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ESOTK Pipeline User Manual

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Authors

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| Affected Section(s) | Changes/Reason/Remarks |
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1 Introduction

1.1 Scope

This document is a guide to the instrument independent recipes as provided by the esotk (ESO Tool Kit) pipeline. It should guide the users through the installation of the software, and bring them quickly to the point where they can use the software tools offered by esotk

1.2 Stylistic conventions

Throughout this document the following stylistic conventions are used:

| | |
|-----------------------|---|
| bold | in text sections for commands and other user input which has to be typed as shown |
| <i>italics</i> | in the text and example sections for parts of the user input which have to be replaced with real contents |
| <code>teletype</code> | in the text for FITS keywords, program names, file paths, and terminal output, and as the general style for examples, commands, code, etc |

In example sections expected user input is indicated by a leading shell prompt.

In the text **bold** and *italics* may also be used to highlight words.

1.3 Notational Conventions

Hierarchical FITS keyword names, appearing in the document, are given using the dot-notation to improve readability. This means, that the prefix “HIERARCH ESO” is left out, and the spaces separating the keyword name constituents in the actual FITS header are replaced by a single dot.



2 Related Documents

2.1 Reference Documents

[RD01] GEN-SPE-ESO-33000-5335 / ESO-044286 8.0 Phase 3 User Documentation - ESO Science Data Products Standard



3 Definitions, Acronyms and Abbreviations

| | |
|--------|-------------------------------------|
| CPL | Common Pipeline Library |
| CCD | Charge Coupled Device |
| DFS | Data Flow System |
| DRS | Data Reduction System |
| ESO | European Southern Observatory |
| EsoRex | ESO Recipe Execution Tool |
| ESOTK | ESO Tool Kit |
| FITS | Flexible Image Transport System |
| FOV | Field Of View |
| GUI | Graphical User Interface |
| OB | Observation Block |
| pixel | picture element (of a raster image) |
| PSF | Point Spread Function |
| QC | Quality Control |
| SDP | Science Data Product |
| SOF | Set Of Frames |
| TBD | To be defined |
| TBC | To be confirmed |
| VLT | Very Large Telescope |
| WCS | World Coordinate System |



4 Overview

The ESO Tool Kit is a collection of in general instrument independent recipes that can be used to apply specific algorithms like fringe correction or stacking of spectra.



5 Quick Start

5.1 The ESOTK Pipeline Recipes

The ESOTK at the moment provides the following recipes:

- Recipes to remove fringes from an image
 - `esotk_mask_create`: Determines the object mask
 - `esotk_masterfringe_create`: Determines the masterfringe frame
 - `esotk_masterfringe_correct`: Scales the masterfringe frame and removes the fringes from the image.
- Recipe to coadd spectra in IDP and non-IDP format
 - `esotk_spectrum1d_combine`: Combines a list of input 1D spectra into a single spectrum.
- Recipes to derive and apply the barycentric correction of an observation.
 - `esotk_barycorr`: Derives and applies the barycentric correction of an observation
 - `esotk_eop`: Retrieves the IERS Earth Orientation Parameter used by the `esotk_barycorr` recipe.

The recipes for fringe correction can be run within a reflex workflow, whereas the other recipes are standalone recipes without a workflow.

5.2 Running the ESOTK Pipeline Recipes

Before being able to call pipeline recipes to process a set of data, the data must be correctly classified, and associated with the appropriate calibrations. The *Data Classification* consists of tasks such as: "What kind of data am I?", e.g., BIAS, "to which group do I belong?", e.g., to a particular Observation Block or observing mode. *Data Association* is the process of selecting appropriate calibration data for the reduction of a set of frames. Typically, a set of frames can be associated if they share a number of properties, such as instrument and detector configuration. Since all the required information is stored in the FITS headers, data association is based on a set of header keywords (called "association keywords") and the process is specific to each type of calibration. The process of data classification and association is known as *data organisation*.

The ESOTK pipeline consists of a set of data processing modules that can be called from different host applications, namely:

- *Reflex* is a graphical tool that helps the user to execute data reduction workflows that contain several recipes. *Reflex* takes care of grouping the different data sets, associating the calibration frames and managing the interdependencies between recipes in the calibration cascade. **Reflex is the recommended software tool for reducing your data.**
- *EsoRex* is a command line tool used to run each pipeline recipe. *EsoRex* commands can be easily scripted.



5.2.1 Getting Started with EsoRex

EsoRex is a command-line tool which can be used to execute the recipes of all standard VLT/VLTI instrument pipelines. With *EsoRex* in your path, the general structure of an *EsoRex* command line is

```
1> esorex [esorex options] [recipe [recipe options] [sof [sof]...]]
```

where options appearing before the recipe name are options for *EsoRex* itself, and options given after the recipe name are options which affect the recipe.

All available *EsoRex* options can be listed with the command

```
1> esorex --help
```

and the full list of available parameters of a specific recipe can be obtained with the command

```
1> esorex --help <recipe name>
```

The output of this command shows as parameter values the current setting, i.e. all modifications from a configuration file or the command line are already applied.

The listing of all recipes known to *EsoRex* can be obtained with the command

```
1> esorex --recipes
```

The last arguments of an *EsoRex* command are the so-called *set-of-frames*. A *set-of-frames* is a simple text file which contains a list of input data files for the recipe. Each input file is followed by a unique identifier (frame classification or frame tag), indicating the contents of this file. The input files have to be given as an absolute path, however *EsoRex* allows the use of environment variables so that a common directory prefix can be abbreviated. Individual lines may be commented out by putting the hash character (#) in the first column. An example of a *set-of-frames* is shown in the following:

```
1> cat bias.sof
/data/iiinstrument/raw/IIINSTRUMENT.2019-03-29T09:48:53.153.fits BIAS
$RAW_DATA/IIINSTRUMENT.2019-03-29T09:50:36.645.fits BIAS
$RAW_DATA/IIINSTRUMENT.2019-03-29T09:52:16.513.fits BIAS
$RAW_DATA/IIINSTRUMENT.2019-03-29T09:53:47.996.fits BIAS
#$RAW_DATA/IIINSTRUMENT.2019-03-29T09:55:04.515.fits BIAS
```

These *set-of-frames* files will have to be created by the user using a text editor, for instance. Which classification has to be used with which recipe is described in section [5.3](#)

Finally, if more than one *set-of-frames* is given on the command-line *EsoRex* concatenates them into a single *set-of-frames*.



5.3 Data Organization

ESOTK includes instrument independent recipes. Therefore the classification tags of the frames are kept general. The tags accepted by the recipes as input and output tags are:

- Recipe `esotk_mask_create`

Input files:

| DO category: | Explanation: | Required: |
|--------------|-----------------|-----------|
| ----- | ----- | ----- |
| RAW | Data | YES |
| RAW_BPM | Bad pixel mask | NO |
| RAW_CONFMAP | Confidence mask | NO |

Output files:

| DO category: | Explanation: |
|--------------|--------------|
| ----- | ----- |
| OBJ_MASK | Object mask |

- Recipe `esotk_masterfringe_create`

Input files:

| DO category: | Explanation: | Required: |
|--------------|-----------------|-----------|
| ----- | ----- | ----- |
| RAW | Data | YES |
| RAW_BPM | Bad pixel masks | NO |
| RAW_ERROR | Error | NO |
| RAW_VARIANCE | Variance image | NO |
| OBJ_MASK | Object masks | NO |
| FRINGE_MASK | Fringe mask | NO |

Output files:

| DO category: | Explanation: |
|----------------------------|-----------------------------------|
| ----- | ----- |
| MASTER_FRINGE | Master-fringe |
| MASTER_FRINGE_ERROR | Error of master-fringe |
| MASTER_FRINGE_CONTRIBUTION | Contribution map of master-fringe |
| MASTER_FRINGE_BPM | BPM of master-fringe |

- `esotk_masterfringe_correct`



Input files:

| DO category: | Explanation: | Required: |
|---------------------|------------------------|-----------|
| ----- | ----- | ----- |
| RAW | Data | YES |
| RAW_BPM | Bad pixel masks | NO |
| RAW_ERROR | Error | NO |
| RAW_VARIANCE | Variance | NO |
| OBJ_MASK | Object masks | NO |
| FRINGE_MASK | Fringe mask | NO |
| MASTER_FRINGE | Master-fringe | YES |
| MASTER_FRINGE_BPM | BPM of master-fringe | NO |
| MASTER_FRINGE_ERROR | Error of master-fringe | NO |

Output files:

| DO category: | Explanation: |
|------------------------|---|
| ----- | ----- |
| FRINGE_CORRECTED | Fringe corrected images |
| FRINGE_CORRECTED_BPM | Bad Pixel Mask of the fringe corrected images |
| FRINGE_CORRECTED_ERROR | Error of the fringe corrected images |

• esotk_spectrum1d_combine

Input files:

| DO category: | Explanation: | Required: |
|----------------------------|-------------------------|-----------|
| ----- | ----- | ----- |
| SPECTRUM_1D | Spectrum in IDP format | YES |
| SPECTRUM_COLLAPSE_WLENGTHS | Destination wavelengths | NO |

Output files:

| DO category: | Explanation: |
|---------------------------|-------------------------------------|
| ----- | ----- |
| ESOTK_SPECTRUM_COMBINED | The combined spectrum |
| ESOTK_SPECTRUM_IDP_FORMAT | The combined spectrum in IDP format |



6 Known Issues



7 Recipe Reference

The ESOTK pipeline process data that are usually products of other data reduction pipelines. These are identified by the value of a DO category the user must provide or adapt before using an ESOTK recipe. In this section we summarize all relevant information to use the various recipes.

7.1 esotk_mask_create

This recipe detects the objects in the input images (`RAW`) and creates an objects mask (`OBJ_MASK`). The latter is then used in the `esotk_masterfringe_create` recipe to exclude the objects when deriving the masterfringe frame.

7.1.1 Short algorithm description

The recipe first estimates the local sky background over the field and tracks any variations at adequate resolution to eventually remove them (if `bkg.estimate=TRUE`). Then it detects objects/blends of objects and keep a list of pixels belonging to each blend. Finally, it flags all pixels belonging to the detected objects. Please note that pixels are weighted in the source detection according to their value in the confidence map.

7.1.2 Input Frames

| Frame Tag | Type | Count | Description |
|-------------|---------|-------|-----------------|
| RAW | raw | 1..n | Data image |
| RAW_BPM | bpm | 1..n | Bad pixel mask |
| RAW_CONFMAP | confmap | 1..n | Confidence mask |

The recipe assumes that all data input frames are either single extension frames with the data in the primary section only, or multi extension frames. If they are multi extension frames the primary extension is supposed to be empty and is not read. Moreover, if optional bad pixel, and/or confidence masks are provided, the number (and dimension) of additionally provided confidential maps (and bad pixel masks) must match the number of data (`RAW`) frames.

7.1.3 Product Frames

| Default File Name | Frame Tag | Description |
|-----------------------------|-----------|-------------|
| esotk_object_mask_0000.fits | OBJ_MASK | object mask |

The product frames are single extension or multi extension frames depending on the input frames. They contain a mask that flags all pixels belonging to an object with unity (1) whereas all other (background) pixels are not



flagged, i.e. they are set to 0¹.

7.1.4 Recipe Parameters

| Parameter | Type | Values | Description |
|-----------------------|---------|----------------------------------|---|
| obj.min-pixels | int | 4 | Minimum pixel area for each detected object. |
| obj.threshold | double | 3. | Detection threshold in sigma above sky. |
| obj.deblending | boolean | TRUE | Deblend overlapping objects if set to true |
| obj.core-radius | double | 5.0 | Value of Rcore in pixels. |
| bkg.estimates | boolean | TRUE | Estimate background from input, if false it is assumed the input is already background corrected with median 0. |
| bkg.mesh-size | int | 64 | Background smoothing box size. |
| bkg.smooth-gauss-fwhm | double | 2.0 | The FWHM of the Gaussian kernel used in convolution for object detection. |
| det.effective-gain | double | 3.0 | Detector gain value. Used to convert intensity to electrons. |
| det.saturation | double | infinity | Detector saturation value. |
| pfm | string | closing, dilation closing | Post filtering mode. This mathematical operation is applied to the object mask after object detection. |
| px | int | 3 | X size of the post filtering kernel. Only odd values are allowed |
| py | int | 3 | Y size of the post filtering kernel. Only odd values are allowed |

7.2 esotk_masterfringe_create

This recipe derives a master fringe frame from the input images. Properly scaled, it can be used to efficiently remove the fringes from single frames and improve their photometric accuracy.

7.2.1 Short algorithm description

The algorithm consists of two main steps: i) Using a Gaussian mixture model the recipe estimates the background (a scalar) and the fringe scaling-factor (amplitude - a scalar) for each image tagged as RAW_BPM. The

¹The flagging follows the CPL convention



background is then subtracted and the amplitude used to normalize the background-subtracted image to the same scale. ii) The resulting images are then collapsed into a master-fringe image. There are different collapsing methods available (for details of the more sophisticated algorithms see appendix A) and they are controlled by the `-collapse` recipe parameters. In other words: the amplitude of the fringes is computed for each input image (RAW) and used to re-scale each of them before stacking.

Different masks controlling the algorithm in different stages can be passed to the recipe:

A) **RAW_BPM**: The bad pixel mask of each single input image (one for each RAW image). Each step in the algorithm takes this mask into account.

B) **OBJ_MASK**: Masks flagging the objects in the input image (one for each RAW image). Each step in the algorithm takes this mask into account.

C) **FRINGE_MASK**: A single mask. This mask is only taken into account in step i), i.e. when computing the image background and fringe amplitude for each RAW image. Step ii), i.e. the collapsing algorithm ignores this mask. Please note that if the fringe mask has mask-data only in the primary extension or only in the first extension but the raw frames are multi-extension files, the mask-data is applied to all extensions. This allows the user to e.g. exclude the borders of all extensions in step i) without the need to create a multi-extension mask-file. Part of the code is paralelised with OpenMP².

7.2.2 Input Frames

| Frame Tag | Type | Count | Description |
|--------------|----------|-------|----------------|
| RAW | raw | 1..n | Data image |
| RAW_BPM | bpm | 1..n | Bad pixel map |
| RAW_ERROR | error | 1..n | Error image |
| RAW_VARIANCE | variance | 1..n | Variance image |
| OBJ_MASK | object | 1..n | Object mask |
| FRINGE_MASK | fringe | 1 | Fringe mask |

The recipe assumes that all data input frames are either single extension frames with the data in the primary section only, or multi extension frames. If they are multi extension frames the primary extension is supposed to be empty and is not read. Moreover, if optional bad pixel, error, variance, and/or object masks are provided, the number (and dimension) of each optional input provided must match the number of data (RAW) frames.

7.2.3 Product Frames

| Default File Name | Frame Tag | Description |
|-------------------------------|---------------------|---------------------------|
| esotk_masterfringe.fits | MASTER_FRINGE | master fringe frame |
| esotk_masterfringe_error.fits | MASTER_FRINGE_ERROR | master fringe error frame |

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²See <https://www.openmp.org>



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|--------------------------------------|----------------------------|---------------------------------|
| Default File Name | Frame Tag | Description |
| esotk_masterfringe_contribution.fits | MASTER_FRINGE_CONTRIBUTION | master fringe contribution mask |
| esotk_masterfringe_bpm.fits | MASTER_FRINGE_BPM | master fringe bad pixel mask |

The product frames are single extension or multi extension frames depending on the input frames. The recipe derives the master fringe frame (`MASTER_FRINGE`), the corresponding error frame (`MASTER_FRINGE_ERROR`), the contribution mask (`MASTER_FRINGE_CONTRIBUTION`) and the bad pixel mask (`MASTER_FRINGE_BPM`). The contribution mask contains the number of pixels that contributed to the creation of the master fringe frame.

7.2.4 Recipe Parameters

| Parameter | Type | Values | Description |
|-----------------------------|--------|--|---|
| collapse.method | string | MEAN, WEIGHTED_MEAN, MEDIAN, SIGCLIP, MINMAX MEDIAN | Method used for collapsing/combining the data to derive the master fringe frame |
| collapse.sigclip.kappa-low | double | 3.0 | Low kappa factor for kappa-sigma clipping algorithm. |
| collapse.sigclip.kappa-high | double | 3.0 | High kappa factor for kappa-sigma clipping algorithm. |
| collapse.sigclip.niter | int | 5 | Maximum number of clipping iterations for kappa-sigma clipping. |
| collapse.minmax.nlow | int | 1 | Low number of pixels to reject for the minmax clipping algorithm. |
| collapse.minmax.nhigh | int | 1 | High number of pixels to reject for the minmax clipping algorithm. |

7.3 esotk_masterfringe_correct

This recipe properly scales the master fringe frame and removes the fringes from the input images.



7.3.1 Short algorithm description

The algorithm consists of two main steps: i) The recipe estimates the background and the fringe scaling-factor (amplitude) for the master-fringe image (`MASTER_FRINGE`) of each image tagged as `RAW`. The required offset and scaling factor is determined using a least-square fit of the master-fringe image to the `RAW` image. ii) The properly scaled (if `rescale=TRUE`) master-fringe frame is then subtracted from each individual `RAW` frame.

Different masks controlling the algorithm in different stages can be passed to the recipe:

A) `RAW_BPM`: The bad pixel mask of each single input image (one for each `RAW` image). Each step in the algorithm takes this mask into account.

B) `OBJ_MASK`: Masks flagging the objects in the input image (one for each `RAW` image). These masks are only taken into account in step i), i.e. when computing the scaling factors between `MASTER_FRINGE` and `RAW`, but ignored for step ii).

C) `FRINGE_MASK`: A single mask. This mask is only taken into account in step i), i.e. when computing the scaling factors between `MASTER_FRINGE` and `RAW`, but ignored for step ii). Please note that if the fringe mask has mask-data only in the primary extension or only in the first extension but the raw frames are multi-extension files, the mask-data is applied to all extensions. This allows the user to e.g. exclude the borders of all extensions in step i) without the need of creating a multi-extension mask-file. Part of the code is paralelised with OpenMP³.

7.3.2 Input Frames

| Frame Tag | Type | Count | Description |
|----------------------------------|---------------------------|-------|------------------------------|
| <code>RAW</code> | <code>raw</code> | 1..n | Data image |
| <code>RAW_BPM</code> | <code>bpm</code> | 1..n | Bad pixel map |
| <code>RAW_ERROR</code> | <code>error</code> | 1..n | Error image |
| <code>RAW_VARIANCE</code> | <code>variance</code> | 1..n | Variance image |
| <code>OBJ_MASK</code> | <code>object</code> | 1..n | Object mask |
| <code>FRINGE_MASK</code> | <code>fringemask</code> | 1 | Fringe mask |
| <code>MASTER_FRINGE</code> | <code>masterfringe</code> | 1 | Master fringe |
| <code>MASTER_FRINGE_BPM</code> | <code>bpm</code> | 1 | Master fringe bad pixel mask |
| <code>MASTER_FRINGE_ERROR</code> | <code>error</code> | 1 | Master fringe error |

7.3.3 Product Frames

| Default File Name | Frame Tag | Description |
|---|-------------------------------------|------------------------------|
| <code>esotk_fringecorrected_n.fits</code> | <code>FRINGE_CORRECTED</code> | fringe corrected frame |
| <code>esotk_fringecorrected_n_err.fits</code> | <code>FRINGE_CORRECTED_ERROR</code> | fringe corrected frame error |

continued on next page

³See <https://www.openmp.org>



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|----------------------------------|----------------------|----------------------------|
| Default File Name | Frame Tag | Description |
| esotk_fringecorrected_n_bpm.fits | FRINGE_CORRECTED_BPM | fringe corrected frame bpm |

The product frames are single extension or multi extension frames depending on the input frames. Additional to the fringe corrected frames (`FRINGE_CORRECTED`) the recipe also determines the corresponding error frame (`FRINGE_CORRECTED_ERROR`), and the bad pixel mask (`FRINGE_CORRECTED_BPM`).

7.3.4 Recipe Parameters

| Parameter | Type | Values | Description |
|-----------|---------|-------------|---|
| rescale | boolean | TRUE | measure fringe amplitude and rescale fringe correction before subtracting?. |

7.4 esotk_spectrum1d_combine

This recipe combines a list of input spectra into a single product spectrum and is currently used by the QC group to create OB-stacked data products⁴. In order to create products that follow the ESO 1D spectroscopic standard⁵ (IDP) the input must be fully compliant with this standard. If this is not the case, there is also the possibility to relax the IDP input checks with a recipe parameter and stack non IDP compliant spectra. Obviously, in this case the output is also not fully IDP compliant.

7.4.1 Short algorithm description

The recipe first resamples (by interpolation) all input spectra (`SPECTRUM_1D`) to a common output grid and then combines/stacks them. The user can choose between different interpolation and combination methods using by dedicated recipe parameters (see table 7.4.4). For the interpolation of the spectrum we rely on the [GSL implementation](#). Moreover, the user can also provide the desired output grid (`SPECTRUM_COLLAPSE_WLENGTHS`), or, if no destination wavelengths are specified, the wavelengths of the first spectrum are used instead.

If the ESO 1D spectroscopic standard should be followed (by setting the recipe parameter `--noIDP` to `FALSE`), the `FLUX` (or `FLUX_REDUCED`) column must contain the spectrum flux, the `ERR` (or `ERR_REDUCED`) column, the spectrum error and the `WAVE` column the wavelengths. The `QUAL` column (optional, controlled by the recipe parameter `--use-quality-column`) indicates a bad pixel if the value is different from 0. See the ESO 1D spectroscopic standard for more information.

If the ESO 1D spectroscopic standard is not mandatory (by setting the recipe parameter `--noIDP` to `TRUE`), the extension and the columns containing the data can be set by appropriate recipe parameters (see section 7.4.4 for the parameter). Moreover, not only the usage of the quality flag is optional in this mode (controlled

⁴See e.g. [OB-stacked data products for GIRAFFE](#)

⁵See [ESO Science Data Products Standard](#)



by `--use-quality-column`) but also the presence of a column containing the error (controlled by the presence or absence of the column name specified by `--noIDP.colname-err` in the table).

In order to be able to combine a very low number of spectra (e.g. $N = 2$) which are affected by cosmic ray events, a preprocessing step was implemented. The preprocessing algorithm first collapses the stack of input spectra by using the median to generate a master spectrum. Then it subtracts the master spectrum from each individual spectrum and derives the bad pixels on the residual spectra by thresholding, rejecting all pixels exceeding the thresholds. This works very well for e.g. GIRAFFE spectra when one sets the lower threshold to such a high value (e.g. $1e6$) that it has no effect and then filter only for cosemics (positive outliers). Usually when combining more than 2 or 3 spectra the preprocessing step is unnecessary because the sigma clipping algorithm (if used) suppresses the cosemics very efficiently.

Additionally to the previously mentioned preprocessing, the user can normalize the input spectra to the flux level of the first input file by setting the recipe parameter `--rescale-spectra` to `TRUE`. The scaling is done by dividing by the median of the flux level. Errors are propagated as appropriate. Please note that the errors reported in the spectrum are used to calculate the error of the scaling factor. As in some cases these errors are extremely high also the error associated with the scaling factor is large, which in turn leads to a decreased SNR of the stacked spectrum. This is not an error in the recipe algorithm but a signature of a problem present in the input spectra.

7.4.2 Input Frames

| Frame Tag | Type | Count | Description |
|----------------------------|------------|-------|-------------------------|
| SPECTRUM_1D | spectrum | 1..n | 1D spectrum |
| SPECTRUM_COLLAPSE_WLENGTHS | wavelength | 1 | Destination wavelengths |

The input file format has to follow the ESO 1D spectroscopic standard.

7.4.3 Product Frames

| Default File Name | Frame Tag | Description |
|-----------------------------------|---------------------------|---------------------------------|
| combined_spectrum.fits | ESOTK_SPECTRUM_COMBINED | combined spectrum |
| combined_spectrum_idp_format.fits | ESOTK_SPECTRUM_IDP_FORMAT | combined spectrum in IDP format |

The main product of the recipe is `ESOTK_SPECTRUM_IDP_FORMAT`, i.e. the combined/stacked spectrum that follows the ESO 1D spectroscopic standard, whereas the second product (`ESOTK_SPECTRUM_COMBINED`) contains mostly the same information but is not following the standard.

Please note that the `ESOTK_SPECTRUM_COMBINED` product is the only product, if the ESO 1D spectroscopic standard is not mandatory (by setting the recipe parameter `--noIDP` to `TRUE`).



7.4.4 Recipe Parameters

| Parameter | Type | Values | Description |
|------------------------|------------------------|--------------|---|
| use-quality-column | boolean | FALSE | If TRUE and quality (QUAL column) exists and is not 0 the pixel is rejected. If FALSE (or if the column does not exist) all the pixels are assumed as valid. |
| rescale-spectra | boolean | FALSE | If TRUE all the spectra are multiplicatively rescaled to the (median) level of the first spectra in the SOF. |
| output-columns | Comma separated string | ALL | Comma separated string specifying the output columns. The "WAVE" column can be omitted as it is a mandatory column. The other columns can be selected (e.g. "FLUX,ERR,SNR"). If ALL is set, all columns computed by the recipe will be saved. |
| continued on next page | | | |



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|------------------------------|------------------------|--|---|
| Parameter | Type | Values | Description |
| copykeys | Comma separated string | | Comma separated string specifying a list of keywords. If a keyword in this list is found in any of the input spectra, the keyword will be propagated to the output spectrum with the prefix HIERARCH ESO STACK and the number of the input file as suffix (e.g. copykeys='ESO.SEQ.CUMOFFSETA,- ESO.TEL.AIRM.START,- ESO.TEL.AIRM.END,- OBSERVER' → HIERARCH ESO STACK SEQ CUMOFFSETA1, HIERARCH ESO STACK SEQ CUMOFFSETA2, ... HIERARCH ESO STACK TEL AIRM START1, HIERARCH ESO STACK TEL AIRM START2, ... HIERARCH ESO STACK TEL AIRM END1, HIERARCH ESO STACK TEL AIRM END2, ... HIERARCH ESO STACK OBSERVER1, HIERARCH ESO STACK OBSERVER2, ...) If the keyword to copy is a HIERARCH ESO keyword, the HIERARCH ESO is stripped before appending. |
| interpolation.method | string | LINEAR, CSPLINE, AKIMA AKIMA | Method used for Spectrum1D interpolation. |
| collapse.reject-bpm | boolean | TRUE | If TRUE rejects an interpolated wavelength whose neighbor (in the original spectrum) is a bad pixel. For the rejection to occur only one bad neighbor is sufficient. |
| collapse.method | string | MEAN, WEIGHTED_MEAN, MEDIAN, SIGCLIP, MINMAX MEDIAN | Method used for collapsing the data. For details of the more sophisticated algorithms see appendix A |
| collapse.sigclip.kappa-low | double | 3.0 | Low kappa factor for kappa-sigma clipping algorithm. |
| continued on next page | | | |



| continued from previous page | | | |
|------------------------------|---------|---|--|
| Parameter | Type | Values | Description |
| collapse.sigclip.kappa-high | double | 3.0 | High kappa factor for kappa-sigma clipping algorithm. |
| collapse.sigclip.niter | int | 5 | Maximum number of clipping iterations for kappa-sigma clipping. |
| collapse.minmax.nlow | int | 1.0 | Low number of pixels to reject for the minmax clipping algorithm. |
| collapse.minmax.nhigh | int | 1.0 | High number of pixels to reject for the minmax clipping algorithm. |
| bpm.enable | boolean | FALSE | If TRUE the recipe tries to detect and mark bad pixels, e.g. cosmics on the single aligned input spectra by following the algorithm described in section 7.4.1. If FALSE the bpm parameters are ignored. |
| bpm.kappa-low | double | 3.0 | Low RMS scaling factor for image thresholding. |
| bpm.kappa-high | double | 3.0 | High RMS scaling factor for image thresholding. |
| bpm.method | string | absolute, relative, error relative | Thresholding method to use for bpm detection. |
| noIDP | boolean | FALSE | If TRUE, the recipe will not check if the input is IDP compliant and will not produce an IDP compliant output. Moreover, the user can specify the extension and the column names - see parameters below. |
| noIDP.extension | int | 1 | Fits extension containing the spectrum table. |
| noIDP.colname-wave | string | WAVE | Name of the column containing the wavelength for a non IDP input. |
| noIDP.colname-flux | string | FLUX | Name of the column containing the flux for a non IDP input. |
| noIDP.colname-err | string | ERR | Name of the column containing the flux error for a non IDP input. |
| noIDP.colname-qual | string | QUAL | Name of the column containing the quality/bpm for a non IDP input. |



7.4.5 QC Parameter

The following QC parameters are written by the recipe:

- **QC.AIRM.AVG:** This keyword is not recalculated frame by frame by `esotk_spectrum1d_combine` but expects that the instrument pipeline itself writes the value in the header of each IDP. The `esotk_spectrum1d_combine` recipe will then average these keywords and write the average to the pipeline product. If the keywords are not in the input frames the default value in the product will be -1
- **QC.IA.FWHM.AVG:** This keyword is not recalculated frame by frame by `esotk_spectrum1d_combine` but expects that the instrument pipeline itself writes the value in the header of each IDP. The `esotk_spectrum1d_combine` recipe will then average these keywords and write the average to the pipeline product. If the keywords are not in the input frames the default value in the product will be -1
- **QC.IWV.AVG:** This keyword is not recalculated frame by frame by `esotk_spectrum1d_combine` but expects that the instrument pipeline itself writes the value in the header of each IDP. The `esotk_spectrum1d_combine` recipe will then average these keywords and write the average to the pipeline product. If the keywords are not in the input frames the default value in the product will be -1
- **QC.CONTRIB.AVG:** This keyword contains the mean contribution of the stacked spectra as derived from the CONTRIB column.
- **QC.CONTRIB.REL:** This keyword contains the relative mean contribution of the stacked spectra as derived from the CONTRIB column, i.e. $QC.CONTRIB.REL = QC.CONTRIB.AVG / \text{Number-of-Frames}$
- **QC.SNR.AVG:** Mean Signal-to-Noise ratio excluding pixels with $SNR \leq 0$
- **QC.SNR.RATIO:** $QC.SNR.AVG / (\text{mean SNR of input frames})$. The mean SNR of the input frames is calculated by averaging the SNR keyword of the input headers
- **QC.SNR.IMPROV:** $QC.SNR.RATIO / \text{sqrt}(\text{number of input frames})$.
- **QC.SQRTNCOM:** $\text{sqrt}(\text{number of input frames})$
- **QC.MAXDEV:** The relative maximum scaling deviation. To calculate this keyword the scaling factors (controlled by the recipe parameter `--rescale-spectra`) are used. The QC parameter is defined as the maximum of the scaling values (i.e. the median of the flux spectrum i) as follows

$$\frac{|scale[i] - \overline{scale}|}{|\overline{scale}|}$$

Please note that whenever there are the standard IDP columns in the table, the normal columns are used to derive the QC parameter, if not, the `_REDUCED` columns are used. Moreover, bad pixels are always excluded in all calculations.



7.5 esotk_barycorr

The recipe derives the barycentric correction of an observation by using the [ERFA](#) (Essential Routines for Fundamental Astronomy) library and saves the correction in the product header using the keyword `ESO.DRS.BARYCORR`. ERFA is a C library containing key algorithms for astronomy, and is based on the [SOFA library](#) published by the International Astronomical Union (IAU).

On request the recipe also applies the barycentric correction to data stored in table format. Moreover, `esotk_barycorr` alters the input headers (primary, extensions) as little as possible to preserve the IDP standard if the input already follows this standard and updates a few wavelength related IDP keywords.

7.5.1 Short algorithm description

The recipe uses the ERFA function [eraApc13\(\)](#) to calculate the barycentric correction of an observation. For details on the implemented algorithm please visit the above mentioned web pages and links therein.

A comparison between the here implemented algorithm and the one implemented in the ESPRESSO pipeline shows a very good agreement. For this about 7000 ESPRESSO IDPs from 2021 were re-analyzed with the ERFA based implementation and the differences read as follows:

- Mean difference : 0.036 m/s
- Median difference: 0.055 m/s
- Standard deviation: 0.281 m/s
- MAD (median absolute deviation): 0.217 m/s
- Maximum deviation: 1.573 m/s

The `esotk_barycorr` recipe allows the user to read the input values (e.g. `ra`, `dec`, ...) requested by the ERFA routine from the header of the frames by specifying the header keywords containing these values. For this the various recipe parameters (e.g. `barycorr.hname-ra`, `barycorr.hname-dec`, ...) can be used.

Please note that the pressure, the temperature, the humidity, and the wavelength (recipe) parameters were always kept to their default value of 0. No tests with other values were performed.

The derived barycentric correction is saved in the product header using the keyword `ESO.DRS.BARYCORR`, in km/s units, e.g.

```
HIERARCH ESO DRS BARYCORR = 18.3512096944018 / Barycentric correction [km/s]
```

This keyword is always saved independent if the user also requests to apply the correction or not.

In order to apply the correction to the data, three prerequisites must be fulfilled:

1. The user requests to apply the correction by setting the recipe parameter `barycorr.apply` to `TRUE`
2. The data are not yet corrected, i.e. the `SPECSYS` header keyword is set to `TOPOCENT` or does not exist at all
3. The input data are stored in table format.



If all prerequisites are fulfilled the correction (*barycorr*) is applied to the wavelength columns (λ) as follows

$$\lambda_{corr} = \lambda_{orig} \times (1 + barycorr/c)$$

with c being the speed of light. The `SPECSYS` primary header keyword is changed into `BARYCENT` and a few IDP related header keywords (e.g. `WAVELMIN`, `WAVELMAX`, ...) are updated accordingly.

7.5.2 Input Frames

| Frame Tag | Type | Count | Description |
|-----------|-------|-------|--------------------------------------|
| RAW | raw | 1..n | Frame containing the data to correct |
| EOP_PARAM | calib | 1 | Earth Orientation Parameter file |

The recipe derives the barycentric correction by using keywords from the primary header of the `RAW` frame. Therefore, the input `RAW` file can be of practically any type (1D-, 2D-, 3D-images, table, ...) as long as the requested keywords are present. When it comes to apply the barycentric correction, only the table format is supported. Moreover, the header of the output product is as close as possible to the header of the input product.

Additionally to the `RAW` frame, the `EOP_PARAM` frame has to be passed to the recipe. The latter contains the [Earth Orientation Parameter](#) as a function of time (`MJD-OBS`). As the time resolution of the file is only one day, the parameters are interpolated by the recipe to have the most accurate values at the time of observation. A EOP file is included as static calibration in the pipeline distribution, but one can also use the recipe `esotk_eop` (see section 7.6) to download the most up to date file from [IERS](#).

Please note that the `SOF` can contain many `RAW` frames that can also be completely independent (even from different instruments). The recipe loops over all files and tries to process them. If for some reason the barycentric correction can not be derived for one file (e.g. a requested header parameter for this file is not present or has a different name) this file is simply skipped and the next one is processed. Obviously there will be a corresponding warning in the log file.

7.5.3 Product Frames

| Default File Name | Frame Tag | Description |
|---------------------------------------|-----------------------------|--|
| <code>esotk_barycorr_0000.fits</code> | <code>ESOTK_BARYCORR</code> | Barycentric corrected file and/or a primary header with the keyword <code>DRS.BARYCORR</code> containing the correction itself |

Depending on the input data and recipe parameters, the product frames contain

- The barycentric corrected data and the correction itself in the header keyword `DRS.BARYCORR`
- A primary header only with the correction itself written to the keyword `DRS.BARYCORR`



7.5.4 Recipe Parameters

The following recipe parameters can be used to control the recipe:

| Parameter | Type | Description |
|--------------------------|---------|---|
| barycorr.hname-ra | string | Name of the header keyword containing the target right ascension (J2000) [deg] |
| barycorr.hname-dec | string | Name of the header keyword containing the target declination (J2000) [deg] |
| barycorr.hname-mjdobs | string | Name of the header keyword containing the mjd-obs, i.e. start of observation [d] |
| barycorr.hname-exptime | string | Name of the header keyword containing the exposure time [s] |
| barycorr.hname-longitude | string | Name of the header keyword containing the longitude of the observatory, i.e. the telescope geodetic longitude (+ = East) [deg] |
| barycorr.hname-latitude | string | Name of the header keyword containing the latitude of the observatory, i.e the telescope geodetic latitude (+ = North) [deg] |
| barycorr.hname-elevation | string | Name of the header keyword containing the elevation of the observatory, i.e. the telescope elevation above sea level [m] |
| barycorr.pressure | double | Pressure during observation, i.e. pressure at the observer [hPa == mbar] |
| barycorr.temperature | double | Temperature during observation, i.e. ambient temperature at the observer [deg C] |
| barycorr.humidity | double | Humidity during observation, i.e. relative humidity at the observer [range 0 - 1] |
| barycorr.wavelength | double | Wavelength during observation, i.e. observing wavelength [micrometer] |
| barycorr.apply | boolean | Apply barycentric correction to the wavelength column. |
| barycorr.extension | int | Fits extension containing the spectrum table. |
| barycorr.colname-wave | string | Name of the table column containing the wavelength to be corrected. |

7.6 esotk_eop

This recipe downloads the latest version of the [Earth Orientation Parameter](#) and DUT⁶ (Difference to Universal Time: UT1-UTC) from [IERS](#). The IERS Earth Orientation Parameters (EOP) describe the irregularities of the earth's rotation. It stores the parameter in a fits-file that is used as input for the computation of the barycentric correction (see section [7.5](#)).

7.6.1 Short algorithm description

Download of the latest version of the [Earth Orientation Parameter](#) and DUT from [IERS](#).

⁶The time correction equal to the difference between Universal Time (UT1), which is defined by Earth's rotation, and Coordinated Universal Time (UTC), which is defined by a network of precision atomic clocks.



7.6.2 Input Frames

No input frame needed - use empty SOF or no SOF.

7.6.3 Product Frames

| Default File Name | Frame Tag | Description |
|----------------------|-----------|---|
| esotk_eop_param.fits | EOP_PARAM | File containing the Earth Orientation Parameter |

The product file contains the EOP table that is used as input for the computation of the barycentric correction (see section [7.5](#)).

7.6.4 Recipe Parameters

The following recipe parameters can be used to control the recipe:

| Parameter | Type | Description |
|----------------|--------|---|
| eop_host | string | Host to retrieve the EOP from. [https://datacenter.iers.org] |
| eop_urlpath | string | URL path of the EOP file to retrieve. [/products/eop/rapid/standard/finals2000A.data] |
| eop_usertag | string | TAG provided by the user. [None] |
| eop_instrument | string | Product header keyword value for INSTRUME. [ESOTK] |



A Statistical Estimators

A.1 Arithmetic mean - Arithmetic weighted mean

The arithmetic mean of a sample x_1, x_2, \dots, x_N is defined as

$$\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i. \quad (1)$$

For a random variable X that is normally distributed ($N(\mu, \sigma)$), the sample mean is the most efficient estimator of the population mean μ . By the central limit theorem this statement holds asymptotically for many noise distributions encountered in practice.

If the noise distribution of X is unknown, its variance can be estimated from the sample as

$$\hat{\sigma}^2 = \frac{1}{N-1} \sum_{i=1}^N (x_i - \bar{x})^2. \quad (2)$$

If X has variance σ then the average (1) has variance

$$\sigma_{av}^2 = \frac{\sigma^2}{N}. \quad (3)$$

This relation can be used in place of Eq. (2) if an *a priori* estimate of the noise in the images is available and is the same for all images (homoscedastic case).

When each image has its own noise image $\sigma_i^2(x, y)$ (heteroscedastic case⁷), then the weighted mean

$$\bar{x} = \left(\sum \frac{x_i}{\sigma_i^2} \right) \left(\sum \frac{1}{\sigma_i^2} \right)^{-1} \quad (4)$$

can be used, giving higher weight to values with lower noise. The variance of the average value at a given pixel is in this case given by

$$\frac{1}{\sigma_{av}^2} = \sum_{i=1}^N \frac{1}{\sigma_i^2}. \quad (5)$$

While the average is computationally efficient, it is also sensitive to the presence of outliers, i.e. sample values which arise from a process which is not included in the $N(\mu, \sigma)$ model of the background noise. Cosmic ray hits and the like that affect single exposures in the set therefore show up clearly in the stacked image. The average fails in the presence of a single outlier in the sample.

A.2 Median

For the computation of the sample median, the sample $\{x_i, i = 1 \dots N\}$ is first sorted such that $x_1 < x_2 < \dots < x_N$. The median is then the 50th percentile of the ordered set, i.e.

$$x_{med} = x_{\frac{N+1}{2}} \quad \text{if } N \text{ is odd} \quad (6)$$

⁷In statistics, a vector of random variables is heteroscedastic if the variability of the random disturbance is different across elements of the vector.



Figure A.1: Sample variance of the median as a function of sample size (left panel). The lower dashed curve is the expected variance of the arithmetic mean, the upper dashed curve the asymptotic variance of the median. The right panel shows the relative error compared to the asymptotic variance. Crosses are for even sample sizes, pluses for odd sample sizes.

and

$$x_{\text{med}} = \frac{1}{2}(x_{\frac{N}{2}} + x_{\frac{N}{2}+1}) \quad \text{if } N \text{ is even.} \quad (7)$$

This definition of the median for even-sized samples ensures that the median is an unbiased estimator of the population mean μ for a Gaussian error distribution or indeed any distribution that is symmetric about its mean.

The sample median has a variance larger than the sample average, i.e. it is less efficient as an estimator of the population mean. It is however robust against outliers in the sample since only the central one or two sample values are actually used for the computation. The median only fails if half or more of the sample values are outliers, i.e. if a given pixel is affected by a cosmic ray hit in half or more of the images in the stacking list.

While the sample distribution of the median (which is not Gaussian) can be written down easily, the computation of its moments and hence its variance is difficult. A scheme to compute it analytically has been described in [2] and exact values for a few sample sizes and a number of parent distributions are given in [3]. However, these are hardly useful for practical purposes. The asymptotic value for the ratio of the variances of mean and median (the *asymptotic relative efficiency* of the median, [1]) in the Gaussian case is

$$\sigma_{\text{med}}^2 = \frac{\pi}{2} \sigma_{\text{av}}^2 = \frac{\pi \sigma^2}{2N}. \quad (8)$$

In Fig. A.1, we determine the variance of the median from simulations by drawing for any given sample size 10 000 samples from a standard normal distribution. The asymptotic value is approached from below, which makes it a conservative choice for an estimate of the median's variance. The relative error, defined as

$$\frac{\pi/2N - \hat{\sigma}_{\text{med}}^2}{\pi/2N}, \quad (9)$$

is plotted in the right hand panel of Fig. A.1. For even sample sizes, the relative error is significantly larger than for odd sizes because the variance is actually lower. For odd-sized samples, the error is below 10% for $N \geq 7$



($N \geq 5$ according to [3]), whereas for even sized samples this threshold is not crossed until $N \gtrsim 12$. However, as mentioned above, the asymptotic value in Eq. (8) is conservative for any N and it is therefore used.

When each image has its own noise image $\sigma_i^2(x, y)$ (heteroscedastic case), then a weighted median can be defined as the point where cumulative weights is equal to $1/2$. Specifically, the weighted median of an ordered sample of N values x_i with weights w_i is

$$x_{\text{wmed}} = \begin{cases} \frac{x_j + x_{j+1}}{2}, & \text{if } \sum_{i=1}^j w_i = 0.5 \\ x_j, & \text{if } \sum_{i=1}^j w_i > 0.5 \text{ and } \sum_{i=1}^{j-1} w_i < 0.5 \end{cases} \quad (10)$$

A.3 Kappa-sigma clipping

In the min-max rejection algorithm, a fixed number of sample values are rejected, regardless whether they can be identified as outliers or not. If one wants to retain all “good” sample values and only reject true outliers, one has to employ an adaptive method which compares each sample value to the distribution of the entire sample.

In the $\kappa\sigma$ clipping algorithm, all values that deviate from the mean by more than κ standard deviations are rejected as outliers. Typically, $\kappa = 3$. The mean is usually estimated from the data, as is the standard deviation if no independent error estimate is available. One can introduce an iteration which stops once no more values are rejected.

Standard $\kappa\sigma$ clipping is not very efficient in removing low-significance outliers because the estimates of the mean and the standard deviation are themselves affected by the outliers. Using more robust estimators of location and scale, like the median and the inter-quartile range (IQR) or the median absolute deviation (MAD), improves the situation and makes $\kappa\sigma$ clipping a robust and easy-to-use adaptive outlier-rejection algorithm. This implementation uses the median and the MAD as robust estimators for the location and scale. For a Gaussian distribution, the standard deviation σ is given in terms of the MAD through

$$\sigma = \text{MAD} \times 1.4826. \quad (11)$$

$\kappa\sigma$ clipping has one parameter, the clipping threshold κ . The value of κ is not critical if outliers are expected to lie far from the sample distribution, as is the case for cosmic ray hits. Weaker effects, such as satellite trails, may require fine-tuning of κ .

The functions that make use of $\kappa\sigma$ clipping have a second parameter, e.g. `niter` which specifies the maximum number of iterations to run.

The method might fail if more than half of the input images are affected by outliers at a given pixel because then the estimate of the MAD might be affected and cause outlier rejection to fail. The method also requires a sufficient number of input images to be able to obtain reasonably accurate estimates of the mean and standard deviation.

The variance of the estimator now varies from pixel to pixel depending on the number of values that are rejected as outliers. Since outliers are not drawn from the same distribution as the “good” data values, the cleaned sample is equivalent to a smaller sample drawn from the noise distribution. In the general heteroscedastic case, the variance is therefore estimated as

$$\sigma_{\kappa\sigma}^2 = \frac{1}{N_{\text{good}}^2} \sum_{\text{good}} \sigma_i^2. \quad (12)$$



B Installation

See: [Installation instructions](#)



C Troubleshooting



- [1] Anirban DasGupta. *Asymptotic Theory of Statistics and Probability*. Springer, New York, 2008. [32](#)
- [2] J. S. Maritz and R. G. Jarrett. A note on estimating the variance of the sample median. *Journ. Am. Stat. Assoc.*, 73:194–196, mar 1978. [32](#)
- [3] Paul R. Rider. Variance of the median of small samples from several special populations. *Journ. Am. Stat. Assoc.*, 55:148–150, mar 1960. [32](#), [33](#)