# Planning and reducing spectral line projects
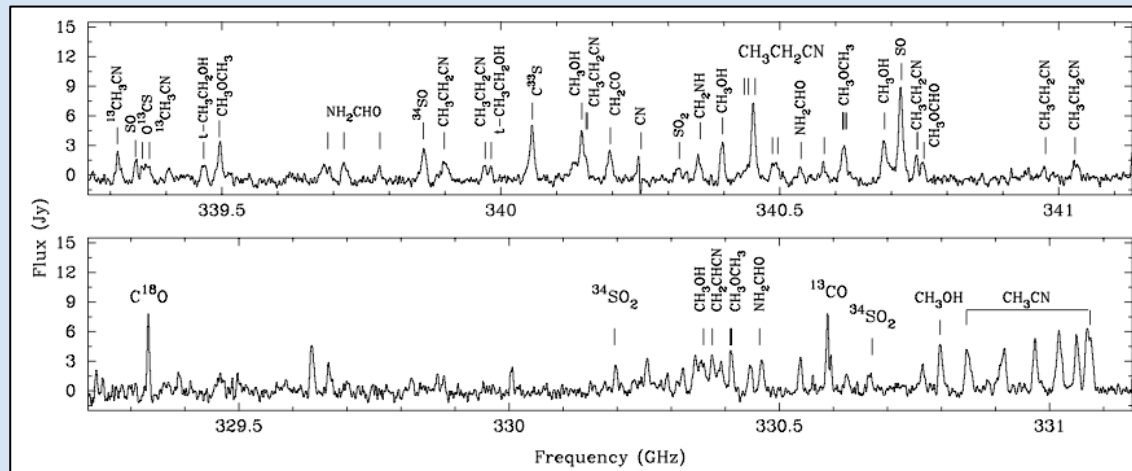
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Based on previous ERIS and NRAO lectures
and book Synthesis Imaging in Radio Astronomy II



*SMA spectrum showing molecular lines in a "hot core" (Rathborne et al. 2008)*

# What is spectral line interferometry?

**Spectral line interferometry...**

*is observing many adjacent frequency channels with an interferometer for an object whose flux changes rapidly with frequency* (analogous to spectroscopy in optical)
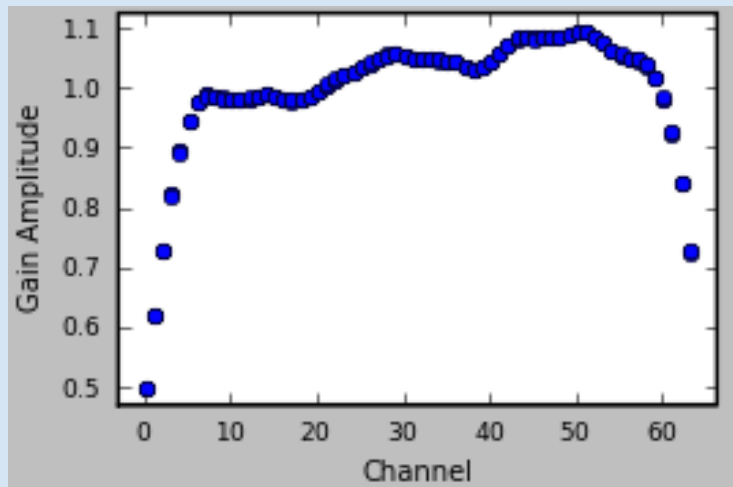
In essence, it gives you a third axis: frequency or velocity
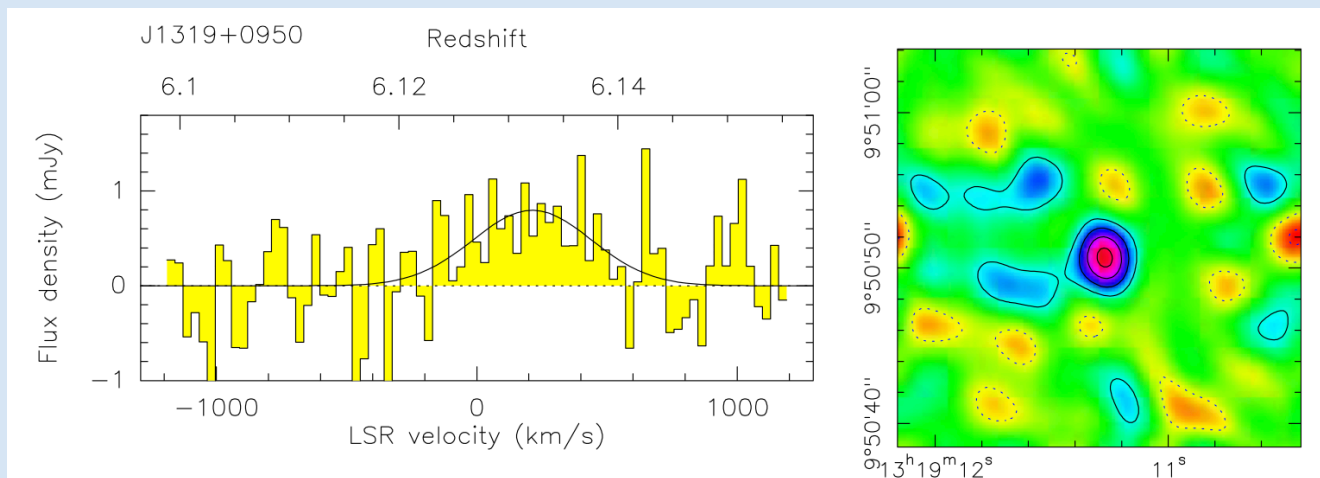


CO(6-5) emission from a high redshift quasar observed with the Plateau de Bure Interferometer (Wang et al. 2011)

# What is spectral line interferometry?

However, today even continuum observations are now often carried out with many channels (called pseudo-continuum)



Plot of response across a band for one VLA antenna as a function of channel, during reduction of **continuum data**

**Therefore, you need to understand spectral line interferometry to do (almost all) interferometry!**

# Outline

Part I: Setting up your observation

Part II: Data reduction

Part III: Image and spectral analysis

# Part I: Setting up your observation

1. Choose your science case and line(s)

2. Choose your source(s) and research its properties

3. Choose your interferometer and configuration

4. Check source velocity reference frame, on-line Doppler tracking

5. Choose the channel width, total bandwidth and number of channels

6. Determine your required channel sensitivity and time on source

7. Choose your calibrators

8. Data rate and size considerations

# 1. Choose your science case and line(s)

**Doppler shifts** → Velocity fields


VLA HI @ 21cm
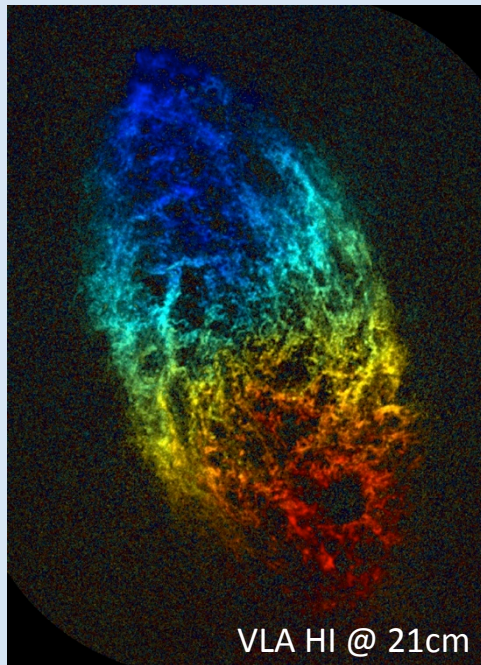
*Velocity field of galaxy M33 in HI line. Colors show Doppler shift of line and brightness is proportional to HI column density (NRAO, Thilker et al.)*

1. **Choose spectral line(s) from science case**
2. **Find which telescopes have bands that contain these lines**

**Physical Properties from lines for science case**

Dynamics            Optical depth

Excitation Temperature

Column density

Density

Turbulent motions

Magnetic field strength

Chemistry

# Commonly observed lines:
# HI line at 21cm (1.4GHz)
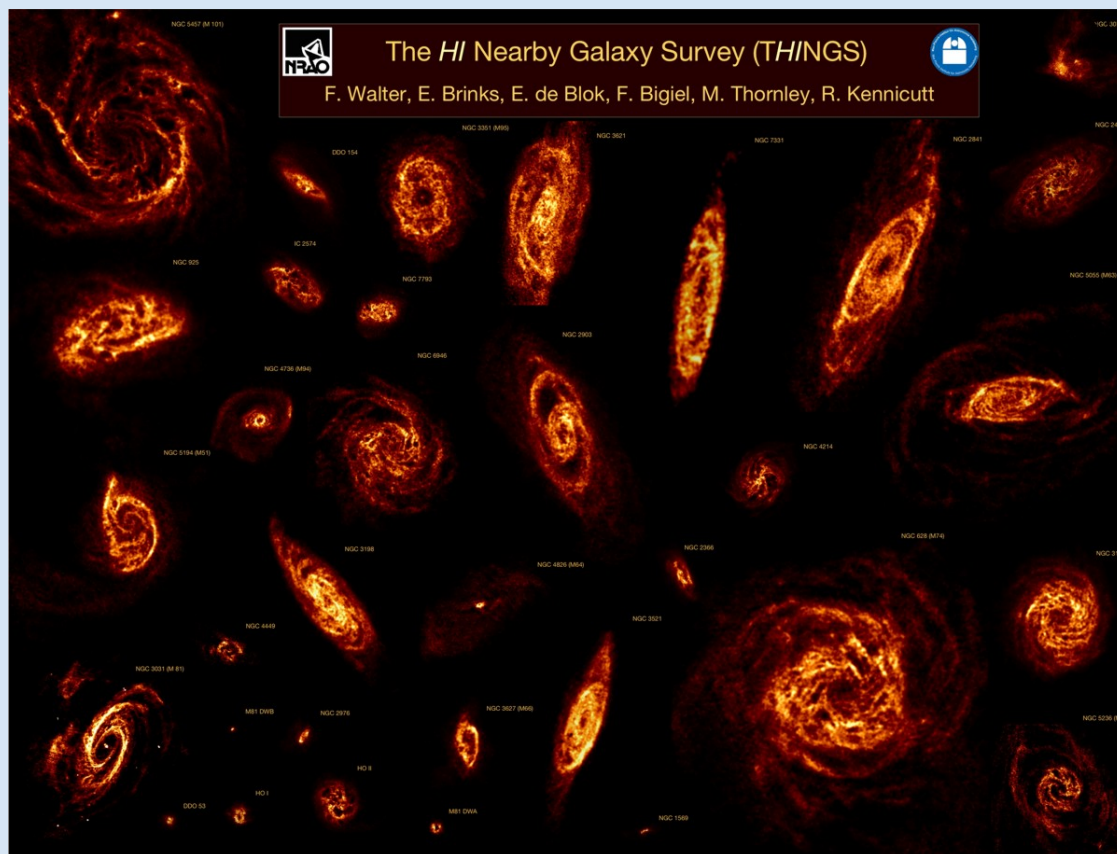


**Can determine:**

- Morphology of atomic gas

- Dynamics of the atomic gas in galaxies
  → gives enclosed mass (including dark matter)

- Column density and mass of optically thin gas

- Temperature of optically thick gas

- Distance via Hubble law

# Commonly observed lines:
# Radio Recombination Lines (RRLs)
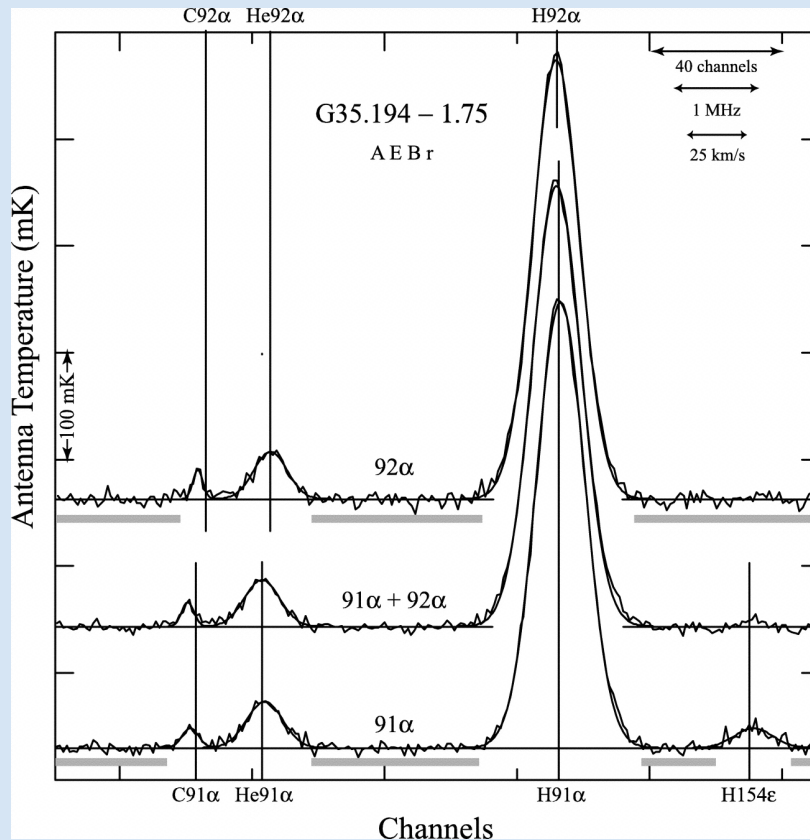


*RRLs for n=91 and 92 for H, He and C in an HII region (Quireza et al. 2006)*

**Can determine:**

- Ionized gas dynamics

- Optical depth and electron temperature (in Local Thermo-dynamic Equilibrium, LTE)

- Gas density from collisional broadening of the lines

- Speed of turbulent motions from linewidths (for low n)

- Abundance ratio H/He/C

- Magnetic field strengths from Zeeman splitting

# Commonly observed lines: Molecular lines

**AGB star R Sculptoris**
CO($J = 3 - 2$)  with ALMA
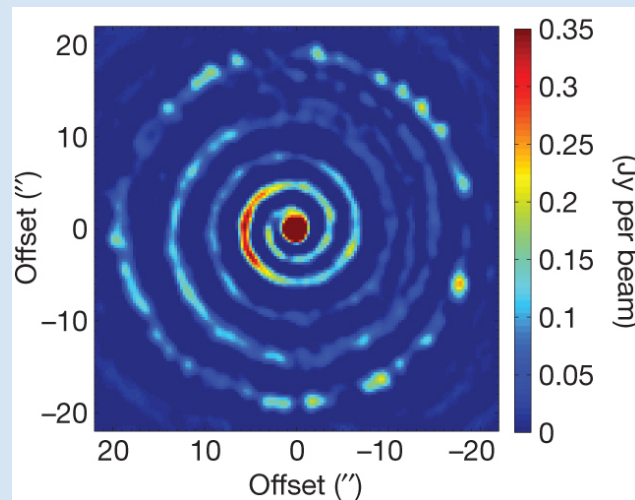


Maercker et al. (2012)

- Common molecular lines:
  **CO, OH, H₂O, SiO, HCN, methanol**

- As well as thermal emission and absorption lines, **masers** (stimulated emission) can be observed

**Can determine:**

- Morpholgy of molecular gas

- Dynamics of molecular gas

- Gas column and volume density

- Optical depth

- Gas temperature

- Abundances

- Magnetic field strengths from Zeeman splitting

- Chemistry

- Presence of shocks (e.g. SiO)

# 2. Choose your source and research its properties

Learn about the object you wish
to study, e.g.

- Position (and equinox)

- Size

- Velocity (and reference frame)

- Estimated brightness

# 3. Choose your interferometer and configuration

Read about telescopes online

(e.g. VLA Observational Status summary)

# 3. Choose your interferometer and configuration

(J)VLA



Part of the ALMA Compact Array



**Larger arrays**: better resolution! Good for absorption studies as want to detect a small, bright background source

**Smaller arrays**:  have better surface brightness sensitivity so easier to detect extended or faint emission

# 4. Check source velocity reference frame

Need to always specify velocity reference frame:

| Rest Frame | Corrected for | Amplitude of Correction (km/s) |
|---|---|---|
| Topocentric | Nothing | 0 |
| Geocentric | Earth rotation | 0.5 |
| Earth-Moon Barycentric | Effect of Moon on Earth | 0.013 |
| Heliocentric | Earth's orbital motion | 30 |
| Solar System Barycentric | Effect of planets on Sun | 0.012 |
| Local Standard of Rest (LSRK/D) | Solar motion | 20 |
| Galactocentric | Milky Way Rotation | 230 |
| Local Group Barycentric | Milky Way Motion | ~100 |
| Virgocentric | Local Group Motion | ~300 |
| Microwave background | Local Supercluster motion | ~600 |

# 4. Check source velocity reference frame

- Optical Barycentric or Heliocentric system often used for extragalactic observations

- Radio Local Standard of Rest (LSR) used for Milky Way observations

# Doppler shift and Doppler Tracking

Full relativistic equation:

$$\frac{v}{c} = \frac{\nu_0^2 - \nu^2}{\nu_0^2 + \nu^2}$$

Radio definition:

$$\frac{v_{\mathrm{radio}}}{c} = \frac{\nu_0 - \nu}{\nu_0}$$

Optical definition:

$$\frac{v_{\mathrm{optical}}}{c} = \frac{\lambda - \lambda_0}{\lambda_0}$$

# Doppler shift and Doppler Tracking

- **On-line Doppler tracking** automatically corrects to a given reference frame during the observation **in real time**

- The tracked or observed frequency is usually called the **sky frequency**

- However, for wide frequency bands (VLA, ALMA, SMA...) on-line Doppler tracking is not done/recommended as correction is only strictly correct at one frequency

- Instead "Doppler Setting" is used, i.e. sky frequency calculated once at the start of the observation

- Further corrections can be made during data reduction and imaging (need >4 channels across the line for good correction)

# 5. Choose the channel width, total bandwidth and number of channels

- Channel width determined by required **spectral resolution** and **sensitivity**

- Total bandwidth should:

  Leave good line free channels at ends of band for continuum subtraction (end channels often bad)

- In a "lag" correlator, total number of channels is conserved, so total bandwidth is directly related to channel width

# Example available correlator setup
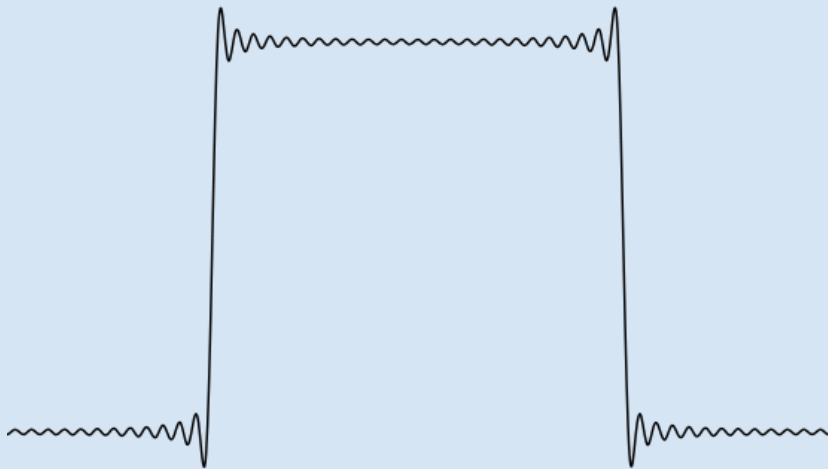
VLA WIDAR Correlator Setup

| Subband Bandwidth and Spectral Resolution Options (without recirculation) | | | | | | |
|---|---|---|---|---|---|---|
| **Subband bandwidth & total velocity coverage** | | **Full polarization products** (RR, RL, LR, LL) $64n_{BIBP}$ spectral channels Channel spacing: | | **Dual polarization products** (RR, LL) $128n_{BIBP}$ spectral channels Channel spacing: | | **Single polarization product** (RR *or* LL) $256n_{BIBP}$ spectral channels Channel spacing: |
| 128 MHz | $38400/v_{GHz}$ km/s | $2000/n_{BIBP}$ kHz | $600/n_{BIBP}/v_{GHz}$ km/s | $1000/n_{BIBP}$ kHz | $300/n_{BIBP}/v_{GHz}$ km/s | $500/n_{BIBP}$ kHz | $150/n_{BIBP}/v_{GHz}$ km/s |
| 64 | 19200 | $1000 / n_{BIBP}$ | $300 / n_{BIBP}$ | $500 / n_{BIBP}$ | $150 / n_{BIBP}$ | $250 / n_{BIBP}$ | $75 / n_{BIBP}$ |
| 32 | 9600 | $500 / n_{BIBP}$ | $150 / n_{BIBP}$ | $250 / n_{BIBP}$ | $75 / n_{BIBP}$ | $125 / n_{BIBP}$ | $37.5 / n_{BIBP}$ |
| 16 | 4800 | $250 / n_{BIBP}$ | $75 / n_{BIBP}$ | $125 / n_{BIBP}$ | $37.5 / n_{BIBP}$ | $62.5 / n_{BIBP}$ | $18.75 / n_{BIBP}$ |
| 8 | 2400 | $125 / n_{BIBP}$ | $37.5 / n_{BIBP}$ | $62.5 / n_{BIBP}$ | $18.75 / n_{BIBP}$ | $31.25 / n_{BIBP}$ | $9.375 / n_{BIBP}$ |
| 4 | 1200 | $62.5 / n_{BIBP}$ | $18.75 / n_{BIBP}$ | $31.25 / n_{BIBP}$ | $9.375 / n_{BIBP}$ | $15.625/n_{BIBP}$ | $4.687 /n_{BIBP}$ |
| 2 | 600 | $31.25 / n_{BIBP}$ | $9.375 / n_{BIBP}$ | $15.625/n_{BIBP}$ | $4.687 / n_{BIBP}$ | $7.8125 / n_{BIBP}$ | $2.344 / n_{BIBP}$ |
| 1 | 300 | $15.625/n_{BIBP}$ | $4.687 / n_{BIBP}$ | $7.8125 / n_{BIBP}$ | $2.344 / n_{BIBP}$ | $3.906 / n_{BIBP}$ | $1.172 / n_{BIBP}$ |
| 0.5 | 150 | $7.8125 / n_{BIBP}$ | $2.344 / n_{BIBP}$ | $3.906 / n_{BIBP}$ | $1.172 / n_{BIBP}$ | $1.953 / n_{BIBP}$ | $0.586 / n_{BIBP}$ |
| 0.25 | 75 | $3.906 / n_{BIBP}$ | $1.172 / n_{BIBP}$ | $1.953 / n_{BIBP}$ | $0.586 / n_{BIBP}$ | $0.977 / n_{BIBP}$ | $0.293 / n_{BIBP}$ |
| 0.125 | 37.5 | $1.953 / n_{BIBP}$ | $0.586 / n_{BIBP}$ | $0.977 / n_{BIBP}$ | $0.293 / n_{BIBP}$ | $0.488 / n_{BIBP}$ | $0.146 / n_{BIBP}$ |
| 0.0625 | 18.75 | $0.977 / n_{BIBP}$ | $0.293 / n_{BIBP}$ | $0.488 / n_{BIBP}$ | $0.146 / n_{BIBP}$ | $0.244 / n_{BIBP}$ | $0.073 / n_{BIBP}$ |
| 0.0325 | 9.375 | $0.488 / n_{BIBP}$ | $0.146 / n_{BIBP}$ | $0.244 / n_{BIBP}$ | $0.073 / n_{BIBP}$ | $0.122 / n_{BIBP}$ | $0.037 / n_{BIBP}$ |

Subband bandwidth and spectral resolution options. Note that the table entries refer to the spacing between spectral channels -- that spacing is *before* any frequency smoothing, so these channels are *not* independent.

- $n_{BIBP}$ is the number of Baseline Board Pairs assigned to the subband.

# Gibbs Ringing and Hanning Smoothing

**Gibbs Ringing**  Fixed by  **Hanning Smoothing**

Smooth data with a running mean
in frequency with weights:

0.5 for central channel
0.25 for adjacent channels

(i.e. triangular smoothing kernel)

**Pro**: reduces ringing
**Con**: reduces spectral resolution
by factor of 2

- See at channel edges
- Also see for bright lines e.g. masers, RFI

# 6. Determine your required channel sensitivity and time on source

- Determine how many channels needed to adequately resolve your line (e.g. >5)

- If **detection important**, need to detect line in **peak channel** with >3-5 sigma

- If **need to resolve emission in different channels** for e.g. dynamics, need to detect line in **faintest of these channels** with >3-5 sigma

- You should determine the estimated flux of the source (May need to convert from brightness temperature $T_b$ or expected column density)

- Use sensitivity calculator to determine required time on-source (e.g. VLA, ALMA, SMA)

# 7. Choose your calibrators
## Bandpass calibration

The bandpass is the spectral frequency response of an antenna to a spectrally flat source of unit amplitude

Phase slope of a few degrees across band from delay errors

Phase

20
10
0
-10
-20

10
0
-10
-20

Amp

1.2
1.0
0.8
0.6
0.4
0.2
0.0

1.2
1.0
0.8
0.6
0.4
0.2
0.0

**Ideal Bandpass
Phase=0, Amp=1**

Nearly flat over inner 75% of band

**Example
Observed Bandpass**

- Shape due primarily to electronics/ transmission systems of individual antenna
- Different for each antenna

Edge roll-off caused by shape of bandpass filters
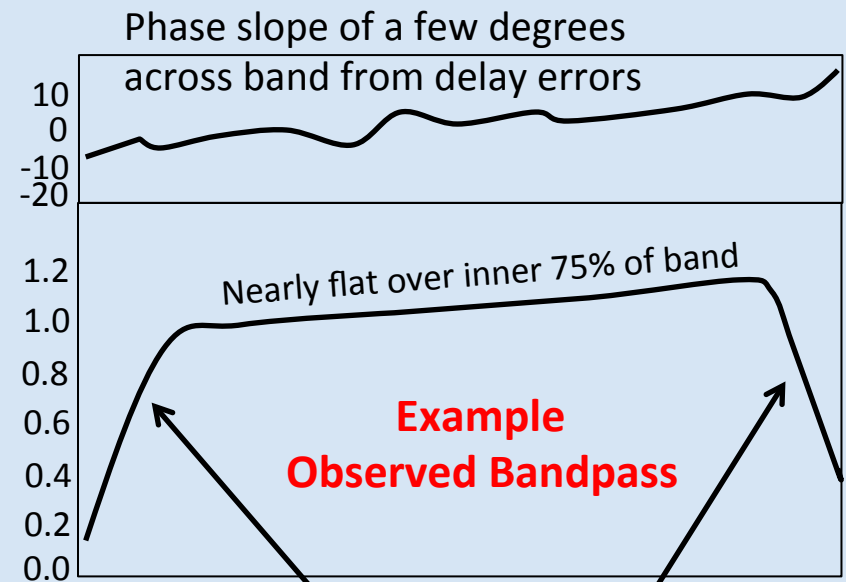
**Bandpass calibration attempts to correct for the deviations of the observed bandpass from the ideal one**

# Why is bandpass calibration important?

The quality of the bandpass calibration is a key limiting factor in the ability to detect and analyze spectral features

ν-dependent amplitude errors:
- limit ability to detect/measure weak emission/absorption lines superposed on the continuum
- may mimic changes in line structure

ν-dependent phase errors:
- may lead to spurious positional offsets between spectral features as a function of frequency, imitating Doppler motions
- Relative positional accuracy in channel images: $\Delta\theta / \theta_B = \Delta\phi / 360^o$ where $\theta_B$ is the synthesized beam and $\Delta\phi$ is the scatter in the phases

For pseudo-continuum experiments conducted in spectral line mode, dynamic range of final images is limited by bandpass quality

# What makes a good bandpass calibrator?

**Select a bright continuum source with**:
- High SNR in each channel
- Intrinsically flat spectrum
- No spectral lines/features
- No changes in structure across band (e.g. point source at all frequencies)

Calibration should not contribute to noise in target spectrum, i.e. in one channel:

    bandpass SNR >> target SNR

Can smooth the bandpass or fit polynomial to increase the SNR.

May need higher SNR for bandpass calibrator if looking for faint lines on strong continuum.



K. Johnston
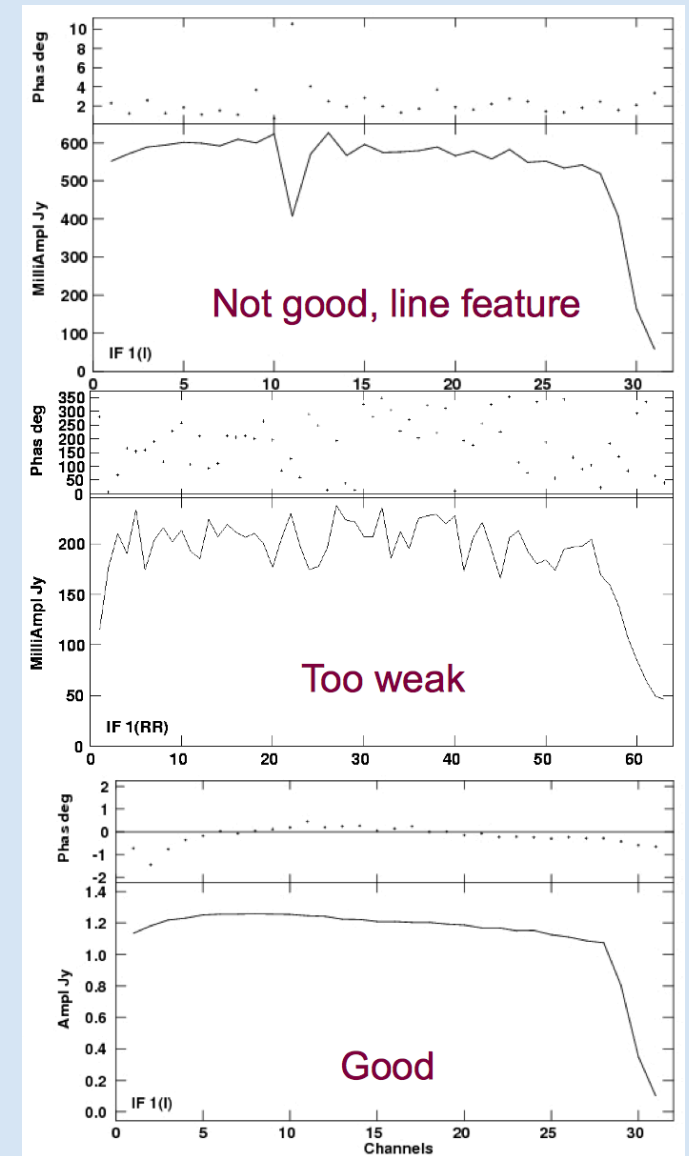
# 7. Choose your calibrators
# Flux calibration

- In mm/sub-mm observing, if using a solar system object with an atmosphere for calibration (Jovian or Saturnian moons, for example), be aware that these objects often have absorption lines.

- Check your calibrator spectrum carefully, particularly if that source is not red-shifted.

- You should exclude affected channels (or even basebands if the absorption is broad).
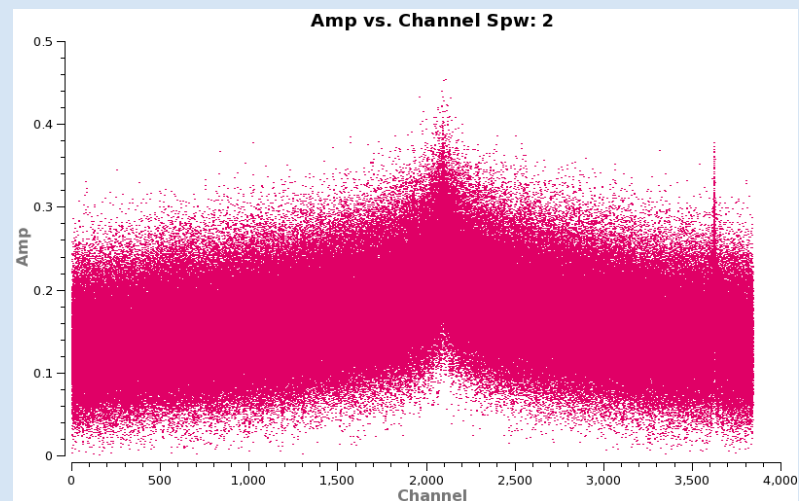


Titan observed in one of the observed spectral windows
(cf. TW Hya Spectral Line Tutorial)

# 8. Data rate and size considerations

Finally, many observatories impose a maximum data rate for a given observation.

For instance, for the VLA the data rate depends on:

- The number of channels
- The number of spectral windows
- The number of polarisations observed
- The length of one integration in seconds
- The number of antennas

Large datasets are difficult to transfer and reduce… only use high spectral and time resolution if you really need it!

# Part II: Data reduction

- Flagging methods
- Bandpass calibration
- Doppler correction
- Continuum subtraction
- Self-calibration
- Imaging of cubes

# Flagging Methods – in frequency

- For large data sets, checking the data channel-by-channel is not practical

- This task can be simplified using approaches such as:
  - Examination of scalar-averaged cross-power spectra: check for dips or spikes
  - Use of automated flagging routines: these can flag data based on deviation from expected spectral behavior (e.g. SERPent for e-MERLIN, AOFlagger)

But… if you are planning to make image cubes then avoid excessive frequency-dependent flagging which changes the uv-coverage across the band

# Flagging Methods – in frequency

Scalar-averaged cross-power spectra can be helpful for spotting narrowband RFI
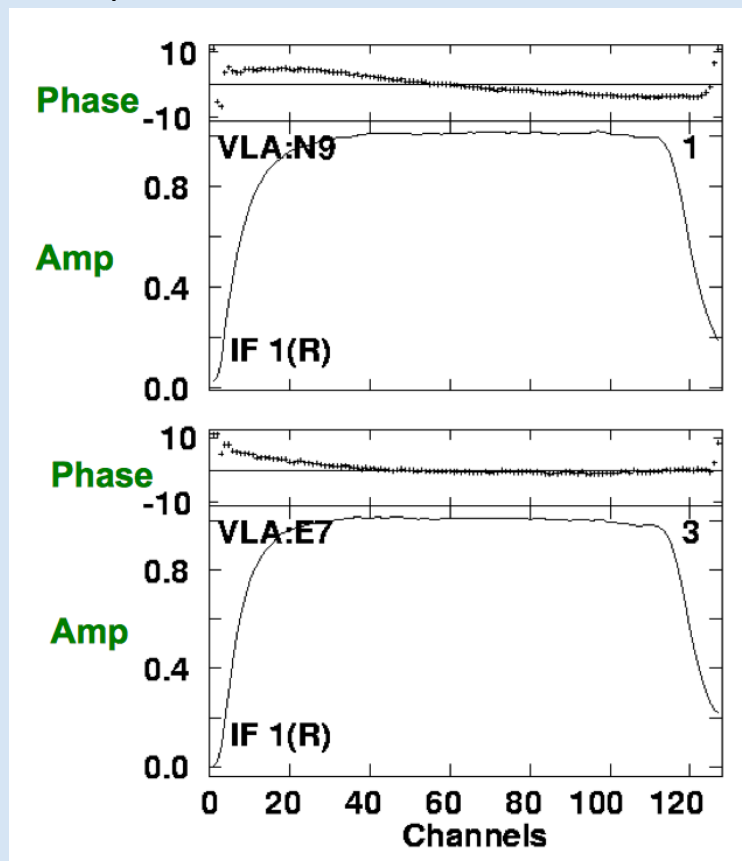


Phase

Amplitude
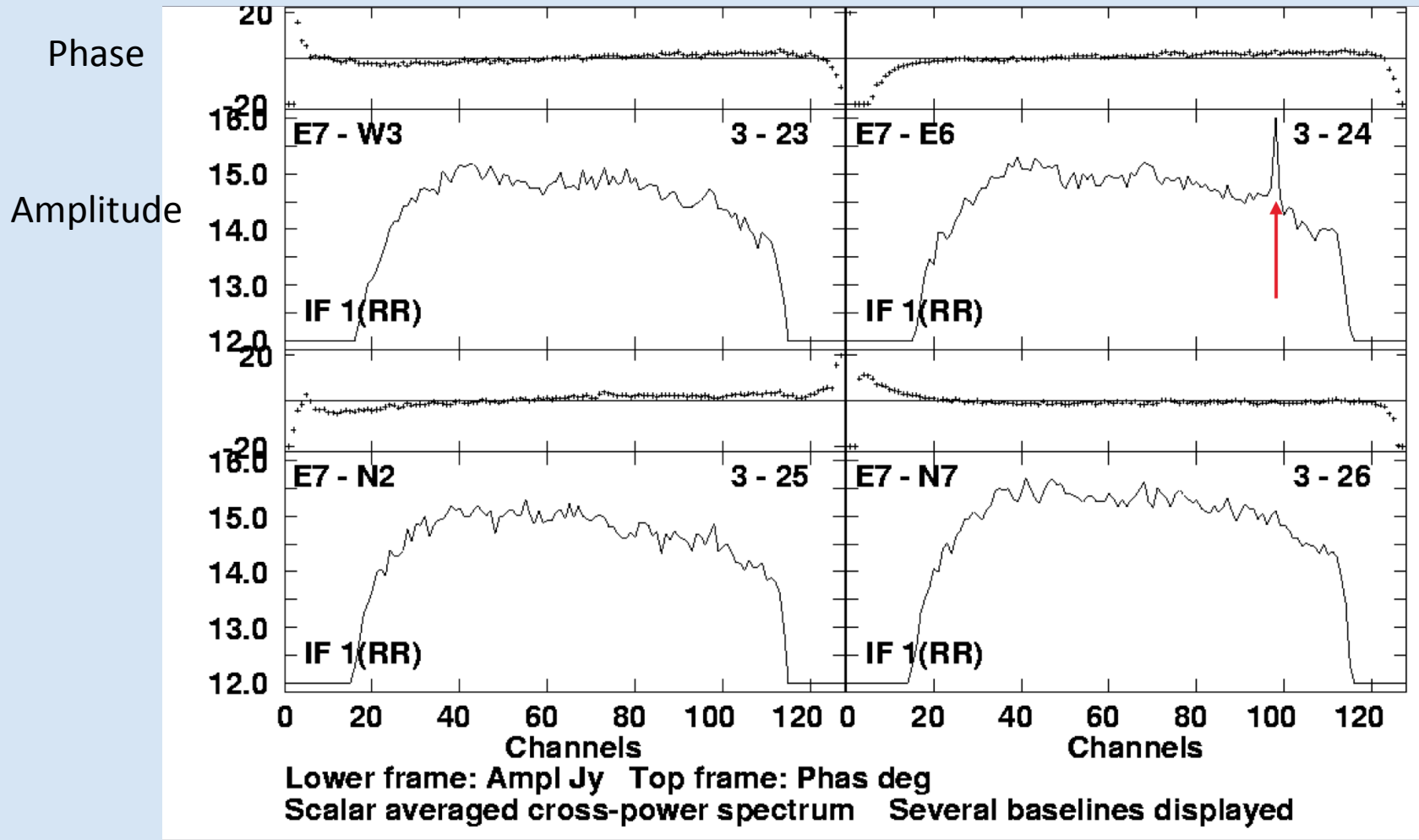
# Flagging Methods – in time

- Can find bad data in time using the vector-averaged central ~75% of channels of the calibrator sources

- Can find problems affecting all frequency channels
  e.g. malfunctioning electronics or mechanical
     problems with a particular antenna

- Resulting flags are then be copied to the line dataset and applied to all spectral channels

# Bandpass calibration

## Has your bandpass calibration gone well?

Bandpass solutions



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 are not dominated by noise

# Bandpass calibration

## Has your bandpass calibration gone well?

Another good way to check: examine cross-power spectra of a continuum (flat spectrum) source with BP corrections applied.
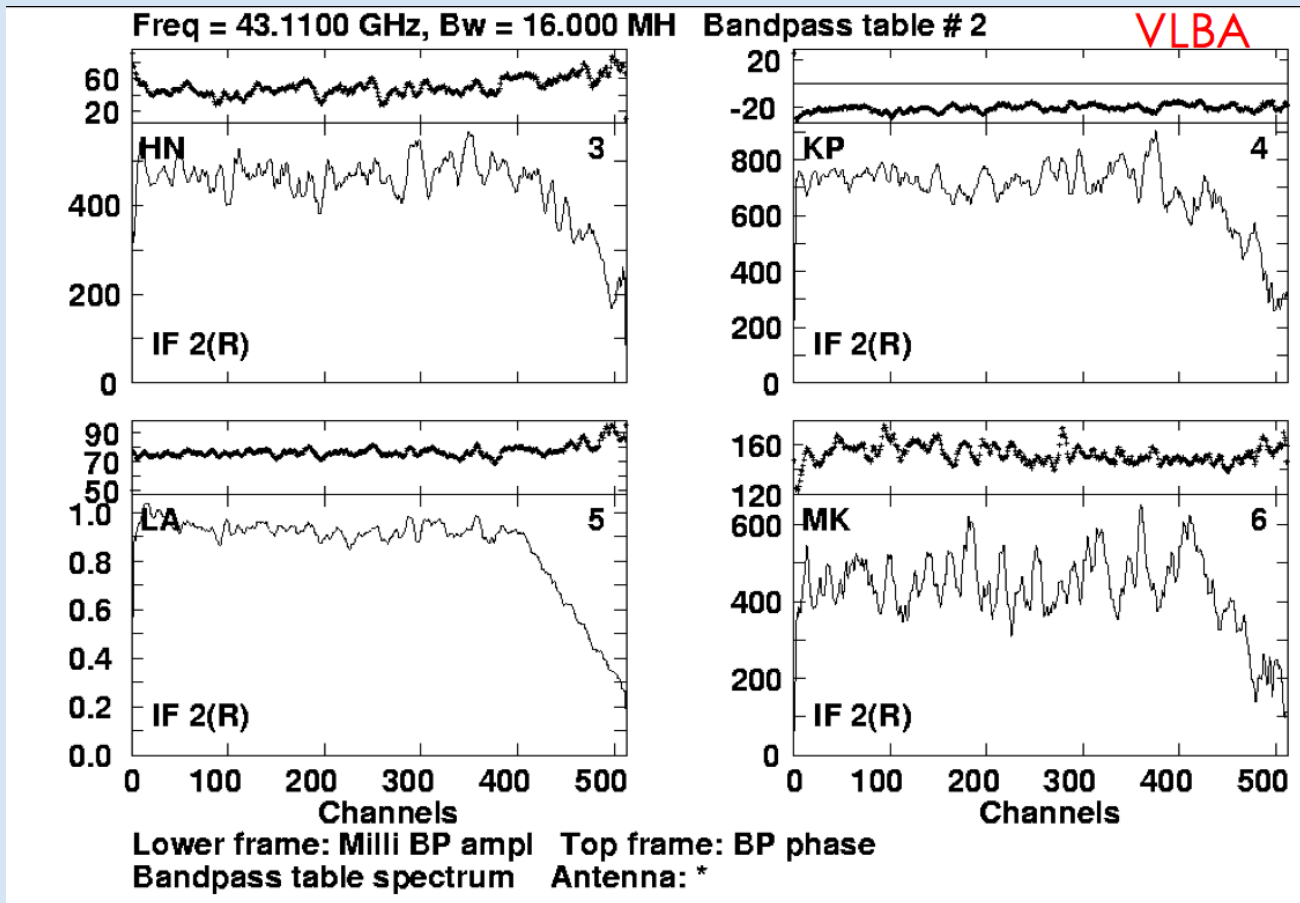
Checklist:

- ✓ Phases are flat across the band
- ✓ Amplitude is constant across the band
- ✓ Corrected data do not have significantly increased noise
- ✓ Absolute flux level is not biased high or low
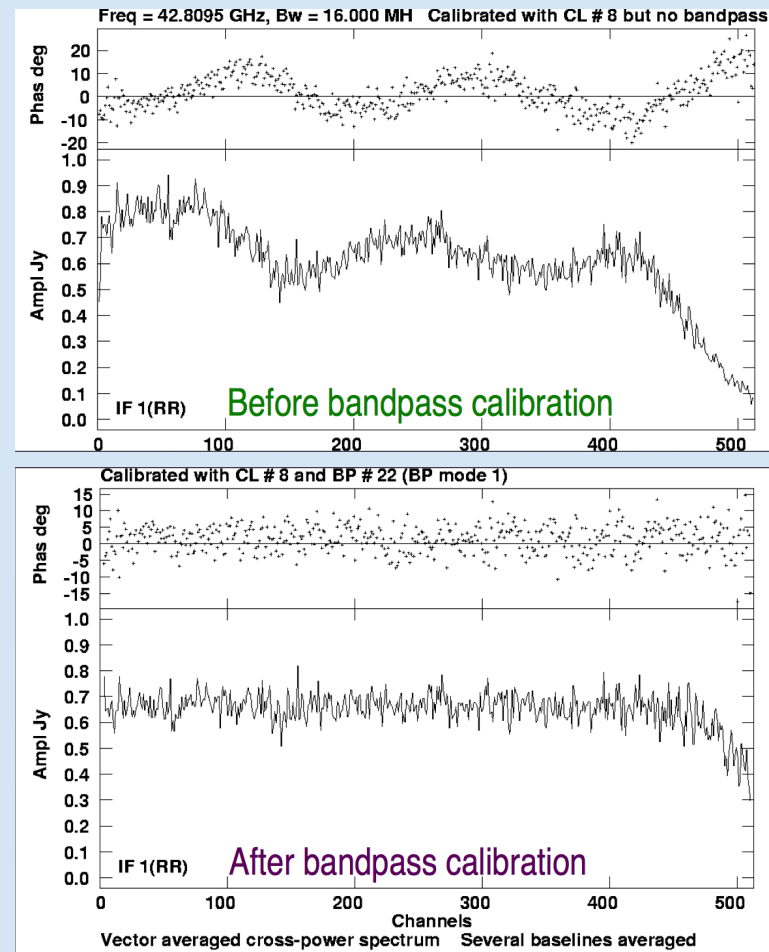
# Bandpass calibration

## When has your bandpass calibration **not** gone well?



Plot of bandpass solutions for four antennas VLBA

**Problems:**

Amplitude has different normalisation for different antennas

Noise levels are high, and are different for different antennas

# Doppler correction

- Often now done using Doppler Setting and further finer corrections during post-processing and imaging (see slides from Part I).

- Within one observation, Doppler Setting can correct for the Heliocentric velocity (~30 km/s), but cannot exactly correct the ~0.5 km/s for the Earth's rotation on its axis.

- Remaining corrections done in e.g. tasks clean or cvel in CASA and task CVEL in AIPS (after bandpass calibration). CASA task plotms can correct on-the-fly (less accurately).

Different colours are different times in the observation

Before and after Doppler correction
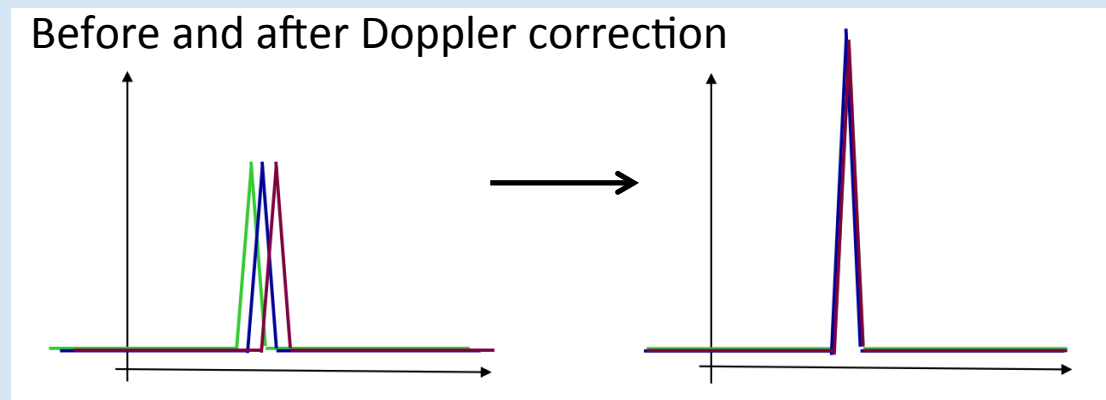
# Continuum subtraction

As well as lines, spectral-line data often contain continuum sources (either from the target or from nearby sources in the field of view)

- This emission complicates the detection and analysis of line data
- Continuum emission limits the achievable spectral dynamic range



from Roelfsma (1989)

m (DEC)

z (VEL)

ℓ (RA) →
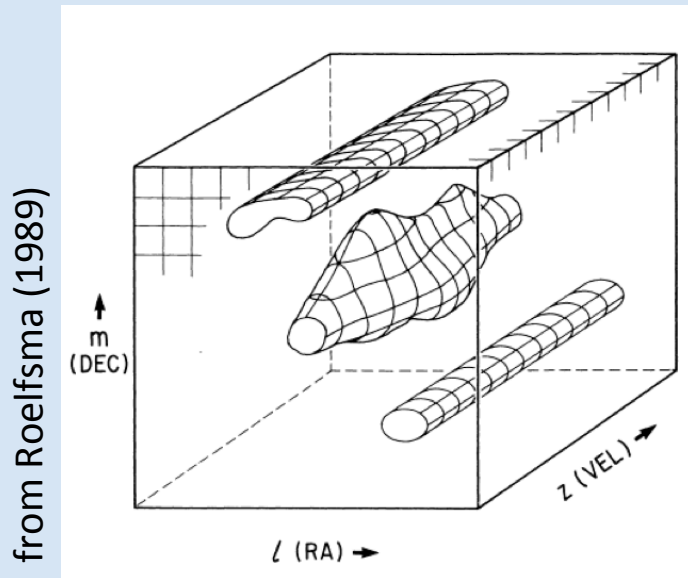
Spectral line cube with two continuum sources (structure independent of frequency) and one spectral line source near the field centre

# Continuum subtraction

Method:

1) examine the data
2) assess which channels appear to be line-free
3) use line-free channels to estimate the continuum level
4) subtract the continuum
5) evaluate the results



Before

After
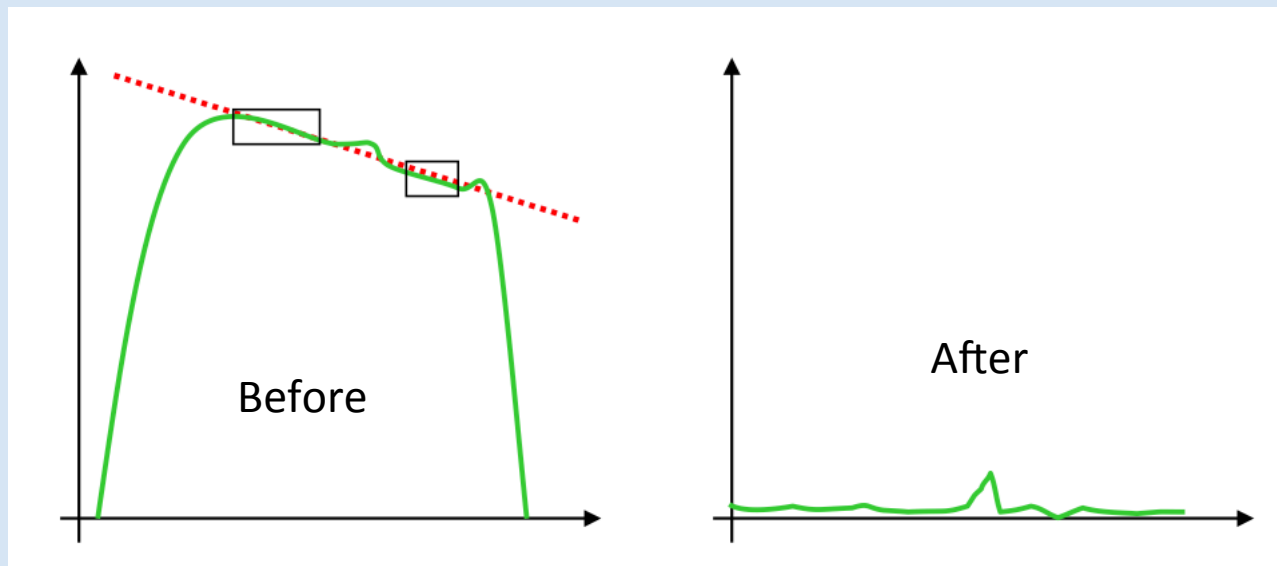
# Continuum subtraction
## Two methods:

1. **In the uv-plane**
   Subtract continuum → clean line & cont. separately
   - Use AIPS task such as UVLIN, UVLSF, UVSUB
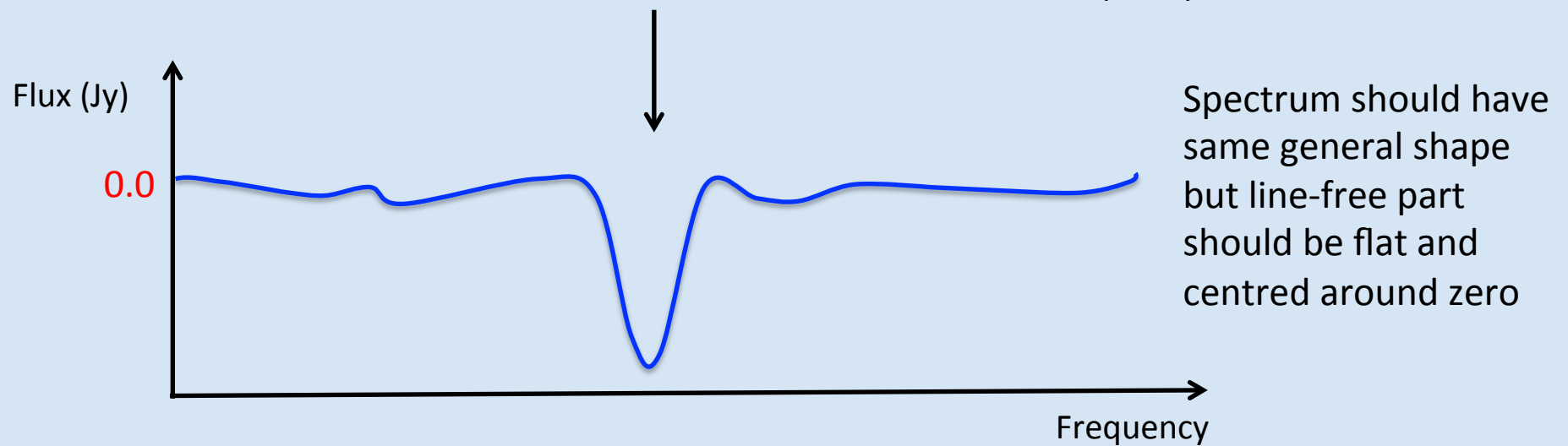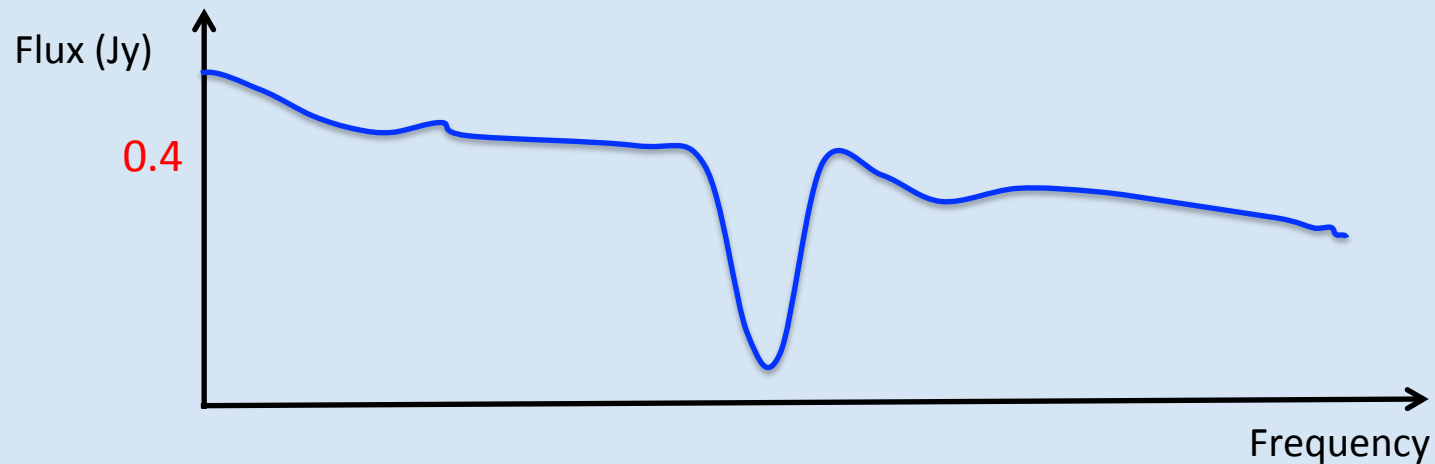   - Use CASA tasks such as uvcontsub

2. **In the image-plane**
   FT data → subtract continuum from 'dirty' cube → clean both cont. & line
   - Use AIPS task such as IMLIN
   - Use CASA tasks such as imcontsub

*No one single subtraction method is appropriate for all experiments!*

# Continuum subtraction
## Did it work?



Flux (Jy)

0.4

Frequency

Flux (Jy)

0.0

Frequency

Spectrum should have same general shape but line-free part should be flat and centred around zero

# Self-calibration

Can apply self-calibration solutions to improve quality of line data

Two cases:
1 ) Strong line emission (i.e. maser)
- Choose a strong channel with "simple" structure
- Self-cal that channel & apply solutions to all other channels
- Allows imaging of weak continuum (& channels) with improved SNR

2) Weak line and strong continuum emission
- Apply solutions from the continuum to individual channels
- Allows imaging of weak lines with improved SNR

Get good positions of line features relative to continuum, but lose absolute positional information

# Imaging of cubes

- Principles for continuum imaging mostly applies to line data as well (cleaning, weighting, etc.)

- But keep in mind that deconvolution of spectral line data often poses special challenges:

  – Cleaning many channels is computationally expensive
     (do you need the full spectral resolution or can average?)

  – Emission *structure* changes from channel to channel
     (may have to change cleaning boxes for each channel)

  – If you are interested in *both* high sensitivity (to detect faint emission) and high spatial/spectral resolution (to study kinematics):
        robust weighting with -1<$R$<1 good compromise

# Part III: Image and Spectral Analysis

After mapping all channels in the data set, we have a spectral line 3D data *cube* (RA, Dec, Velocity or Frequency)

To visualize the information we usually make 1-D or 2-D projections providing different analysis methods:

- Line profiles (1-D slices along velocity axis)
- Channel maps (2-D slices along velocity axis)
- Moment maps (integration along the vel. axis)
- Position-velocity plots (slices along spatial dimension)
- Movies (2-D slices along velocity axis)

**See Tutorial T10C on Wednesday!**

# Line profiles
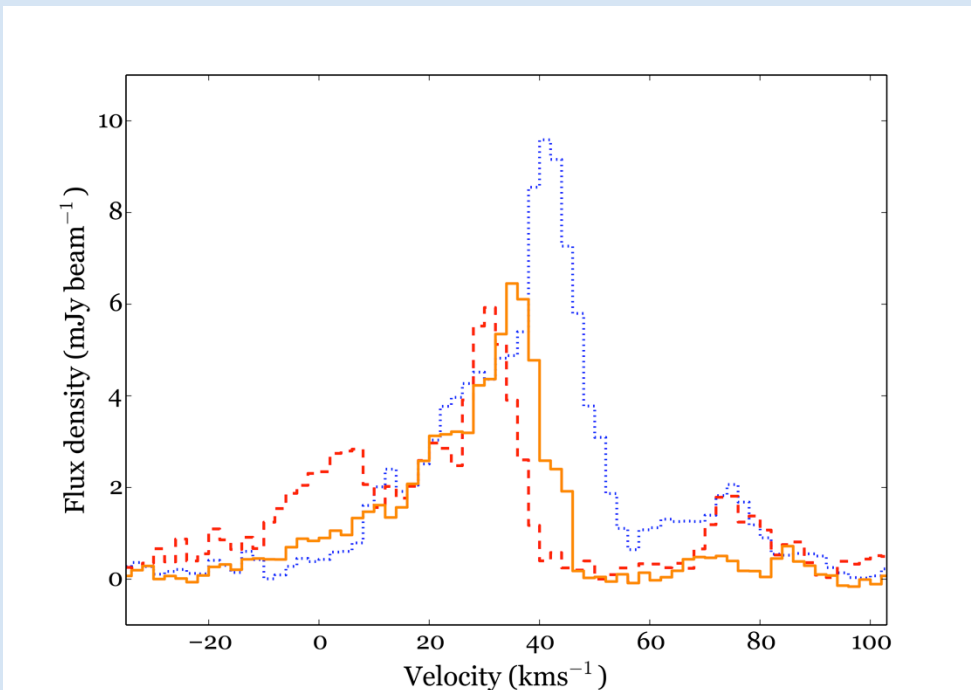


Johnston et al. (2014)

Spectra taken at different positions in a cube of $^{13}CO$ (J=2-1) emission.

The cube was created by combining SMA and IRAM 30-m data.

Use AIPS task ISPEC and the Spectral Profile tool in the CASA viewer

# Channel maps

Channel maps of $^{13}$CO (J=2-1) emission from a Cloud near the Galactic Centre

Channels are from -10 to 85 km/s (in steps of 5km/s)

Coloured ✚ show the positions where the spectra on the previous slide were measured

Increasing velocity

Increasing velocity
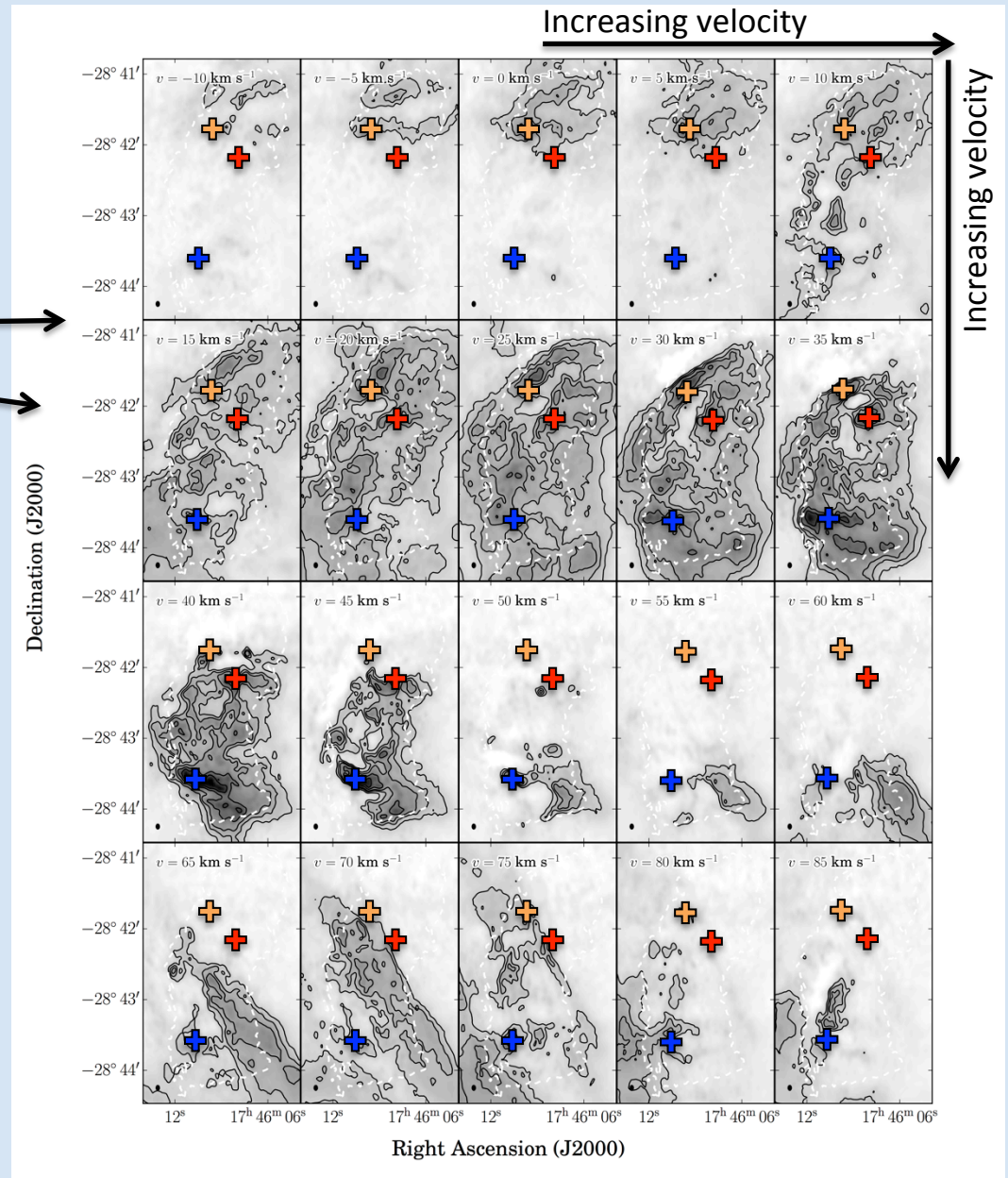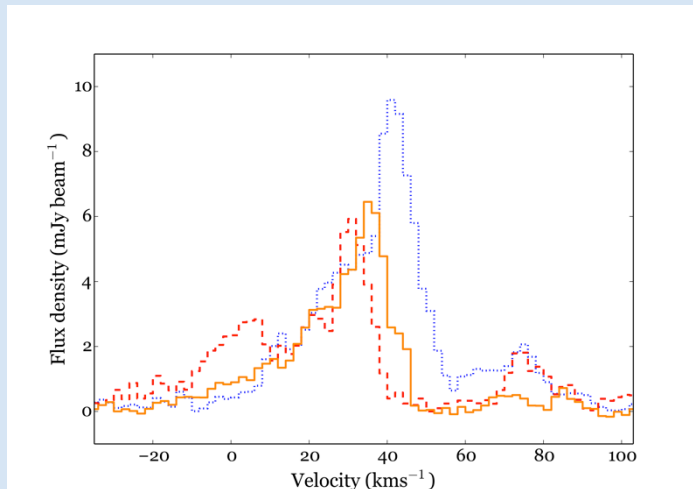
Johnston et al. (2014)

# Moment maps

Use moment maps to derive parameters such as integrated line intensity, centroid velocity and line widths as function of position:

$$I_{\text{tot}}(\alpha, \delta) = \Delta v \sum_{i=1}^{N_{\text{chan}}} S_{\nu}(\alpha, \delta, \nu_i)$$

Total intensity
(Moment 0)

$$\overline{v}(\alpha, \delta) = \frac{\sum_{i=1}^{N_{\text{chan}}} v_i \, S_{\nu}(\alpha, \delta, \nu_i)}{\sum_{i=1}^{N_{\text{chan}}} S_{\nu}(\alpha, \delta, \nu_i)}$$
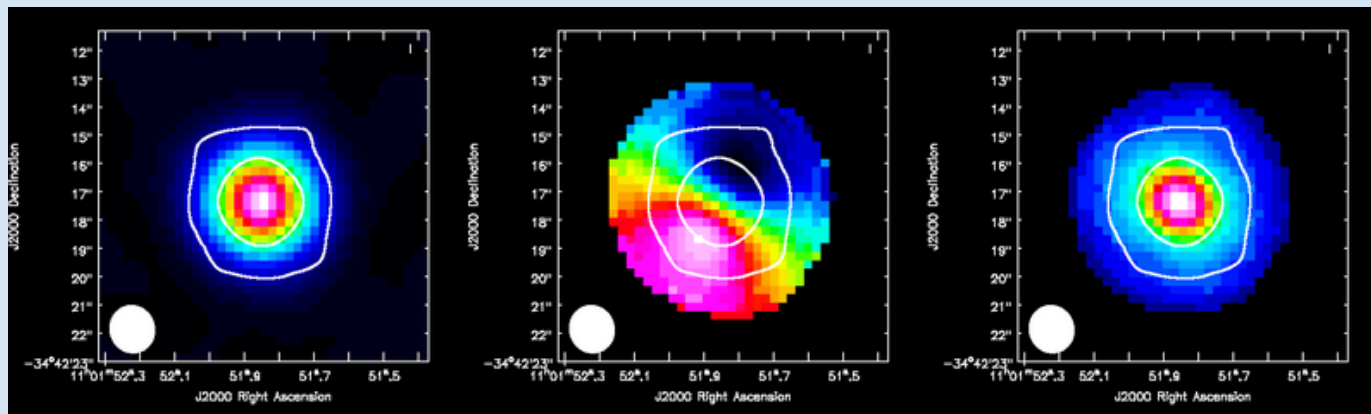
Intensity-weighted velocity
(Moment 1)

$$\sigma_v(\alpha, \delta) \equiv \sqrt{\langle (v_i - \overline{v}(\alpha, \delta))^2 \rangle}$$

$$= \sqrt{\frac{\sum_{i=1}^{N_{\text{chan}}} (v_i - \overline{v}(\alpha, \delta))^2 \, S_{\nu}(\alpha, \delta, \nu_i)}{\sum_{i=1}^{N_{\text{chan}}} S_{\nu}(\alpha, \delta, \nu_i)}}$$

Intensity-weighted
velocity dispersion
(Moment 2)

Can be made with AIPS task MOMNT and CASA task immoments

# Moment maps

HCO$^+$(4-3) moment maps of TW Hya with ALMA (white is continuum)



|   |   |   |
|---|---|---|
| Zero Moment | Moment 1 | Moment 2 |
| Integrated flux | Mean velocity | Velocity Dispersion |

Moments are sensitive to noise so clipping is required:
- Sum only over the planes of the data cube that contain emission
- Since higher order moments depend on lower ones (so progressively noisier), set a conservative intensity threshold for 1st and 2nd moments
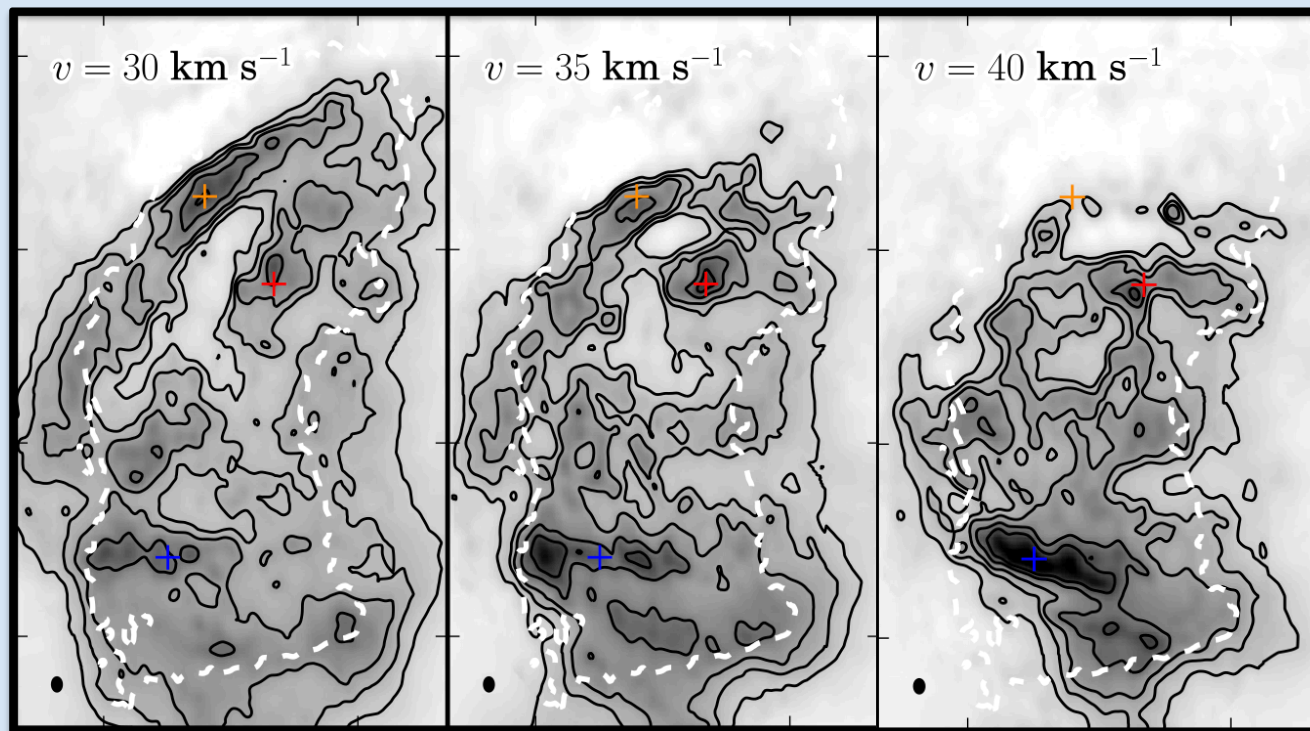
# Position-Velocity (PV) diagrams

PV diagrams take a slice out of a cube along a
"PV cut" (e.g. red line shown below)





$^{12}CO(3-2)$ PV diagram of TW Hya

Velocity (km/s)

Offset

channel

Dec

R.A.
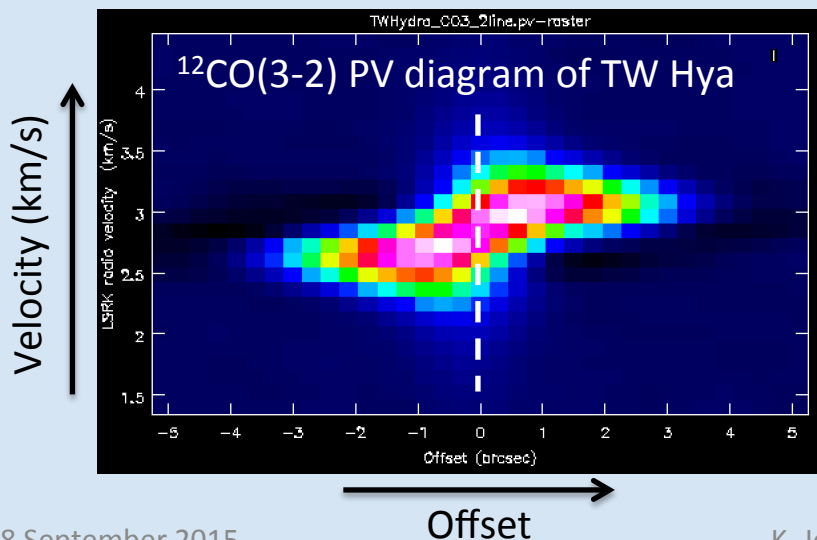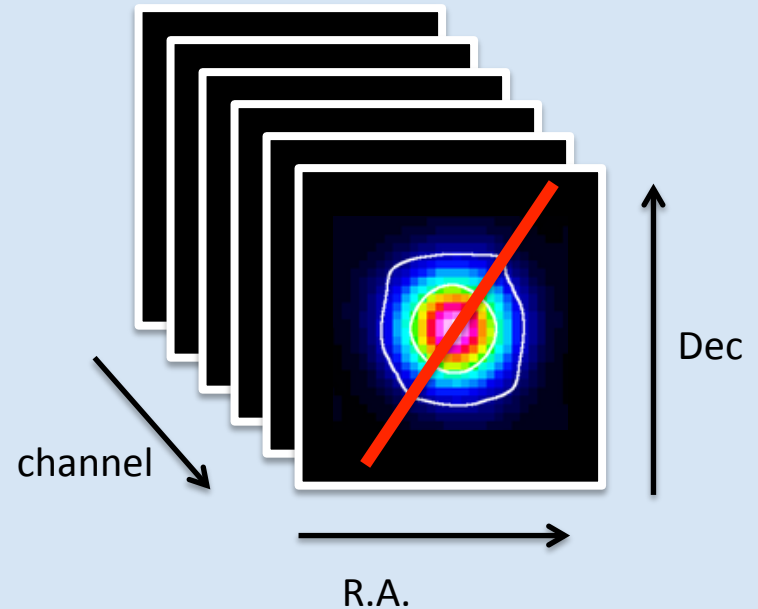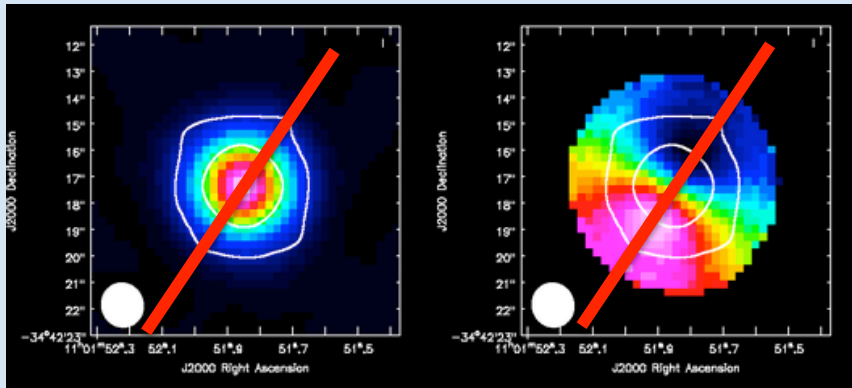
You can produce PV diagrams directly in CASA using task impv, or using the task IMMOMENTS, by collapsing the RA or DEC axis

# 3D visualisations…

Three channels from the $^{13}$CO (J=2-1) channel map



Can use tools like 3D Slicer to make 3D visualisations…

# Line identification/fitting and modelling

Line identification and Gaussian line fitting can be done interactively in CASA viewer or more complex fitting using task specfit

Available external line fitting/modelling programs:

- CASSIS (http://cassis.irap.omp.eu )

- Weeds (Maret+ 2011)

- XCLASS: eXtended CASA Line Analysis Software Suite (Möller+ 2015)

Screenshot of CASSIS
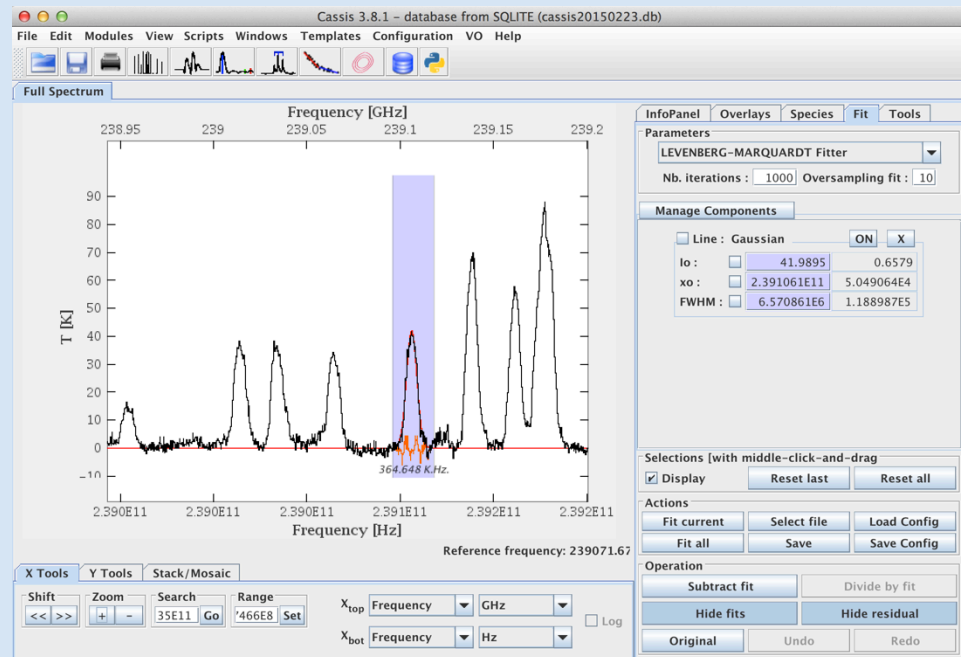
# Summary

Having a third axis (frequency or velocity) provides you with a lot of extra information about the physics of your observed source.

To recap, we covered:

- Setting up your observation
- Data reduction
- Image and spectral analysis

**You're now ready to do some spectral line proposing, observing and reduction!**

**(see you in Tutorial T5 later)**