Follow-up on Cross-Instrument Spectrometer

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With inputs from I. Valtchanov and E. Puga
Objectives of the splinter

- **Summary of plenary sessions on spectrometer**
  - Cross-Instrument I: Cross-instrument simple spectrum
  - Cross-Instrument II: Cross-instrument spectroscopic maps

- **Multi-instrument spectroscopy**
  - Cross-calibration (consistency of absolute intensity scales)
  - Cross-comparison (consistency of spectral information)
  - Instrument combination (spectra/maps concatenation, line ratio, etc)
  - Typical use-case: HIFI/SPIRE/PACS cross-comparison of IRC+10216

- **Record all limitations/missing functionalities encountered during the above exercises**
  - Have experts discussing solutions during splinter
  - What other use-cases should be covered?
  - Agree on work-plan (SxRs, who does what, priorities – maybe after splinter)
Cross-Instrument I: HIFI summary

- **Data access and saving**
  - Turn `getObservation` into a GUI task – e.g. embed overview of available pools to chose from, and available obsids in pool (see also “Obs. Mngt” sessions)

- **Re-pipelining (esp. with new CalTree)**
  - Issue to identify CalTree version available on HifiCalibrationWeb at HSC
  - CalTree version in reprocessed data appears as “IA_CAL_USER_HEAD”

- **Flagging is not user-friendly enough**
  - Available flag codes in flagPixels task should show on a drop-down menu
  - Manual flagging offers long list of opaque names (some not applying to HIFI)

- **SpectrumFitterGui is not user-friendly enough**
  - Is it a documentation issue? Refurbishment along those lines already took place.

- **Data averaging / combining**
  - `polarPair in doc` now `PairAvg` (for 2 DS, re-sampling to common grid needed)
  - Combination of multiple obsid, or DF within an obsid:
    - prototype in CHESS project – but no specification collected broadly
    - Could consider an upgrade of PairAvg (more than two DS, dynamical size adjustment), although a more general combiner tool (not only HIFI) would be more interesting
Re- PACS user perspective: re-pipeline spectra

- HIPE workflow to re-pipeline spectra
  - **Adapt interactive pipeline to user needs works well!**
    - loop over OBSIDs and cameras
    - flux cal: apply latest CalTree, run flat-field task, use calBlock response and dark estimates, do point-source beam correction if applicable
    - change product export format (save rebinned 5x5 cubes, also for separate nod positions)
  - **Conclusion:** HIPE syntax is unintuitive (even worth not stable) and sometimes fishy but top-level coding around Tasks is doable

- **Interactive data inspection works in practice but the workflow has still not yet crystallized**
  - Flat-field (correct for response variations between 16 pixels)
  - Examine OFF-position line contamination
  - **Outlier spectral segment masking (was not addressed)**
  - Pointing offset check/correction
  - **Conclusion:** available tasks are used, problems revealed (important test feedback) but adequacy and impact on science is not completely clear, probably because not well documented. Always check (i.e. overplot) result spectra obtained from interactive tasks!
Re- PACS user perspective: interactive tasks

- Flat-field
  - **Short-range (line) case**
    - Do always, overplot, no need to change parameters
    - Improvement is quite on a solid basis in v8.0
    - Alternative algorithms will be available in the toolbox which may further improve FF
  - **Long-range case**
    - Continuum RMS is reduced but not sufficiently for Nyquist sampled spectra
    - Continuum is estimated by a poly-fit (5th order by default) what may distort continuum shape after FF (especially in a full R1 SED coverage)
    - Consider to split-up long-range spectra into parts
    - Do baseline removal in the leakage areas before fitting a line
    - Always check/overplot FF results on original data!

5th order poly-fit could be severely distort the continuum in full R1 range FF because of the leak shape
Re- PACS user perspective: interactive tasks

• OFF-position examination
  – Check contamination in chop off-fields
    • Uses a total-power reduction without any subtraction
    • Due to very strong residual RSRF wriggles faint contaminating lines could remain hidden (contaminating line peak-to-continuum below ~10 Jy!)

– Check contamination in nod A and B
  • ON-OFF (nod A) and OFF-ON (nod B) subtracted data
  • A-B is an estimate of flux difference of contaminating line between the two chop-off positions
  • In case the contaminating line is weak (≤10 Jy p2c) and its strength is similar in the two off-positions then it can be only found inspecting the two nods separately
Re- PACS user perspective: optimal flux extraction and visualization

• Line fitting, flux extraction done in IDL
  – SpectrumExplorer can do the job but workflow is not clear and some level of coding is required
  • Fit line + continuum model or
  • Do (non-parametric) continuum subtraction first and fit line model
  – For mapping observations flux extraction should be done in HIPE as in some cases it is more advantageous to project fit parameters instead of flux density values

• Footprint visualization
  – Very important to check flux distribution on the 25 spaxels before total source flux is derived (pointing offset and/or source extendedness)
  – Work in HIPE v8.0 but maybe not as nice as in IDL
Cross-Instrument I: SPIRE summary

• Dark field correction
  – Apparently needs intervention from ICC member. Is there a “generic” way to do this assessment? If so, what is the prospect to have this offered within HIPE?

• Baseline residual artefacts
  – Is it a limitation of the current pipeline? What would be needed to improve this?

• Data analysis outside of HIPE
  – SINC fitting Done in IDL. Same thing available in HIPE but needs to be better explained (dedicated user script to be added in HIPE)

• Intensity comparison with ground-based telescope data
  – Conclusion is that ground-based telescope are missing a lot of line flux. Any chance this is the other way around (SPIRE calibration issue?)
Cross-Instrument II (mapping): summary

• Wish list
  – Easily visualise entire cube in 3D / View spectra from single cube/different cubes
  – Fit spectra over whole cube
    • Be interactive for single spectra, semi-interactive for cubes
    • Results as table, maps, ASCII – Save model fits
    • Refit easily and track work – Include errors in fitting
    • Limit and/or tie fits together
  – Spectral maths on cube
  – Extract sub cube/spectra/images
  – Compare whole cube with single spectrum
  – Control the spectral/spatial gridding
  – Simple/more thorough convolution/deconvolution

• Cross-instrument comparison
  – Needs same physical unit (not particular to maps), same grid (doGridding can do this with common WCS), convolution in both spatial/spectral domain
  – Parameters for convolution kernels (defaults at least) should be easily accessible

More follow-up during Alain’s and Jeroen’s splinters
Instrument cross-calibration

• Use information from another instrument to verify consistency of or correct absolute intensity scale
  – Within Herschel, overlapping ranges between HIFI bands 1a-5b and SPIRE, HIFI bands 6a-7b and PACS, SPIRE and PACS in ~193-210 um
  – Outside Herschel, overlapping ranges between Planck HFI and SPIRE (photometer), PACS and Spitzer, HIFI and ALMA, SOFIA, APEX, etc

• Requirements: Cross-calibration plan and use-cases (HSC-DOC-1720)
  – Use cases for cross calibration between the three Herschel focal plane instruments
  – Primary checks on the stellar, asteroid and planetary models used in the Herschel mission
  – Use cases for cross-calibration with data from the Planck mission
  – Flux X-Calibration need to address:
    • Long-term temporal variability affects X-instrument (e.g. change in responsivity)
    • Line-flux dependent X-calibration
    • Wavelength dependence
    • Continuum check between PACS&SPIRE (may help for PACS in the leak regions)
    • Systematic effects in point-source beam correction or map reconstruction

• Implementation: Instruments routine phase calibration plan – coordinated efforts needs to be followed-up after re-consolidating the spectrometers’ X-Cal plan
Instrument cross-calibration

- **Implementation**: summary of observations done so far for PACS
  - The goal is to establish and verify a consistent line and continuum flux calibration between the PACS spectrometer and the SPIRE and HIFI spectrometers
  - Post-AGB stars & PNe with CO lines and [NII] have been observed: NGC 7027, AFGL 4106, CRL 618 and AFGL 2688
  - Total of 11.6 hrs in cal-cycles from #31 to #37 so far

<table>
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<th>ID: RPSpecFlux</th>
<th>Measurement description</th>
<th>AOT/CUS</th>
<th>basic duration (h)</th>
<th>repetitions, parameter variations</th>
<th>total time (h)</th>
<th>sources</th>
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<td>A</td>
<td>chopped range scans 172 – 220 μm, Nyquist sampling, medium chopper throw, 2 range repetitions</td>
<td>AOT</td>
<td>1.1</td>
<td>4 SPIRE-S – HIFI cross-calibration sources</td>
<td>4.4</td>
<td>post-AGB stars &amp; PNe with CO lines &amp; [CII] and [NII] lines AFGL 2688, CRL 618, AFGL 4106, NGC 7027</td>
</tr>
<tr>
<td>B</td>
<td>chopped range scans 195 – 210 μm, high sampling density, medium chopper throw</td>
<td>AOT</td>
<td>1.8</td>
<td>4 SPIRE-S – HIFI cross-calibration sources</td>
<td>7.2</td>
<td>same as A</td>
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**Instrument cross-calibration**

- **HIFI calibration monitoring program** (part of routine Calibration plan)
  - A set of ~15 sources observed every 3-4 months – overlap with PACS sources in leak region only (CO (13-12))

<table>
<thead>
<tr>
<th>NGC7027</th>
<th>IRC+10216</th>
<th>Ep Aqr</th>
<th>VY Cma</th>
<th>R Dor</th>
<th>CRL618</th>
<th>3x3 raster</th>
<th>G34.3</th>
<th>NGC7023</th>
<th>OTF LChop maps</th>
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<td>CO(8-7)</td>
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<td></td>
<td>CO(10-9)</td>
<td>CO(13-12)</td>
<td></td>
<td>CO(10-9)</td>
</tr>
</tbody>
</table>

- **SPIRE calibration monitoring program**
  - Set of AGB in common with HIFI, e.g. NGC7027, CRL618, AFGL2688, AFGL4106 – how often are these observed? What’s the complete source list?
  - Some dedicated observations performed on sources observed in full Spectral Scans with HIFI by KP (e.g. AFGL2591)
Instrument cross-calibration

- X-Cal implementation & design, possible room for improvement
  - Nyquist sampled range in the 172-220 µm range, high-sampling density in 195-220 µm range
    - The Nyquist-sampled range is very poorly sampling the line profile, off-pointed observations usually do not reveal skewed line profiles
    - The [NII] 205 µm line should be used to internally cross-check PACS profiles in Nyquist vs. high sampling modes
    - Beyond ~190 µm PACS suffers of leakage contamination but actually this part of the spectra could be cross-calibrated with SPIRE (i.e. PACS broad-band RSRF corrections if needed)
  - Recently discovered temporal line variability (especially for C-rich stars) on a timescale of 6 months has been measured up to ~300% (e.g. IRC10216 for lines of H$_2$O, HCN, SiS, SiO, CCH…), X-Cal observations need to be taken in a single cal-cycle close as possible. (Line variability could also effect photometric broad-band continuum but not PACS/SPIRE spectrometer continuum measurements)
    - Single line observations needed on a more frequent base and close in epoch. Probably [CII] and [NII] dedicated line-spectroscopy scans
  - No mapping X-Cal dedicated observations: raiding the archive for good cases?
**Instrument cross-calibration**

- Summary of investigations done so far (*to our knowledge*)
  - Comparison of integrated intensities of isolated lines between HIFI and SPIRE in evolved stars (M. Olberg/P. Imhof/I. Avruch) – application for SPIRE point-source intensity correction (NGC7027)
  - Comparison of HIFI spectra with APEX spectra – comparison with SOFIA on-going
  - Comparison of integrated intensities of [CII] lines in Carina (WADI KPGT)
  - Very limited comparison yet on broad spectral ranges (but see later slides)

*HIFI vs SPIRE IRC+10216 Band 5a*
Instrument cross-calibration

HIFI vs APEX CO (6-5)

HIFI vs PACS [CII] WADI

Follow-up Cross-Instrument Spectrometer – HIPE Forum 2011 - page 15
Instrument cross-calibration

HIFI versus SPIRE integrated line intensities in AGB – use for non-point source correction (P. Imhof, FTS and SDAG report)

Latest baseline subtraction & fit by Michael Olberg:

CO(10-9)

CRL 618: $2.1 \times 10^{-15}$ W/m²
NGC 7027: $1.5 \times 10^{-15}$ W/m²
CRL 2688: $2.7 \times 10^{-15}$ W/m²

Latest line fits from David & Gibion (ifgm fitting):

CRL2688 OK!
CRL618 great!
NGC7027 not very good (slightly extended?)

SPIRE line fitting (non-apodised) on NGC7027

Follow-up Cross-Instrument Spectrometer – HIPE Forum 2011 - page 16
Instrument cross-comparison

• Use information from another instrument to verify consistency of spectral information
  – Particularly useful for broad range surveys: are all lines seen in both instruments?
  – Assessment of detection feasibility based on existing data in another instrument
  – Cal-aspects: systematic properties of spectra need to be taken into account if multi-instrument data are combined (resolution-matched spectra becomes sensitive to different noise frequencies)

• Minimum set of tools for cross-cal/cross-comparison includes
  – Transform spectral/spatial/intensity scales into a common one
    • A priori knowledge of kernels is needed
    • Intensity calibration and/or scale transformation do assumptions on source geometry
    • Spatial convolution needs minimum mapping coverage
    • Spectral convolution needs minimum spectral range
    • Baseline fitting also with very crowded line spectra
  – Needs assessment of absolute noise levels on common scales, or SNR
  – Use output container able to encompass multi-set of data
Instrument combination

- One should be able to combine spectroscopic information collected by different instruments with, or without spectral or spatial overlap
  - Concatenate spectra over a large spectral range (e.g. PACS + SPIRE + mid-IR spectrum, HIFI+mm spectral scans, HIFI multi-obsids, HIFI+PACS spectrum)
  - Concatenate spectral maps over complementary spatial coverage (e.g. HIFI + PACS [CII] maps on close-by/overlapping regions)

- Minimum set of tools for this includes
  - Import data from other observatories into HIPE, and have them all in the same spectrum container
  - Otherwise, same as for X-Cal/X-Comparison
Example: multi-instrument spectral survey of IRC+10216

• Available data:
  – Full HIFI spectral survey (bands 1a to 7b) – GT1_jcernich + CAL (PUBLIC)
  – Full SPIRE coverage in High-Resolution – DDT_jcernich (PROPRIETARY !)
  – Full PACS range spectroscopy – DDT_jcernich (PROPRIETARY !)

• Exercises
  – Over-plot SPIRE and degraded HIFI data in bands 1a-1b and 5a-5b
  – Over-plot PACS and degraded HIFI data in bands 7a-7b
  – Check PACS vs SPIRE in 193-210 um area (leakage correction ?)

Follow-up Cross-Instrument Spectrometer – HIPE Forum 2011 - page 19
Use-case 1: HIFI bands 1a-1b and SPIRE

• Work flow
  1. Retrieve pipelined (HIPE 6.1) level-2 HIFI data in band 1a (*getObservation*)
  2. Clean fringes and baseline removal – both done together (*fitHifiFringe*)
     • Line auto-masking
     • 3 fringes considered
     • Continuum subtracted – *Would have liked to “divide” it but not available*
  3. Repeat above steps for HIFI data in band 1b
  4. Run deconvolution for both bands together (multi-obsids) – (*doDeconvolution*)
  5. So far, all steps treat H and V separately – then combine:
     1. Need to resample onto common (e.g. H) grid (*resample*)
     2. Average the two (*pairAvg*)

Product here is a *Spectrum1d*, calibrated in K (Ta*), versus GHz
Easy case here because no need for spur removal or fancy baseline correction
Use-case 1: HIFI bands 1a-1b and SPIRE

• Work flow (cont’d)
  1. Convert frequency scale in wavenumber (convertWavescale)
  2. Retrieve pipelined (HIPE 7.0) level-2 SPIRE data (getObservation)
  3. Extract either apodized or non-apodized SLW spectrum
  4. Resample/smooth HIFI data to SPIRE resolution – two approaches considered:
     • Smooth function (smooth): assumed Gaussian kernel size: 0.06 cm-1 for apodised (i.e. HR x 1.5)
     • Resample function (resample): re-project onto SPIRE grid
       • Apodised: Gaussian function with “params” = 0.06 cm-1
       • Non-apodised: SINC function with “params” = 0.04 cm-1
  5. Convert temperature scale into Jansky
     • Task (convertK2Jy) does not work yet on Spectrum1d (but will in 7.1- HIFI-3899)
     • Task needs to access multiple LO Freq. to assign applicable efficiency
     • For this exercise, we multiplied manually by the applicable value: 488 Jy/K
  6. Subtract continuum from SPIRE
     • No existing task – did some attempt with polynomial fit but line density too high
     • In the end, subtracted an average value applicable to the HIFI band 1 range (10 Jy)
Use-case 1: HIFI bands 1a-1b and SPIRE

SPIRE apodized minus 10 Jy: total = 8.8e-15 Wm-2
HIFI native (x10): total = 8.9e-15 Wm-2
HIFI re-sampled with Gaussian: total = 8.6e-15 Wm-2
HIFI smoothed: total = 8.4e-15 Wm-2

Flux (Jy)

Wavenumber (cm⁻¹)

Following Cross-Instrument Spectrometer – HIPE Forum 2011 - page 22
Use-case 1: HIFI bands 1a-1b and SPIRE

SPIRE non-apodized minus 10 Jy: total = 9.4e-15 Wm-2
HIFI native (x10): total = 8.9e-15 Wm-2
HIFI re-sampled with SINC: total = 8.9e-15 Wm-2
Use-case 2: HIFI bands 5a-5b and SPIRE

SPIRE apodized minus 55 Jy: total = 2.7e-14 Wm-2
HIFI native (x10): total = 2e-14 Wm-2
HIFI re-sampled with Gaussian: total = 2e-14 Wm-2
HIFI smoothed: total = 2e-14 Wm-2

Assumed conversion: 588 Jy/K

Flux (Jy)

Wavenumber (cm⁻¹)
Use-case 3: HIFI bands 7a-7b and PACS

- Same work flow as for bands 1 and 5 leads to worse baseline quality because of residual spurs and non-standard fringes
- Re-sampling at PACS resolution is not straight-forward
  1. The \textit{resample} function can be used to resample onto PACS grid. However ideally the PACS resolution element has a width function of wavelength
  2. In the example given, simple variable width kernel convolution applied but need to be recoded in the Fourier space (~800 HIFI channels per PACS bin!)
  4. Residual from de-convolution on imperfect data-set contaminate the smoothed HIFI data. Need to work from data processed by KP experts
Use-case 3: HIFI bands 7a-7b and PACS

HIFI native (x10)
HIFI resampled (x50 !)

PACS minus 70 Jy
PACS minus cont
HIFI re-sampled
Other use-cases

• Combine HIFI data with other ground-based telescope or HIFI data processed outside of HIPE
  1. Data import can be done via Class-export into FITS
     • Very limited header information
     • In practice, get a collection of individual spectral segments as flux versus frequency
     • Needs to feed data into common container compatible with further analysis through the SE or CSAT, etc. I could not find doc. on how to fill in a Spectrum1d e.g.
     • Combination with other HIFI obsids not yet straight-forward
  2. Beam dilution correction (different dish size) has to be done manually for single pixel case – any need to provide more guidance for this?

• PACS/SPIRE cross-comparison in 194-210 um
  • Point-source correction not yet applied on PACS (x2 expected)
  • Some ghost features in PACS, but also some SPIRE features with no PACS counterpart?
HIFI SScan versus SPIRE/PACS: conclusions

• Intrinsic limitations
  – Considered data-set not collected for this purpose – in particular, SNR not necessarily compatible for proper comparison
  – Absolute intensity calibration still has a limited accuracy
  – Source variability makes HIFI/SPIRE taken at different epoch more complex

• Overall spectra comparison: line density consistency and intensities
  – Overall, all strong lines have a match, albeit with intensity incompatibility depending on the wavelength
  – Native HIFI and SPIRE data have good agreement in full integrated intensity, although worse in band 5 (35% difference – inaccurate cont. subtraction ?)
  – SPIRE point-source correction may not be valid for all lines in IRC+10216 (some will have somewhat extended emission) – cf NGC7027 case
  – Pointing accuracy very critical for PACS observations – data-set considered here not corrected for this (works only for point sources) – question is whether HIFI/PACS-S X-Cal can be done at all on extended sources
HIFI SScan versus SPIRE/PACS: conclusions

- Data transformation tasks
  - Overall, re-sampling/smoothing functions seem to conserve flux consistently
  - Kernel options in GUI interface do not cover all those available in cmd-line (is it a more general GUI issue?)
  - Re-sampling function does not seem to check for overlap in spectral range (at least, error message not explicit) – but it fails if no overlap!
  - Convolution with SINC function not conclusive (wrong kernel size?)
  - Use of smooth function does not seem appropriate (at least with chosen kernel)
  - Baseline removal over broad wavelength ranges not straightforward
  - PACS resolution is function of wavelength: HIFI wavelength scale may need to translate into a fixed Kernel size in order to do a fast FFT-based convolution

- Programmatic
  - We need MANY more test cases to build statistics on e.g. systematics – DB mining for existing candidates, and better coordination for future cal obs.
  - E. Puga (HSC) will look into this as prime task, in collaboration with the ICCs
Proposed improvements / new tasks

1. Data transformation
   • Current re-sampling task should be more explicit in error message when trying to
     resample data that do not overlap in wavelength/frequency (no a priori checks ?)
   • Need for re-sampling task/function taking into account a variable Kernel width
     convolution (esp. for PACS, but probably true for other facilities). A generic tool should
     be able to convolve any non-equidistant grid with wavelength dependent kernel size.
   • Implement “standard” intensity conversion task between Herschel instruments (output
     scale as user input – e.g. K, Jy) – users should not have to look for conversion factors
     (BUT source size will matter…) Could be used for VO export?
   • Mapping observations have to be translated into Jy/pixel units on the same spatial (and
     wavelength) grid

2. Data analysis
   • Is the SpectrumFitterGui not (yet) user-friendly enough ? Or is documentation unclear ?
   • Baseline correction / continuum subtraction for PACS/ SPIRE: prototype with
     multiresolution tools shows promising results
   • De-fringing tool should allow to “divide” by baseline too (not only subtract), as in the
     fitBaseline
     • As an extension, need to discuss why “divide” option in fitBaseline returns a baseline
       normalised to 1 (this is e.g. not what Class is doing)
Proposed improvements / new tasks

2. Data analysis (con’td)
   • Improve flagging task: usually users just want to get rid of a range of channels: it should be easy to simply exclude channels from any further processing – is it already but no well documented?
   • More user-friendly integrated intensity task (current statistics task not sufficient)?
     • Chose unit of integrated area (GHz, wavelength, cm-1, etc)
     • Chose integrated windows
     • Chose unit of output intensity scale (e.g. K.km/s, K.Hz, Jy.cm-1, W.m-2, etc)
     • Allow beam dilution in a given dish (comparison with other facilities)

3. Data combination (complementary to VO? Redundant?)
   • Need for a tool allowing to combine data-sets from different obsids (same instrument), different spectra within an obsid (e.g. sub-set of DF in HIFI SScan), or from different instrument
     – As “idiot-proof” as possible through basic consistency checks
     – Size of container should be dynamically adjustable to “append” new data ad libitum
     – Options for overlapping regions (stitching) TBD
     – How “easy” to have this working for cubes as well?
Proposed improvements / new tasks

4. Data re-pipelining
   • Better version management/information for CalTree: refer to Calibration Framework splinter
   • OFF-chop contamination (both HIFI/PACS): refer to User and Advanced Scripts sessions

5. Data I/O: refer to the Observation Management splinter

6. Documentation: several “failed” attempts in some tasks applied along the workflow
   • Usually solved on the HIPE 8 track
   • Otherwise, treat as normal maintenance work (JIRA)