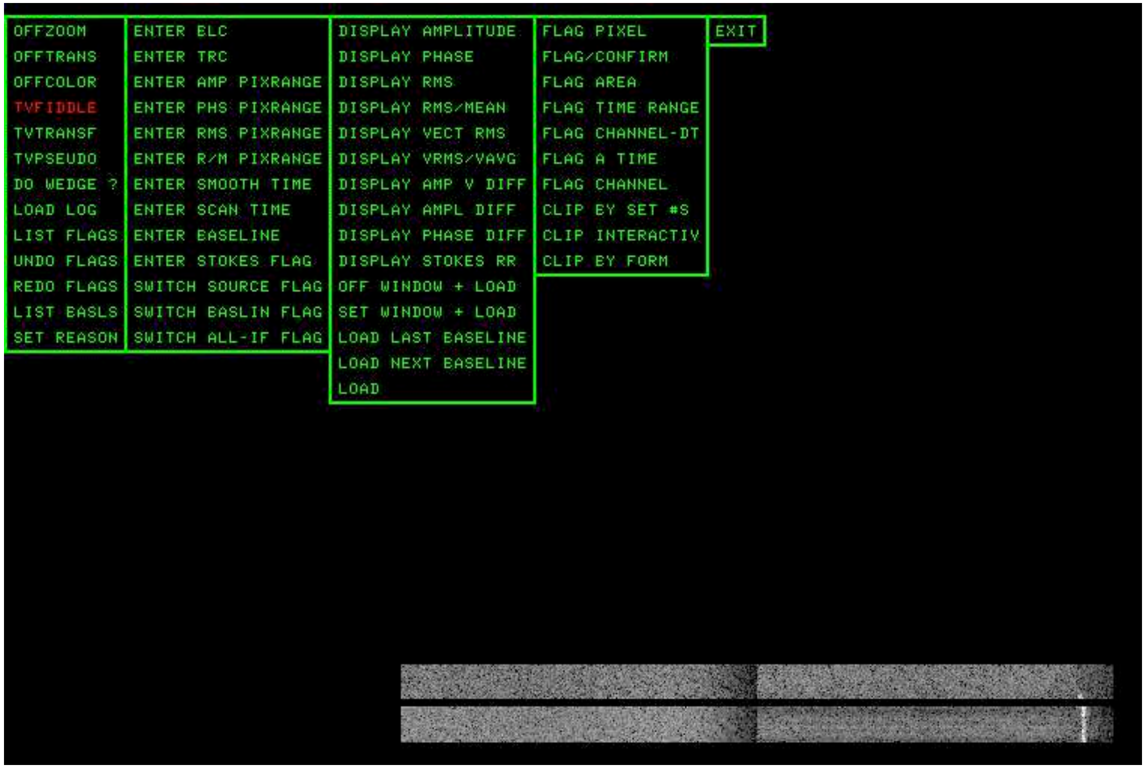


Scalar averaging helps to identify RFI features

- 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 (SPFLG/Viewer)

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



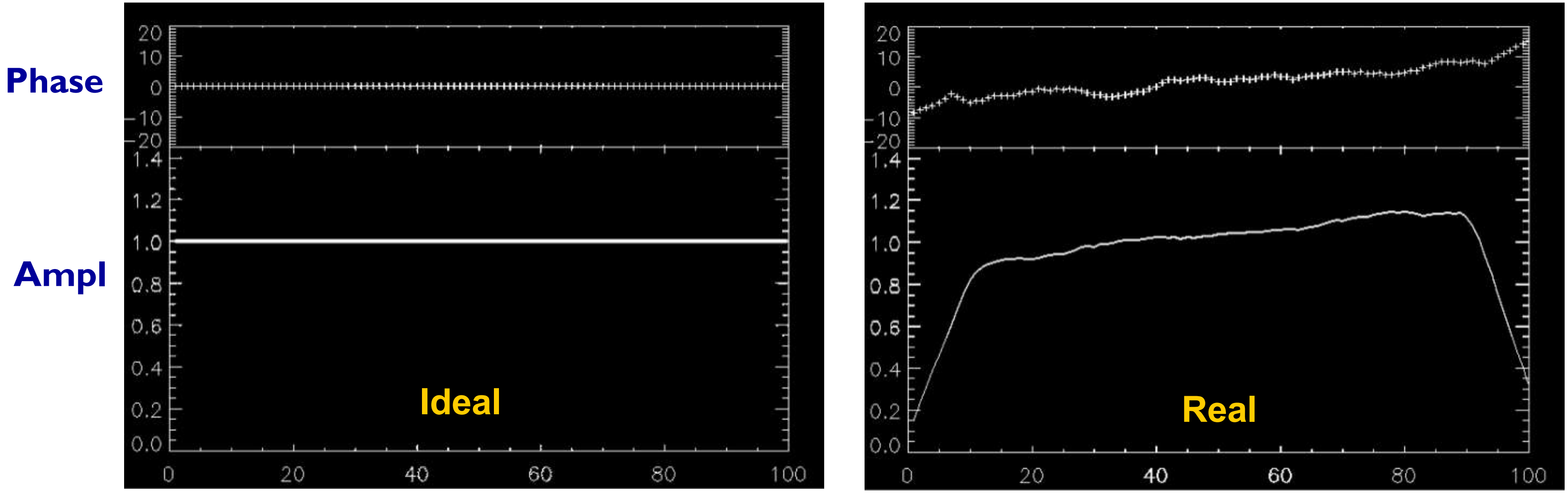
Bandpass calibration: Why?

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 (baseline based functions)

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

  - 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

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

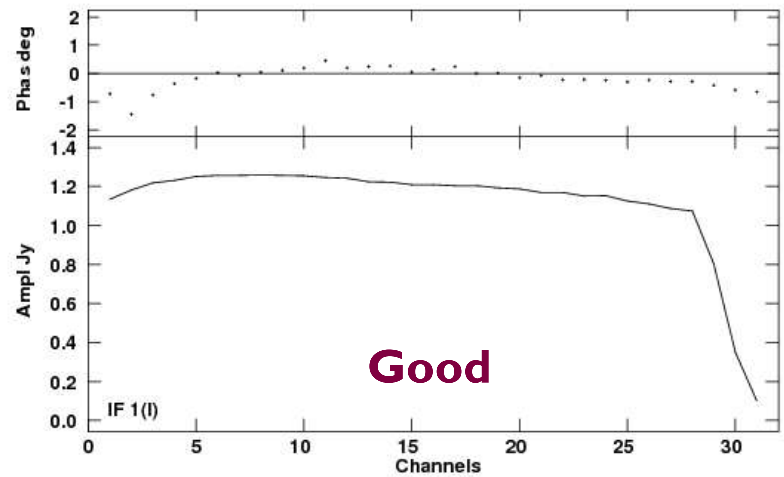
  which then results in an integration time:

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

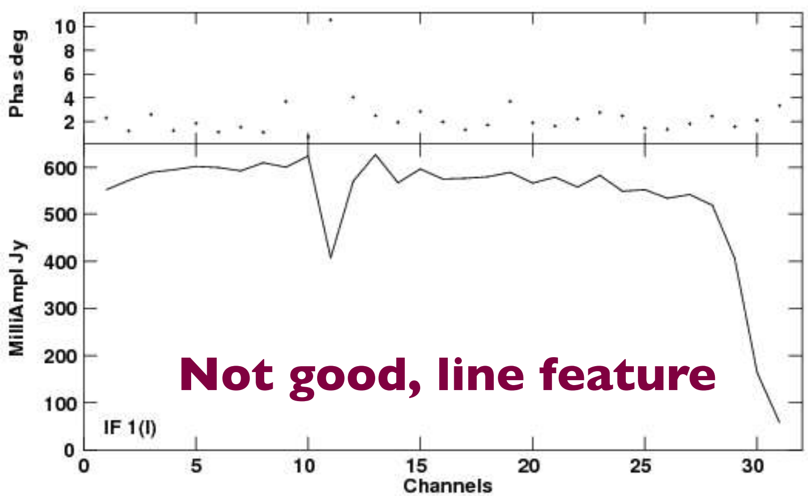
- If long observations, include several scans of the BP calibrator in your experiment to account for slow time variations

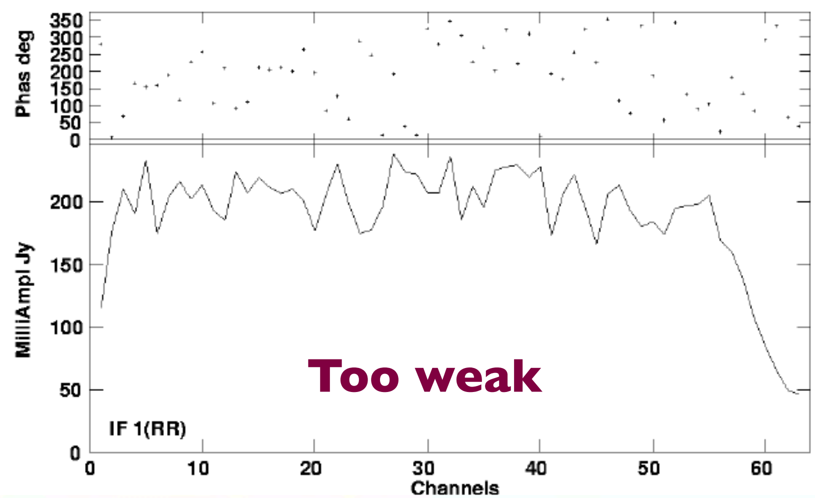
The BP calibrator

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



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

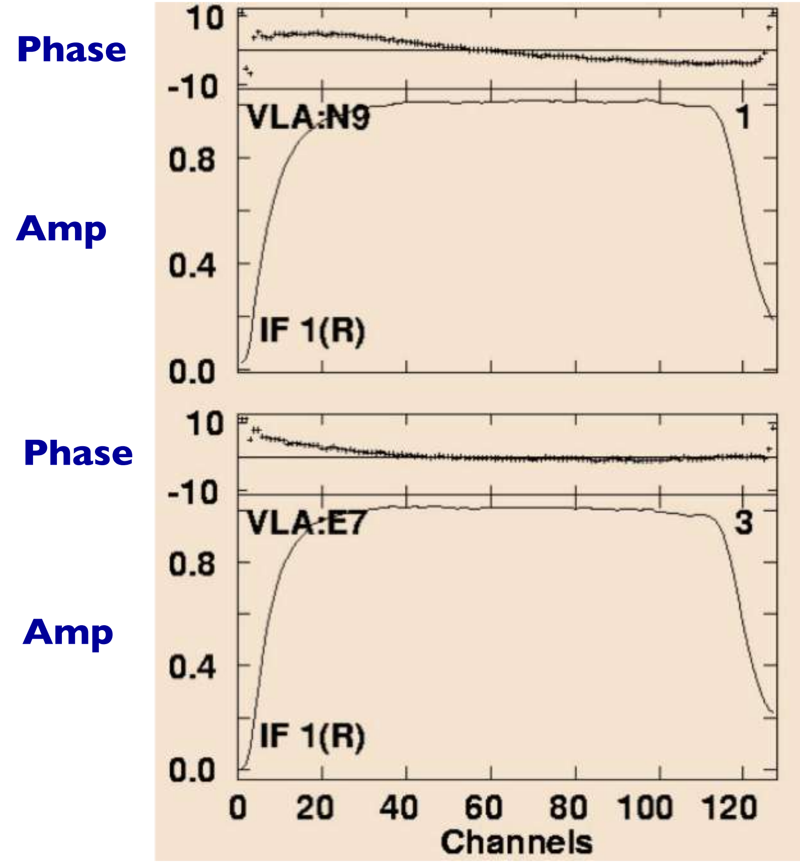




Good quality bandpass calibration

Examples of good-quality bandpass solutions for 2 antennas:

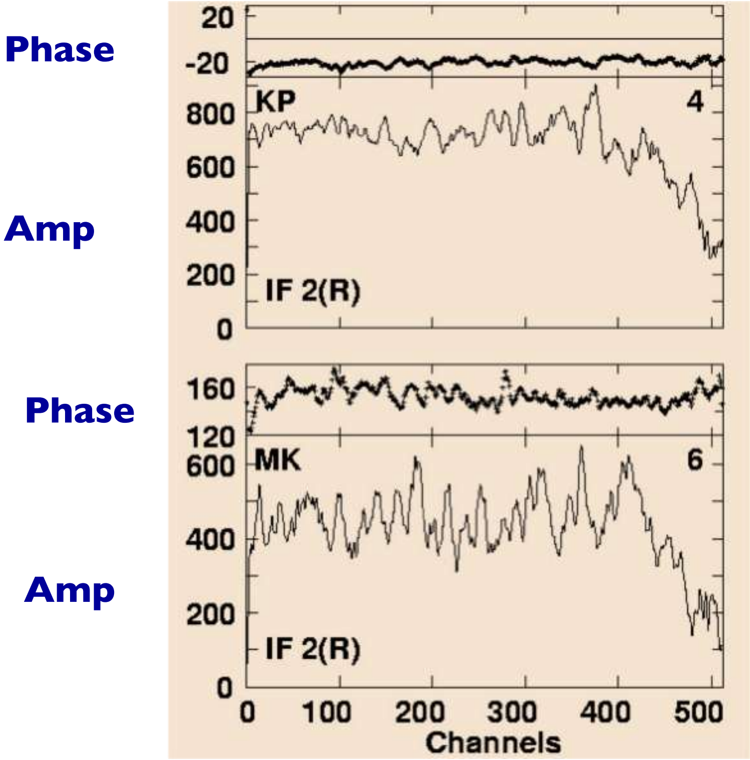
- Solutions should look comparable for all antennas
- Mean amplitude ~1 across useable portion of the band.
- No sharp variations in amplitude and phase; variations not controlled by noise



Bad quality bandpass calibration

Examples of bad-quality bandpass solutions for 2 antennas:

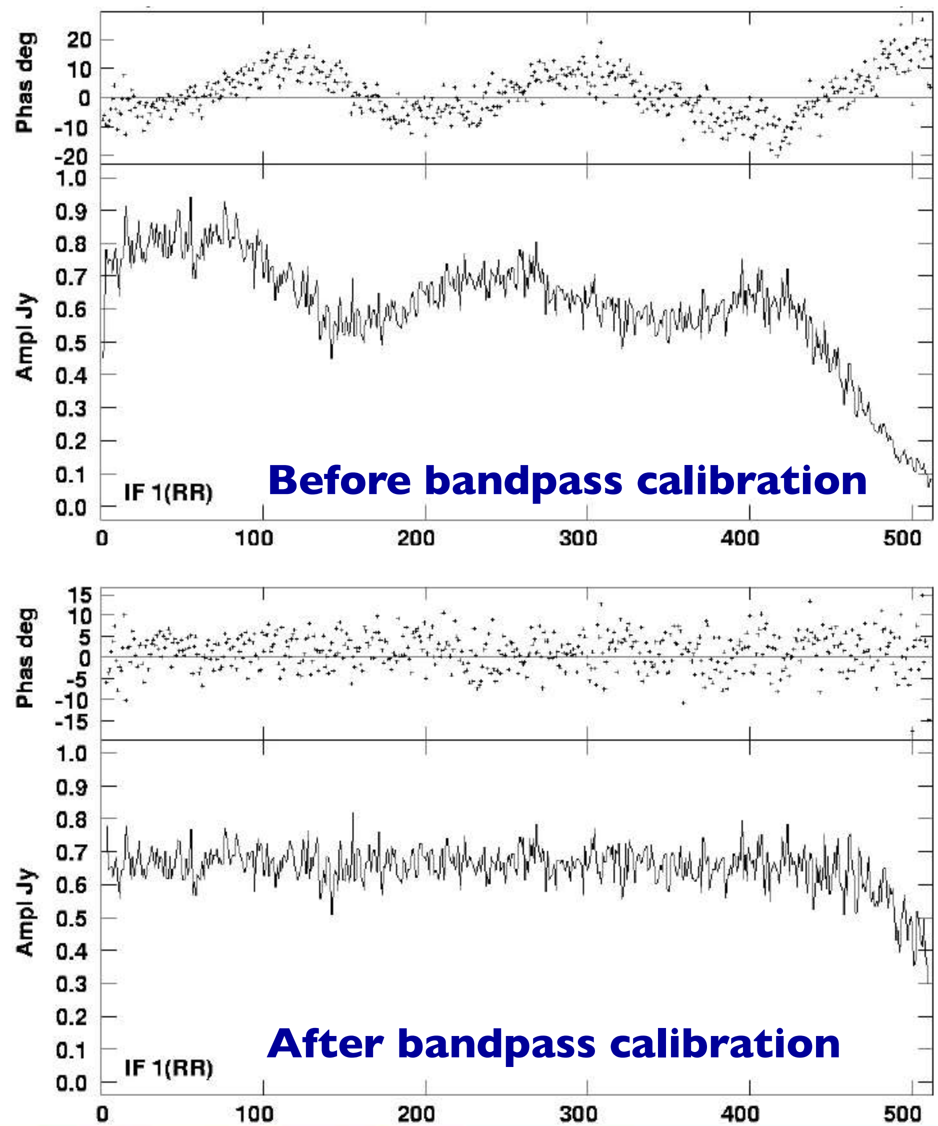
- Amplitude has different normalization for different antennas
- Noise levels are high, and are different for different antennas



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: XF correlator

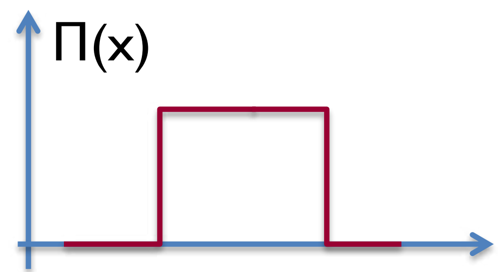
For spectroscopy in an XF correlator (VLA) lags are introduced

- Correlation function is measured for a large number of lags.
- FFT gives the spectrum.

We don't have infinitely large correlators (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: FX correlator

ALMA, VLBA, EVN SFXC:

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

Spectrum at each antenna formed from sample with limited time extent, hence also a truncated signal

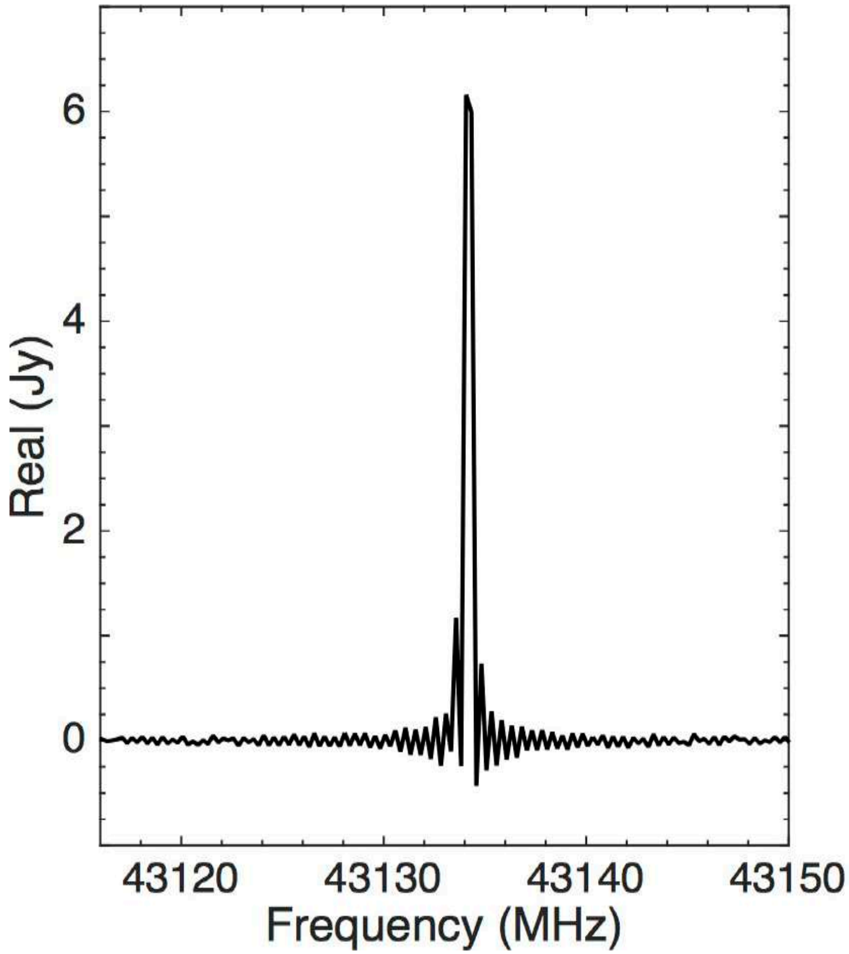
- Each antenna spectrum multiplied with a boxcar function

FT of the product = convolution of the FT of each function

FT of $\Pi(x)$ = sinc(x) => Total response $\mathrm{sinc}^2(x)$

Gibbs ringing

- Produces a "ringing" in frequency called the Gibbs phenomenon.
- Occurs at sharp transitions:
  - Narrow banded spectral lines (masers, RFI)
  - Band edges

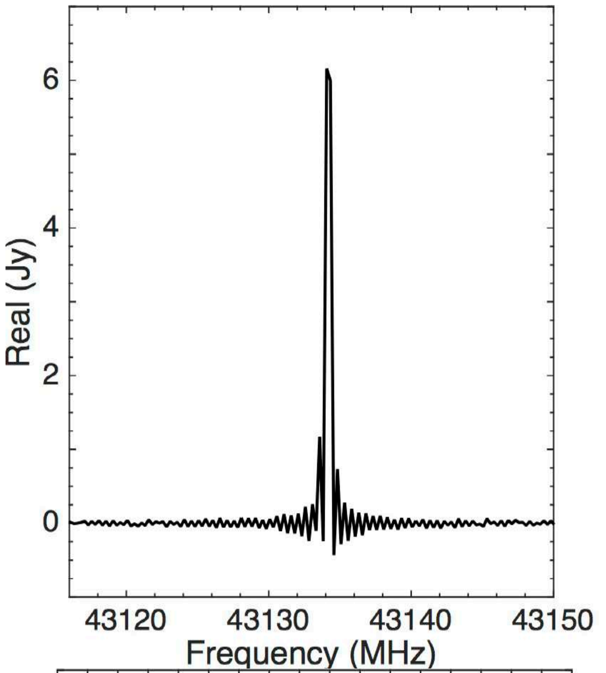


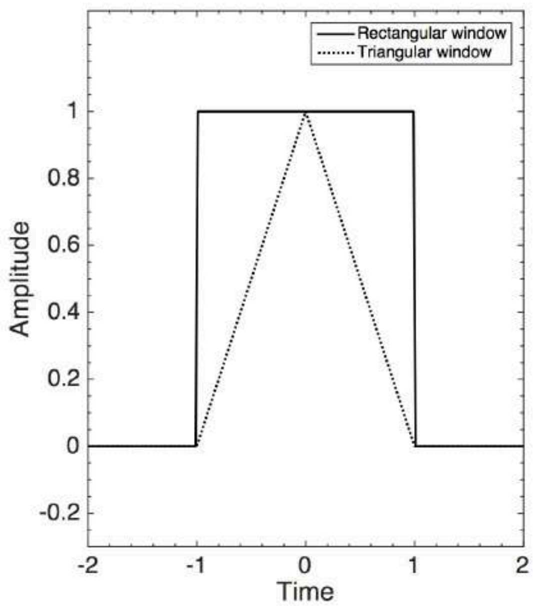
Gibbs ringing

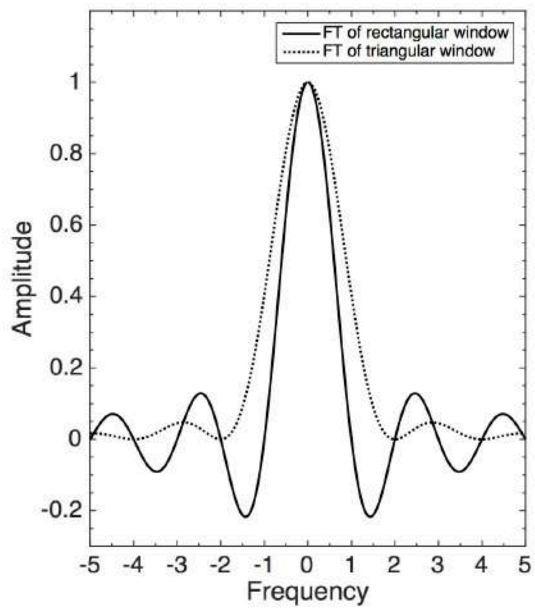
To reduce effects, window functions can be applied

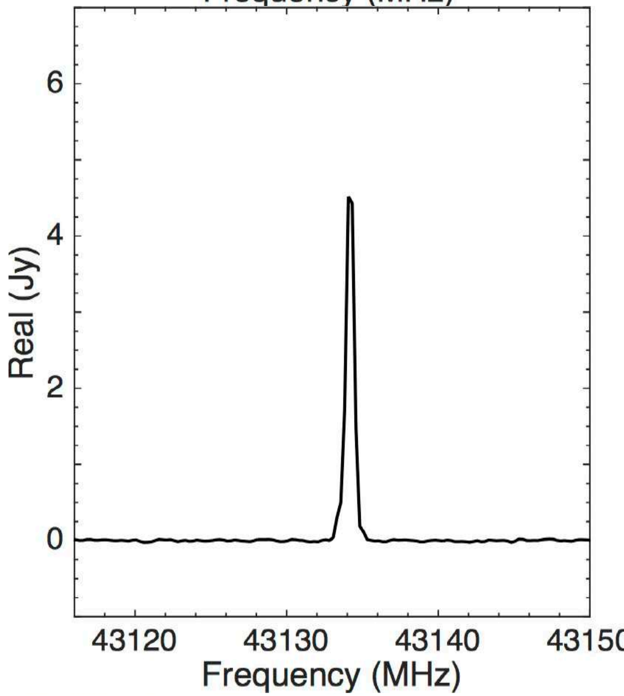
- FX correlator applies triangular weighting function
- Reduces sidelobes at the expense of main peak resolution
- Can also smooth in post-processing (often Hanning window applied)

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



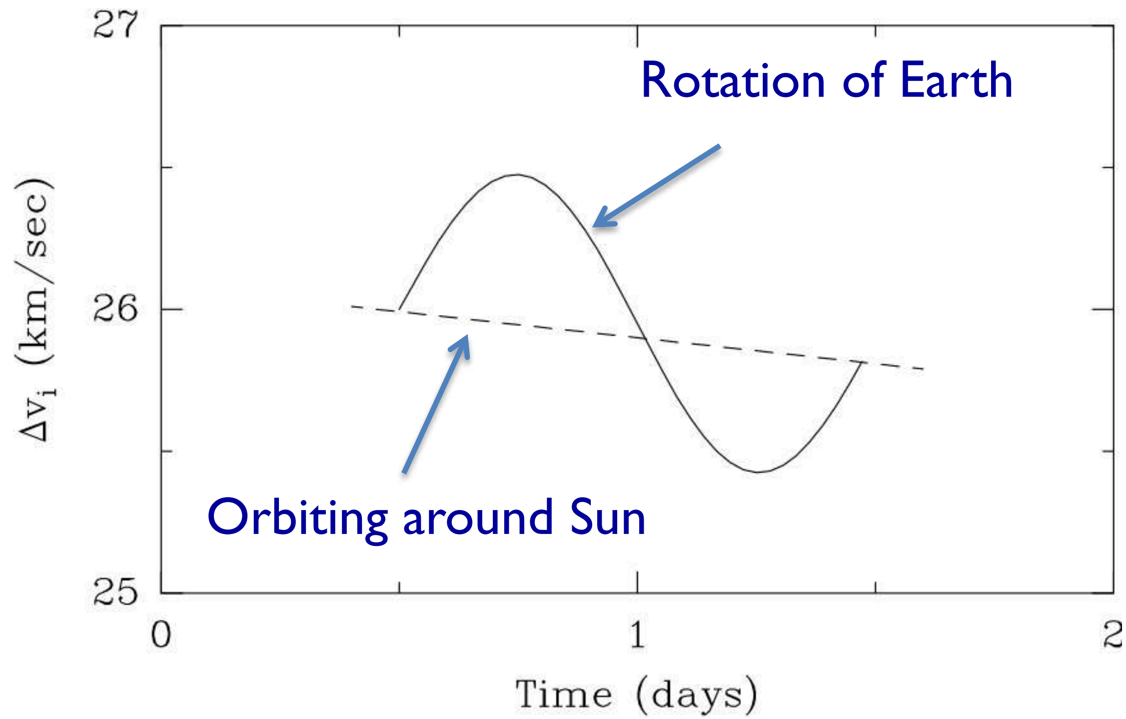






Doppler tracking/setting

- 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

- 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:

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

- 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, the successively transform to other frames.
Transformations standardized by IAU.

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

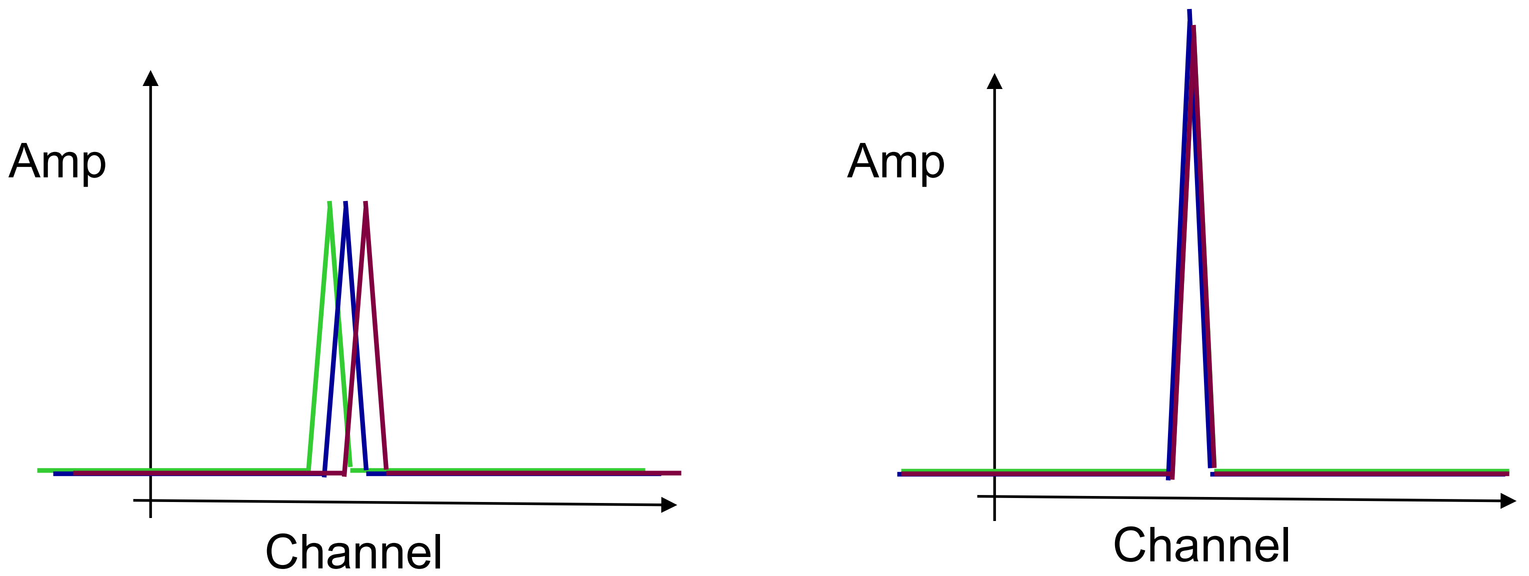
- Applying Doppler tracking will introduce a time-dependent and position dependent frequency shift.

- 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

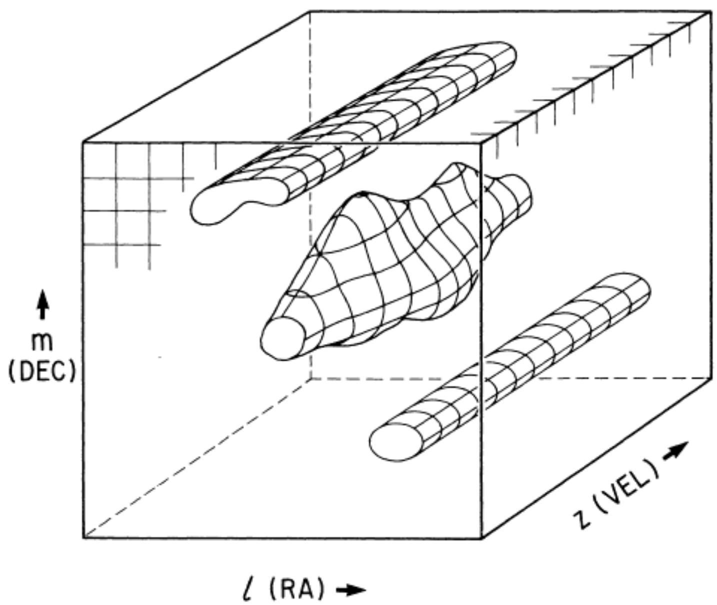
Before imaging

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

- 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

- 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.
- Deconvolution is non-linear: can give different results for different channels since *u,v* - coverage and noise differs
  - results usually better if line is deconvolved separately
- 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 do flagging automatically (based on residuals on baselines)
  - Can produce a continuum data set

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

UVLIN/uvcontsub

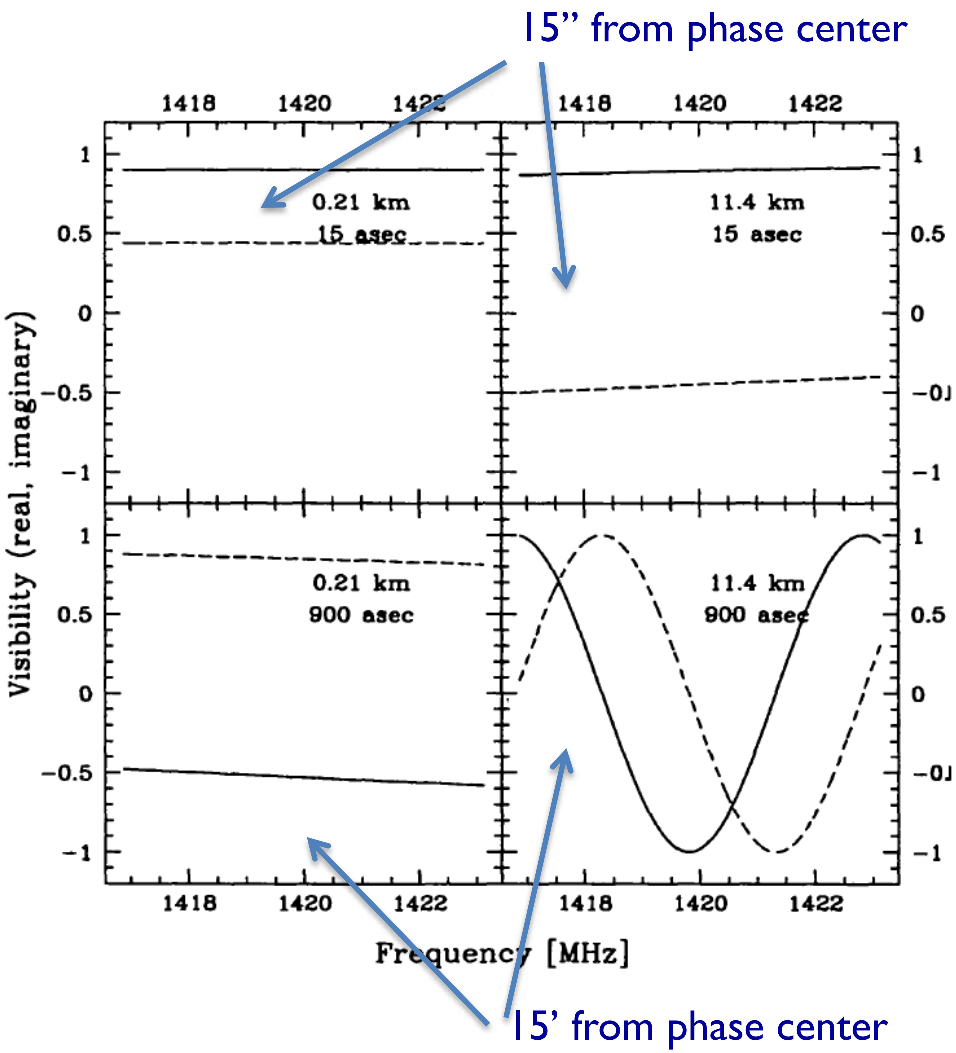
Restriction: small FOV

- 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.*



Imaged based

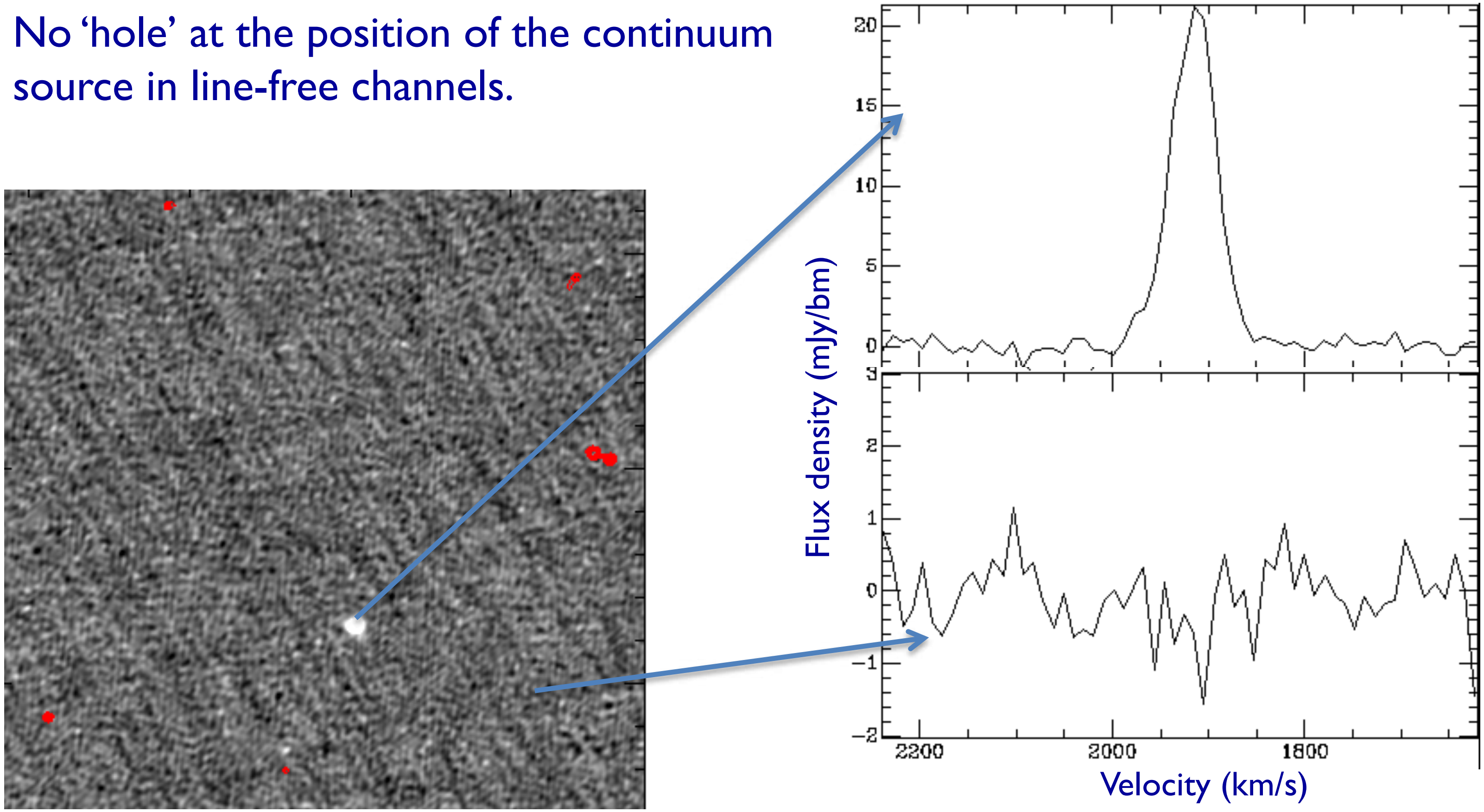
- Fit and subtract a low order polynomial fit to the line free part of the spectrum measured at each spatial pixel in cube.

- 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

- 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 spacings to estimate flux

Challenges include:

- Emission structures 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 with $-1 < \mathcal{R} < 1$ 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.

- 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

Visualizing 3-D

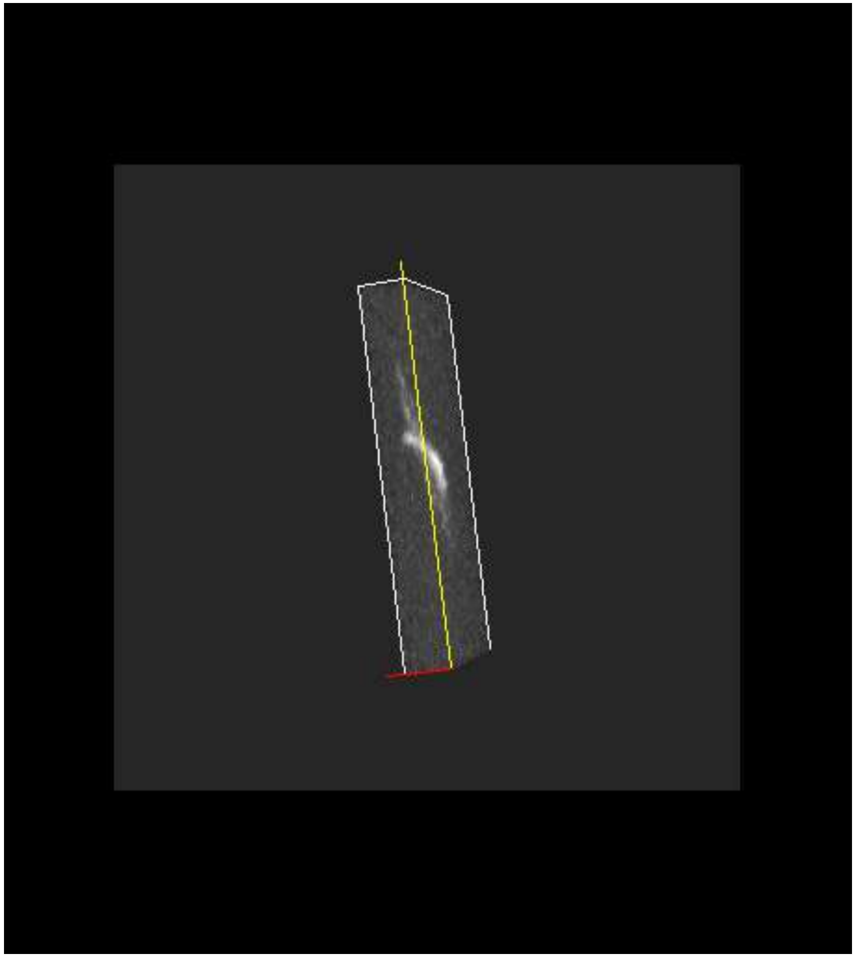
Some software allows 3-D visualization of cubes:

SAOimage DS9:

http://ds9.si.edu/site/Home.html

Karma package:

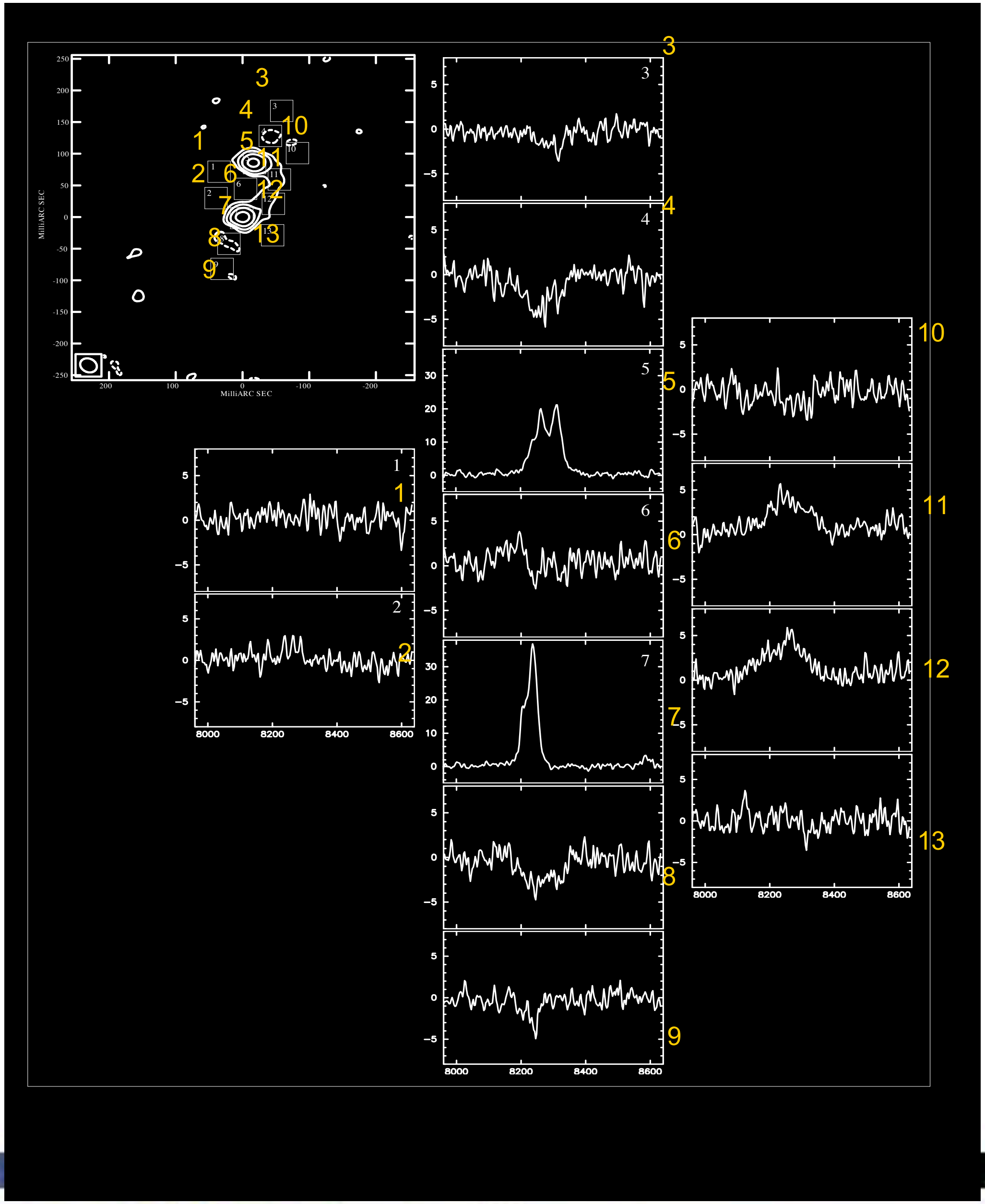
http://www.atnf.csiro.au/computing/software/karma/



Karma package; L. Matthews

1-D line profiles

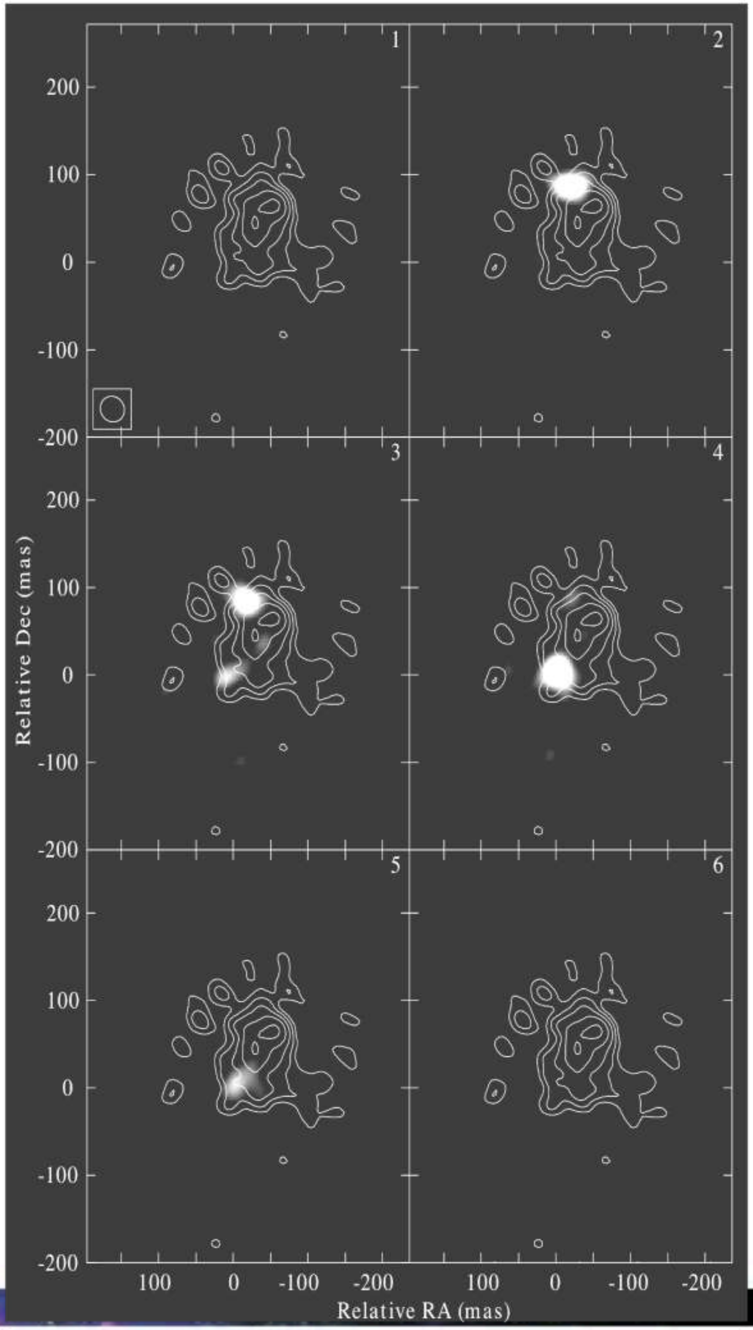
- Line profiles show changes in line shape, width and depth as a function of position.
- Can give information of relative position of features (absorption in front)
- Velocity width



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

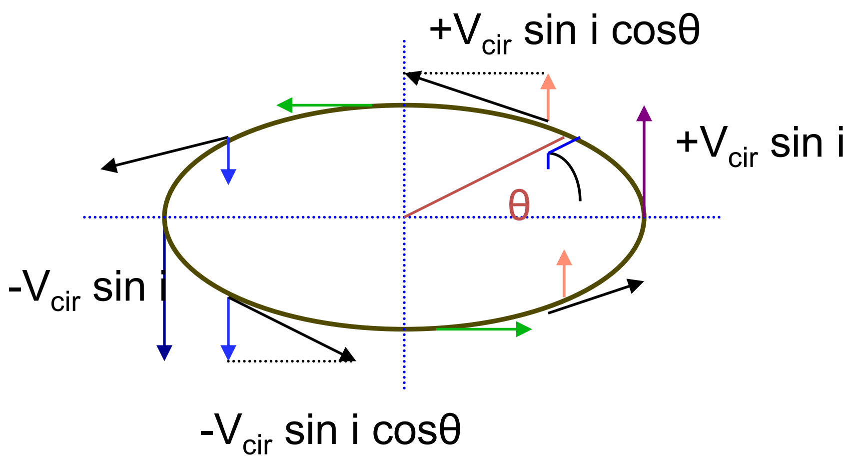
2-D channel maps

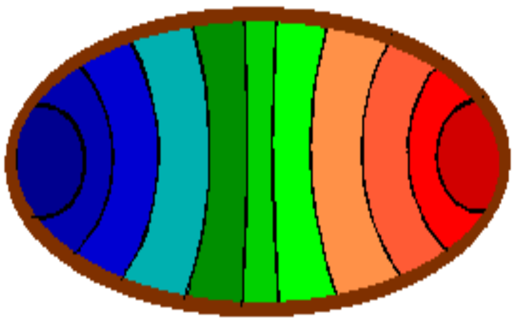
- Channel maps show how the spatial distribution of the line feature changes with frequency/velocity.
- Information about kinematics.



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

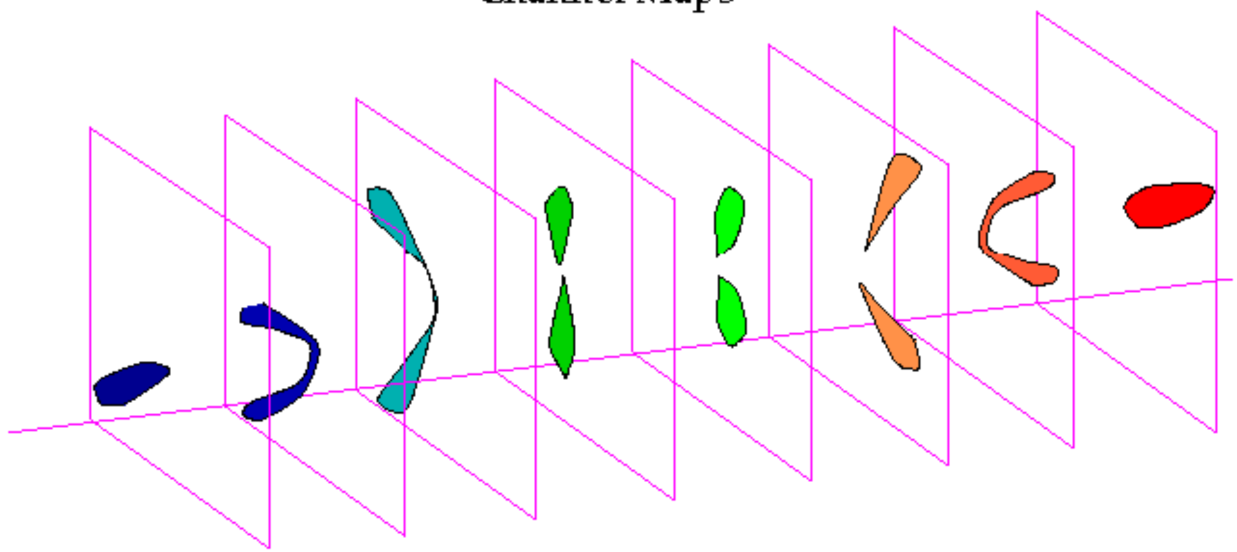
Rotating disk model





Mean Velocity Field

Channel Maps

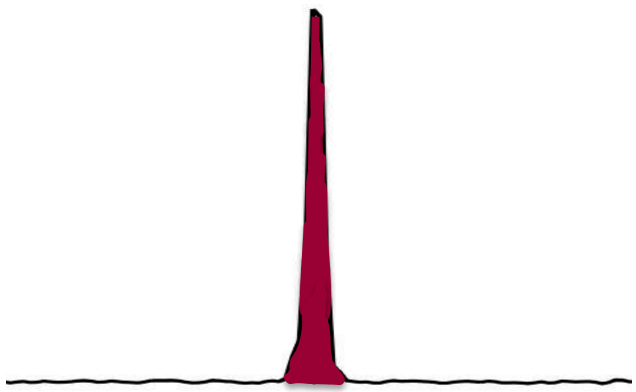


Moment analysis

- 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:

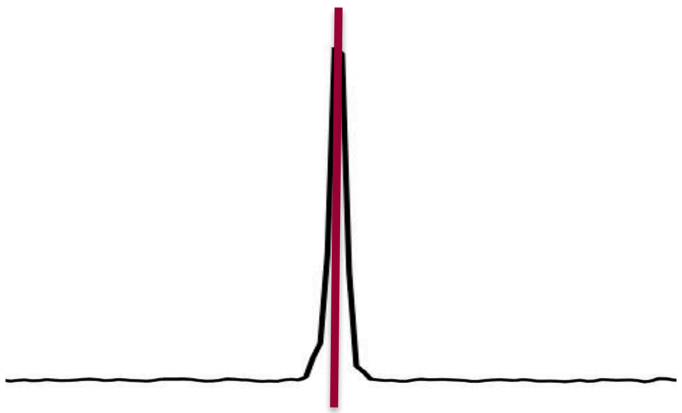
- Integrated intensity

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



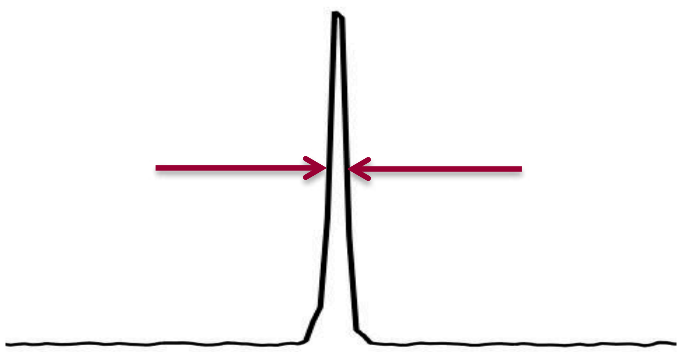
- Intensity weighted velocity

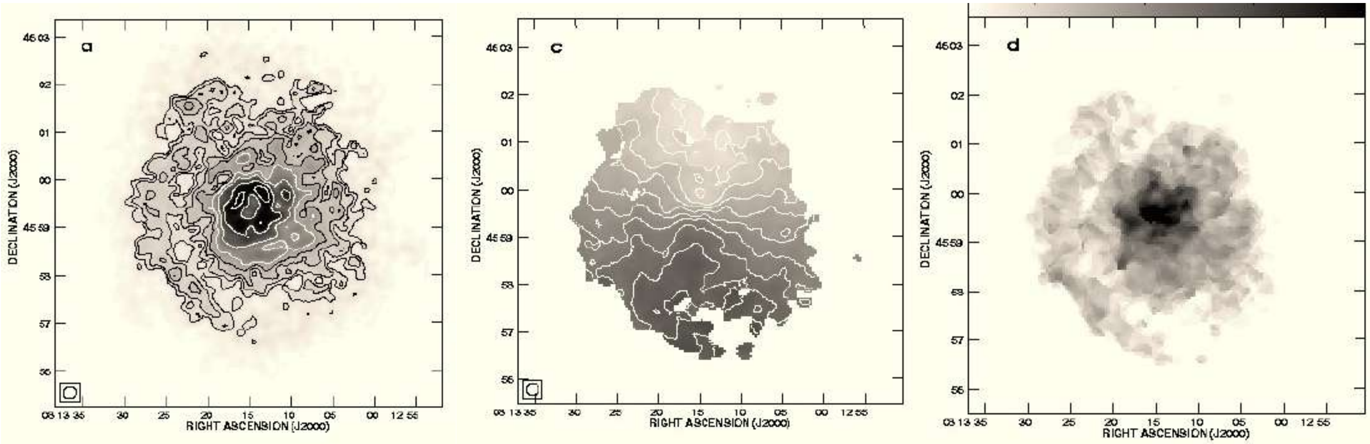
$$\text{Moment 1} = \langle V \rangle = \frac{\int S_v v\, dv}{\int S_v\, dv}$$



- 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

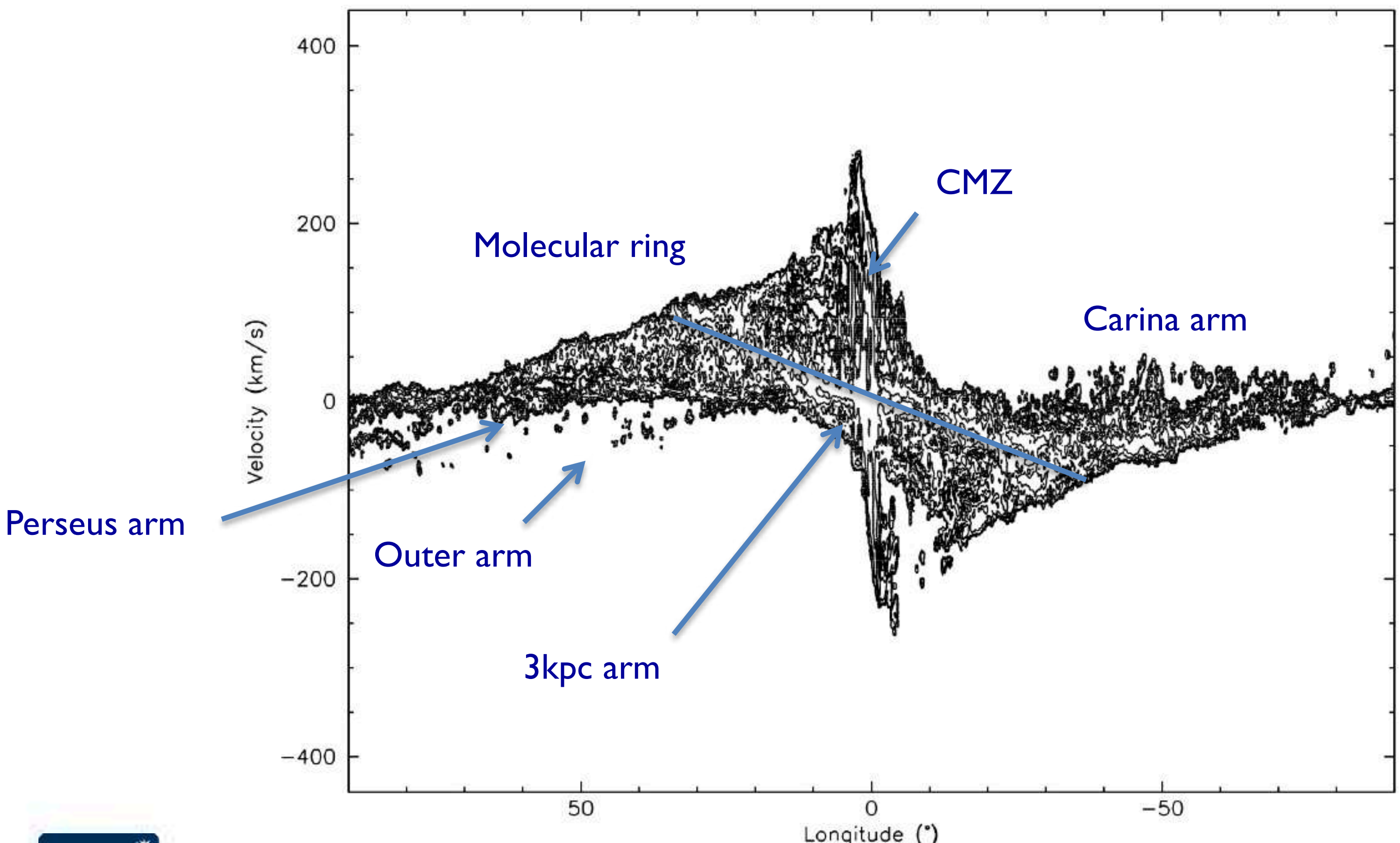
- Can be demanding to interpret correctly:
  - Both emission and absorption may be present
  - Velocity patterns can create misleading moment maps
  - Biased towards regions of high intensity
  - Complicated error estimates: number or channels with real emission used in moment computation will greatly 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)
  - "Maxmaps" show emission distribution (finding the max in each x,y pixel through the cube).

Position-Velocity diagrams

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



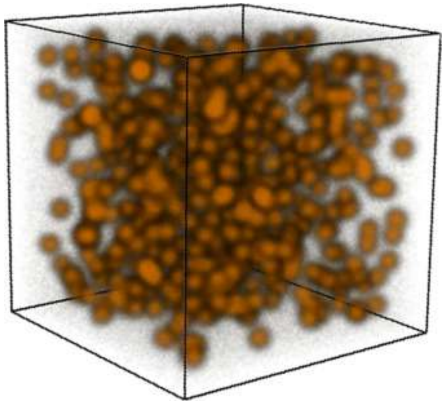
CO(1-0) as a function of longitude in the Milky Way, from Dame et al. (2001).

Going deeper

There exists programs to help with the analysis, not only doing the plotting/visualization:

Example:

- 'Clumpfind':
  - Searches for peaks of emission in cubes, then follows down to lower intensity levels
  - Decomposes the cube into 'clump' units
  - http://www.ifa.hawaii.edu/users/jpw/clumpfind.shtml; Williams et al. (1994, 2011), 2D and 3D
- 'CUPID', Berry et al (2007, 2013)

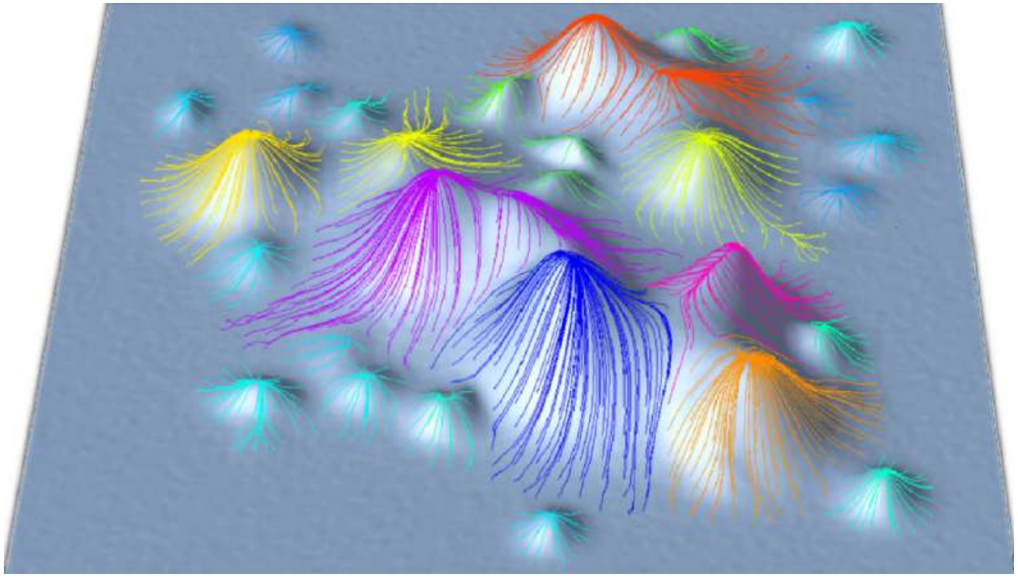


Going deeper

There exists programs to help with the analysis, not only doing the plotting/visualization:

Example:

- 'FellWalker'
  - Similar algorithm to Clumpfind, Berry (2014), 3D



Going deeper

Further consider different statistical methods to analyze and quantify your data in detail:

- To quantify similarities and differences in images, e.g., to compare different line distributions ('correlation analysis'):
  - Factor Analysis
  - Principal Component Analysis

- Statistical methods for astronomers, http://astrostatistics.psu.edu (has example data sets including spectral sets).

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

With most instruments now observing in high resolution, multi-channel mode we must consider:

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

Better, it also implies:

- Ability to avoid line contamination – kinematical details revealed
- Much improved line searches
- Multi-frequency synthesis enabled

The End