Spectral Line Interferometry

(A bit of) Science, (some) theory, and (mostly) practice

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Grateful to previous lecturers at ERIS and NRAO Interferometry Workshops (L. Matthews, Y. Philstrom, H. Van Langevelde, R. Beswick, A. Richards)

Lecture's Outline

- I. Why doing spectral line interferometry?
 - Science driven: science depends on frequency
 - Spectroscopy: Emission and absorption lines, atomic and molecular lines, thermal and maser lines
- II. Planning and observing a line experiment
 Science goals, lines, observational setup, instruments
 Scheduling blocks (target, calibrators, etc.)

III. Data Calibration, Visualization, and Analysis

- Differences with continuum calibration: RFI, Bandpass, Doppler correction, Continuum subtraction, etc.
- Analysis & Visualization: spectral profiles, channel & moment maps, pv-diagrams, etc.

<u>Part I</u>

Why doing spectral line interferometry? Science!

Radio Spectroscopy Atoms and Molecules

Atomic interstellar medium

- Widespread and diffuse, dominated by HI, atomic hydrogen
- Uniquely observable by 21cm hyperfine transition
- Some places (e.g. HII regions): recombination lines
 H186α H50α (radio), H42α H22α (mm)

✤ Molecular Clouds: H₂

- Similar total mass as HI, but more condensed
- Dense and cold gas heated and shocked by young stars
- Dominated by H_2 , but no dipole, largely undetectable
- Molecular Clouds: Other molecules (other than H_2)
 - Several simple linear molecules have large dipole moments, typically leading to simple ladders at 40 – 100 GHz (CO, SiO, HCO⁺, CS, HCN)
 - Non-symmetric molecules have more complex rotational spectra, with 2 or 3 quantum numbers/levels (H₂O, H₂CO, CH₃OH, SO₂)
 - A special case is provided by NH₃: inversion doublets from oscillations of the N nucleus through the plane of the three H nuclei (22-36 GHz or 1cm)

Line Interferometry gives you a 3rd axis

.....Which implies lots of extra information:

- Velocity information (kinematics and dynamics!)
- Column density (amount of gas!)
- Excitation conditions (temperature and density)
- Chemical history (gas composition)
- And magnetic fields, distances, etc.

....Result is not a map, but a cube

- 3 axes: α , δ , ν or v

...The price to pay is more complexity to handle

- Large data sets: 4096² pixels x 4000 channels = 250 Gb!
- <u>Visualization</u>: channel and moment maps, movies, 3D rendering, ad hoc visualization softwares...
- <u>Analysis</u>: model for structure & kinematics, excitation (collisions vs radiation, masers), etc.

More Physics and more Science!



Types of spectral lines

I. Thermal Emission Lines

- e.g. HI, CO, SiO, NH₃, CH₃CN, etc.
 - Low T_B often implies lower resolution required to map extended emission (e.g. HI or CO) but depends on line excitation (e.g. CH_3CN) see next slide

II. Absorption Lines

- e.g. HI, OH, NH₃, etc.
 - Requires a background source
 - High T_B of the background source implies can be observed at high resolution (e.g. EVN, ALMA, MERLIN, JVLA, etc.)

III. Maser Lines (stimulated emission)

- e.g. OH, CH₃OH, H₂O, SiO, etc.
 - Stimulated emission requires specific (often extreme) physical conditions
 - Can be very high T_B, which implies can be observed at highest angular resolution with VLBI (e.g., EVN)

Observations of Spectral Lines

Angular resolution achievable with interferometers

- HI emission: ~>5"
 JVLA, WSRT, etc.
- mm molecular lines (CO, SiO, HNC, CH₃CN, etc.): ~>0.1-1"
 - IRAM, CARMA, SMA, ATCA, e-MERLIN etc.
 - But ALMA is gonna give 0.01" at 600 GHz or 0.5 mm
- Via Absorption (HI, OH, NH₃, etc) :
 - ~1"-0.001"

IRAM-PdBI

- WSRT, ATCA, JVLA, e-MERLIN, VLBI, etc?
- Masers (e.g. OH, H₂O, CH₃OH, SiO):
 ~1"-0.001"
 - VLBI, JVLA, e-MERLIN, etc. ALMA





Part II

Planning and Observing a Line Experiment

Planning a line experiment

- Assess your Science Goals
 - Science justification in the Proposal (Tutorials T6 on Thursday and T9 on Friday)
- Lines to be observed
 - Molecular tracer(s) and transition(s)
 - Choose the correct observing frequency (Doppler Shift)
- Instruments
 - Which observe the correct frequency?
 - Resolution requirements?
 - Sensitivity requirements?

An example experiment

- I want to probe hot gas accreting close to a massive protostar (e.g., NGC7538, D~2kpc)
- Since the protostar is surrounded by a thick envelope/disk, I need an optically thin tracer to get as close as possible to the star
- NH_3 inversion lines are an excellent temperature probe and the dusty envelope is thin at cm- λ :
 - $=> NH_3$ is gonna be my tracer!



Q1. Which frequencies?

We want to probe hot gas very close to the protostar, so we need optically thin lines with high-excitation.

Table 1:	LISU OF INH	3 Drefas	stable inversi	on transition
(J,K)	Rest	$E_u^{(a)}$	Lab	Sky
	Freq.		Intensity ^(b)	Intensity ^(c)
	(MHz)	(K)	(cm^{-1})	Jy
ORTHO (7,7)	25715.18	539	$2.7 imes 10^{-4}$	
(8,8)	26518.91	687	$2.0 imes 10^{-4}$	0.39
(10, 10)	28604.74	1037	$9.0 imes 10^{-5}$	0.56
(11,11)	29914.49	1238	5.5×10^{-5}	0.37
(13, 13)	33156.85	1693	1.7×10^{-5}	0.085
PARA (6,6)	25056.03	408	$6.9 imes10^{-4}$	
(9,9)	27477.94	853	$2.8 imes 10^{-4}$	0.69
(12, 12)	31424.94	1457	$6.2 imes 10^{-5}$	0.26

 $E_{\rm u}$ from 500 K up to 1500 K is the best tool to unveil heating sources Q2. Emission or absorption?

VLA

2cm

NGC 7538

Effelsberg

- Emission expected to be very weak
- is there a strong background continuum? \bullet
- is there absorption detected from single-dish?

Choose an interferometer

Q3. What angular resolution do we need?

- Need sub-arcsec resolution (<2000 AU)
 - VLBI? these arrays do not have brightness temperature sensitivity to detect $\rm NH_3$
 - So let's observe with a connected-element interferometer

Q5. But which interferometer can tune these frequencies?

Table 1: List of NH₃ metastable inversion transitions $E_u^{(a)}$ Lab (J,K)Rest Sky Intensity^(b) Intensity^(c) Freq. (MHz) (K) (cm^{-1}) JyORTHO(7,7)25715.18 5 39 2.7×10^{-4} 7 2.0×10^{-4} (8,8)26518.91 $\mathbf{6}$ 0.3937 9.0×10^{-5} 0.5610.10) 28604.741:38 5.5×10^{-5} 29914.49 0.37(13.13) $593 \quad 1.7 \times 10^{-5}$ 33156.850.085PARA (6,6) 6.9×10^{-4} 08 25056.0385327477.94 2.8×10^{-4} (9,9)0.691457 6.2×10^{-5} (12.12)31424.94 0.26

25 GHz to 33 GHz

The JVLA with the new K and Ka-band receivers can tune all these transitions and easily achieve the required angular resolution (in B-conf, $9\sim0.2$ ") and sensitivity for a 100 mJy line So let's observe NH₃ in absorption with the JVLA B-Array

Choose a spectral setup

JVLA Spectral Line Capabilities:

- 2-4 basebands (2-8 GHz tot max)
- 16 (8 dual) tunable subbands per baseband with between 0.03125 – 128 MHz
- Up to 2000 channels per subband (up to 16,384 per baseband)



Dual Polarization

Sub-band BW (MHz)	Number of channels/poin product	Channel width (kHz)	Channel width (km/s at 1 GHz)	Total velocity coverage (km/s at 1 GHz)
128	128	1000	300/v(GHz)	38,400/v(GHz)
64	12 8	500	150	19,200
32	128	250	75	9,600
16	12 <mark>8 Up to 2000</mark>	125	37.5	4,800
8	123	62.5	19	2,400
4	121	31.25	9.4	1,200
2	128	15.625	4.7	600
1	128	7.813	2.3	300
0.5	128	3.906	1.2	150
0.25	128	1.953	0.59	75
0.125	128	0.977	0.29	37.5
0.0625	128	0.488	0.15	18.75
0.03125	128	0.244	0.073	9.375

Choose a spectral setup Q6. Which Bandwidth/spectral resolution do we need?

- Need to fully cover line and provide additional non-line channels for continuum
 - The line is 5-10 km/s so one SB with 30 km/s is enough, but we have also HP components (at ±30 km/s), so we need 3 SBs. The remaining 5 SBs for continuum
- Need enough channels (i.e. spectral resolution) to sample the line
 - 0.3 km/s well enough to sample the line (≤ 10 km/s)
- Need enough sensitivity per channel (*not* for the whole bandwidth)
 - 5 mJy rms enables snr=10 for a 50 mJy line
 - Dual Polarization



WIDAR correlator baseband with subbands

Sub-band BW (MHz)	Number of channels/poin product	Channel width (kHz)	Channel width (km/s at 1 GHz)	Total velocity coverage (km/s at 1 GHz)
128	128	1000	300/v(GHz)	38,400/v(GHz)
64	128	500	150	19,200
32	128	250	75	9,600
16	128	125	37.5	4,800
8	128	62.5	19	2,400
4	128	31.25	9.4 /30=0.3 km/s	1.200 / 30 = 40 km/s

So let's observe NH3 inversion lines paired in 2 basebands with 8 subbands of 4 MHz each and 128 channels, and 31 KHz channel resolution

Observations Preparing Scheduling Blocks

- Check observing frequency/velocity for the target (Doppler/Redshift)
- Make sure you ask for enough time to reach the required sensitivity/uv-coverage on target (1.5h on-source, rms~2 mJy, track-sharing)
- Include scans on calibrators
 - Possibly multiple scans through the run
 - Flux calibrators
 - Phase calibrators: need to be nearby (a few degrees) from target
 - Bandpass (BP) calibrator
 - see Part III on how to choose a good BP calibrator



Data calibration & analysis

III. Data calibration & analysis

- * Spectral line observations use several channels of width δv , over a total bandwidth Δv
 - => much like continuum but with more channels!
- Data calibration is not fundamentally different from continuum observations, but a few additional elements must be considered:
 - a) Presence of RFI (data editing as a function of v)
 - b) Bandpass calibration
 - c) Doppler corrections
 - d) Continuum subtraction
 - e) Self-calibration of line (or continuum)
 - f) Imaging of a data cube
 - g) Visualisation & analysis of cubes

a) Editing spectral line data

- Start with identifying problems affecting all channels (e.g., malfunctioning electronics or mechanical probls with a particular antenna), by using a frequencyaveraged data set (the 'Channel 0' in the old VLA).
 - Has better SNR.
 - Apply flags to all spectral channels.
- Then check the line data for narrow-band RFI that may not show up in averaged data.
 - identify features by using cross-power spectra e.g., use POSSM in AIPS, PLOTMS in CASA.
 - Flag based on the feature (limited in time, to specific telescope or baseline?)
 e.g., use SPFLG or TVFLG in AIPS, FLAGDATA in CASA.

a) Editing spectral line data Flagging RFI: Primarily a low frequency problem Produce scalar-averaged cross-power spectra of calibration (i.e. <u>continuum</u>) sources to spot narrowband RFI.

RFI at the JVLA L-Band



ower frame: Log10(Amp) Jy calar averaged cross-power spectrum Baseline: ea04 (03) - ea08 (05) imerange: 00/00:30:00 to 00/00:31:00

Avoid known RFI if possible, e.g. by constraining your bandwidth (Use RFI plots posted online)

Plots made with AIPS task POSSM.

RFI at the EVN L-Band



By inspecting different baselines, you can identify individual channels affected by RFI to flag

a) Editing spectral line data

Once identified the RFI in our passband, we can study the real line emission from our target



Example: SiO maser spectra on different VLBA baselines

b) Spectral Bandpass Calibration Definition

• The general goal of calibration is to find the relationship between the observed visibilities, V_{obs} , and the true visibilities, V:

 $V_{ij}(t,v)_{obs} = V_{ij}(t,v)G_{ij}(t)B_{ij}(t,v)$

- where t is time, v is frequency, (i,j) refers to a pair of antennas (i.e., one baseline), G is the complex "continuum" gain, and B is the complex frequency-dependent gain (the "bandpass").
- Bandpass calibration is the process of deriving the frequencydependent part of the gains, Bi j(t,v)
- Bij may be constant over the length of an observation, or it may have a slow time dependence (much slower than atmospheric gain or phase terms)

b) Spectral Bandpass Calibration Definition

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



Shape due primarily to electronics/ transmission systems of individual antenna

Edge roll-off caused by shape of baseband filters

Different for each antenna

Bandpass calibration attempts to correct for the deviations of the observed bandpass from the ideal one

b) Spectral Bandpass Calibration Why is it important?

- The quality of the bandpass calibration is a key limiting factor in the ability to detect and analyze spectral features
 - v-dependent amplitude errors limit ability to detect/measure weak emission/absorption lines superposed on the continuum
 - v-dependent amplitude errors may mimic changes in line structure
 - v-dependent phase errors may lead to spurious positional offsets between spectral features as a function of frequency, imitating doppler motions.
- For continuum experiments conducted in spectral line mode, dynamic range of final images is limited by bandpass quality

b) Spectral Bandpass Calibration How BP calibration is performed?

- Bandpass calibration is typically performed using observations of a strong continuum source (at least once in the experiment).
- The most commonly used method is analogous to channel by channel self-calibration (AIPS task BPASS)
 - The calibrator data is divided by a source model or continuum (Channel 0), which removes any source structure effects and any uncalibrated continuum gain changes
 - Most frequency dependence is antenna based, and the antenna-based gains are solved for as free parameters.
- What is a good choice of a BP calibrator?

b) Spectral Bandpass Calibration

Cross-power spectra of three potential calibrators

How to select a BP calibrator?

Select a continuum source with:

- High SNR in each channel
- Intrinsically flat spectrum
- No spectral features
- a point source (not required but helpful since the SNR will be the same in the BP solutions for all baselines)



b) Spectral Bandpass Calibration How long to observe a BP calibrator?

- Applying the BP calibration means that every complex visibility spectrum will be divided by a complex bandpass, so noise from the bandpass will degrade all data.
- Need to spend enough time on the BP calibrator so that SNR_{BPcal} > SNR_{target}. A good rule of thumb is to use

$$SNR_{BPCal} > 2 \times SNR_{target}$$

which then results in an integration time: $t_{BPCal} = 4 \times (S_{target} / S_{BPCal})^2 t_{target}$

b) Spectral Bandpass Calibration Assessing quality of BP calibration

Example of good-quality bandpass solutions for a JVLA antenna



- Solutions should look comparable for all antennas.
- Mean amplitude ~1 and phase~0 across useable portion of the band.
- No sharp variations in amplitude or phase; variations are not dominated by noise.
- Flat phase across the band (Phase slope across the band would indicate residual delay errors).

Plots made with CASA task PLOTCAL

b) Spectral Bandpass Calibration Poor-quality bandpass solutions for 4 VLBA antennas

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



Plots made with AIPS task POSSM

b) Spectral Bandpass Calibration Bandpass quality: apply to a continuum source

- Before accepting the BP solutions, apply to a continuum source and use cross-correlation spectra to check:
 - That phases are flat across the band
 - That amplitudes are constant (for continuum sources)
 - That the noise is not increased by applying the BP
 - Absolute flux level is not biased high or low



c) Doppler Correction Line observing frequency: Rest Frames

- The redshifted/blueshifted velocity of a source is a crucial number as this sets the sky frequency at which a line is observed.
- Source velocities need to be corrected relative to a rest frame:

Correct for	Amplitude	<u>Rest frame</u>
Nothing	0 km/s	Topocentric
Earth rotation	< 0.5 km/s	Geocentric
Earth around Sun	< 30 km/s	Heliocentric
Sun peculiar motion	< 20 km/s	Local Standard of Rest
Galactic rotation	< 300 km/s	Galactocentric

Conventions:

Radio-LSR $V_{radio}/c = (v_{rest}-v_{obs})/v_{rest}$ - Mainly Galactic workOptical-heliocentric $V_{opt}/c = (v_{rest}-v_{obs})/v_{obs} = cz$ - Extragalactic work(approximations to relativistic formulas, differences become large as redshift increases)

c) Doppler Correction Line observing frequency: Doppler tracking

- Observing from the surface of the Earth, our velocity with respect to astronomical sources is not constant in time or direction.
- Doppler tracking can be applied in real time to track a spectral line in a given reference frame, and for a given velocity definition (e.g., radio vs. optical)
- Correcting these motions done in array model

c) Doppler Correction

Doppler Setting and fixed frequency

- Note that the BP shape is really a function of frequency, not velocity!
 - Applying Doppler tracking will introduce a time-dependent and position dependent frequency shift.
- VLBI is done with <u>fixed frequency</u>
- The current interferometers (JVLA, SMA, ALMA, etc.) have wider bandwidths, so online Doppler setting is done <u>but not tracking</u> (this would be correct only for a single frequency)



Doppler tracking must be done in post-processing (AIPS/CASA: CVEL/CLEAN) =>Want well resolved lines (>4 channels across line) for good correction

d) Continuum subtraction

- Spectral-line data often contain continuum sources (either from the target or from nearby sources in the field of view) as well as line data.
 - Note this continuum also contains valuable science!
- This continuum emission should be subtracted in your spectral-line data set before deconvolution

Line and continuum should be cleaned separately.



Spectral line cube with two continuum sources (no change in structure with frequency) and one spectral line source (near the field center).

Roelfsema 1989

(RA) →



- Use channels with no line features to model the continuum
- Subtract this continuum model from all channels
- The process of continuum subtraction is iterative

d) 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!

d) Continuum subtraction Method 1: In the uv-plane

·····

 A low order polynomial is fit to a group of line free channels in each visibility spectrum, the polynomial is then subtracted from whole spectrum

• <u>Pros</u>:

- Fast, easy, robust
- Corrects for spectral index slopes across spectrum
- Can do flagging automatically
- Can produce a continuum data set
- <u>Cons</u>:
 - Channels used in fitting must be line free (a visibility contains emission from all spatial scales)
 - Only works well over small field of view $\theta << \theta_{\rm s} \, \nu$ / $\Delta v_{\rm tot}$

d) Continuum subtraction Method 2: In the image-plane

- Fit and subtract a low order polynomial fit to the line free part of the spectrum measured at each pixel in cube.
- <u>Pros</u>:
 - Fast, easy, robust to spectral index variations
 - Better at removing continuum sources far away from phase center
 - Can be used with few line free channels.
- <u>Cons</u>:
 - Can't flag data since it works in the image plane.
 - Line and continuum must be simultaneously deconvolved.

d) Continuum subtraction Results

NH₃(6,6) JVLA



Spectrum should have same shape, different scale after continuum subtraction.

e) Self-calibration

Same as continuum, but two cases:

- a) 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 >snr
- b) Weak line and strong continuum emission
 - > Apply solutions from the continuum to individual channels
 - > Allows imaging of weak lines with >snr

f) Imaging: cleaning and deconvolution

- What you learned about imaging for continuum 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
 - Emission distribution changes from channel to channel
 - Emission structure changes from channel to channel

• One is often 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

g) Analysis of Line Cubes

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

- 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)
 - Movies (2-D slices along velocity axis)
 - Moment maps (integration along the vel. axis)
 - Position-vel. plots (slices along spatial dimension) Tutorial T8 on Friday!

Example: line profiles

Line profiles may show changes in line shape, width and depth in different portions of your source.



g) Visualization of Line Cubes Contour maps (channel-by-channel)

Channel maps show how the spatial distribution of the line emission changes with frequency/ velocity

DECLINATION (J2000)

This cube shows SiO (J=5-4) line (217 GHz) emission imaged with ALMA in a massive protostellar outflow in Orion.



Movies

Cube produced in CASA Movie created with DS9



"Movie" showing a consecutive series of channel images from the same data cube as previous slide (168 channels, 0.7 km/s velocity resolution).

g) Analysis of Line Cubes Moment analysis

You might want to derive parameters such as integrated line intensity, centroid velocity and line widths as functions of positions

$I_{ m tot}(lpha,\delta)$	=	$\Delta v \sum_{i=1}^{N_{\mathrm{chan}}} S_ u(lpha,\delta, u_i)$	Total intensity - (Moment 0)
$\overline{v}(lpha,\delta)$	Ξ	$rac{\sum\limits_{i=1}^{N_{ ext{chan}}} v_i S_ u(lpha, \delta, u_i)}{\sum\limits_{i=1}^{N_{ ext{chan}}} S_ u(lpha, \delta, u_i)}$	 Intensity-weighted velocity (Moment 1)
$\sigma_v(lpha,\delta)$	Ξ	$\sqrt{\langle (v_i - \overline{v}(\alpha, \delta))^2 \rangle}$	Intensity-weighted velocity
	-	$\sqrt{\frac{\sum_{i=1}^{N_{\text{chan}}} (v_i - \overline{v}(\alpha, \delta))^2 S_{\nu}(\alpha, \delta, \nu_i)}{\sum_{i=1}^{N_{\text{chan}}} S_{\nu}(\alpha, \delta, \nu_i)}}$	dispersion (Moment 2)

g) Analysis of Line Cubes Moments Maps

ALMA Cycle 0 CSV CO(3-2) moment maps of a proto-planetary disk (white contours continuum)



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

g) Analysis of Line Cubes Position-velocity plots

elocity

 PV-diagrams show, for example, the line emission velocity as a function of radius. Here along a line through the disk major axis.

ALMA Cycle 0 CSV CO(3-2) image of a proto-planetary disk

Velocity ↑ Right Ascension ≁ Declination → Keplerian Profile V « VR

Colors convey intensity of the emission.

You can produce pV diagrams directly in CASA using task IMPV, or using the task IMMOMENTS, by collapsing the RA or DEC axis

Concluding remarks

Spectral line imaging gives you more information and hence <u>more science</u>
 – 3-D (RA, DEC, vel) rather than just 2-D images

- Gas physics!

- This comes at a price, in terms of complexity of data reduction and analysis
- Enjoy tutorial T3 this afternoon!