Spectral Lines

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SIW 21 (2026)

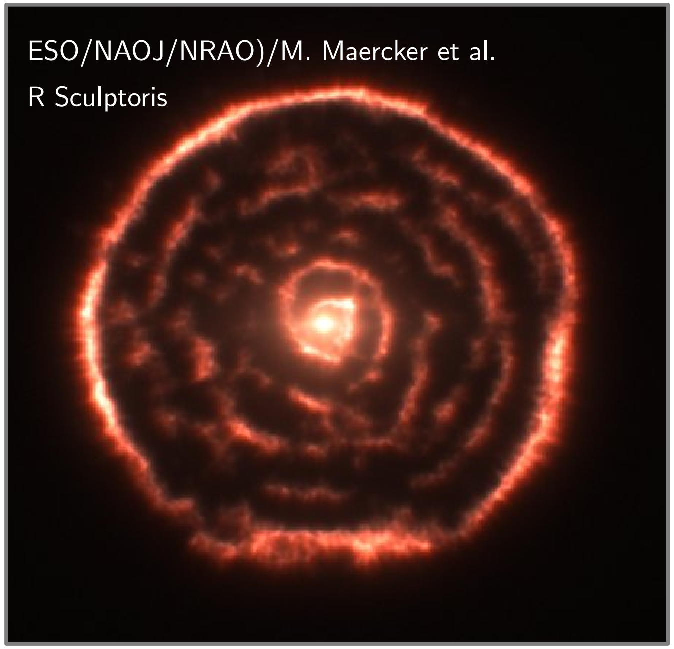
Resources for spectral line observers

- Relevant chapters in Synthesis Imaging in Radio Astronomy II (the “White Book”):
  - **Ch. 11** by D. Westpfahl “Spec. Line Obs. I: Intro.”
  - **Ch. 12** by M. Rupen “Spec. Line Obs. II: Cal. & Analysis”
  - **Ch. 24** by M. Reid “Spectral Line VLBI”
- Chapters in works by *Condon & Ransom*; *Thompson, Moran, & Swenson*; *Wilson, Rohlfs, & Huttemeister*.
- NRAO CASA guides for VLA, VLBA, and ALMA.
- Documentation for CASA (casadocs) and AIPS (memos).
- Past SIW lectures by **Y. Pihlstrom** (esp. 2018, 2022, 2024)

Overview

- **Spectral line science**
  - Science highlights, emission mechanisms, analysis techniques.
- **Frequency dependent effects**
  - bandwidth smearing, instrument response, atmospheric profile, narrow-band interference
- **Calibration**
  - editing, bandpass, Hanning smooth, Doppler correction, continuum subtraction
- **Imaging**
  - cube imaging, deconvolving extended emission automated masking.

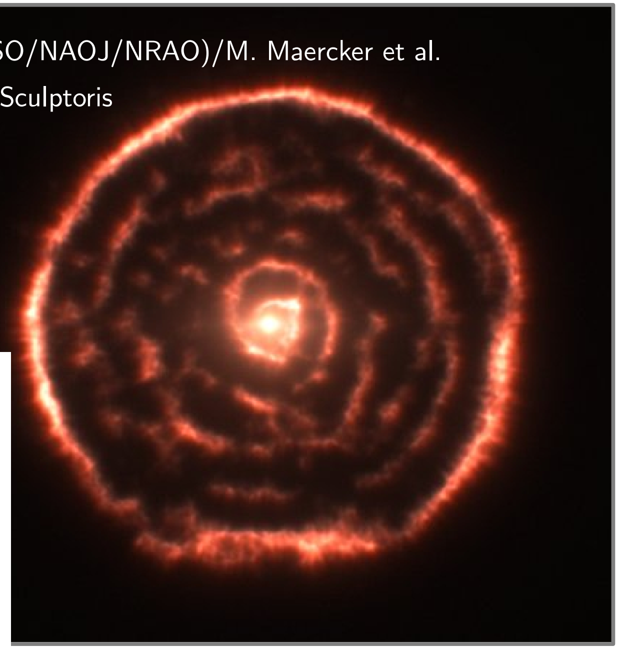
Science with lines



ESO/NAOJ/NRAO)/M. Maercker et al.

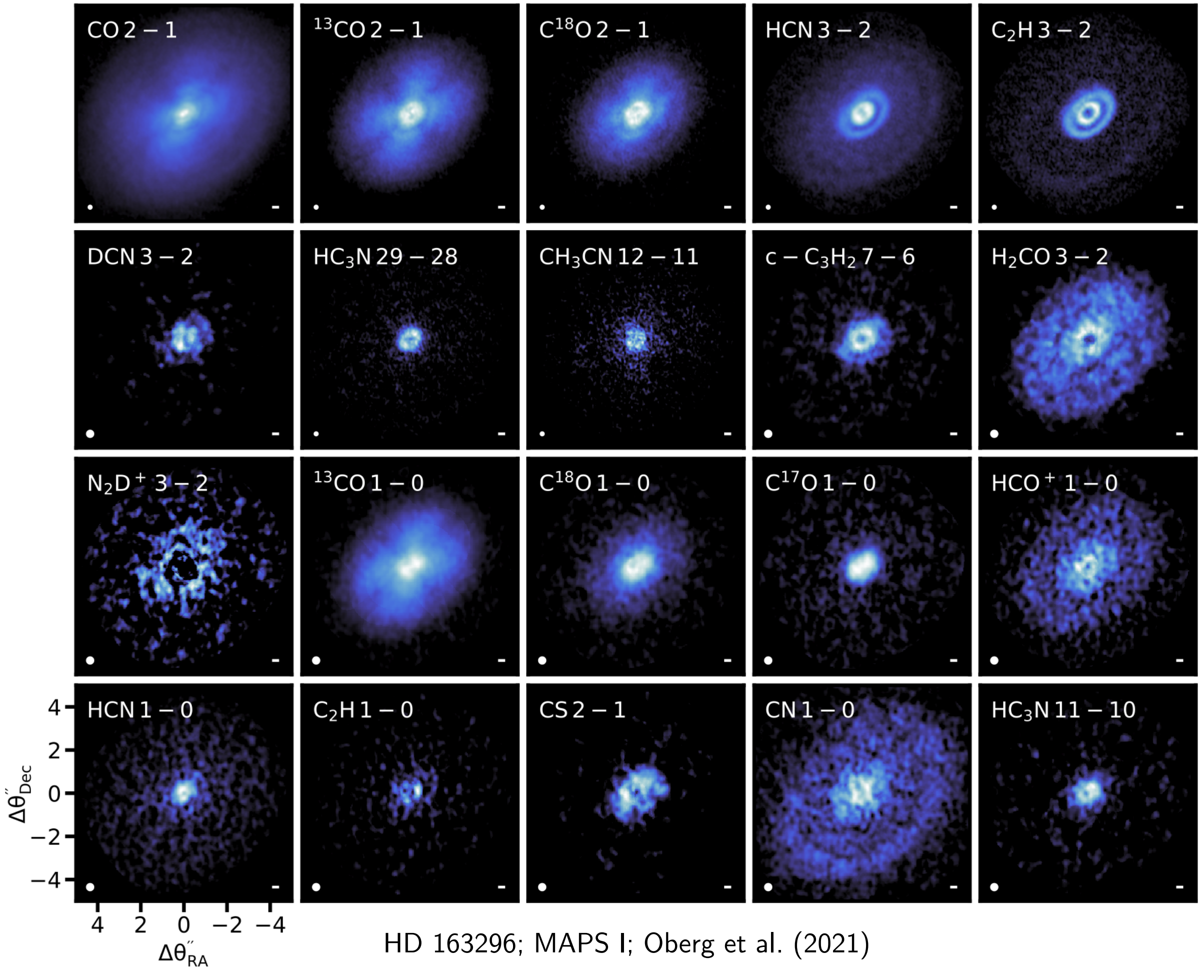
R Sculptoris

Science with lines



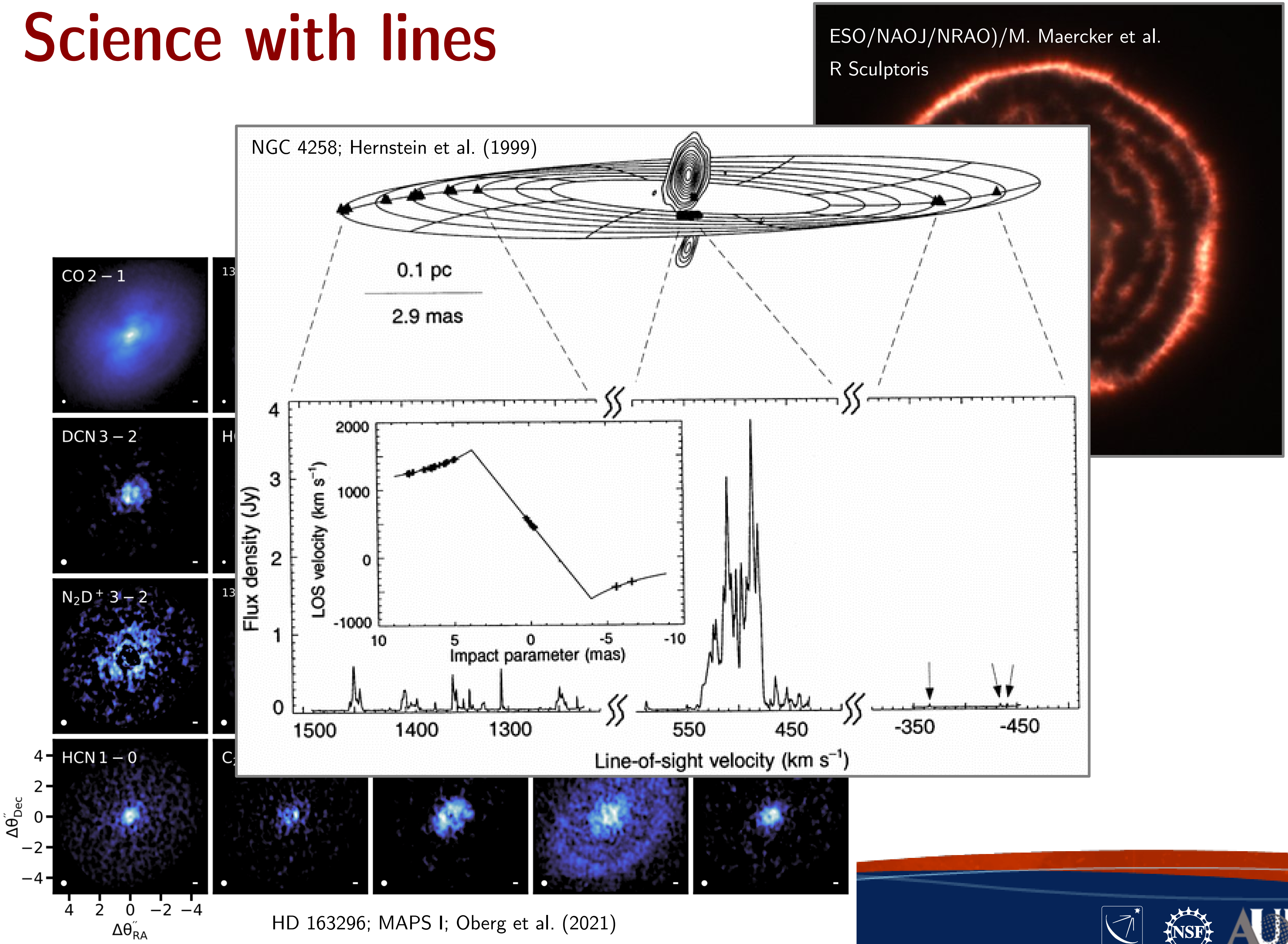
ESO/NAOJ/NRAO)/M. Maercker et al.

R Sculptoris



HD 163296; MAPS I; Oberg et al. (2021)

Science with lines



ESO/NAOJ/NRAO)/M. Maercker et al.

R Sculptoris

NGC 4258; Hernstein et al. (1999)

HD 163296; MAPS I; Oberg et al. (2021)

Science with spectral lines: details

Spectral line transitions of atoms and molecules allow us to probe the physics of ionized, atomic, and molecular gas. Observations applicable to almost all domains that observe these gas phases.

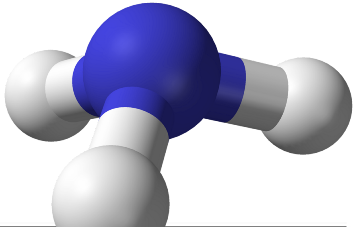
- *Molecular rotational lines:* CO J=1-0 → "Dense gas"
- *Molecular inversion lines:* NH3 (1,1) & (2,2) → "Thermometer"
- *Atomic fine structure:* [CII] → Cooling rate and "CO dark gas"
- *Atomic hyperfine structure:* HI → Column density, rot. curves
- *Radio recombination lines:* H, He, C → Ionization rate
- *Masers:* H2O, CH3OH, SiO → Parallax distances, proper motion
- *Zeeman splitting:* HI, OH, CN ... → Magnetic field strength
- *Multiple species* → Abundances, astrochemistry

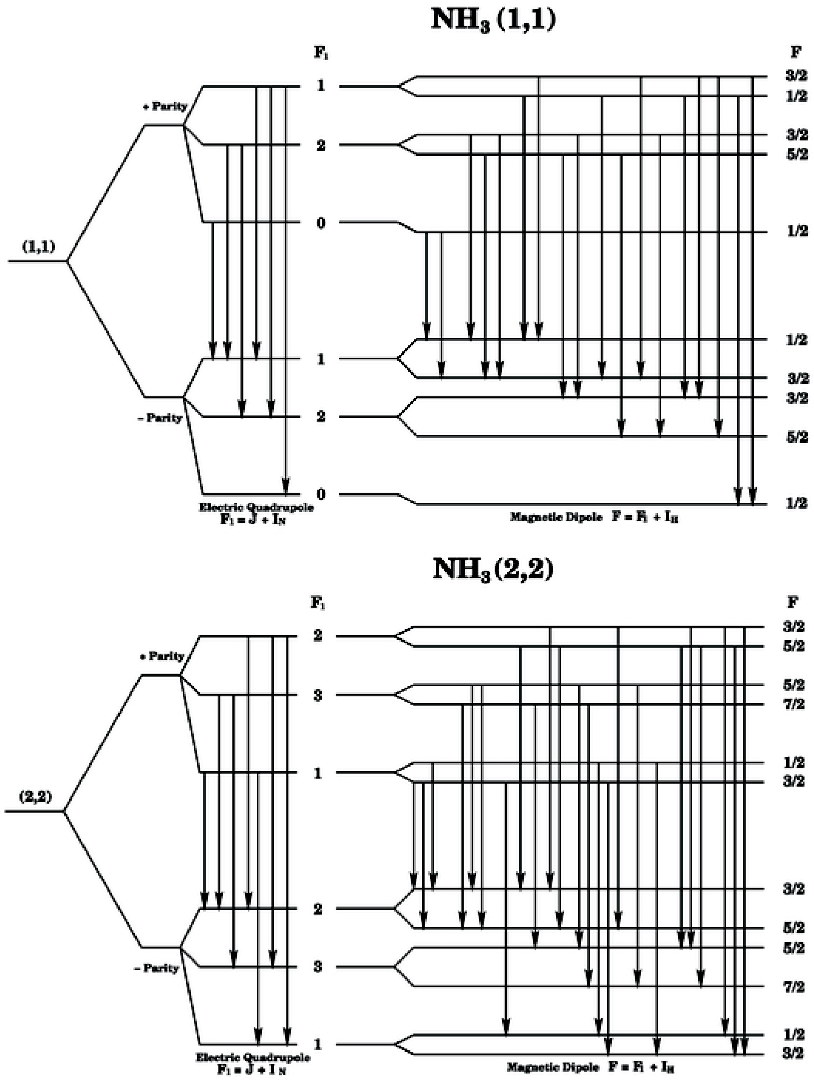
Emission mechanisms

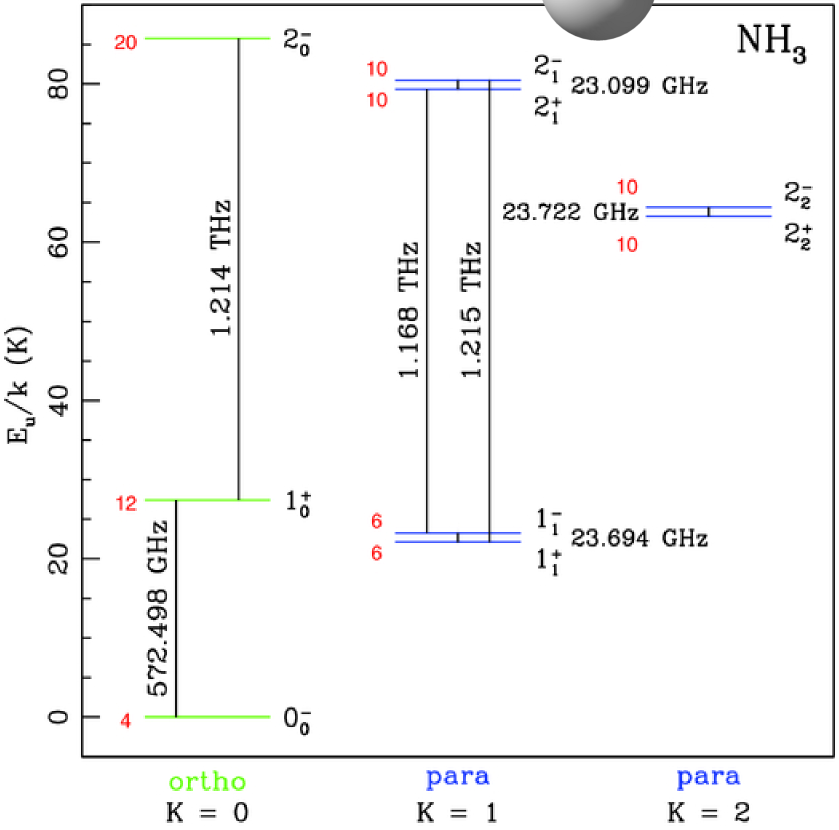
The most common transitions observed in the cm/mm are recombination lines, HI, and molecular rotation lines.

- Quantum systems have discrete levels in energy & momentum.
- Level populations are set due to radiation and collisions.
- LTE: level populations are set via the *kinetic temperature*.
- Non-LTE: sub-thermal populations or inversions, the observed levels define the *excitation temperature*.
- Statistical equilibrium: level populations are stationary.
- Excitation mechanisms: spont./stim. radiation, collisions.
- Coupling of angular momenta produce many forms of line spitting: fine, hyperfine, l- & Λ-doubling, Zeeman/Stark...
- **Good news:** multiplicity means we can often invert the measured intensities to infer gas temperatures and densities!

Example: ammonia inversion trans.



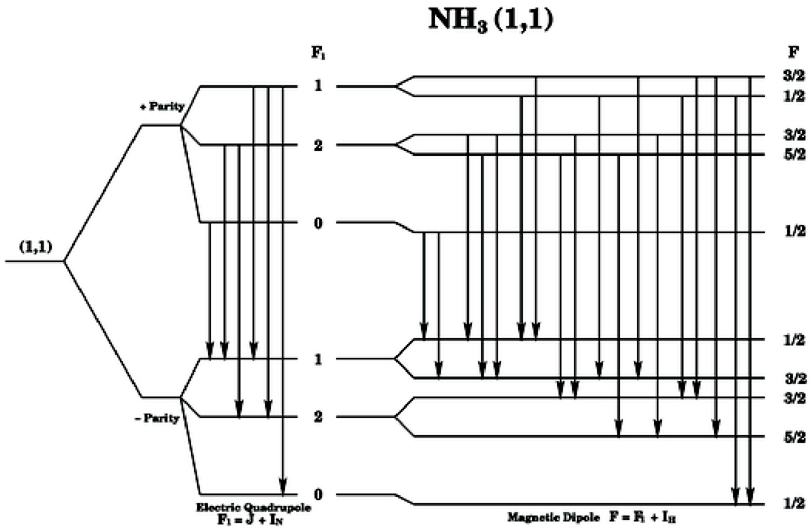


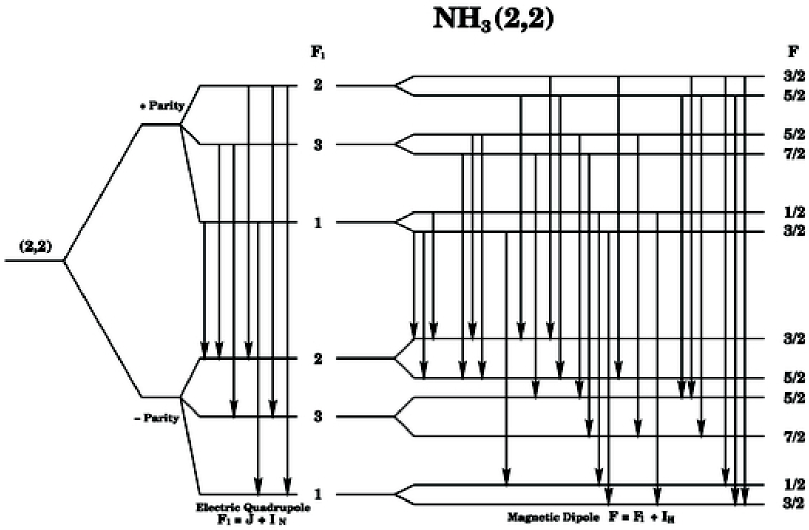


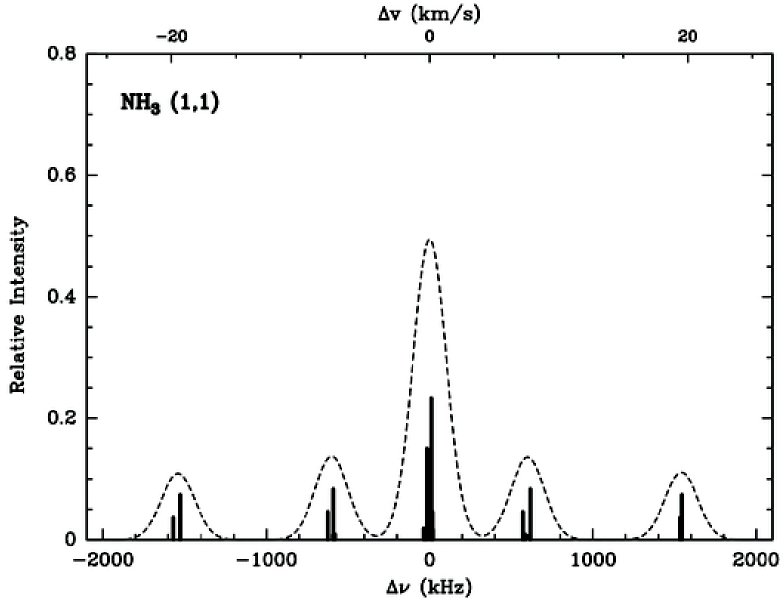
Mangum & Shirley (2015)

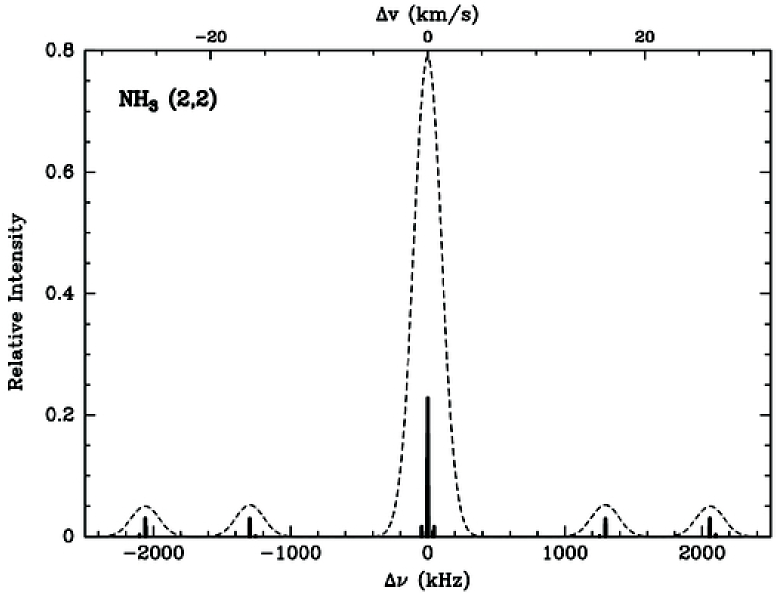
Mangum & Shirley (2015)

Ammonia inversion ...









Historical note

- Chap. 11 by M. Rupen in *SIRA II* (the "White book") details the historical distinction between "continuum" (1 chan/IF) and "spectral line" (multi-channel) observations.
- Effectively all modern interferometers now observe with multiple channels. *We are all "spectral line" observers!*
- Frequency dependent effects impact *all* observations, but spectroscopy focused projects more so in specific ways.
- Channel dependent calibration is required for continuum observations too in order to achieve high-dynamic range and mitigate bandwidth smearing and RFI.
- Spectroscopic projects require careful channel dependent calibration for stable spectral baselines, proper weighting, continuum subtraction, and attention to reference frames.

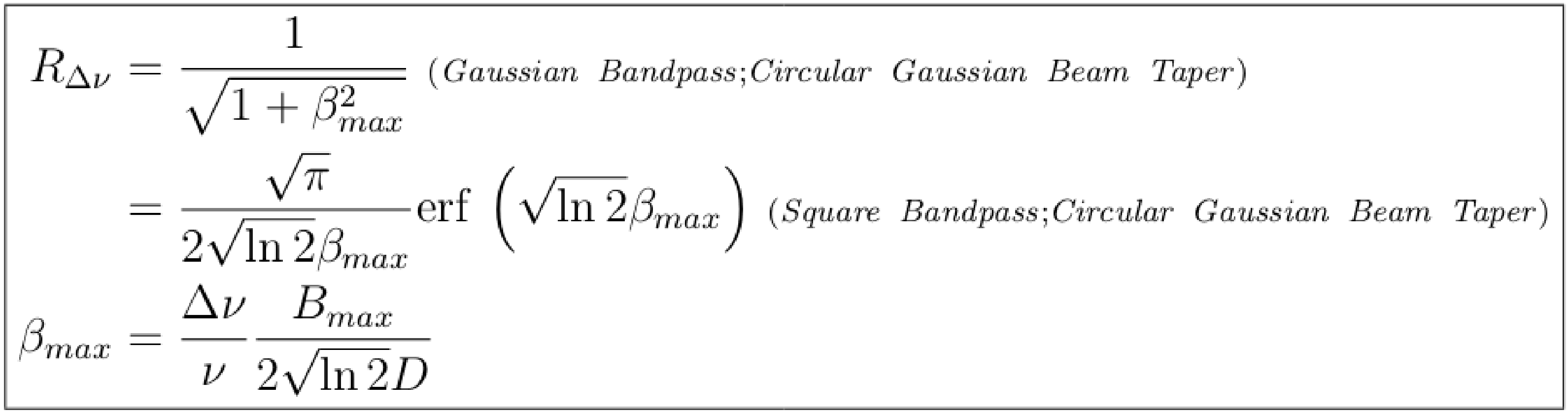
Frequency dependent effects

There are several frequency dependent calibration effects that impact spectroscopic projects (and continuum too)

- bandwidth smearing (chromatic aberration)
- atmospheric opacity profile (e.g., telluric lines)
- narrowband RFI
- standing waves (generally minimized for interf. obs viz. sd)
- front-end: amplifiers, analog filters
- back-end: sub-band filters, aliasing, Gibbs phenomenon

Bandwidth smearing

When visibilities from a finite bandwidth are gridded as if monochromatic, aberrations in the image will result. These take the form of radial smearing which worsens with increased distance from the delay-tracking center.



$$\begin{aligned}
R_{\Delta\nu} &= \frac{1}{\sqrt{1+\beta_{max}^2}} \quad (Gaussian\ \ Bandpass;Circular\ \ Gaussian\ \ Beam\ \ Taper) \\
&= \frac{\sqrt{\pi}}{2\sqrt{\ln 2}\beta_{max}} \mathrm{erf}\left(\sqrt{\ln 2}\beta_{max}\right) \quad (Square\ \ Bandpass;Circular\ \ Gaussian\ \ Beam\ \ Taper) \\
\beta_{max} &= \frac{\Delta\nu}{\nu}\frac{B_{max}}{2\sqrt{\ln 2}D}
\end{aligned}$$

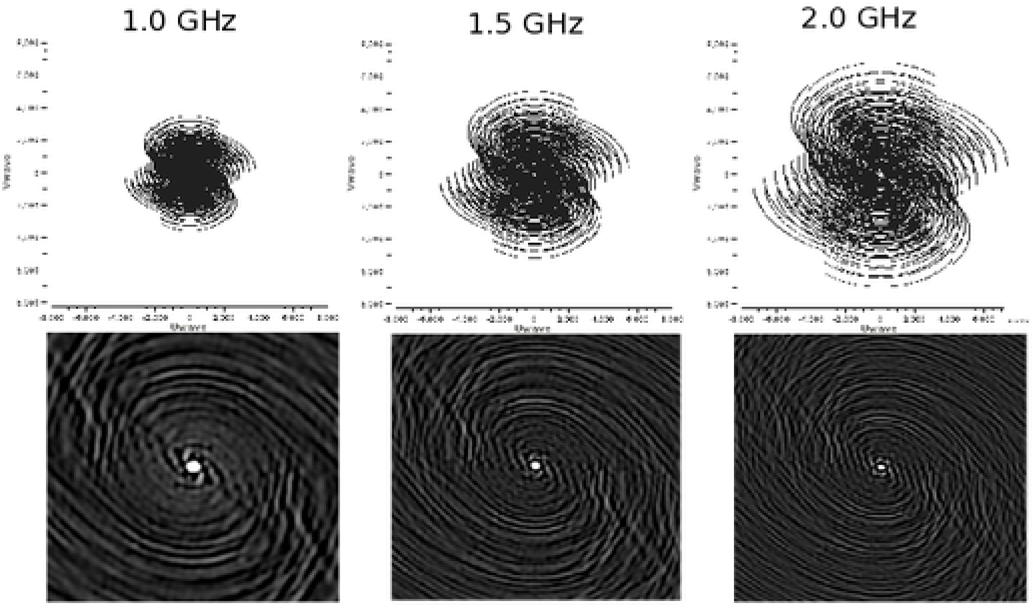
Mangum (2020): "How to calculate bandwidth smearing in radio synthesis measurements"

Reduction factor R as a function of maximum baseline, fractional channel bandwidth, and antenna diameter.

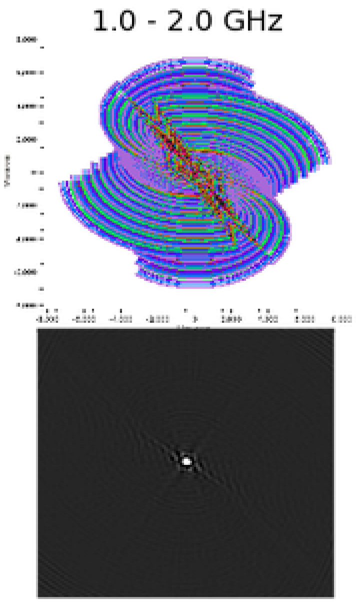
For VLA: 2 MHz, 5 GHz, 30 km, 25 m → ~0.96 at HPBW

Bandwidth smearing

When visibilities from a finite bandwidth are gridded as if monochromatic, aberrations in the image will result. These take the form of radial smearing which worsens with increased distance from the delay-tracking center. But with MFS, improves *uv*-coverage!



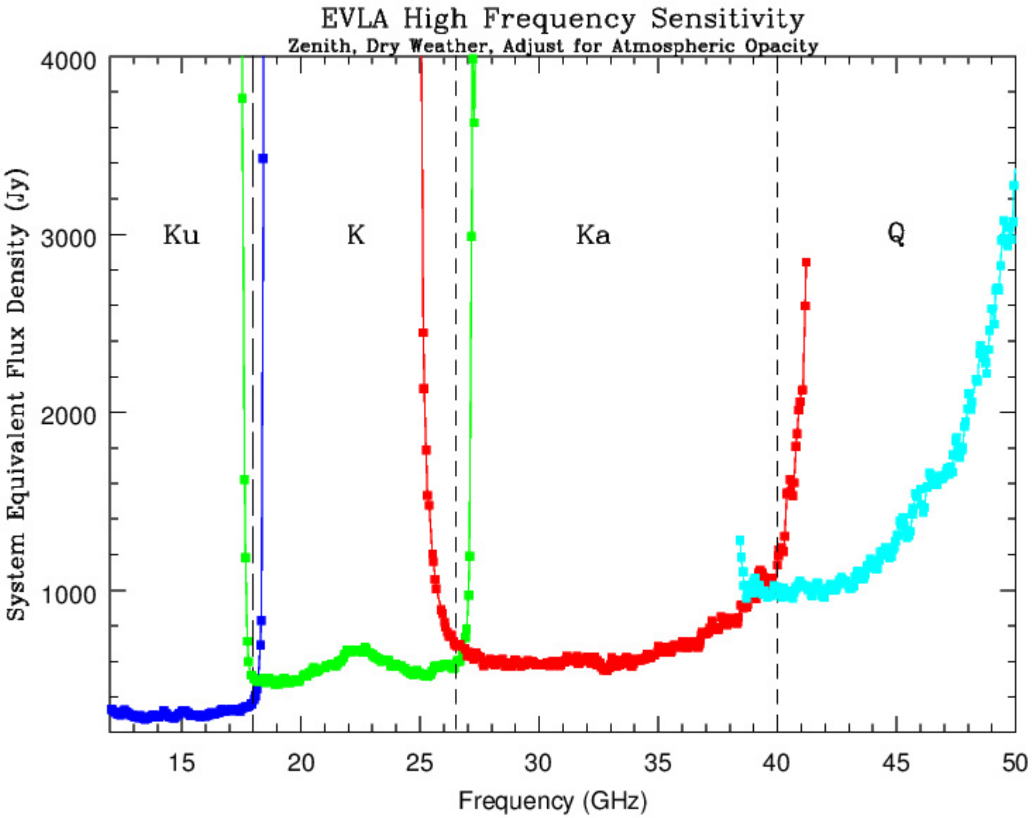
Observed image : $I_{\nu}^{obs} = I_{\nu}^{sky} * PSF_{\nu}$



$$I_{wb}^{obs} = \sum_{\nu} \left[I_{\nu}^{sky} * PSF_{\nu} \right]$$

Instrument frequency response

Impact of all system components as a function of frequency: antenna optics, receiver, amplifiers, back-end electronics, etc.



VLA Observing Guide.

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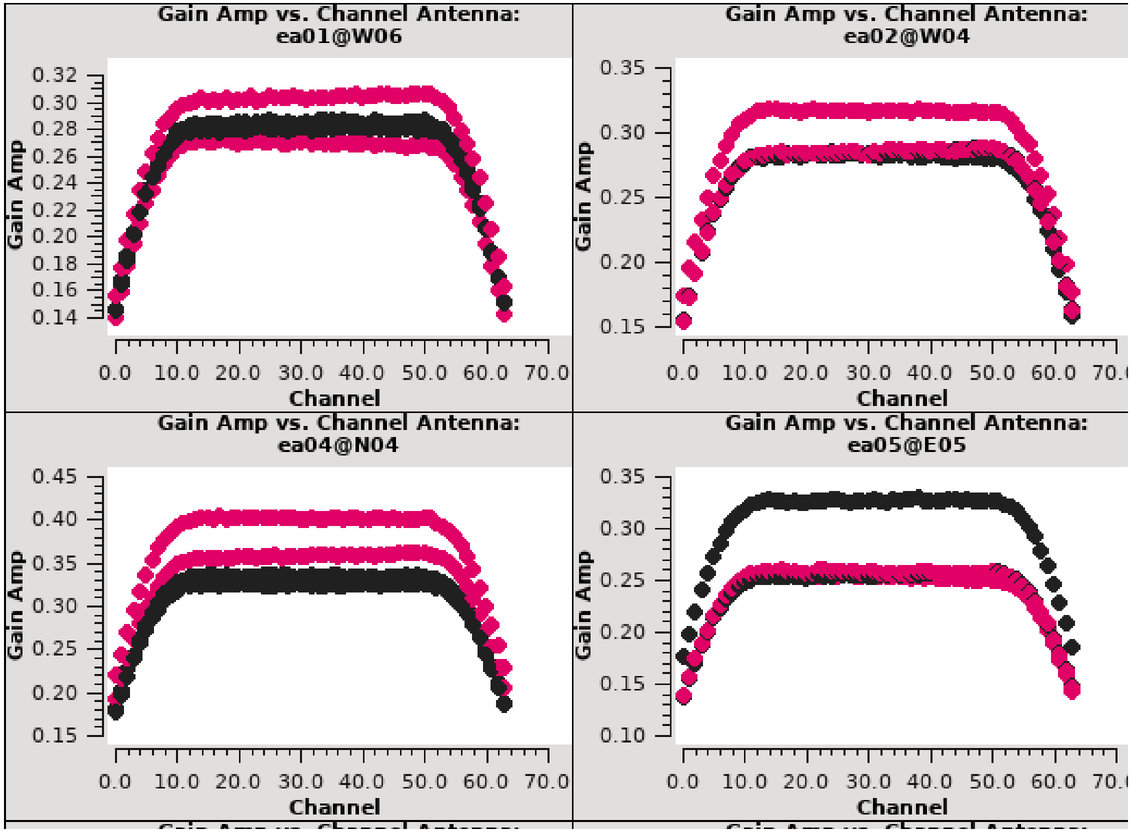


VLA IRC+10216 CASA Guide

Atmospheric opacity

The atmospheric opacity varies as a function of frequency with the primary contribution at cm & mm wavelengths from water (H2O), molecular oxygen (O2), and ozone (O3).

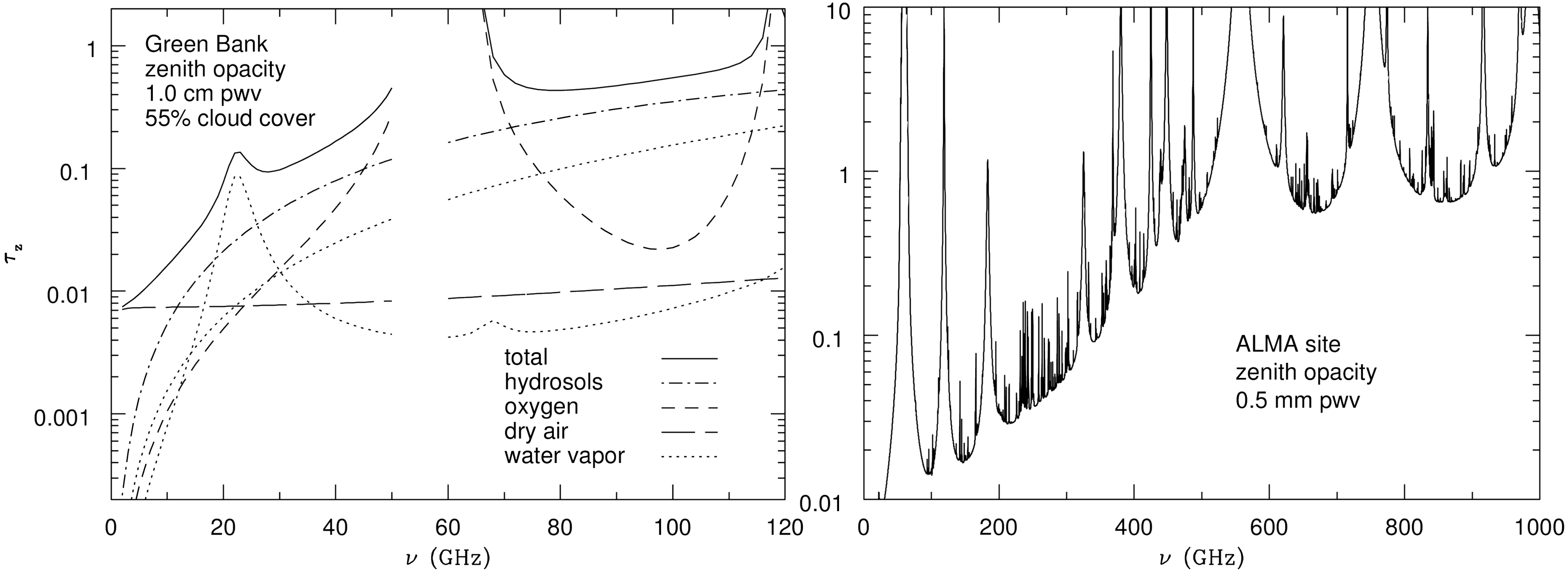
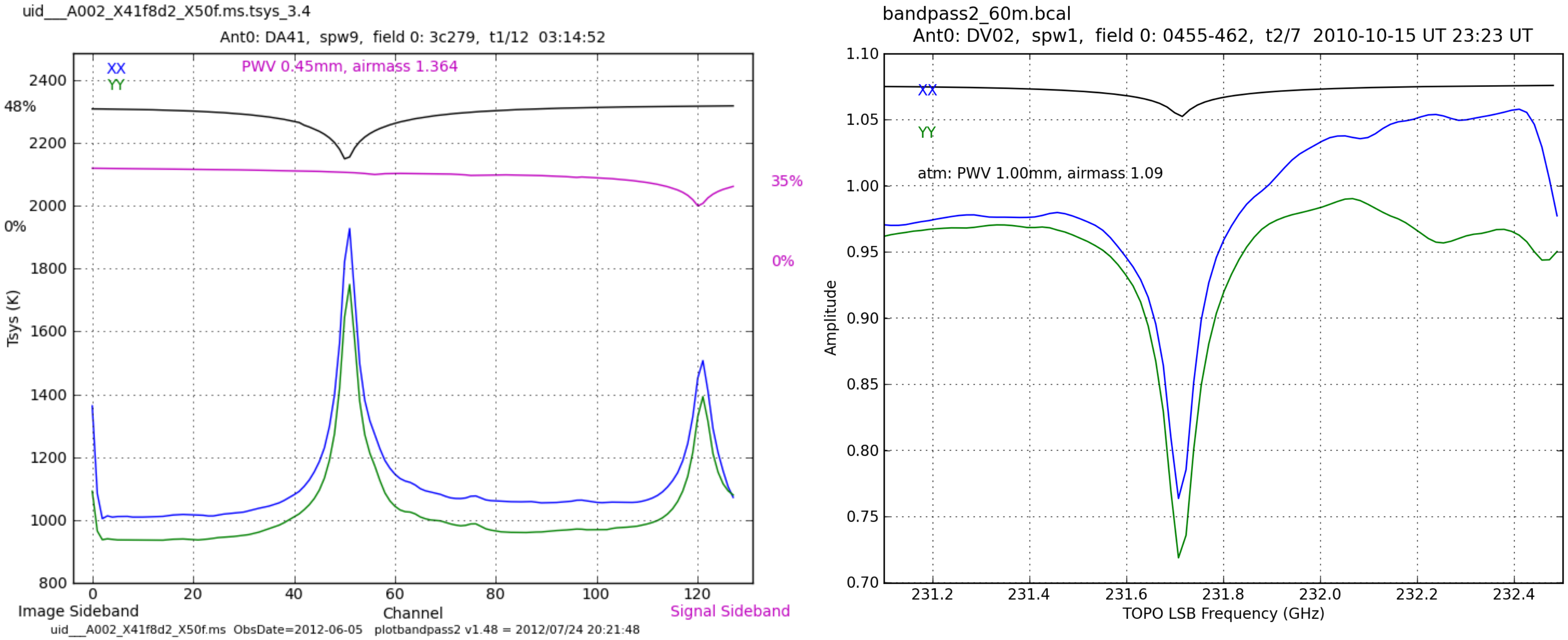


Figure credit: Condon & Ransom "Essential Radio Astronomy" Figs. 1.2 & 1.3

Atmospheric opacity

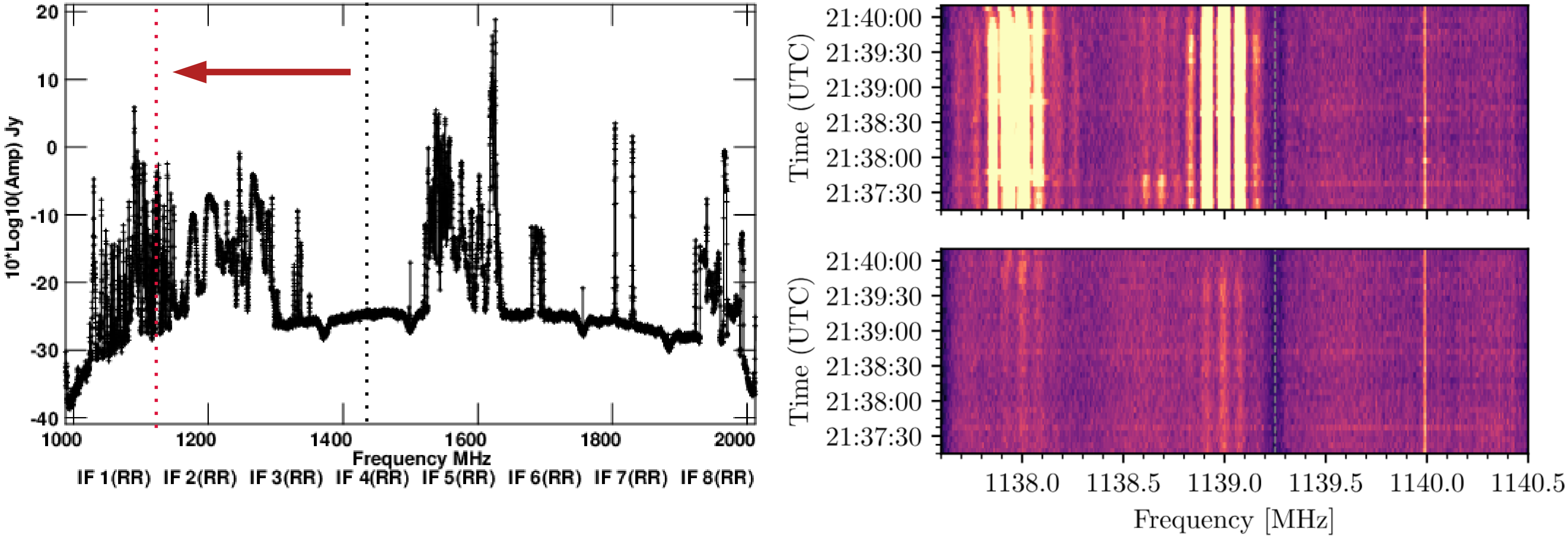


This ozone line near 231.7 GHz impacts the system temperature (left) and the bandpass solution (right), nearly doubling the system temperature and dropping the transmittance by ~30%!

Figure credit: https://casaguides.nrao.edu/index.php?title=Plotbandpass

Radio frequency interference (RFI)

Unlike continuum observations, lines must be observed at particular sky frequencies dictated by the rest frequency and source velocity.



(Left) VLA L Band RFI sweep from 2025. Ouch! Observable redshifts for HI are strongly impacted by the presence of RFI. This makes pre-correlation RFI mitigation (viz. flagging) important for lines.

Figure credit: NRAO VLA RFI page; Svoboda et al. (2023; IEEE Xplore)

Calibration

Concrete calibration steps for typical, modern multi-channel interferometer observations focused on spectroscopy:

- RFI flagging (post correlation data flagging and editing)
- Bandpass calibration
- Correlator effects (Hanning)
- Doppler corrections and reference frames
- Continuum subtraction

RFI flagging

RFI post-correlation flagging is necessary for most datasets below 15 GHz, but can be present at higher frequencies.

- Consider what the science goals require. Does a heavily impacted subband require careful flagging for only modest continuum bandwidth recovery? or are your target lines directly impacted and RFI *must* be flagged? (e.g., L Band OH @ 1612 MHz)
- Carefully review calibrator data: tends to be smaller quantities of data and cal tables are easier to quickly inspect than visibilities.
- Review calibrator data using time-frequency (“waterfall”) plots to identify narrowband RFI. Use calibrator data to tune parameters for automated flagging (e.g., tfcrop/aoflagger). Spot check results on the science target; perform expensive aggregations as needed.

RFI flagging in CASA: flagdata & tfcrop

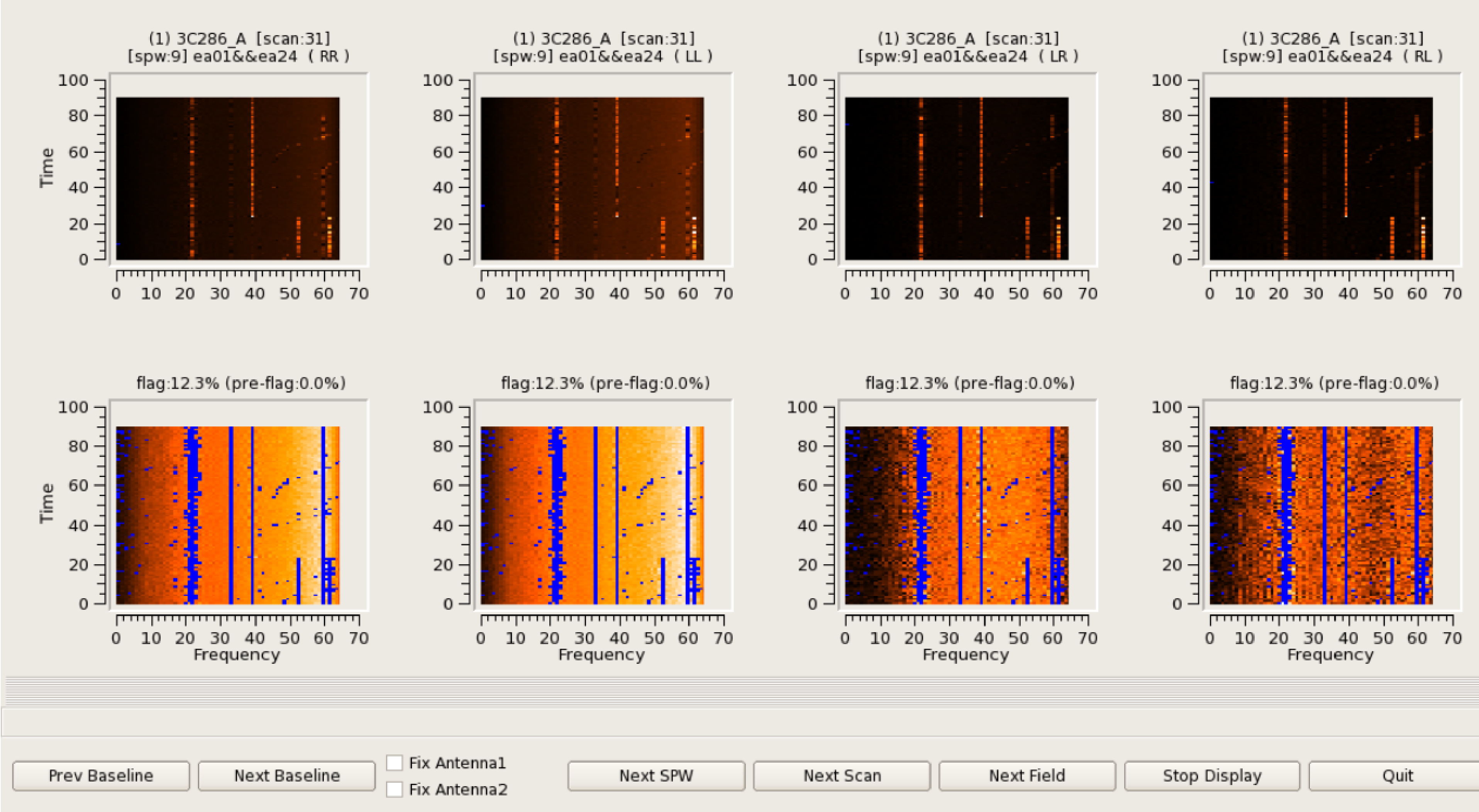


Figure credit: Urvashi Rao, 2013 Data Reduction Workshop

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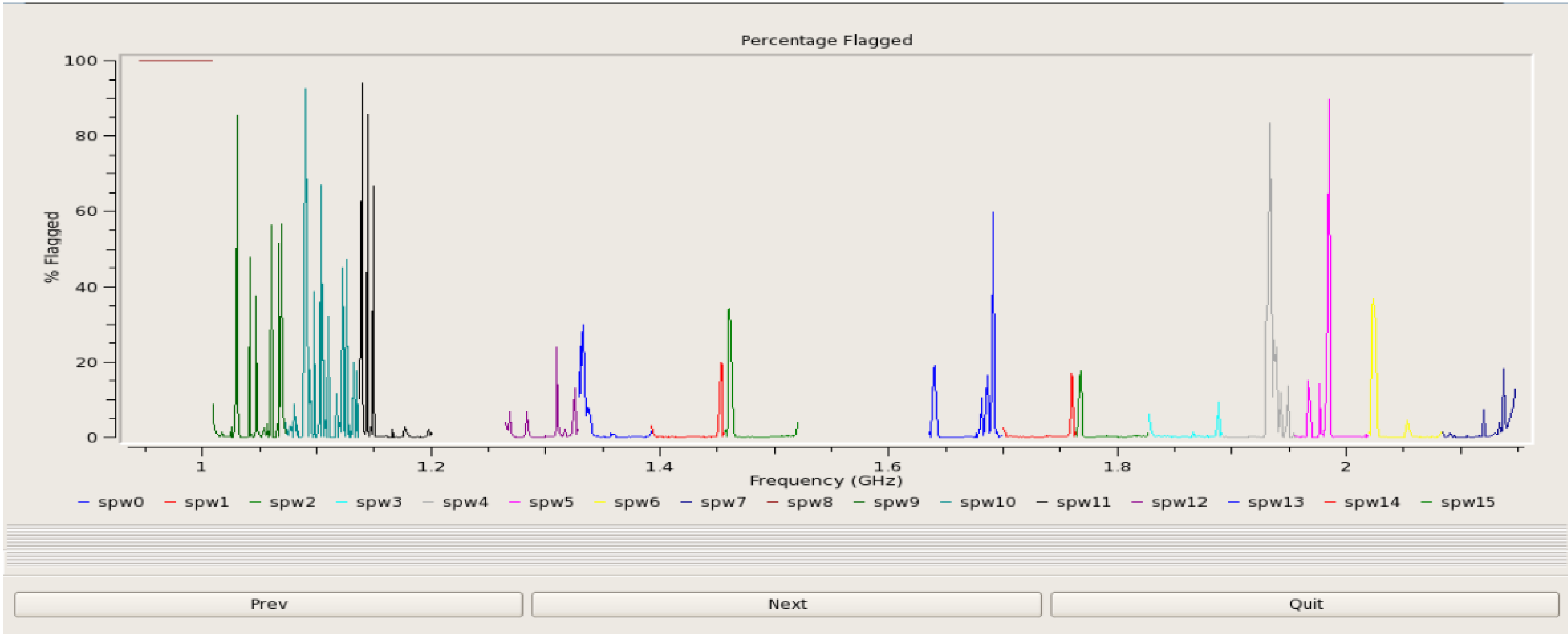

Figure credit: Urvashi Rao, 2013 Data Reduction Workshop

Bandpass calibration

Spectroscopy aims to detect and analyze spectral features, thus:

- Frequency dependent amplitude errors limit the ability of detecting weak emission and absorption lines.
- Frequency dependent amplitude errors can imitate changes in line profile shapes.
- Frequency dependent phase errors can lead to spatial offsets between spectral components, imitating motion.

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

Bandpass calibration: theory

The bandpass is the relative gain of an antenna (or baseline) as a function of frequency. Our aim with bandpass calibration is to correct for the discrepancy between the measured and ideal cases. We parametrize this scaling using complex gains.

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

Our instrumental effects vary on hour to day timescales, factor these into two terms for quickly-varying frequency-independent (G', e.g., the atmosphere) and slowly-varying frequency-dependent (B, e.g., analog filter response) terms.

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

SIRA II: Chap. 11 by M. Rupen, eq. 12.1

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

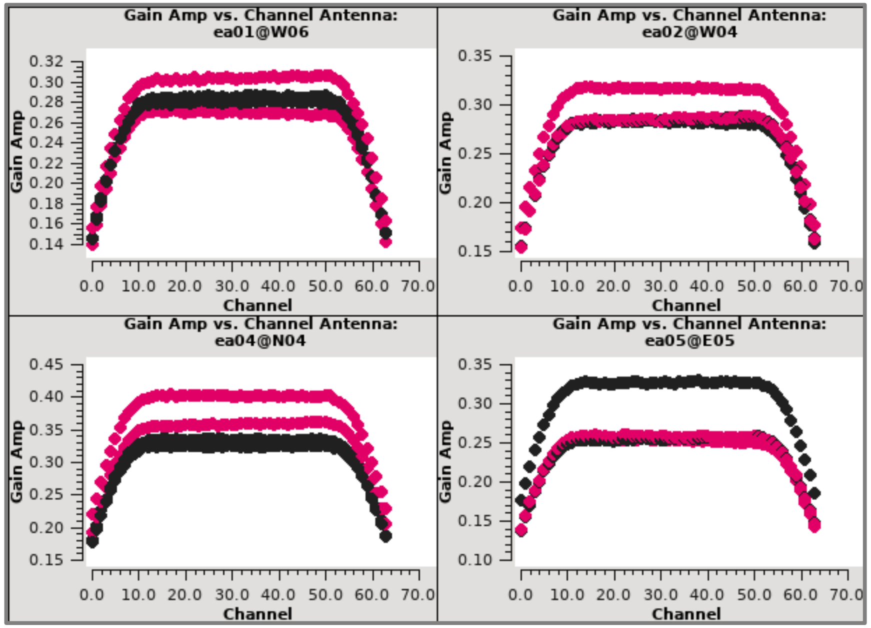
We further factor the bandpass terms into antenna based terms (viz. baseline based). This works well because the most significant sources of uncertainty **are** antenna based, it also improves SNR in the optimization.

$$B_{i,j}(t,\nu) \approx B_i(t,\nu) B_j^*(t,\nu)$$

SIRA II: Chap. 11 by M. Rupen, eq. 12.1

Bandpass calibration: practice

For the EVLA, the bandpass is mostly due to the electronics of individual antennas: analog filters of the front-end (ripples on tens of MHz scales) and subband filter roll-off (edges).



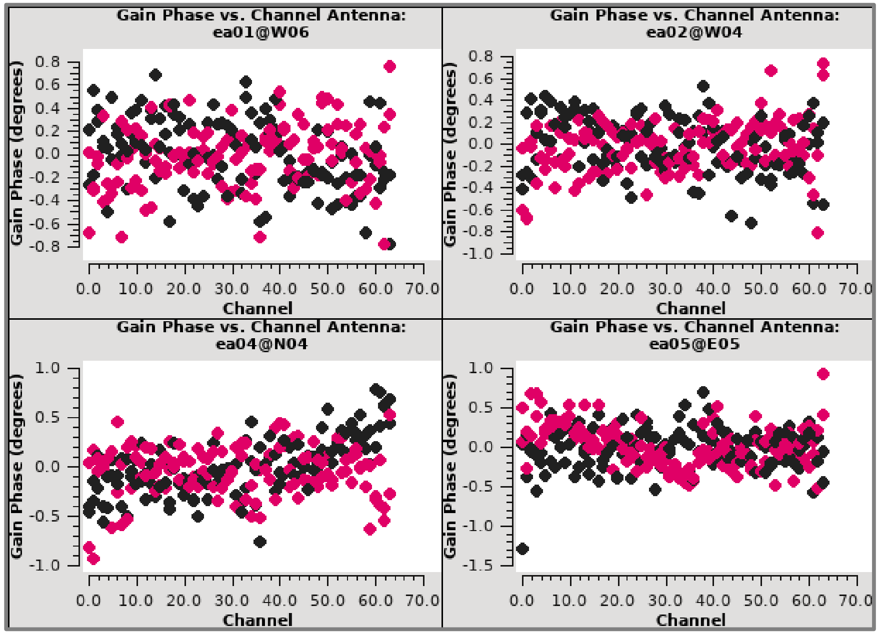


Figure credit: CASA Guide "VLA high frequency Spectral Line tutorial - IRC+10216"

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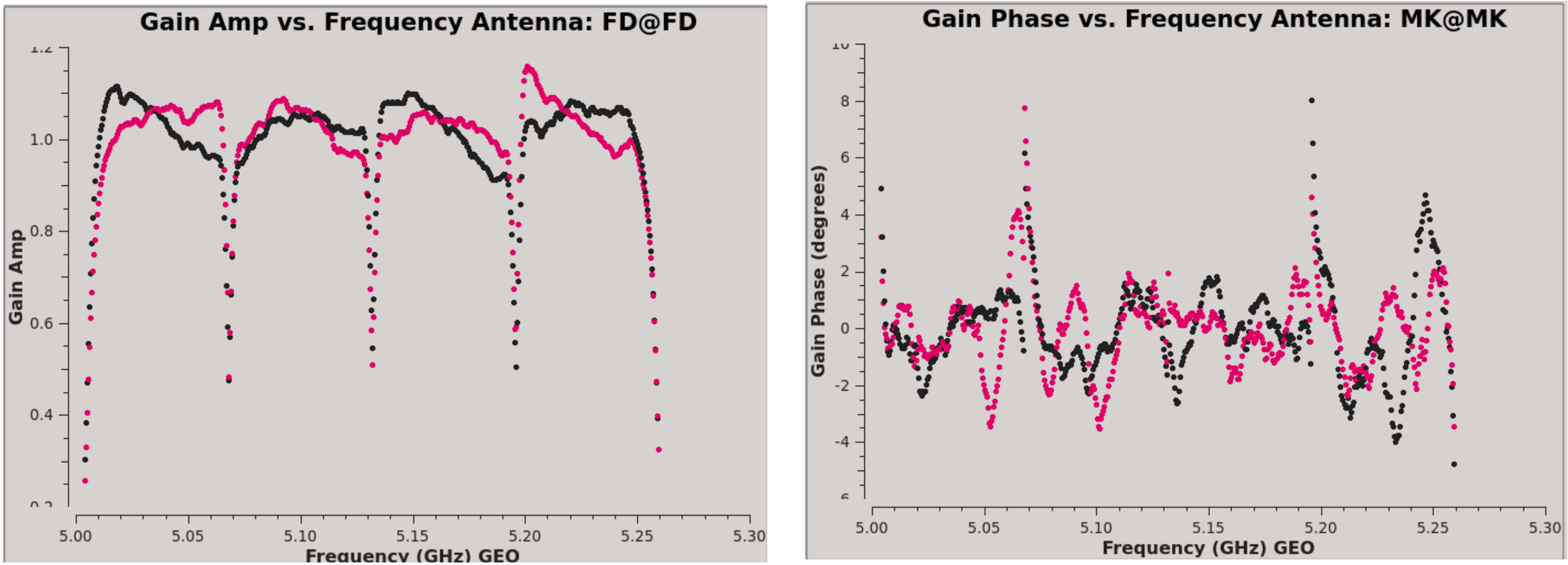


Figure credit: CASA Guide “VLBA Basic Phase-referencing Calibration and Imaging”

What to look for in a good bandpass?

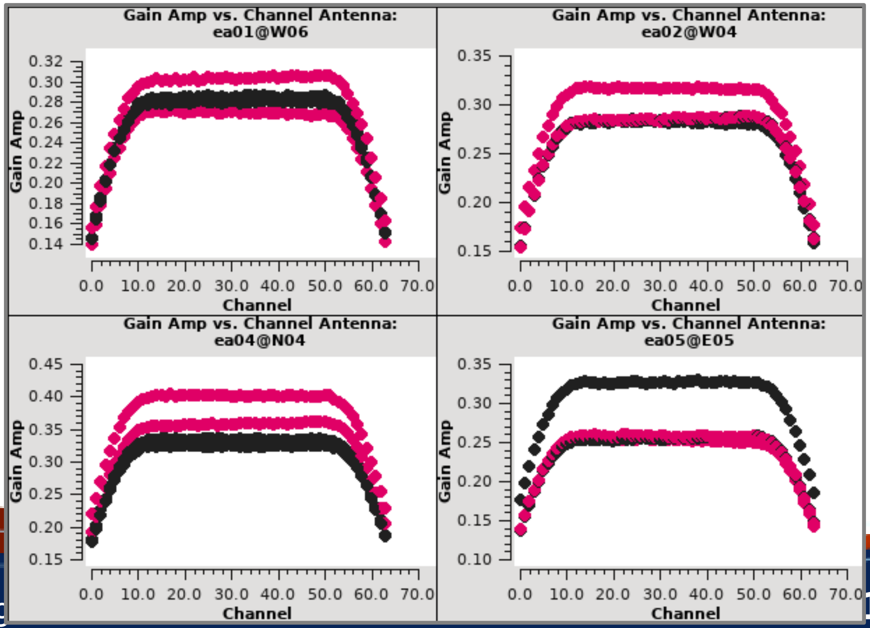
Flat gain amplitudes across center.

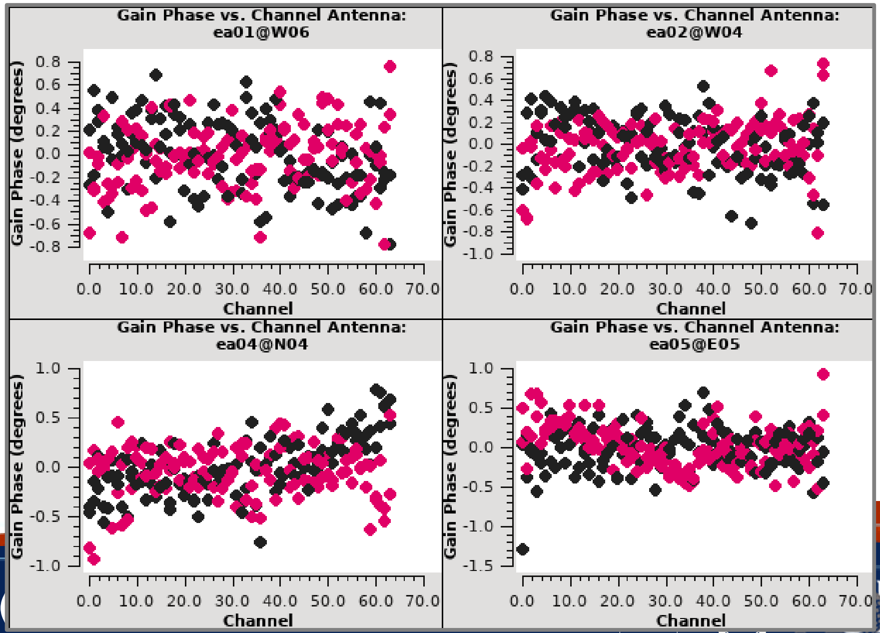
Near zero gain phase with modest slope.

Solutions comparable across antennas.

No obvious statistical noise.

No absorption lines or spikes.





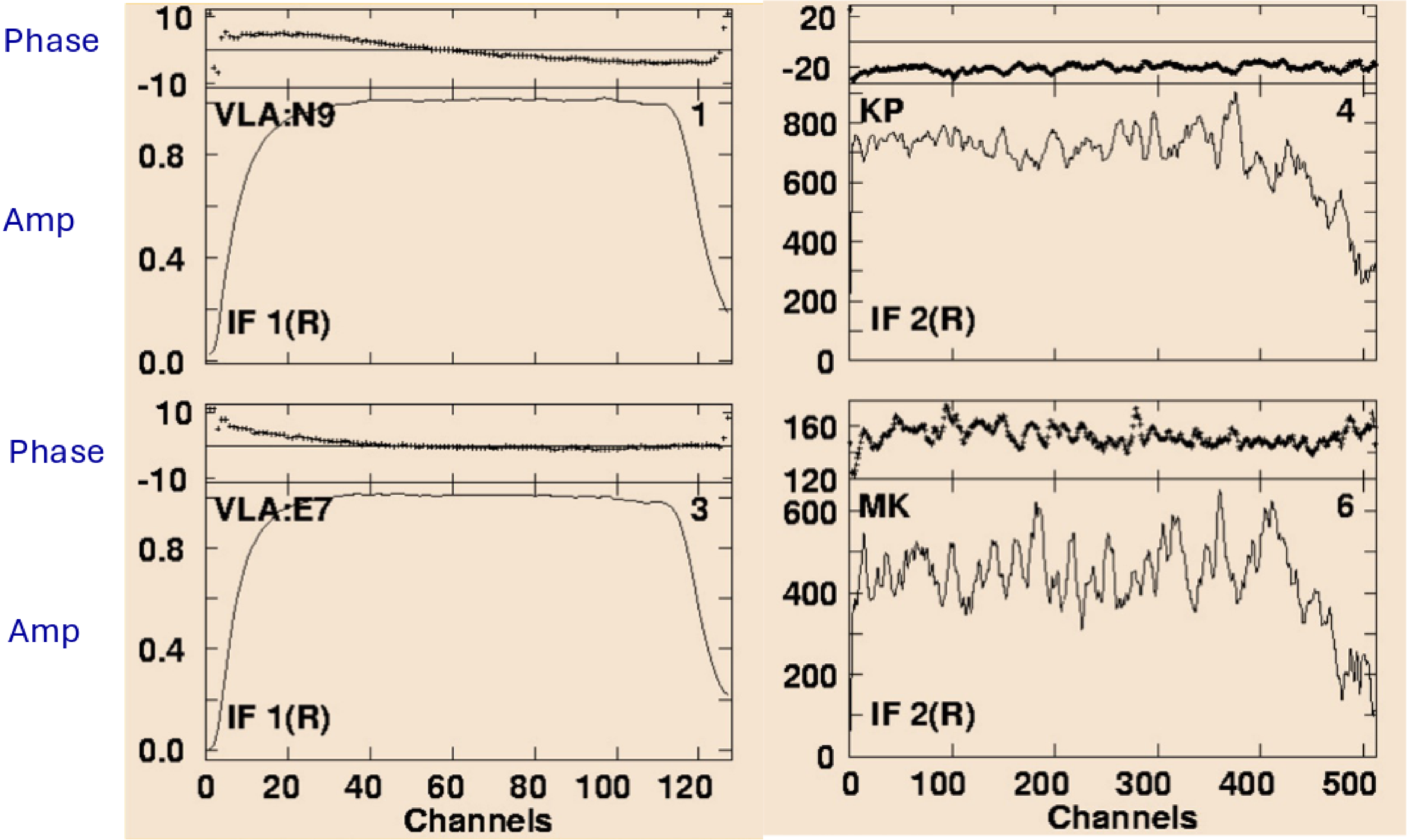


Figure credit: Ylva Pihlstrom SIW 2024

How can I get good bandpass calibration?

Simple: observe a bright calibrator for long enough! In detail, all of your target and secondary calibrator observations will be divided by bandpass, so it needs to be measured at high-enough SNR that it doesn't introduce appreciable noise.

A good rule of thumb when preparing your observations is:

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

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

Presumes channel-independent solutions, although can gain some sensitivity with polynomial fitting. Bright masers can be an exception if they are narrow (bandpass is smooth).

Doppler correction

In order to tune to the appropriate sky frequency we must account for the relative motion between the observer frame (Earth surface, topocentric) and the source frame (e.g., a velocity known in LSRK).

The primary contributors are the Earth's rotation and orbital motion around the Solar System barycenter. If unaccounted for, lines may fall outside of observed subbands!

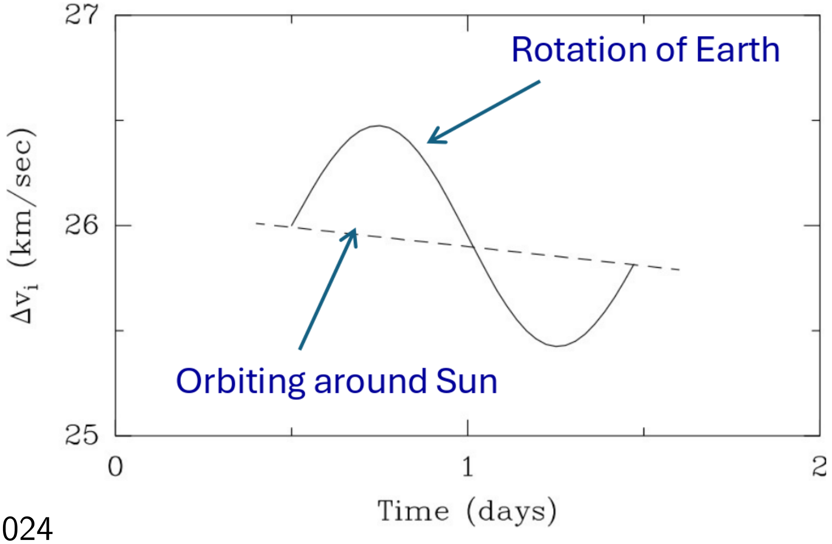


Figure credit: Ylva Pihlstrom SIW 2024

Doppler correction: reference frames

Rest Frame	Corrected for...	Amp. of correction
Topocentric	Nothing!	0.0
Geocentric	Earth rotation	0.5
Earth-Moon Barycentric	Effect of the Moon on Earth	0.013
Heliocentric	Earth’s orbital motion	30
Solar System **Barycentric**	Effect of planets on the Sun	0.012
Local Standard of Rest	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

See Table 11-1 SIRA II Chap. 11 by D. Westpfahl

Doppler correction: velocity definitions

Velocity values depend on either the “radio” or “optical” definitions in order to convert from a measured frequency and a rest frequency.

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

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

Make sure to use the correct definition for your target! The differences can be significant for extragalactic sources.

See Eqs. 11-5 & 11-7 SIRA II Chap. 11 by D. Westpfahl

Doppler correction: online and offline

The VLA performs Doppler *setting* rather than *tracking* by applying an offset for the appropriate frame, source velocity, and direction at the start of the observation.

Post-processing tasks like `tclean` apply Doppler correction on the fly, but some tasks such as `gaincal` when used for self-calibrating on a single, narrow channel of a strong maser require velocity coordinate transformations up-front (e.g., using `cvel2`).

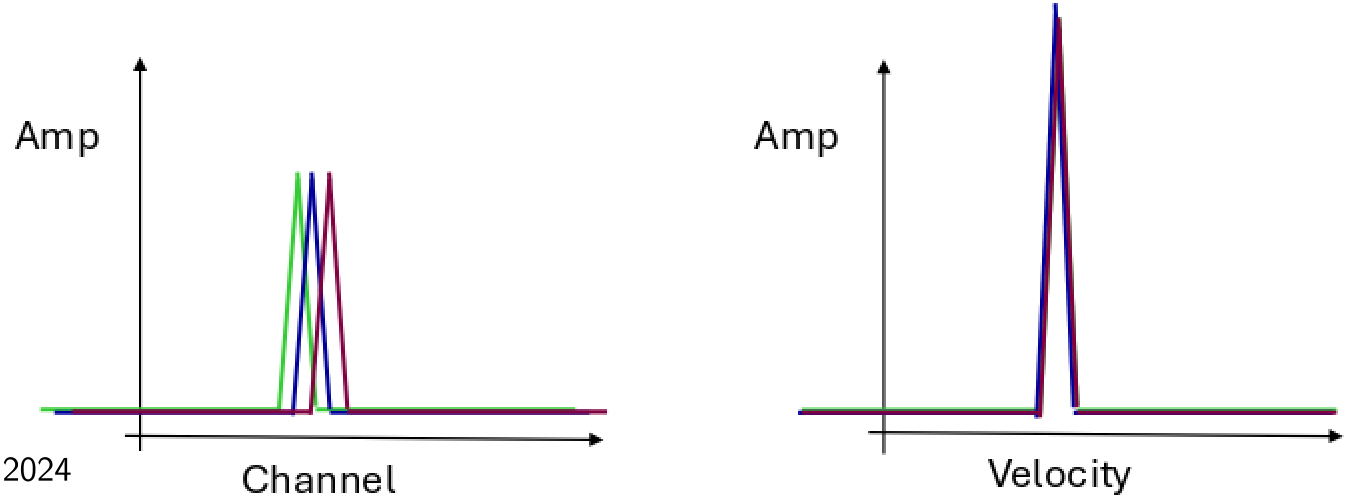


Figure credit: Ylva Pihlstrom SIW 2024

Continuum subtraction

Spectral line analysis techniques often require subtracting the continuum contribution to the flux, leaving just the spectral line emission. This can be done in CASA via three main strategies:

- **`uvcontsub`** – performs continuum fitting and subtraction in the *uv*-domain. The continuum fit degrades with distance from the phase center and may not be suitable for multiple bright sources.
- **`imcontsub`** – estimate and subtracts continuum emission in the image domain. Requires deconvolving the continuum plus lines in one cube.
- **`uvsub`** – Image continuum, save model, and subtract the resulting model directly from the visibilities. Most accurate method.

Note that while the `*contsub` tasks produce continuum fits, continuum images should be made through multi-frequency synthesis CLEAN on the line-free channels.

Continuum subtraction: trade-offs

All methods require some trade-off in terms of accuracy versus convenience. The CASA notebook “UV Continuum Subtraction” provides in-depth discussion on the topic.

- Subtraction in the *uv*-domain is desirable if continuum emission dominates the source: deconvolution of the line emission will be more robust if it is not subject to the deconvolution errors of the brighter continuum.
- There is also a performance penalty to deconvolving each channel’s continuum contribution in a cube.
- However, fitting a polynomial to the *visibility spectrum* is only a good approximation for a single source near the phase center, otherwise it can produce artifacts due to bandwidth smearing.
- Cornwall+ (1992), Sault (1994): *uv*-domain based algorithms in detail.

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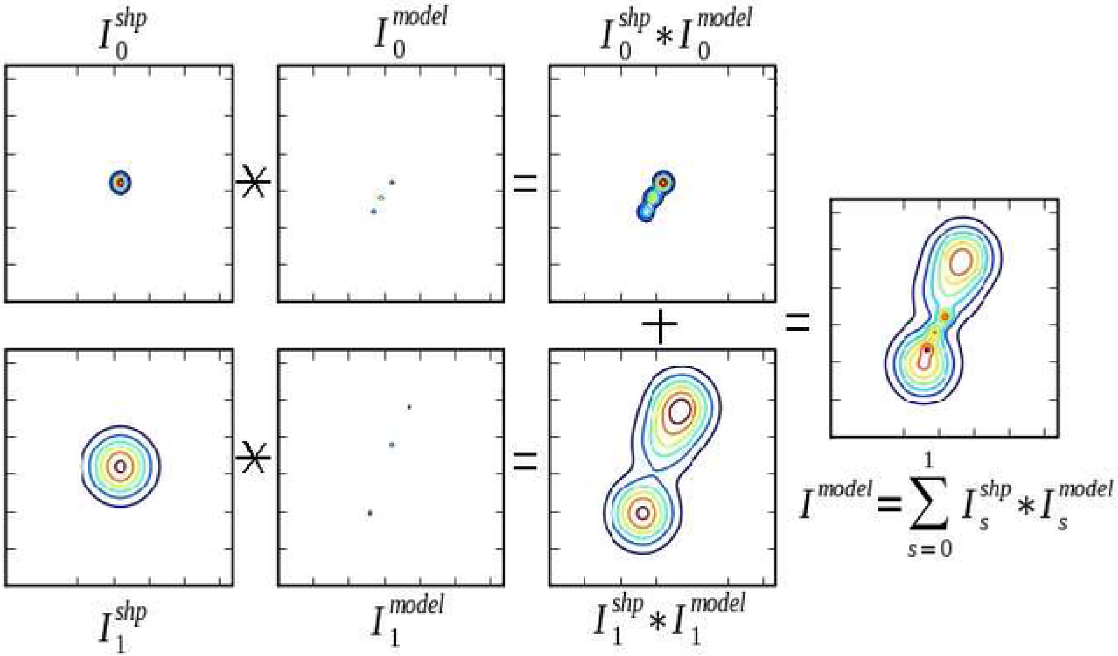
Use **`uvcontsub`** if emission is bright, compact, and mostly nearly the phase center.

Use **`imcontsub`** if emission is extended across the primary beam and is relatively weak.

Generate a continuum model and subtract it with **`uvsub`** if bright, complex continuum is present. If self-calibrating the continuum, this method comes nearly for free.

Imaging extended emission

Although not unique to spectral line data, line emission is often spatially extended. Multiscale CLEAN and adaptive-scale pixel (ASP) CLEAN both provide better deconvolution of extended emission than the standard Cotton-Schwab/Hogbom CLEAN.



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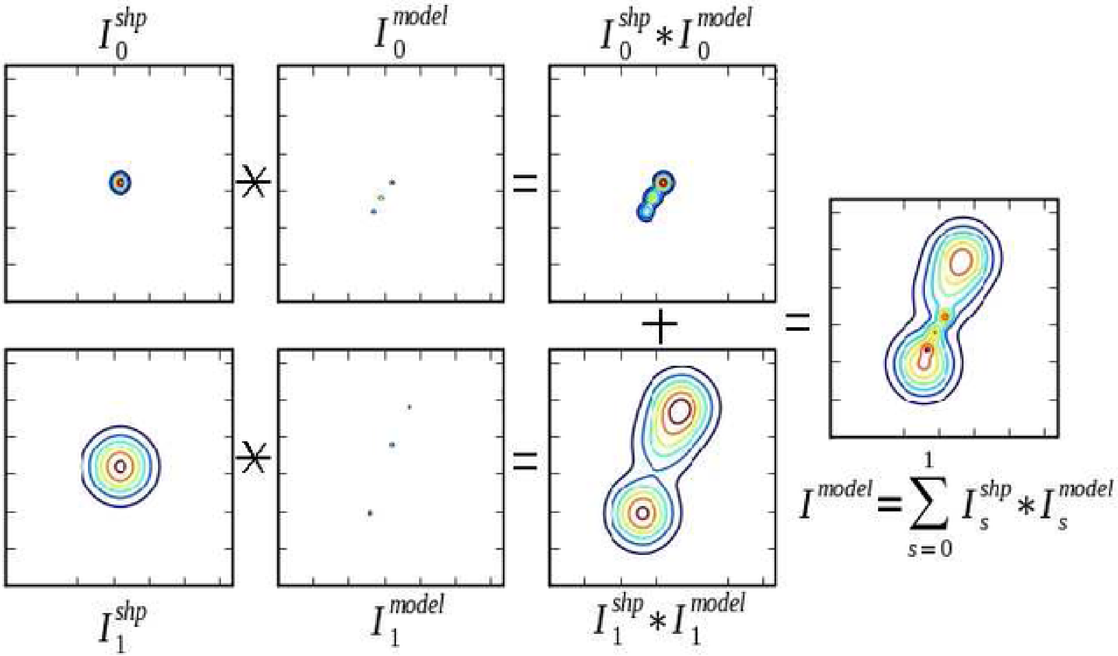

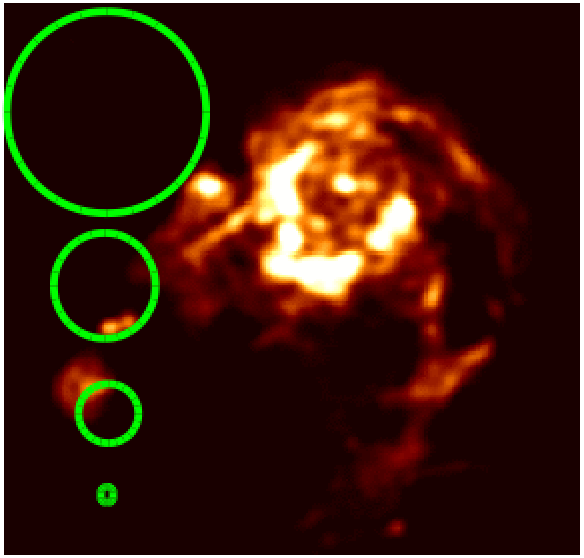

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```
tclean(
    ...
    deconvolver='multiscale',
    scales=[0, 3, 9],
)
```

Described in Cornwell (2008), multiscale CLEAN uses Gaussian model components in addition to pixel size delta-functions to model extended emission.

The `scales` parameter defines the width of the component Gaussians in pixels. The 0 scale corresponds to a delta-function.

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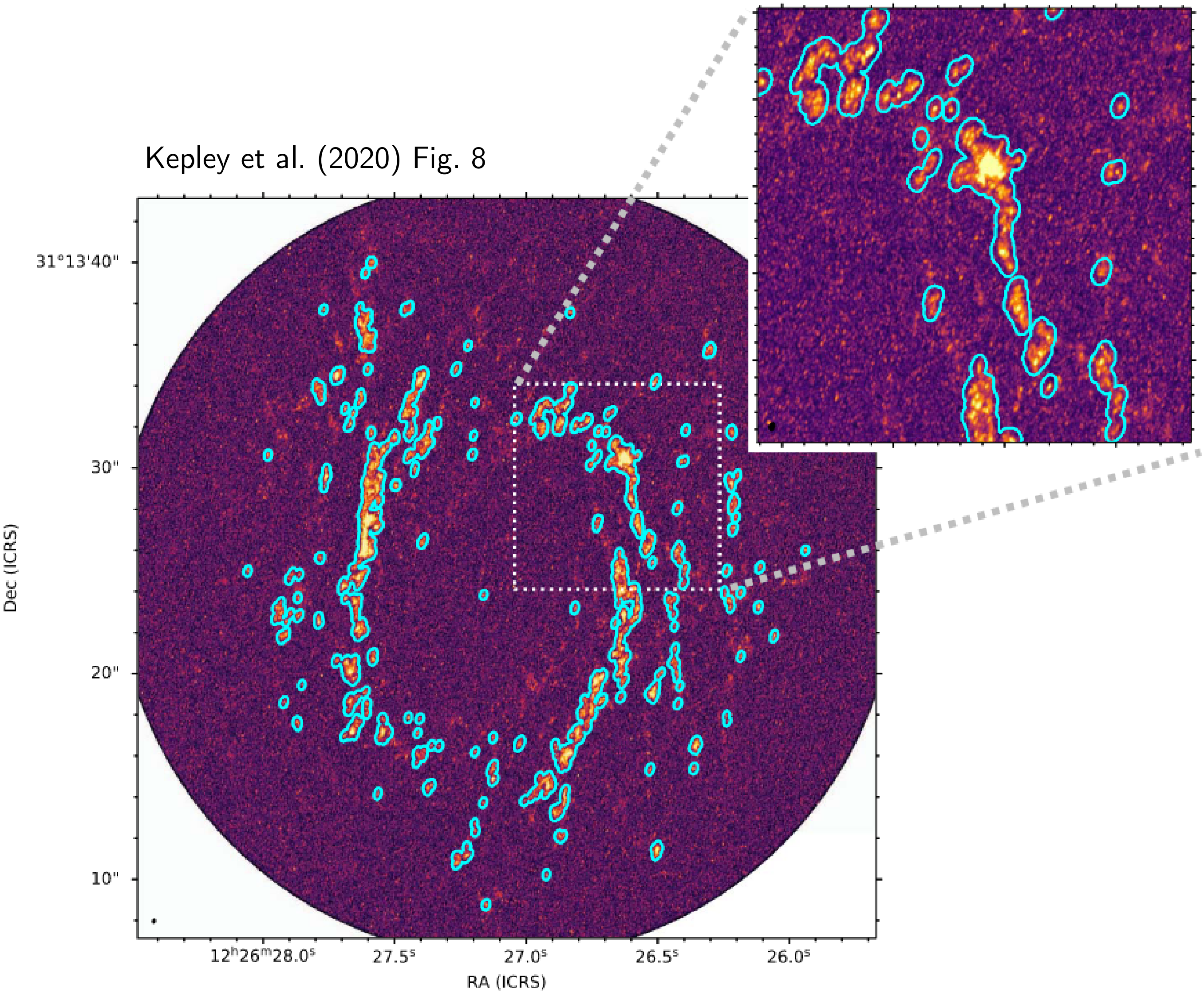
```
tclean(
    ...
    deconvolver='asp',
)
```

Described in Bhatnagar & Cornwell (2004), ASP CLEAN adaptively selects the scale sizes and unlike multiscale CLEAN they do not need to be explicitly set.

Kepley et al. (2020) Fig. 8



Automasking with auto-multithresh

The auto-multithresh algorithm iteratively grows a CLEAN mask based on the SNR and sidelobe thresholds in the image. This method mimics the manual masking process of masking significant emission and increasing it encompass fainter emission as one CLEANs more deeply.

CASA Guide – https://casaguides.nrao.edu/index.php/Automasking_Guide

Kepley et al. (2020) – `DOI 10.1088/1538-3873/ab5e14`

Automasking with auto-multithresh

The auto-multithresh algorithm iteratively grows a CLEAN mask based on the SNR and sidelobe thresholds in the image. This method mimics the manual masking process of masking significant emission and increasing it encompass fainter emission as one CLEANs more deeply.

`usemask=''auto-multithresh''` – enable auto-multithresh

`noisethreshold` – SNR threshold above which emission is masked

`sidelobethreshold` – sidelobe threshold above which emission is masked

`minbeamfrac` – minimum region size as fraction of the beam size

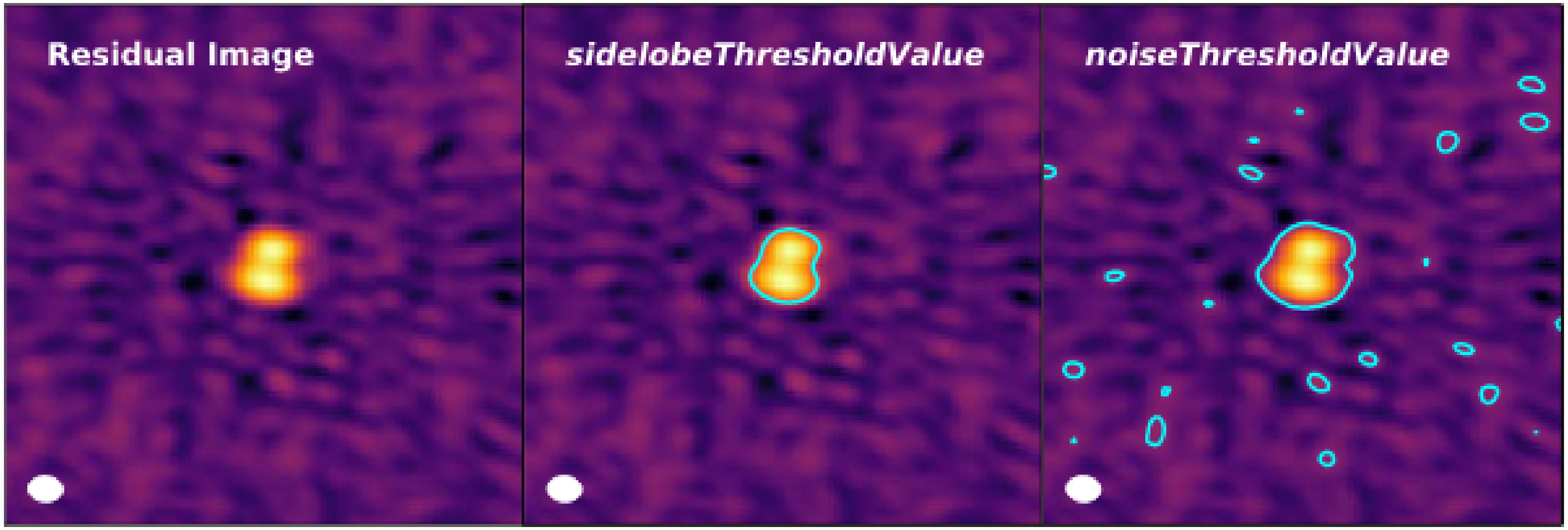
`lownoisethreshold` – SNR threshold that mask is grown down to

`negativethreshold` – SNR threshold for absorption features to be masked

See the automasking guide for further description of secondary parameters.

Automasking: multiple thresholds

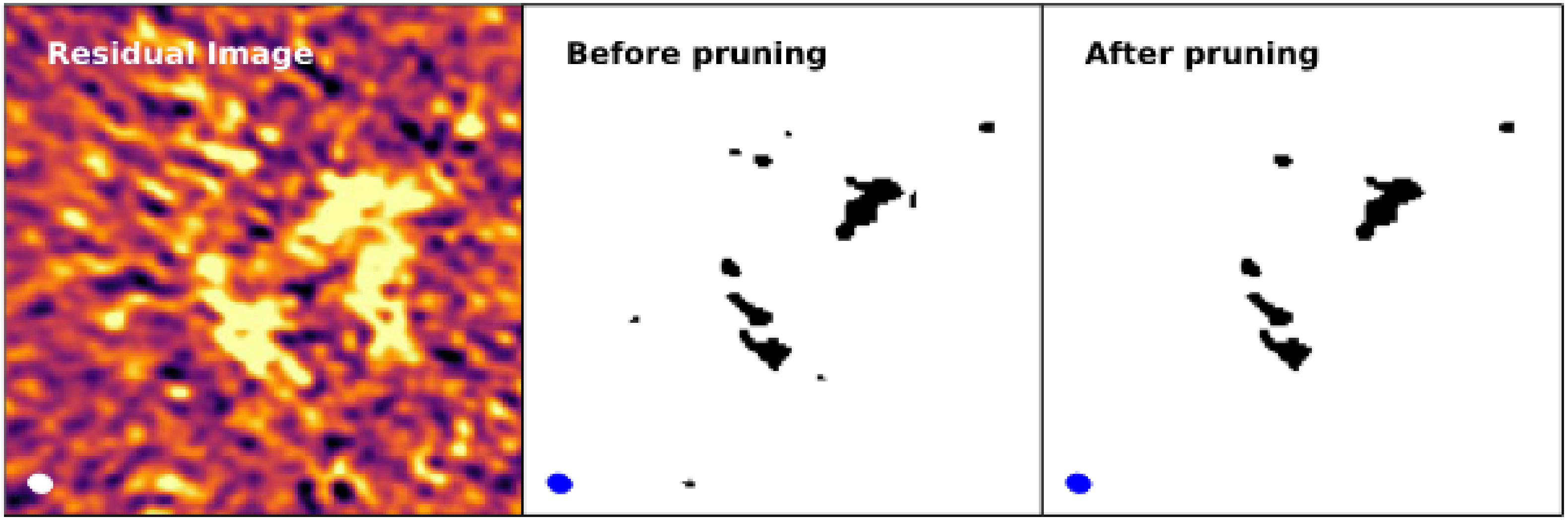
Auto-multithresh estimates two image thresholds and determines which is greater. The threshold based on the side-lobe level of the peak residual is likely to be greater initially. The second threshold, based on a multiple of the image RMS, is likely to be greater after partially CLEANing the image.



Kepley et al. (2020) Fig. 2

Automasking: pruning small regions

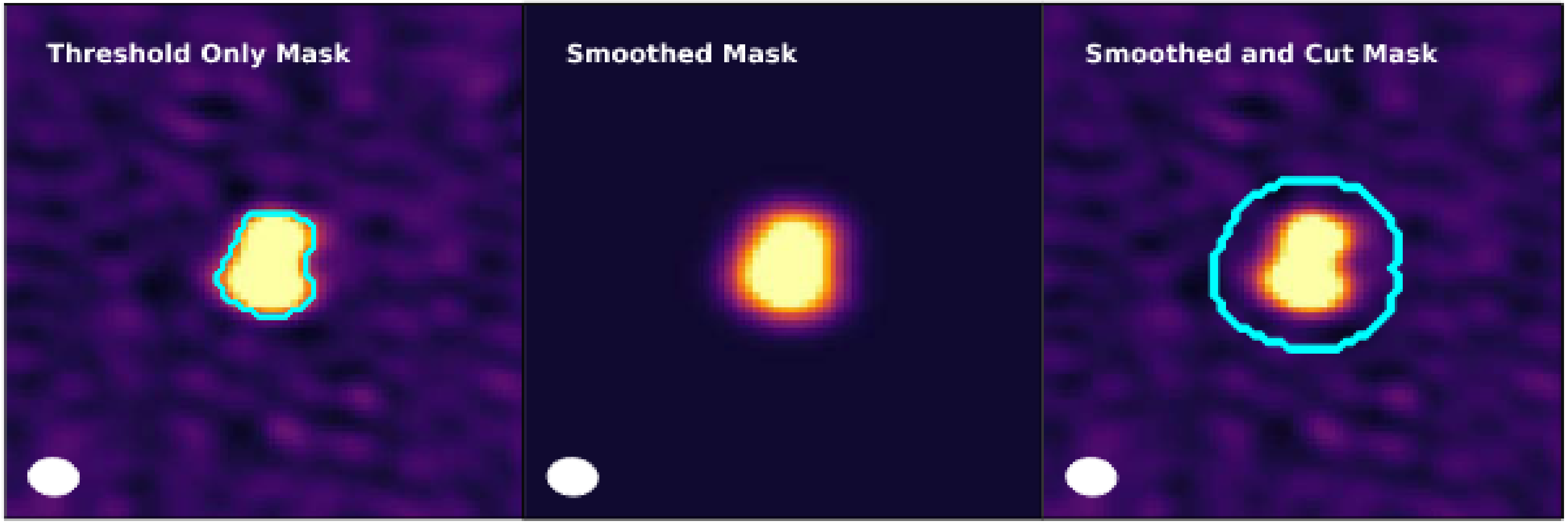
The noise-based threshold is likely to suffer from false positives by masking small noise spikes. Regions in the mask are pruned based on if they are smaller than a minimum area relative to the synthesized beam (in blue below). Typical values are 0.1 to 0.3.



Kepley et al. (2020) Fig. 3

Automasking: growing the mask

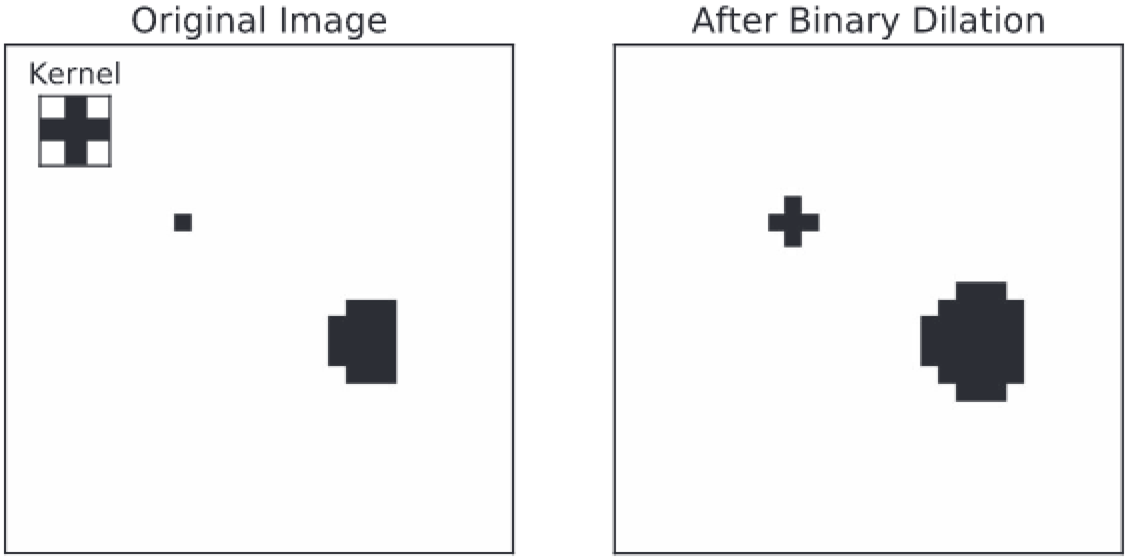
The selected and pruned mask is then smoothed and cut to extend partially beyond the initial masked region. These are secondary parameters that may need to be tuned in rare circumstances.



Kepley et al. (2020) Fig. 4

Automasking: growing the mask

The smoothed mask is then iteratively grown through a technique "binary dilation" in imaging processing. This process is similar to convolution and is used to grow the mask down to a configurable low-noise threshold. Typical values of the low-noise threshold may be one or two times the image RMS.

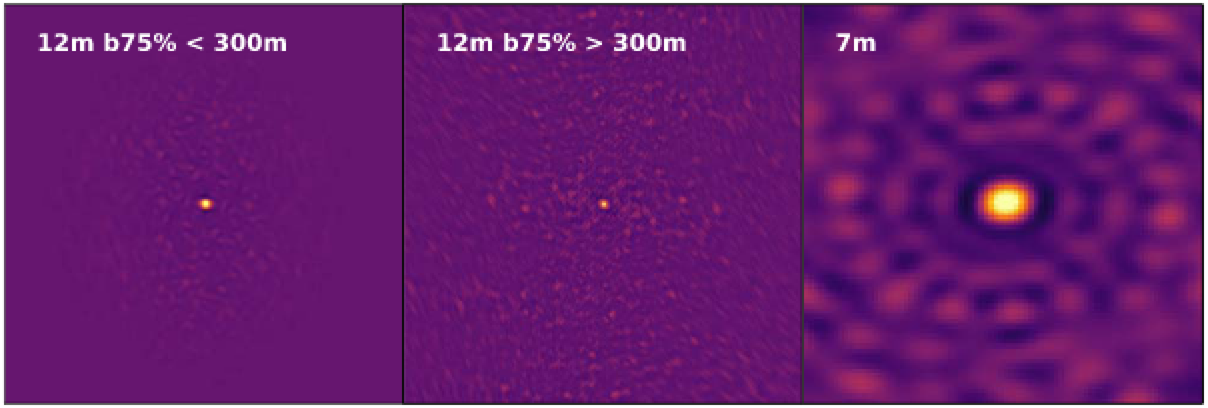


Kepley et al. (2020) Fig. 5

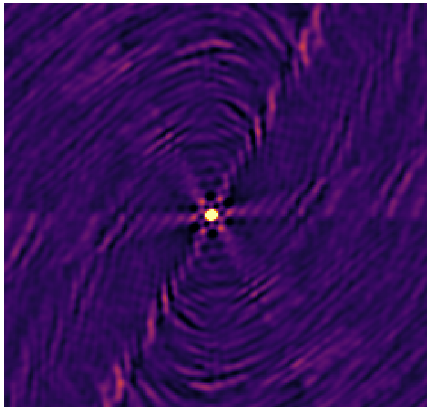
Automasking: parameter tuning

To achieve optimal results, the parameters for auto-multithresh need to be tuned. The parameters are particularly sensitive to the PSF.

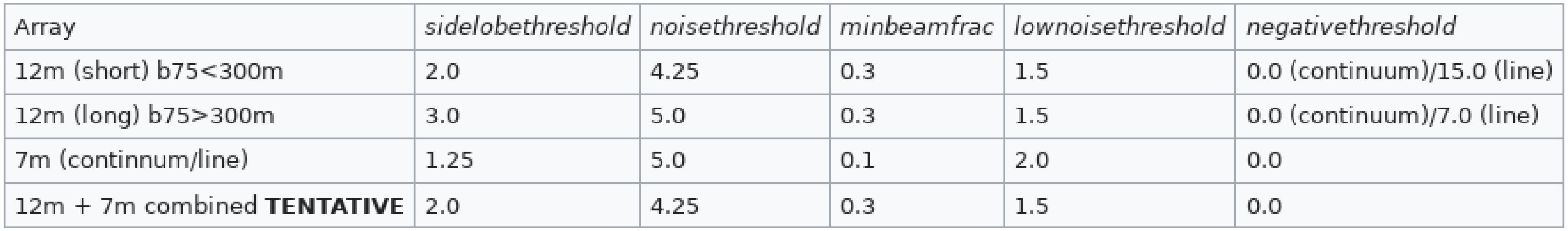
ALMA short baselines, long-baselines, and ACA 7m array



VLA Ka low-dec for 2hr



Kepley et al. (2020) Fig. 10



Array	*sidelobethreshold*	*noisethreshold*	*minbeamfrac*	*lownoisethreshold*	*negativethreshold*
12m (short) b75<300m	2.0	4.25	0.3	1.5	0.0 (continuum)/15.0 (line)
12m (long) b75>300m	3.0	5.0	0.3	1.5	0.0 (continuum)/7.0 (line)
7m (continnum/line)	1.25	5.0	0.1	2.0	0.0
12m + 7m combined **TENTATIVE**	2.0	4.25	0.3	1.5	0.0
Above VLA dataset	0.5	4.0	0.1	1.0	1000.0

Tools for analyzing spectral lines

While analysis is highly goal dependent, inspection of **moment maps**, **PV diagrams**, **line frequency querying**, **spectral smoothing**, and **line model fitting** are common practices.

- CARTA (user interface examples)
- Python community tools: `astropy`, `pyspeckit`, `spectral-cube`
- CASA, AIPS, etc.
  - Moment maps: `immoments`, `ia.moments`, `specflux`
  - PV diagrams: `impv` (casaviewer)
  - Gaussian fitting: `specfit` (casaviewer)
  - Spectral smoothing: `specsmooth` (casaviewer)
  - Line querying: casaviewer

CASA: moment maps and aperture sums

Moment maps can be generated in CASA using the `immoments` task. For more complex masking and smoothing use the `ia.moments` task.

```
rms = 0.003  # Jy
inf = 1e8
immoments(
    imagename=’my.image’,
    moments=[0,1,2,8],
    includepix=[4*rms,inf],
    outfile=’my_moments’,
)
```

$$M_0 = \Delta v \sum_i I_i$$

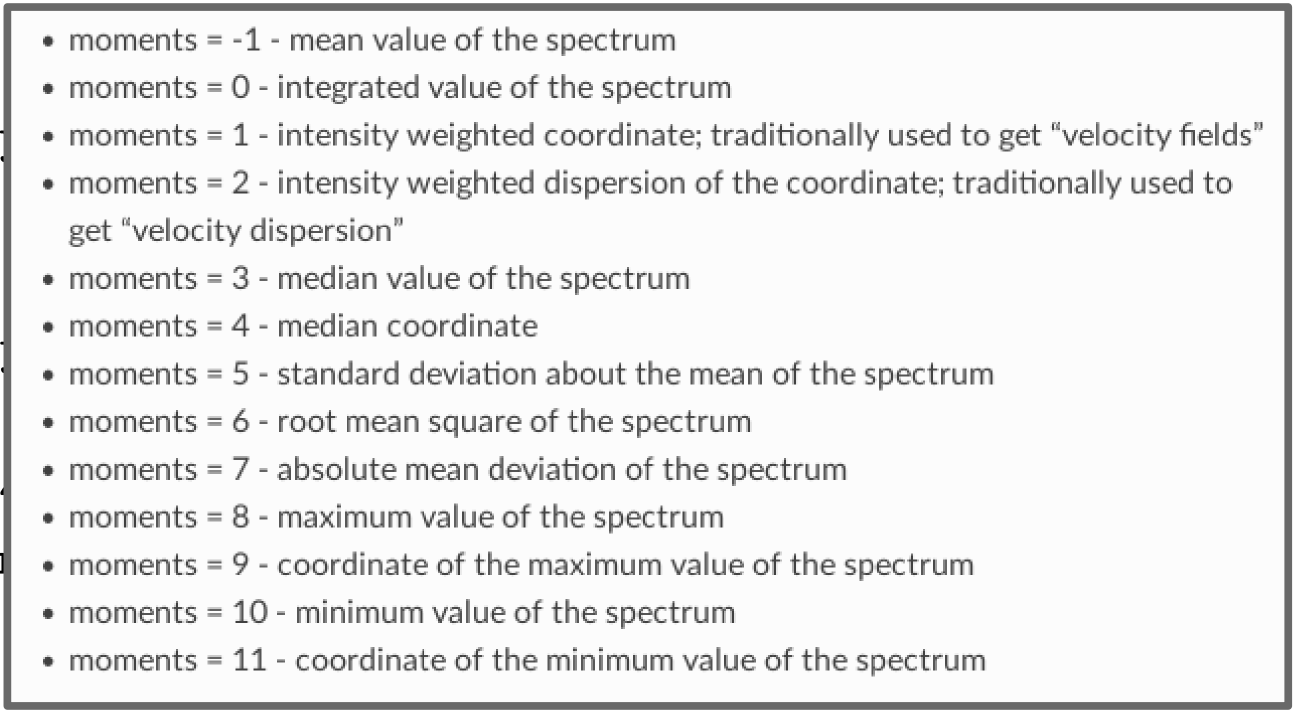
$$M_1 = \frac{1}{M_0} \sum_i I_i v_i$$

$$M_2 = \sqrt{\frac{1}{M_0} \sum_i I_i \left(v_i - M_1\right)^2}$$

CASA: moment maps and aperture sums

Moment maps can be generated in CASA using the `immoments` task. For more complex masking and smoothing use the `ia.moments` task.

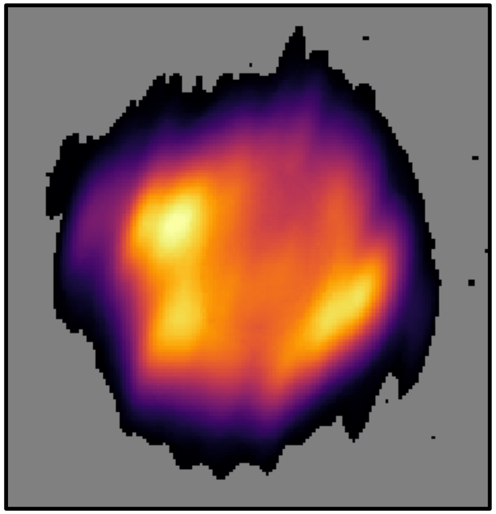
```
rms = 0.003  # J
inf = 1e8
immoments(
    imagename='m
    moments=[0,1
    includepix=[
    outfile='my_
)
```



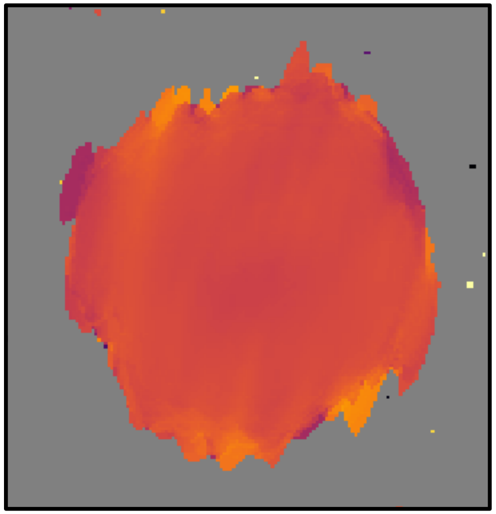
- moments = -1 - mean value of the spectrum
- moments = 0 - integrated value of the spectrum
- moments = 1 - intensity weighted coordinate; traditionally used to get "velocity fields"
- moments = 2 - intensity weighted dispersion of the coordinate; traditionally used to get "velocity dispersion"
- moments = 3 - median value of the spectrum
- moments = 4 - median coordinate
- moments = 5 - standard deviation about the mean of the spectrum
- moments = 6 - root mean square of the spectrum
- moments = 7 - absolute mean deviation of the spectrum
- moments = 8 - maximum value of the spectrum
- moments = 9 - coordinate of the maximum value of the spectrum
- moments = 10 - minimum value of the spectrum
- moments = 11 - coordinate of the minimum value of the spectrum

CASA: moment maps and aperture sums

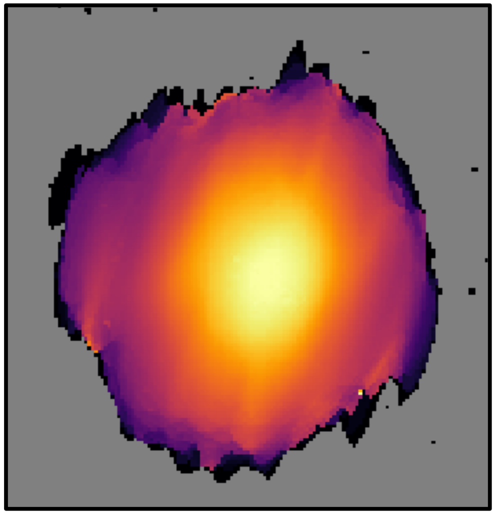
Moment maps can be generated in CASA using the `immoments` task. For more complex masking and smoothing use the `ia.moments` task.



Moment 0

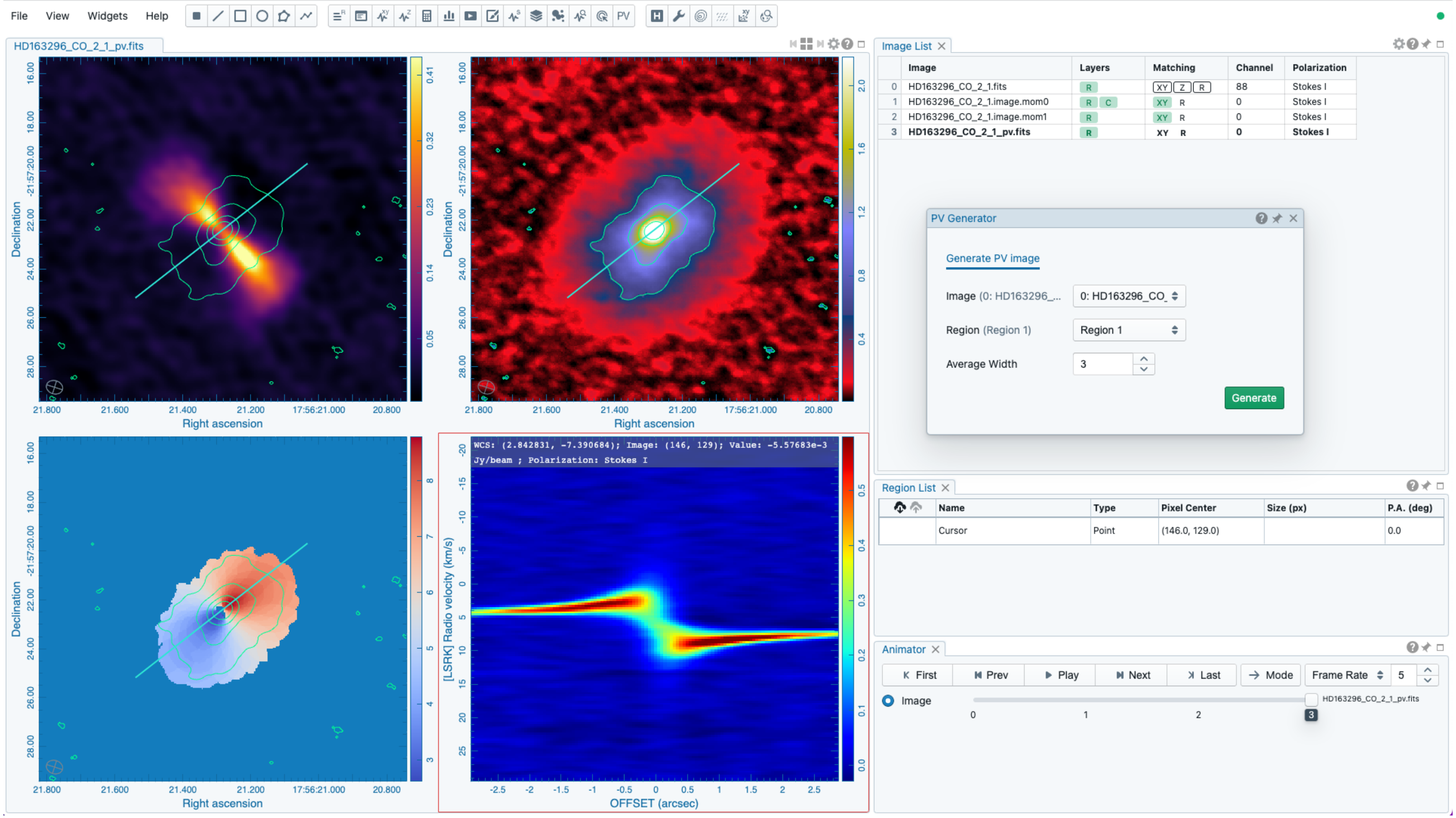


Moment 1



Moment 2

CARTA: position-velocity image generator



WCS: (2.842831, -7.390684); Image: (146, 129); Value: -5.57683e-3 Jy/beam ; Polarization: Stokes I

	Image	Layers	Matching	Channel	Polarization
0	HD163296_CO_2_1.fits	R	XY Z R	88	Stokes I
1	HD163296_CO_2_1.image.mom0	R C	XY R	0	Stokes I
2	HD163296_CO_2_1.image.mom1	R	XY R	0	Stokes I
3	**HD163296_CO_2_1_pv.fits**	R	XY R	**0**	**Stokes I**

PV Generator

Generate PV image

Image (0: HD163296_... : 0: HD163296_CO_

Region (Region 1) : Region 1

Average Width : 3

Generate

Name	Type	Pixel Center	Size (px)	P.A. (deg)
Cursor	Point	(146.0, 129.0)		0.0

Frame Rate: 5

Summary

Spectroscopic science is extremely rich and varied. Maser parallax, astrochemistry, galaxy rotation curves, protostellar jets, and more!

We are all spectral line observers... although particular calibration requirements may change for projects focused on spectroscopy.

Basic considerations are for frequency dependent effects, but today these are handled by standard calibration techniques. It's important to have properly configured observations from the start: sufficient channelization, integration time on your bandpass calibrator, and RFI mitigation.

Imaging and analysis tends to have a focus on cube processing and deconvolving extended emission.

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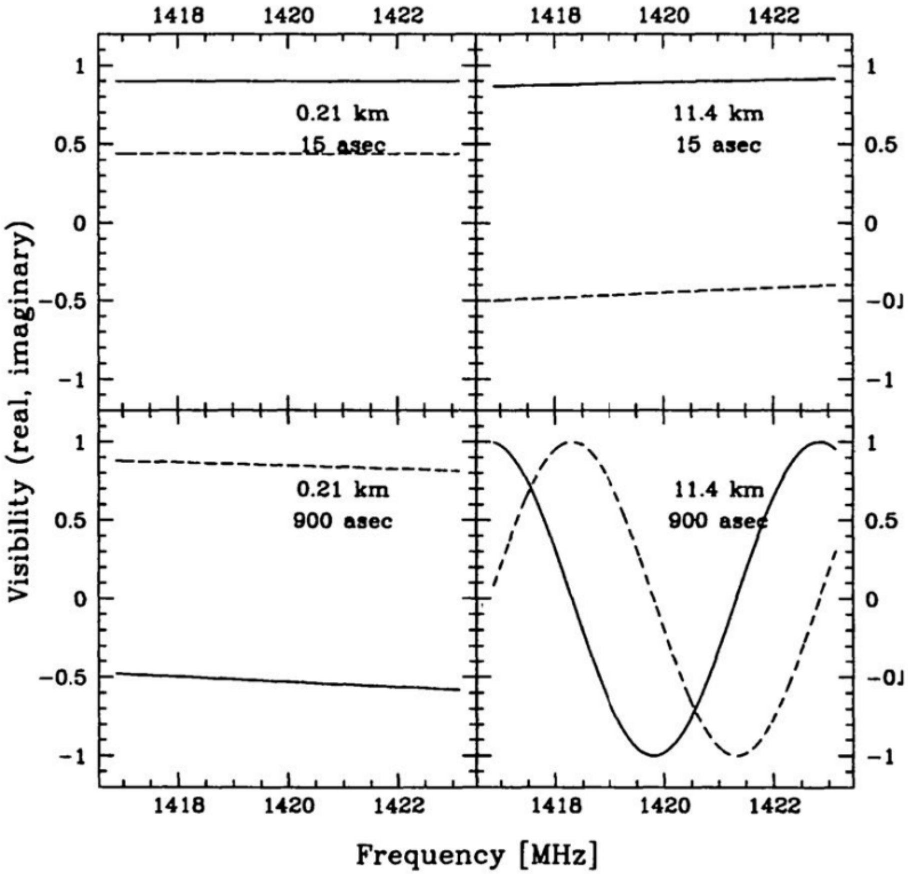
Continuum subtraction: trade-offs

$$\eta = \frac{\Delta\nu_{\rm M}}{\nu}\frac{\ell_0}{\theta}$$

$$V = \cos\frac{2\pi\nu b\, l_0}{c} + i\sin\frac{2\pi\nu b\, l_0}{c}$$



SIRA II: Chap. 11 by M. Rupen, eq. 12-4, Fig. 12-5