Dealing with Point Sources Observed with PACS Spectroscopy
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1 INTRODUCTION

This user note is to guide users through working with PACS spectroscopy observations of point sources.

It is important to realise that for point sources observed with PACS spectroscopy, the observed spectra require point-source corrections to be performed. It is generally not enough to simply sum up the flux of the point source in the observed field. The reason for this is that aperture extractions from a cube do not correct fully for the flux “falling between” spaxels. These gaps are a consequence of the uneven illumination of the PACS FoV. This is corrected for by the PACS flux calibration only for fully extended sources: any other source morphology will require extra flux corrections. More detail on this uneven illumination can be found in the PACS Handbook and the user note on working with extended sources. A simple aperture extraction also does not correct for the flux falling outside of the spaxel(s) where the point source falls (because the beam is larger than a spaxel: in fact its wings even extend slightly beyond the $47'' \times 47''$ FoV of a single pointing). Therefore, it is necessary to apply the provided point-source corrections to all observations of point sources performed with PACS spectroscopy.

The standard calibration of PACS spectroscopy calibrates fully only the extended sources. Point and small sources, for which the calibration can be very different, need specific corrections. It is clear from the name that the “point-source” corrections are for point sources. Nonetheless, sources that are very close to being a point will probably also benefit from these corrections. However, the “very close to” limit has not been established, and hence it is up to the user to decide whether or not these corrections are suitable for their source. For more information about dealing with semi-extended sources, see the user note on semi-extended sources that can be found in Herschel Explanatory Legacy Library (PACS section). The calibration scheme of PACS is explained in the PACS Handbook.

Before reading this release note you should be familiar with PACS spectroscopy, in particular with the various observing modes that were used and different types of cubes that were produced. These are explained in the Quick-Start Guide, and in more detail in the PACS Products Explained and the PACS Handbook, all of which can be found in the Herschel Explanatory Legacy Library (PACS section). To follow the advice given in this user note, the user should have at least read the Quick-Start Guide. Definitions are provided at the end of this release note, but to understand the terms defined, it is necessary to read the other documentation. Additionally, the tasks discussed in this note are explained, and their parameters defined, in the Help documentation available from HIPE, in particular the PACS Data Reduction Guide (spectroscopy) and the Users Reference Manual.
2 PRE-REQUISITES

The first pre-requisite is that the user knows that their target is a point source at the PACS wavelengths. This is something that cannot be determined from the PACS data alone, although information obtained from the PACS data, together with information from other wavelengths, can be used to determine if a source is consistent, or not, with a point source.

The second is that the user knows the observing mode. This is important when discussing which products to use, what issues to be aware of, and the calibration uncertainties. This information can be obtained from various sources: the FITS header keywords of the final-level cubes in an observation, a spreadsheet of keywords for all observations, and the PACS Observation Summary which is provided in all observations (but can only be read in HIPE; although it may soon also be provided on the HSA search results page). How to find this information is explained in the PACS Products Explained.

The third is that the user knows how to open a cube in HIPE. The Spectrum Explorer is especially useful for working with cubes, and for the type of cubes that are used in the point-source corrections, it provides capabilities that are very difficult to find outside of HIPE. The PACS Footprint Viewer is also a useful tool that is very difficult to replicate outside of HIPE.

Finally, it is necessary that spectrum of the point source is not contaminated by another source (e.g. a background). The point-source corrections are multiplicative, and they are only fully applicable if the observed spectrum is from the point source alone. If your point source is blended with another source, your choices are to either accept the additional uncertainty (which you will also have to calculate yourself, as it is highly dependent on the nature of the blended emission), or to remove the contamination, e.g. subtract it out before applying the point-source corrections to the cubes. See Appendix 1 for advice on removing contamination.

The point-source corrections discussed are applied to the re-binned cubes, which are provided for all observations and are the main science end-product for pointed observations. It was always assumed that observers of point sources would use the pointed observing mode, and this assumption is found in this user note also. If you have a mapping observation instead you simply need to apply the corrections to the re-binned cube in the raster in which the point source is located at, or at least close to, the central spaxel of that cube.

3 THE POINT-SOURCE CORRECTIONS

3.1 What do they do?

The calculation of the point-source corrections is explained in the PACS Handbook. The
corrections are held in the calibration file PCalSpectrometer_PointSourceLoss_FM_v4.fits. They were computed from knowledge of the full size and shape of PACS beam (that of the central spaxel) at the key wavelengths.

The corrections perform two functions:

1. **Correcting for the size of the full beam.** The blue beam and the footprint of the PACS IFU is shown in Fig. 1: it can be seen that the beam extends over the entire 47”x47” FoV – in fact, the beam actually extends a bit beyond this. However, in most observations of point sources, the target is visible mainly in a single spaxel + the immediately adjacent spaxels: thus the observed flux covers a smaller area than the point source (= the beam) actually does. The point-source curves, also shown in Fig. 1, correct for this missing flux: taking the spectrum extracted from the central spaxel or from the central 3x3 spaxel box to the actual flux of the point source as contained within the full beam.

2. **Correcting for the flux lost “between spaxels”**. The footprint of the PACS IFU is an irregular 5x5 grid of nominally 9.4” spaxels, as is shown in Fig. 1. However, the illumination of the IFU is in fact *not* uniform. This means that the 9.4” spaxels are effectively not contiguous: measurements show that their illumination pattern makes them closer to 8” in size. The point-source curves correct for this lost flux because they were computed from a beam constructed from a mapping observing pattern that “filled in” the gaps. This uneven illumination is explained in the PACS Handbook and the user note on working with extended sources.

![Figure 1 Left: the PACS beam at 75 μm with the footprint of the PACS integral field unit. Right: the point-source correction curves to take the flux of the central spaxel or the central 3x3 spaxels to the total flux of a point source.](image)

The correction curves were computed from the beam. In fact, the beams of each spaxel are slightly different to each other, and so the correction curves for each spaxel should also be slightly different to each other. However, the corrections have only been computed from the
central spaxel and so, strictly-speaking, they are only applicable to sources located in the
centre of the central spaxel. Even an offset of a few arcsec can result in a slightly incorrect
calibration. Fortunately, the uncertainty arising from slight off-centring has been folded into
the calibration errors (see e.g. the Quick-Start Guide), and so for small offsets (a few arcsec)
the calibration errors cover the consequent uncertainty.

3.2 How are they applied?

There are two sets of tasks that apply the point-source corrections. Both are applied to the re-
binned cubes created at the end of the pipeline – from Level 2.5 for the un-chopped range
scan observations, and at Level 2 for all others. The re-binned cubes are those that have the
footprint of the native PACS IFU (Fig. 1).

The main point-source task – extractCentralSpectrum – produces three spectra, c1, c9, c129,
and some diagnostic information:

1. The spectrum c1 is created from the first point-source calibration developed by PACS.
The spectrum of the central spaxel is corrected with the central-to-total curve (Fig. 1). This is the basic correction for point sources.

2. The spectrum c9 is created from the second point-source calibration of PACS. This was
done because it was realised that for point sources suffering pointing jitter during the
observation, or for which slight (a few arcsec) pointing offsets moved the source from
the centre of the FoV, the calibration using the sum of the central 3x3 spaxels was
more robust than that using central spaxel only.

3. The spectrum c129 was developed for cases where the SNR of the spectrum from the
central spaxel is superior to that from the central 3x3 spaxels. Here, the spectrum from
the central spaxel, “s1”, is scaled to the flux level of the point-source spectrum c9, to
keep the SNR of the first but the more correct fluxes of the second.

The diagnostics provided are two plots and some correction values:

1. A central9/central plot shows two curves and the data they were smoothed from. The
first curve is the ratio c9/s1, where s1 is the (uncorrected) spectrum of the central
spaxel. This is the scaling curve used to create c129 from s1. The second curve is the
ratio s1/s9 computed from the data, to that same ratio expected for a perfectly centred
point source. Any value larger than 1.2–1.3 indicates that the source is not a point
source and/or is not centred. The effect of off-centring and a non-point-like nature on
this ratio are the same, so you cannot distinguish the two from each other.

2. The mean value of the second curve is printed to the HIPE console, together with the
data error of that value and RMS of the data the mean value was taken from.

3. A plot of the three spectra produced, together.

This task is to be used on all sources that are located within the centre of a cube.
The second task – which is in fact a set of three tasks – produces $c_1$ but extracted from any spaxel in the cube, not only the central spaxel. It is aimed at sources that are offset from the central spaxel, as explained later in this note.

The task extractCentralSpectrum is written into all of the interactive pipeline scripts that are provided in HIPE, and moreover a user script to demonstrate the use of this task on re-binned cubes taken from a downloaded observation can be found in HIPE (i.e. it is not necessary to run the entire pipeline to apply the point-source corrections). The task works on the re-binned cubes only, not on any of the mosaic cubes that are also provided in any PACS spectroscopy observation.

For all pointed observations, the output $c_1$, $c_9$, and $c_{129}$ (this latter not for un-chopped observations) are provided in the HSA download at Level 2.5 or 2, in a spectrum table. More details about this product – HPSSPEC[B|R] – can be found in the PACS Products Explained. If you have a pointed observation, it may therefore not be necessary to use HIPE to get a point-source calibrated spectrum. However, it is still necessary to read this user note and inspect your data so it is clear which point-source spectrum to use and what the associated uncertainties may be. Running the task is HIPE may also be useful because of the diagnostic information it produces, especially the value that indicates the centring/point-like nature of the source.

### 3.3 Additional and alternative paths

There is one additional path a user can follow for any observation of a point source, and one alternative path that a user can follow for off-centred point sources. The details of running these tasks and what sort of point sources they are suited for are given later: first an introduction.

**The additional path** is to run the “Pointing Offset Correction” (POC) pipeline script in HIPE. This is a full data-reduction script, ending with $c_9$ and $c_{129}$ produced by extractCentralSpectrum. It can be only be run any chop-nod observation – the calibration scheme it uses is inapplicable to un-chopped observations. In this pipeline, extra tasks that measure the location of the point source in the FoV and then correct the flux distribution of the central 3x3 spaxels to account for that, are included. By running this pipeline, users can produce spectra that are at least as good as, and can be better than, those taken from the Level 2 data gotten from the HSA. For sources that are offset from the central spaxel, it is *definitely* worth trying this pipeline. For sources that are centred but which suffered pointing jitter during an observation, it is also worth trying this pipeline. (Although it is unfortunately very difficult to tell from the Level 2 data whether or not there was any pointing jitter during that observation.)
This POC pipeline has been run on all pointed chop-nod observations to create an HPDP (highly-processed data product) that can be downloaded from the HSA. The products of the HPDP are the c9 and c129 spectra and the diagnostics created in the POC script (pointing determinations and the output of extractCentralSpectrum). The release note provided with this HPDP explains what the pipeline does and what its diagnostic outputs show, and is recommended reading for everyone who wants to use the HPDP or run the POC script for themselves. Note: at the time of writing this user note, this HPDP is still in the process of being created. Once completed, this HPDP will be available from the HSA and from the HPDP cosmos page.

The alternative path is for point sources offset from the central spaxel. Here you extract the point-source calibrated spectrum of the central part of the cube using extractCentralSpectrum, but then you apply an additional correction – that of an off-centred point source. The task is called specExtendedToPointCorrection: it was written for use on slightly extended sources, but it can also be used to correct for off-centred point sources. For some cases it can create a better-calibrated spectrum that you can get from extractCentralSpectrum alone.

The options and the conditions under which to use the additional and alternative routes are discussed next. After reading this advice, please also read Appendix 2, where some examples of running extractCentralSpectrum on a centred and off-centred source, taken from cubes created by the standard and the POC pipeline, are given. Along with the discussion of these results, some practical advice on how to interpret the results is given.

4 WHAT TO DO FOR YOUR POINT SOURCE

Here we give advice about what to do for point sources with various degrees of offset from the centre of the FoV.

The advice given here is based on the extensive testing of the point-source corrections, since these corrections were part of the flux-calibration determination for PACS spectroscopy (the calibrators used were point sources themselves). The advice concerning the limits of the tasks for faint/bright centred/off-centred sources are based on a smaller set of tests carried out on raster observations of NGC 5315 and HIP 21479 (calibration observations which can be reduced by anyone in HIPE: obsids 1342182744-9 and 1342184661-3) and on simulated observations. However, these sources are bright, and so it was not possible to fully test the limits of the recommendations, especially with respect to source brightness.

It is not easy to determine – especially from a pointed observation – how offset a point source is from the centre of the FoV. However, it is important to have some idea of this offset in
order to understand the associated uncertainties. Some advice is offered in Appendix 3.

4.1 Centred point sources: extractCentralSpectrum

For sources that are centred in or very close to the centre of the FoV, i.e. in spaxel 2,2, the recommendations are clear:

1. For faint sources, where only the central spaxel has signal, use c1
2. For sources bright enough to spill out into the adjacent spaxels, but which are still centred in the centre of that spaxel (to within ~2″), use c129 (however, see the very important advice given in Appendix 2, where examples from real data are shown, and the use of c129 over c9 receives more attention)
3. For bright sources which are offset by >~3″, use c9

We note that for perfectly-centred point sources, c1 and c9 should have the same flux levels. In reality, a source is rarely exactly centred, and even an offset 2″ or 3″ will result in the flux of c1 being less than that of c9, and noticeably so for bright sources (in fact, this will be equally true for faint sources, but here the difference is harder to see as it is hidden below the noise and uncertainties). Note that for such small offsets, the calibration uncertainties cover the corresponding flux losses.

In Sec. 4.4, the conditions under which it is recommended to use the POC pipeline for centred point sources is given. We note here that the advantages of the POC output over the SPG output for centred point sources are generally not so high.

Example spectra showing the output of extractCentralSpectrum on a centred point source can be found in Appendix 2.

4.2 Off-centred point sources: extractCentralSpectrum

The situation for off-centred point sources depends on the brightness of the source, and how much and in which direction it is offset. The brightness is important because it is less clear which output of extractCentralSpectrum is the best to use for faint sources than it is for bright sources, and the flux uncertainties are higher for faint source than for bright sources. The direction of the offset is important because the amount of flux lost between spaxels (due to the uneven illumination explained in Sec. 3.1) depends on where the source falls in the FoV, not just how far it is from the centre.

In Sec. 4.4, the conditions under which it is recommended to run the POC pipeline rather than use the SPG products for off-centred point sources is given. The results from the POC pipeline for point sources are at least as good as those taken from the HSA, but for off-centred sources they can be noticeably better.

Some spectra resulting from tests on offset sources are show in Appendix 2: the output of
extractCentralSpectrum for a slightly offset point source; c1 and c9 for various offsets; c9 and c129 from the SPG and the POC pipelines compared for various offsets and to each other.

4.2.1 Offsets of ~2″–3″
For sources offset from the central spaxel by about 2″ or 3″, the spectrum c1 will capture less flux from the source, and it is usually then not the recommended spectrum to use. In this case, the spectra c9 or c129 will be the better option. Note that c9 is based on the sum of the central 9 spaxels: if the spectra from many of these 9 spaxels are faint, the SNR of c9 will be lower than that of c129. However, for offsets around the 3″ mark, the spectrum c129 starts to become less recommended than c9, as this much of an offset makes the scaling used to create the spectrum (s1-to-c129) less reliable. Generally, the spectrum with the highest flux levels (in the spectral line if that is your point of interest) is the one to use. However, see the very important advice given in Appendix 2, where examples from real data are shown and where the use of c129 vs c9 receives further attention.

For sources with only a small offset, the c9 spectrum taken from the observation is not very different from that produced by the POC script. The point at which the POC results can be better than the SPG results is somewhere around the 4″–5″ mark.

4.2.2 Offsets of >~3″–4″
As the offset becomes larger, the amount of flux lost from c1 also becomes larger and it is definitely recommended to use not c1. For these offsets, the s1-to-c129 scaling used to create c129 becomes invalid, and it is therefore also not recommended to use this spectrum. For these large offsets, c9 is then the recommendation.

From the tests that were carried out on NGC 5315 and HIP 21479, it was found that when the source is located at the edge of the 3x3 spaxel box (i.e. an offset of 8″–10″), the flux loss in the emission lines in c9 were around 20% in the bright emission lines (flux > 100 Jy and good SNR) and up to 50% in the faint/low SNR line (flux ~10s of Jy but SNR quite low). Consider especially that when the source is at the edge of the 3x3 box, then some of its flux will fall outside of the 3x3 box and will not be included in the creation of c9. Consider also that the point-source corrections applied to c9, as well as to c1, are only fully correct if the source is centred.

For sources located well outside of the central spaxel, it is strongly recommended to try the POC script (Sec. 4.4). The E2P task (Sec. 4.5) can also be tried for sources with such large offsets.

4.3 Offsets outside of the 3x3 box
For sources located at the edge of the FoV, the only option is to use a set of tasks that apply the same correction used to create c1, but here on a spectrum taken from any spaxel. These tasks are undoExtendedSourceCorrection, extractSpaxelSpectrum, and…
pointSourceLossCorrection and their use is demonstrated in a user script in HIPE (“Point-source loss correction: any spaxel”). They start with the re-binned cubes taken from Level 2.5/2 of the HSA download.

The spectral flux from this task will almost always be an underestimate: the single-spaxel correction is less than 3x3-spaxel correction unless the source is exactly centred in a spaxel (i.e. c1 is usually < c9, but these tasks only produce the equivalent of c1). In addition, and as explained previously, while the beams of each spaxel of the PACS IFU differ slightly, the point-source corrections were only calculated for the central beam: this results in an additional (un-measured, although not great) inaccuracy in the point-source correction applied to sources taken from a spaxel other than the central.

4.4 Centred and off-centred point sources: the POC script

The Pointing Offset Correction script is a pipeline script with additional tasks to calculate the position of a source (specifically, its offset with respect to the centre of the cube) and to correct the flux levels of the summed central 3x3 spaxel box for this. This script will only work on chop-nod observations. The science outputs from this script are the spectra c9 or c129 created by extractCentralSpectrum.

Before trying the pipeline, yourself, you can consult the PACS spectroscopy HPDPs: an HPDP to provide POC point-source calibrated spectra for all chop-nod pointed observations is currently being created. This HPDP will be available from the HSA and it will be possible to obtain them from the HPDP cosmos page. The release note explains how the POC pipeline works and which outputs should be taken for science.

4.4.1 Centred point sources

For centred point sources, the output of the POC script is mainly useful if there was much pointing jitter during the observation, as this task should reduce the consequent spectral noise. This is mostly useful for targets with faint and/or wide spectral features. It is unfortunately not possible to know what the pointing jitter was from the reduced data taken from the HSA, however in the POC script, the task plotPointingOffset will produce a plot of the measured pointing offsets that can be consulted: if the scatter in this plot is low, then there is probably no need to carry on with that pipeline script. (Note: these plots form part of the POC HPDP.)

If you have lines of decent SNR, there is no need to run the POC script for point sources that are pretty well centred in the central spaxel.

4.4.2 Off-centred point sources

For sources that are offset by ~4" to a full spaxel width (~9"), running the POC script is highly recommended. For the (bright) and highly-offset point sources it was tested on, while
there was clearly some flux loss in spectrum c9 when the sources were located at the extreme offsets, this flux loss was less than found in the spectrum c9 created from the HSA download, i.e. as produced from the SPG pipeline.

For faint sources (fainter than ~10 to a few 10s of Jy) the POC tasks will have more problems determining the offsets and hence the results become less useful. The diagnostic outputs from the POC pointing-determination tasks (a plot called “pjitter” and values printed to the console, by the task plotPointingOffset) will show this: the dots representing the measured positions of the point source taken from the observation’s data-blocks will show very little scatter if the tasks were successful in measuring the pointing offsets. If the scatter in the pjitter plot is high, the results of the pipeline should be treated with caution. This plot is explained in the release note of the POC HPDP.

In general, c9 and c129 arising from the POC script are similar; if they are not, or if the scaling curve that is used to create c129 (and which is plotted by the extractCentralSpectrum) looks “odd”, c9 is to be preferred.

4.5 Off-centred point sources: the E2P correction

For a point source offset by ~4″ or more (but which is still located in the central 3x3), an alternative – and not particularly difficult – option to using the POC pipeline is to model the source and its offset. The advantage here is that you do not need to run a full pipeline, as the task runs on the re-binned cubes gotten from Level 2/2.5 of the observation. Another advantage is that, unlike the POC pipeline, this task will work on un-chopped observations.

The steps are to take the output of extractCentralSpectrum created from the cubes (c9 is the best when the offset is so large); create a model of the source (a narrow Gaussian with a specified offset in RA and Dec from the centre of the FoV); and run the task specExtendedToPointCorrection. This task will compute a correction to the input c9 based on the difference in the surface brightness distribution of a centred point source (c9) and the input model (here, an off-centred point source). This correction should be divided into the input c9 to obtain the final spectrum. This task was written for use with semi-extended sources, but can also be used on offset on point sources. An example script can be found in Appendix 4.

For large offsets, the results of the E2P task will still suffer an uncertainty due to the fact that the correction applied by extractCentralSpectrum is based on the beam of the central spaxel only, although that computed by specExtendedToPointCorrection (aka E2P) uses the beams of the central 3x3 area. Tests show that for large offsets the results are often better than c9 derived from the SPG products, but not better than c9 derived from the POC pipeline A word of warning however: it was found that the flux uncertainty for the E2P results are both plus and minus: for all other tasks discussed in this user note, the errors caused by an offset are in
the direction of a flux loss, but in this case sometimes an offset spectrum modelled by the E2P can be given a flux gain. Therefore, the POC script is to be preferred over the E2P option, and the E2P results should always treated with some caution. It is not possible to state reliably what the uncertainty here is, but a value of ± 20% (additional to the standard uncertainties) should certainly be assumed, and for unfortunate cases (large offsets and/or the star is in a very low-response part of the FoV) a value of ± 50% should be assumed.

Tests were conducted to see how sensitive the E2P correction is to the accuracy of the input source size and offset. The source size should be set to 0.2″ when modelling a point source, but a value of 2 was tested, and offset values wrong by up to 6″ were tested. Getting the source size and the offsets wrong clearly produced incorrect results but not in a predictable way. This is probably because the uneven illumination of the FoV plays a large part in the uncertainty of the point-source corrections for off-centred sources, and so the results depend on in where in the FoV the source actually is. On the whole, the errors in the emission line peaks produced by an incorrect model were 10–20%, but occasional 50% error levels were also found.

5 MAPPING OBSERVATIONS

As stated previously, the information in this user note is applicable to pointed and mapping observations, as long as the re-binned cube in which the point source is centrally-located is used. Why is it not possible to use the mosaic cubes, created for all mapping observations, to work with point sources? The answer lies in the nature of the point-source corrections. The corrections go from what you get within the central or central 3x3 spaxels, to what you would have had if the PACS detector was perfect and covered a larger FoV. However, the mosaic cubes produced for mapping observations are a different starting point: their spatial pixels are the combinations of several input native spaxels (one for each pointing) and the spatial grid has been resampled. In the mosaic cubes from mapping observations, some of the flux gaps that are due to the uneven illumination of the FoV will have been filled in – whereas they are instead corrected for by the point-source task – and the spatial distribution (spaxel sizes and the grid) of the cube is also different. For these reasons, the point-source curves shown in Fig. 1 are only suitable to use on re-binned cubes.

6 DOING YOUR OWN TESTING ON SIMULATED CUBES

If you wish to test the uncertainties and limits of the point-source corrections for different pointing offsets and spectral SNR, you could create re-binned cubes containing simulated spectra of point sources located wherever you want in the FoV. To create a re-binned cube with a simulated point source, a script is given in Appendix 4.
1. The script starts by defining the point-source model. The visualisation part (imageModelInPacsSpecFromModel) is not necessary, but is useful.

2. Define the model – a narrow Gaussian with a spectrum consisting of an emission line and a continuum. If you wish the flux of the spectrum to be based on a real observation use c9 from extractCentralSpectrum: input the values of the line peak and continuum flux from this spectrum. The values then have to be normalised to the area (i.e. the area of a point source). (Note that you may need to iterate to get a match of the model to the data.)

3. Create the model – inputting the scaled fluxes, offsets, size of the source (0.2\" for a point source), and you can also inspect an image of the model (specify the size and wavelength of the image).

4. Get the observation (e.g. the one used to create the model). The sliced re-binnedCubes from Level 2 or 2.5 are used for the RA and Dec, not for their data, or you can enter the coordinates yourself (read the Users’ Reference Manual in the HIPE Help to learn more about the parameters of the task). It is necessary that the wavelength of the spectral line modelled in step 2 has to be within the wavelength range in the cube.

5. Finally, create the re-binned cube with the simulated source+spectrum. This re-binned cube can then be processed extractCentralSpectrum or specExtendedToPointCorrection.

Note: if you want to simulate real data and how the tasks behave with real fluxes, you will need to add noise to the simulated cube.
Appendix 1 How to remove contamination

If your point source is contaminated by another source of emission – most likely a background – this should be removed this before running extractCentralSpectrum. Since this task works on re-binned cubes, it is on these that you need to work. To subtract out the contamination you can fit and subtract it with the Spectrum Toolbox of the Spectrum Explorer. This toolbox is explained in the HIPE help documentation (the Data Analysis Guide): the steps are to find the nicest-looking spectrum in the cube, fit the unwanted spectral feature (e.g. a continuum) of that single spectrum, and then use the “MultiFit” part of the toolbox to fit the entire cube with that model. The output is a set of cubes: the model (e.g. the continuum fit), the total model (the continuum fit if you only defined that as a single model, but all models if you defined multiple models), and the residual (data – model). This residual is then the point source with the contamination removed.

However, you cannot use the residual cube directly. The reason is that the class of output that the fitter creates is a SpectralSimpleCube, and this is not the correct class of cube for extractCentralSpectrum to work on (the task requires a Pacs re-binnedCube), i.e. it loses much of the structure and layers of the re-binned cube that was fitted. The work-around is the following:

```python
obsid = 1342....
obs=getObservation(obsid,useHsa=1)
slicedRe-bnnedCubes = obs.refs["level2"].product.refs["HPS3DRB"].product
# For you: a security copy, as slicedRe-bnnedCubes itself is changed below
slicedRe-bnnedCubes_cp = slicedRe-bnnedCubes.copy()
# Get the first cube in slicedRe-bnnedCubes
cube = slicedRe-bnnedCubes.get(0)
# Open the Spectrum Explorer and from there the Spectrum Toolbox. Do your fitting
# The outputs from the multifitting in there are, for a single model
# (polynominal) fit, are:
==
HIPE> # Added variable: FitResult
HIPE> # Added variable: SFGResultsContext
HIPE> # Added variable: MultiFit_Residual
HIPE> # Added variable: MultiFit_TotModel
HIPE> # Added variable: MultiFit_Parms
HIPE> # Added variable: MultiFit_ParameterCube
HIPE> # Added variable: MultiFit_M1
==
# Get the "image" array from the residual - the fluxes
image = MultiFit_Residual["image"].data
# Replace the fluxes in cube with those from MultiFit_Residual
cube.setImage(image)
# Then push cube back into slicedRe-bnnedCubes – slice 0 (and then 1, 2...)
slicedRe-bnnedCubes.replace(0,cube)
# Repeat for however many cubes in slicedRe-bnnedCubes you want to work with
```
Appendix 2 Examples of c1, c9, c129 for a centred and an off-centred point source

Here we show some examples of the output of `extractCentralSpectrum`. The source is R Doradus, a red giant star that is a point-source to PACS photometry (this can be seen from the tri-lobal shape of the source in Fig. 2). The observation is a calibration observation, obsid 1342186652 (fully reduced by the SPG pipeline, and public in the HSA) that was taken to look at how the flux distribution changes as the source moves over the IFU (the observation is a raster with steps of 7x7 steps of 2.5″). In Fig. 2 we show a PACS photometry image of the source, with the spectroscopy footprints of two of the positions in the raster over-plotted (this was done with the PACS Spectral Footprint Viewer). In one pointing the source is fairly well centred and most of the flux falls in the central spaxel, and the other it is off-centred where just less than half of the flux falls outside the central spaxel.

![Image](image.png)

*Figure 2 Left* is the raster position where R Dor is centred in the FoV. *Right* is the one where it is off-centred. The PACS IFU footprint is plotted on a blue PACS image of the star. In the image, the point at which the flux is ½ of the peak is about 2 map pixels (≈3″) from the peak. Note that the sizes of the spaxels is only approximately represented here: they are shown to be “9.4″ in diameter, but in reality they behave as if they closer to 8″ in diameter (see Sec. 3.1).

In Fig. 3 are the plots that are produced by `extractCentralSpectrum` for these two pointings.
Figure 3 Top are the plots from `extractCentralSpectrum` on R Dor in a centred pointing. Bottom are the same plots for an off-centred pointing. See also Fig. 2.

Top left and right are the plots produced for the pointing where the source is centred close to the centre of the central spaxel.

- The left plot shows two diagnostic curves: the ratio of \( s_9/s_1 \) observed compared to that ratio for a perfectly-centred point source (light grey data and blue smoothed curve); and the ratio of \( c_9/s_1 \) (dark grey data and green smoothed curve). [Key: \( s \)=the spectrum taken from the spaxel, with no extra corrections applied, \( c \)=point-source corrected spectrum, \( 1 \)=from the central spaxel, \( 9 \)=from the central 3x3 spaxels.] The value for the blue curve is also printed to the HIPE console, for our example being: (median) correction: 1.107. Values lower than 1.2—1.3 means the source can be considered to be consistent with a centred point source. The green curve shows the
scaling factor that is applied to the $s_1$ to create $c_{129}$ (remembering that $c_{129}$ is the spectrum $s_1$ scaled to the flux of $c_9$). Bear in mind that it is the green curve – the smoothed version of the $c_9/s_1$ data (the smoothing parameters can be adjusted in `extractCentralSpectrum`) – that is used to create $c_{129}$: for this source it is clear that the correction is dominated by the continuum. Hence it is especially important for the validity of $c_{129}$ that the continuum originates only from the point source, and not also from field contamination.

- **The top right plot** shows $c_1$, $c_9$, and $c_{129}$ as produced by `extractCentralSpectrum`. It is clear that the spectra differ from each other. For a perfectly-centred point source, $c_1$, $c_9$, and $c_{129}$ should yield very similar results, and the only choice you need to make should be: which has the better SNR? However, in the example shown here, the continuum of $c_1$ and $c_9$ differ by about 20 Jy ($\sim13\%$; $c_1<c_9$), the line flux by $\sim2\%$ ($c_1>c_9$), the continuum of $c_{129}$ equals that of $c_9$ (which makes sense, since the $c_{129}$ scaling is dominated by the continuum), but the line flux of $c_{129}$ is greater than both that of $c_1$ and $c_9$ (by about $12\%$). The question here is not between $c_1$ and $c_9$, since their emission line fluxes are so similar, but whether to use $c_{129}$. For $c_{129}$ it is clear that the scaling of the spectrum $s_1$ is different in the emission line than in the continuum: look again at the top left plot, where for both grey curves the values are slightly different in the line (which is at $66.45\ \mu m$) than the continuum.

- **While this difference lies within the calibration uncertainties, it is however something to bear in mind.** As a check on the scaling (dark grey) and diagnostic (light grey) curves for other point sources, we looked at the plots of `extractCentralSpectrum` produced for observations of R Dor (obsid 1342246385; source is nicely centred), NGC 5315 (calibration observation 1342182744, taking the cube slice in which the source is centred), Neptune, and Uranus (obsids 1342197026 and 1342199888; centred sources): for the first two sources the curves look like those shown here, but for the second two sources there is no difference in the line and continuum, the two curves are flat.

It turns out that a slight difference between the lines and continuum has indeed sometimes been observed in the correction/diagnostic curves of point sources observed with PACS spectroscopy. The effect is known and is linked to a very slight difference in the apparent PSF width at the level of spectral lines. However, as the effect was small and not repeatable, no further investigation was carried out.

Therefore, whether to use $c_9$ or $c_{129}$ is a choice for the data-user to make. If you are working on a large set of point sources the use of $c_9$ is recommended, since $c_{129}$ will not be valid as the offset gets larger (Sec. 4.2.2): by always using $c_9$ you are at least being consistent. For small offsets (Sec. 4.2.1), $c_{129}$ may be better than $c_9$, however you should check to see if there is a difference with $c_9$ and if so, include that in your estimates of the uncertainties.

In any case, is strongly advised that you check these plots before using the results, even if that means working in HIPE yourself. A blind use of the products is never a
good idea.

Bottom left and right are the plots produced for the pointing where the source is off centred.

- **The left plot** is again of the scaling and diagnostic curve. The scaling value of ~1.4 and more obviously the footprint image (Fig. 2) show that the source is not centred. Therefore, c1 is not the spectrum to use.

- **The right plot** shows that the difference between c1 and c9/c129 is larger than for the centred source. Again, c1 is not the spectrum to use for science, and moreover, since this is an off-centred source, c129 is also not the spectrum to use for science. The only result you can use here is c9. However, comparing the flux of c9 to that in the top plot (which comes from the pointing where the source is centred) shows that even for what appears to be a rather small offset (1/2 spaxel), even c9 has lost some flux. The amount of flux that is lost depends on where the source falls in the FoV (Sec. 3.1), since e.g. the uneven illumination has a greater effect at the corners of spaxels than in the middle of a spaxel.

In Fig. 4 are further examples of the output of extractCentralSpectrum, this time on obsid 1342182748. This is a calibration observation of the point-like planetary nebula NGC 5315, taken as a 7x1 raster of 2”x2” steps. Unfortunately, the data were not reduced by the automatic pipeline and if you get them from the HSA, only the Level 0 are provided. However, this was because of a missing meta datum in the Observation Context: if you want to use this data for your own testing, they will reduce perfectly well with the interactive pipelines in HIPE. The plots here show the c1, c9, and c129 as derived from cubes produced by the standard (i.e. the SPG) pipeline (it is the “telescope normalisation” script in HIPE) and those from the POC pipeline. The plots show how the spectra vary between the two pipelines and with offset: for large offsets, the POC c9 and c129 “retain” more of the source flux than do the same spectra from the SPG pipeline. The plots also show the skew that the spectral lines develop (Appendix 5) as the point source moves from one spaxel to another in the dispersion direction.
Figure 4 The output of extractCentralSpectrum from a raster observation of NGC 5315 (1342182748). The raster started with the source in spaxel 2,3 and moved it down to spaxel 2,1 (plots moving left to right). Values on the y-axis indicate the offset with respect to the first raster position; the source is best centred in the fourth position. **Top 7:** c1 from the SPG cubes in blue, c9 in red. The emission line in c1 at the edges of the raster have a skew. **Middle 7:** c129 from the SPG cubes in blue, from the POC pipeline in red. The skew can be seen in SPG spectrum but not from the POC one, this because of the way the POC pipeline corrects the spectra in the cubes. **Bottom 7:** c9 from the SPG cubes in blue and the POC pipeline in red.
Appendix 3 Measuring the offset of a point source

It is very difficult to measure the offset of a point source from a pointed PACS observation, because the spatial sampling (the 9.4″ of a spaxel) is less than the FWHM of the beam (which varies from 9″ to 14″ over the wavelength range of PACS). For source bright enough to have flux outside of a single spaxel, an offset of ¼ of a spaxel can usually be seen via the flux distribution over the neighbouring spaxels. However, it is more difficult the measure that offset in RA and Dec (or in instrument Y and Z). Inspecting the interpolated cubes, which are also provided for pointed observations, can provide a slightly better view because the spatial pixels of an interpolated cube are smaller and the image is plane regular, although even with this the spatial sampling is still limited by the 9.4″ spaxel size of the re-binned cube it is made from.

Another clue can come from the spectra: if the spectral lines from your point source show a skew (Sec. 5) then it is probable that the point source is offset from the centre in the Y direction. However, neither here can the amount of the offset be measured from the skew (as that calibration was not done by the PACS team).

The best method for measuring the location of a source in a PACS re-binned cube is to compare the footprint of the cube to an image of the FoV. This can be done in HIPE. Get an image of your target – for example, a PACS image – and open the PACS footprint viewer. Drag and drop the re-binned cubes from the Variables pane of HIPE onto the viewer, and the footprint of the cube will be drawn over the image. You can then determine the source’s RA and Dec (move the cursor over the source and read off the coordinates) and the cube’s spaxel coordinates (which are printed on the image). The use of this tool is explained in the PACS Data Reduction Guide for Spectroscopy, and Fig. 5 is a screenshot.

Figure 5 The PACS spectral footprint viewer, showing the spaxels and their coordinates printed over an image of the same source
If you cannot use this tool, a final option is to run the POC pipeline, at least up to the point where the task plotPointingOffset produces the plot “pjitter”. The location of the source in the IFU plane (axes Y and Z, not RA and Dec) is plotted, and the mean values (in arcsec) are printed to the HIPE console. Comparing the spaxel coordinates from the plot to the coordinates (spaxel and sky) available when viewing the cube in the Cube Viewer or the Spectrum Explorer, will allow for an estimate of the position of the source in spaxel coordinates and sky coordinates.
Appendix 4 Example scripts

##### Script for Sec. 6: Creating a rebinned cube from simulated data Part 1

from herschel.pacs.spg.spec.ExtractCentralSpectrumTask import *
from herschel.pacs.spg.spec.beams import ExtendedSpectralSourceAdapter
from math import *

class MyGaussSpectral(ExtendedSpectralSourceAdapter):
    fwhm = 0.0
    offRa = 0.0
    offDec = 0.0
    contFlux = 0.0
    contSlope = 0.0
    lineAmplitude = 0.0
    lineCenter = 0.0
    lineWidth = 0.0
    # REQUIRED:
    def __init__(self,fwhm,offRa,offDec,contFlux,contSlope,lineAmplitude,lineCenter,lineWidth):
        self.sourceSize = fwhm/2.3548
        self.offRa = offRa
        self.offDec = offDec
        self.contFlux = contFlux
        self.contSlope = contSlope
        self.lineAmplitude = lineAmplitude
        self.lineCenter = lineCenter
        self.lineWidth = lineWidth
        # REQUIRED:
    def getFlux(self, relRa, relDec, wavelength):
        r = sqrt((relRa-self.offRa)**2 + (relDec-self.offDec)**2)
        spectrum = self.contFlux + self.contSlope * \
        (wavelength-self.lineCenter)
        spectrum += self.lineAmplitude * exp(-0.5 * ((\n        wavelength-self.lineCenter) / self.lineWidth)**2)
        flux = spectrum * exp(-0.5 * (r / self.sourceSize)**2)
        return flux
        # OPTIONAL:
    def getFluxImage(self,relRa,relDec, wavelength):
        r = sqrt((relRa-self.offRa)**2 + (relDec-self.offDec)**2)
        spectrum = self.contFlux + self.contSlope * \
        (wavelength-self.lineCenter)
        spectrum += self.lineAmplitude * exp(-0.5 * ((\n        wavelength-self.lineCenter) / self.lineWidth)**2)
        self.fluxImage = spectrum * exp(-0.5 * (r / self.sourceSize)**2)
        return self.fluxImage
        # OPTIONAL:
    def renderGaussLayer(self, size=109, dpix=0.5, wavelength=66.38):
        self.image=Double2d(size, size)
        for y in range( size ):
            for x in range( size ):
                xim = -dpix)*(x-(size/2))
                yim = (dpix)*(y-(size/2))
                self.image.set(y,x, self.getFluxImage(xim, yim, wavelength))
        return self.image
        # OPTIONAL:
    def getSourceModelImage(self, size=109, dpix=0.5, wavelength=66.38):
        return self.renderGaussLayer(size, dpix, wavelength)
For Sec. 6: Creating a re-bnned cube from simulated data Part 2

# Model visualisation OPTIONAL

def imageModelInPacsSpecFromModel(naxis, pixAngSize, wave):
    sourceModellmage_01 = \
    SimpleImage(image=sourceModel.getSourceModellmage(naxis*5, \
               pixAngSize/5, wave))
    res = Double2d(naxis,naxis)
    for i in range(naxis):
        for j in range(naxis):
            iflux = 0.0
            for p in range(5):
                for q in range(5):
                    i2=i*5+p
                    j2=j*5+q
                    flux += sourceModellmage_01.image[j2,i2]
    sourceModellmage_05 = SimpleImage(image=res)
    return sourceModellmage_05

calTree=getCalTree()

## Point source with no offset

sourceSize = 0.2 # arcsec
offRa = 0.0
offDec = 0.0
contFlux = 200.0/(2*Math.PI*(sourceSize/(2*SQRT(2*LOG(2))))**2)
# Area normalisation of continuum surface brightness
contSlope = 0.0
lineAmplitude = 200.0/(2*Math.PI*(sourceSize/(2*SQRT(2*LOG(2))))**2)
# Area normalisation of line surface brightness
lineCentre = 63.18
lineWidth = 7.8E-3
sourceModel = MyGaussSpectral(sourceSize,offRa,offDec,contFlux,contSlope,lineAmplitude,\
                              lineCentre,lineWidth)
d=Display(imageModelInPacsSpecFromModel(109, 0.5, 66.38), \
          title='continuum layer Gaussian model')

## Example observation

obsid = 1342250905
obs = getObservation(obsid, useHsa=1)
camera = 'blue'
level2 = obs.level2
slicedRe-bnnedCubes = level2.getCamera(camera).rcube.product

## Create simulated cubes. An input slicedRe-bnnedCubes is necessary,
## but only for the source coordinates
obsRe-bnned = slicedRe-bnnedCubes.copy()
simRe-bnned = pacsSpecFromModel(obsRe-bnned, sourceModel, calTree=calTree)
Appendix 5 Skewed emission lines

Unresolved lines from off-centred point sources will have skewed Gaussian profiles rather than the Gaussian otherwise found. If a point source is offset from the centre of a spaxel in the dispersion direction (the Y-axis on the jitter plot that is produced by plotPointingOffset from the POC script), the spectral lines will develop a skew in their profile. For example, if a point source is located between spaxel 2,2 (the centre) and 2,3 (one up in the Y direction), the spectrum taken from spaxel 2,2 will have lines with a skew towards the longer wavelengths (i.e. a line “leans” to the right); for a source located between spaxels 2,2 and 2,1, the skew for the spectrum taken from spaxel 2,2 will be towards the shorter wavelengths. To know in which direction your source is offset, you should open the cube with the Spectrum Explorer or use the PACS Spectral Footprint viewer.

When summing up the spectra of all 9 spaxels of the 3x3, the merged skews will result in the spectral lines having a broader profile than those from the spectrum taken from the central spaxel alone. This will be noticeable when comparing c9 and c129, or comparing the c129 from the POC script to that from the SPG data, as shown Appendix 2. The effect of skew is to shift the centre of the line slightly, and to broaden the FWHM over that of a standard Gaussian.

Appendix 6 Additional uncertainties for un-chopped data

For un-chopped observations, the continuum uncertainty is of the order ±20 Jy, in each spaxel of a re-binned cube. Note then that the continuum uncertainty of c9 – which is based on the sum of 9 spaxels – is very high indeed. This means that the continuum level of c9 should be treated with extreme caution. The emission lines are unaffected by this extra uncertainty.

The spectrum c129 is not to be used for un-chopped data, since the s1-to-c129 scaling that is used is invalid for un-chopped observations. The POC script, as mentioned already, will not work on un-chopped data as the calibration scheme used in this pipeline is only applicable to chop-nod observations.
Appendix 7 Glossary

Chop-Nod observing mode: Two ways were provided by PACS to sample the background from an off position. These are explained in the PACS Handbook. The chop-nod mode was the most used because it produced data with a better continuum reliability and slightly better SNR. In this mode the telescope chopped between an on-source and off-source location at two nod positions.

FoV: field of view

HSA: Herschel Science Archive

HIPE: Herschel Interactive Processing Environment

HPDP: Highly-Processed Data Product, which can be obtained via the HSA and via the HPDP cosmos page

Mapping observing mode: Two pointing modes were offered for observing with PACS. Mapping observations were performed as a raster of pointings.

Mosaic cubes (Interpolated, Projected, Drizzled): Mosaic cubes are those created by combining individual cubes taken in a mapping observation: separate and slightly-offset pointings combined to observe either a larger field or to improve the spatial sampling of the source.

Pointed observing mode: Pointed mode observations were on a single FoV, and the primary science products are re-binned or interpolated cube, and point-source tables.

POC: pointing offset correction pipeline script, provided with the interactive pipelines in HIPE and applicable to chop-nod observations.

re-binned cubes: “re-binned cubes” are the final fully-calibrated native cubes that are produced by the pipeline: one cube per requested wavelength range and, for mapping observations, per raster position. It is from the re-binned cubes that the mosaic cubes are produced – these mosaic cubes being the end product for most mapping observations and one possible end product for pointed observations. (The re-binned cubes have the 5x5 grid of 9.4″-sized spaxels that is the native sky footprint of the PACS IFU, while the spatial grid of the mosaic cubes depends on the mapping field requested by the observer and the size chosen for the mosaicked spatial pixels.)

SPG: Standard Product Generator, short-hand for the automatic pipeline run at the HSC for all Herschel observations. The SPG download/products are the “pipeline” products that a user downloads from the HSA after an archive search.

Spatial Pixel/Spaxel: Both are the name given to the pixels of a cube, each of which contains a full spectrum for a small patch of sky. The difference is that spaxel usually refers to the pixel of a native cube (for PACS that is the re-binned cube) with an area that is determined only by the instrument (i.e. 9.4″ for PACS); spatial pixel refers to the pixel of a mosaic cube, and it can have any size – the ideal size depends on the mosaicking algorithm and the pointing pattern of the observation (how many overlapping spaxels are there in each spatial pixel?).

Un-chopped observing mode: Two ways were provided by PACS to sample the background from an off position. These are explained in the PACS Handbook. The Un-chopped mode was offered for observations of crowded sources where the off-position had to be especially chosen. A block of on-source was followed by a block of off-source observing.