HIFI Pipelines and Data Products

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\[ \text{CH}_3\text{CN at 765.5 GHz WBS-H} \]
• HIFI instrument and AOTS
• HIFI pipeline structure (see also posters!)
• HIFI data reduction: how to run the pipeline
  – Standard Product Generation (SPG)
  – Interactively
• HIFI Data Products
HIFI: most powerful and versatile heterodyne instrument in space for observing molecular and atomic lines in FIR/submm at ultra-high spectral resolutions

- Single pixel on the sky

7 dual-polarization mixer bands
- 5 x 2 SIS mixers: 480-1250 GHz, IF 4-8 GHz
- 2 x 2 HEB mixers: 1410-1910 GHz, IF 2.4-4.8 GHz

14 LO sub-bands
LO source unit in common
LO multiplier chains

2 spectrometers
- Auto-correlator (HRS)
- Acousto-optical (WBS)

IF bandwidth/resolution
- 2.4 and 4 GHz (in 2 polarizations)
- 0.14, 0.28, 0.5, and 1 MHz
- Velocity discrimination 0.1-1 km/s

Angular Resolution (w/ telescope): 11” .3 (high-freq. end) to 40” (low-freq. end)

Sensitivity
Near-quantum noise limit sensitivity

Calibration Accuracy
10% radiometric baseline, 3% goal

AOT Schemes

Reference scheme

1 - Position Switch

2 - Dual Beam Switch

Optional continuum measurement

3 - Frequency Switch

Optional sky measurement

4 - Load Chop

Optional sky measurement

HIFI Pipeline Concept

Processing HIFI observations similar to ground-based telescopes with heterodynes, e.g., CSO, JCMT, IRAM, KOSMA

- **Spectrometer Pipeline (level 0 → 0.5):** initial processing backends
  - AOT mode independent
  - Each spectrometer and polarization separately: WBS-H, WBS-V, HRS-H, HRS-V
  - *Users can run automatically and interactively, changing options, but unlikely need to*

- **Generic Pipeline (level 0.5 → 1):** applying AOT mode-specific calibrations
  - Spectrometer independent
  - Intensity calibration using Hot/Cold loads
  - Reference spectrum subtraction (on-off sky DBS, position switch, freq. throw, load)
  - *Users can run automatically and interactively, changing options, but unlikely need to*

- **Extended Pipeline (level 1 → 2):** remove additional instrumental effects
  - e.g. Standing waves, Baseline offset and slope, Sideband deconvolution
  - *Most interactive step for users*
Overall Pipeline Structure

Raw Telemetry
- Conversion to Dataframes and HK (basic reformatting)

Spectrometer Branch
- Level 0 Timeline Product
  - WBS H/V
  - HRS H/V
  - Spectrometer Calibrations

Generic Branch
- Single Point
  - AOT Type
    - Spectral Map
      - Calibrations

Level 1 Product
- Single Point
  - Calibrations
  - Ripple removal
    - Baseline fitting
      - Band stitching, etc.

Level 2 Product
- Single Point
  - Calibrations
  - Ripple removal, etc.

Level 1 Product
- Spectral Scan
  - Calibrations
  - Map construction, etc.

Level 2 Product
- Level 2 Product

Level 0.5 Product

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Spectrometer Pipelines (Level 0 → 0.5)

WBS Level 0 Product

- Find and Flag Bad Pixels
- Subtract Dark Current Levels
- Non-Linearity Correction
- Zero Level Subtraction
- Frequency Calibration
- Derive Attenuator Setting Corrections
- Sub-band Splitting

Output: Level 0 Product

Green: optional user input

- Calibration file in/output
- Quality check file in/output

HRS Level 0 Product

- Compute Offset and Power
- Normalize Correlation Function
- Correct for A to D Quantization
- Gain Non-Linearity Power Correction
- Hanning Smoothing
- Autocorrelation Funct. Symmetrization
- Spectrum in Freq Domain and Scale
- IF Non-Linearity Flux Correction

Output: Level 0.5 Product

- Calibration file in/output
- Quality check file in/output

<table>
<thead>
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<th>Green: optional user input</th>
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- dark pixels?
- Interpolation method?
- Time domain?
- WBS comb or HRS?
- Green: optional user input
- Quality check file in/output

Generic Modules
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Generic Pipeline (Level 0.5 → 1)

Previous spectrometer pipeline

Level 0.5 Product: frequency calibrated

Data as expected for AOT mode?

Frequency drifts?

Tsyst and band pass from Hot and Cold

Determine channel weights

Subtract reference spectrum

Make OFF spectrum

Subtract OFF spectrum

Apply hot/cold band pass:

T_A * calibration

Level 1 Product: frequency and intensity calibrated

Level 2 pipeline

Green: optional user input

Calibration file in/output

Quality check file in/output

drift tolerance [Hz/sec]?

weights from time, variance or Tsys?

smooth over channels?

ref spectrum? e.g. if one chop has line contamination

average, smooth or fit to reduce noise in OFF data?

interpolation method?

(Off spectrum drift over time)

interpolation method?

(band pass drift over time)

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Level 2 processing is most user-interactive. Several steps are optional.
How to Run these Pipelines?

• Pipelines generate level 0, 0.5, 1, and 2 products that can be retrieved from Herschel Science Archive, including all auxiliary and calibration products.

• Observers have all software and can run pipelines on laptop/desktop: automatically, interactively, or with own algorithms.

• Level 2 processing especially interactive, some steps are optional.

• Extensive help on running pipeline available in HIPE, written in 'how-to' fashion.
Running the Pipeline: SPG

- **Basic** HIFI SPG pipeline form (selected with window->Show View->HifiPipeline and click on hifiPipeline in Tasks pane).

- Data (previously retrieved from Herschel Science Archive) to be re-processed is dragged and dropped from ObservationContext in Variables pane on right.

- Click on 'Accept' to run all pipelines or selection thereof.
HIPE: Running Pipeline 'Lights Off'

**Expert** HIFI SPG pipeline form offers possibility of user-defined pipeline algorithms (written in jython).
HIPE: Interactive Pipeline

Both spectrometer and generic pipelines can be run step-by-step. Allows for modification of parameters by user, though rarely necessary.

Example: WBS dark subtraction: even and odd channels have different dark levels.
HIPE: Interactive Pipeline

WBS frequency calibration on comb spectrum, fitting Gaussians. Initial values from Cal file or user input.

If comb spectrum fit fails, equally good solution can be obtained using simultaneous HRS spectrum. Note: although user can intervene using HIPE form, pipeline will likely work fine in 99.9% of cases.
HIPE: Interactive Pipeline

- Generic pipeline somewhat more interactive than Spectrometer pipelines, although defaults will work well for almost all observations.

- Example doChannelWeights():

  - Weight per channel can be calculated by entering in definition box:
    - 'integTime': integration time
    - 'variance': variance in moving window
    - 'radiometric': integration time/$T^2_{sys}$

  - Result can be smoothed as function of channel using box car or Gaussian convolution.

  - Note command-line equivalent in console window.
Level 1 → 2 Processing

- Frequency regridding (available - demo)
- Averaging spectra (available - demo)
- Band stitching (in development)
- Coupling correction, point and extended sources (in development)
- Sideband gain correction (in development)
- Bad channel flagging and interpolation (in development - demo)
- Baseline fitting and subtraction (available – demo)
- Dual sideband deconvolution of spectral scans (available - demo)
- Residual standing wave removal (in development)
- Producing cubes of mapping data (available - demo)
SPG pipelines produce “ObservationContext”, contain products of pipeline levels, calibration files, pointing, spacecraft velocity, quality products, pipeline history, and meta data (observing mode, time, band, etc).
HIFI Data Products: TimelineProduct

- **HifiTimelineProduct** is the fundamental container of spectra and metadata in ObservationContext.

- At level 0 contains all observed spectra in time sequence including hot and cold loads, combs, on and off integrations.

- At level 1 HifiTimelineProduct cleaned from calibration data, and only science spectra remaining.
HIFI Data Products: TimelineProduct

Individual integrations stored in HifiTimelineProduct and user can list and view them in HIPE in several ways.

**Level 0.5 on-source**

**Level 2**
Summary

- Pipeline within HIPE to reproduce the Standard Product Generation of the Herschel Science Archive
- Can step through the pipeline interactively from any level (expect mostly level 1 → 2)
  - Change processing defaults
  - Change calibration files
  - Ensure steps requiring assessment (e.g. fitting baselines) are done to your satisfaction
- Can run pipeline with your own algorithm (must be jython)
- Get used to terms “ObservationContext” and “HifiTimelineProduct”

- Pipelines in place, have been (and are being) extensively tested against various simulator and real-instrument data from various campaigns. Much effort going into level 2 software development.
Supplemental Slides

Backup slides
Science Analysis Tools

Level 2 data ALL instrument signatures removed. Science analysis tools available for HIFI users:

HIPE has Spectrum Toolbox of Astrolib-like applications for

- Conveniently displaying maps, spectral scans: See Russ Shipman presentation tomorrow
- Gaussian, polynomial fitting (and more functions), interactively and in scripts

Line intensity and shape fitting (outside HIPE):

- CASSIS  http://cassis.cesr.fr/ (might be called within HIPE)
- MASSA  http://www.damir.iem.csic.es/mediawiki-1.12.0/index.php/Portada#MASSA

Imaging tool (in HIPE) MADCUBA:

- http://www.damir.iem.csic.es/mediawiki1.12.0/index.php/Portada
- Regrid irregularly spaced data (time, position) to a regular grid
- Production monochromatic images, and cube of images.
- Different interpolation methods depending on desired spatial scale:
  - Nearest Neighbor (coarse but fast)
  - Linear Interpolation with windowing, with selective distance weighting and filtering
Level 1 → 2: Standing Waves Removal

- Standing wave removal needed for all HIFI AOTs, either as a residual (e.g. chopped/nodded spectra) or if OFF sky not taken with FSwitch or LoadChop modes.

- Robust sine wave fitting routine for ISO/SWS and Spitzer/IRS defringing available in IDL. Fits multiple sine waves, using Bayesian statistics. Little user interaction. Contains line blanking routine.

- Tool being developed in HIPE. May be used for PACS and SPIRE spectra as well.
Level 1 → 2: Standing Waves Removal

'Fringes'-diagnostic plot --- $\chi^2$ vs frequency, with clear minimum (red)

- Standing waves successfully removed in gas cell spectra. (residual) standing wave patterns likely different in space. However, algorithm very flexible! Initial guesses easily adjusted.
- Bands 6+7 non-optical standing waves, non-sinusoidal. Strength and shape power-dependent. Well reproduced in laboratory spectra with similar power: remove empirically.
At any given LO frequency, two sidebands of 4 GHz IF coverage each (2.4 GHz bands 6+7), separated by 8-16 (4.8-9.6) GHz in sky frequencies are overlaid on top of each other in DSB spectrum, with mirrored freq. scales.

Sideband deconvolution especially important to spectrally complex regions.


See demo Steve Lord this afternoon
Level 1 → 2: Sideband Deconvolution

Deconvolved (SSB) result, methanol with HIFI in the lab, viewed in HIPE with TablePlotter.

HIPE GUI frontend (beta) for decon tool I/O and hooks to view intermediate results, fit statistics

See demo Steve Lord this afternoon

More pretty examples of real HIFI data in the Supplemental Slides
Level 2 pipeline produces data cubes of maps, which can be displayed and manipulated in HIPE.
Level 1 → 2: Masking Bad Data

- Spurious response ('spurs') in some LO chains observed, arising from strong harmonics or oscillations in bias circuitry.
- Spurs may affect hot/cold calibrations, deconvolution solution, and spectral lines.
- Spur detector will be included in pipeline, but user may also flag spectral ranges

Spur list generated by prototype spur detector

Different spur types, e.g. up/down type, where spur has moved in frequency between calibration steps
Updates expected this December (Thermal Vac)
HIFI Data Interfaces

Where are Users?

HIFI ICC data interface definitions
(P. Roelfsema, HIFI PM)

HSpot

HSpot ICD

HIFI Observers’ Manual

HIFI Tele Command ICD

HIFI instrument to ground ICD

HIFI Data Frame definition

HIF Observe's Manual

HIFI Tele Command ICD

HIFI House Keeping TM ICD
HIFI Science TM ICD

HIFI Data Frame definition not formally listed as ICD

HIFI Tele Command ICD

HIFI Tele Command ICD

HIFI House Keeping TM ICD
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HIFI Data Frame definition not formally listed as ICD

HIFI DP Users’ Manual and Lore

HIFI DP Users’ Manual and Lore

HIFI standard data product specification
Generic Herschel product definition

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HIFI Layout and Optics

HIFI is aimed at the cool and cold Universe of Molecules (120 species known), neutral and ionic lines occurring at TeraHerz ($10^{12}$ Hz) frequencies with very high velocity discrimination (0.1-1 km/s).
So-called M6 mirror, workhorse of Dual Beam Switching and Load Chop Observing Modes to

- Equivalently chop the telescope secondary to move the beam on the sky
- Redirect the instrument's optical beam to internal hot (100 K) and cold (10 K) thermal loads.

Chopping of the telescope beam at fixed 3’ throw, up to 5 Hz.

Chopping to the thermal loads at extreme rotation (4°.6 limit).
HIFI on the “sky”

Beams optically re-imaged (simulating telescope M2) at SRON.

Beams sizes / waist properties are nominal.

FWHM 40\textdegree$$^{2}$$

Measured focal plane spots projected on M3

(TElescope axis out)
H and V polarizations are well aligned orthogonally. Some deviations from linearity in the optics chain, losses are very small.

H and V beams are separated on the sky by up to few arcsec; each are acquired and combined in the automated pipeline.
OCS in the cell, LO is at ~564GHz, picking up simultaneously the J=46-45 and 47-46 transitions in each side-band (OCS has transitions every 12GHz, so it is a dual side-band ratio measurement in one go. In the middle of the IF are all the isotopes and some vibrational transitions. S/N > 100, Tsys ~ 70K. The apparent side-band ratio = 1.5, but requires correction for baseline, some known LO ripple issues, etc. Sideband ratio is closer to 1.1 or less.
Acetonitrile, Methanol

CH$_3$CN at 765.5GHz WBS-H

Methanol at 1016GHz WBS-H
SO with HRS and WBS

SO2 at 1696.5GHz HRS-H
(2.4 GHz IF)

SO2 at 1696.5GHz WBS-H
Start automated HIFI pipeline task ('SPG'): window->Show View->HifiPipeline and click on hifiPipeline in Tasks on right pane
Spectrometer and generic pipelines can be run separately (not sure if showing this makes sense, as level 0.5 of the pipeline task shown before does the same thing)
HIFI Pipelines and Data Products: ObservationContext

SPG pipelines produce “ObservationContext”, wrapping products of pipeline levels, calibration files, pointing, spacecraft velocity, quality products, pipeline history and meta data with observing mode, time, etc.