

EUROPEAN SOUTHERN OBSERVATORY

Organisation Européenne pour des Recherches Astronomiques dans l'Hémisphère Austral

Europäische Organisation für astronomische Forschung in der südlichen Hemisphäre

VERY LARGE TELESCOPE

Reflex FLAMES-UVES Tutorial

VLT-MAN-ESO-19500-XXXX

Issue 6.6.2

Date 2026-05-22

Prepared:	ESO UVES Pipeline Team	2026-05-22	
	Name	Date	Signature
Approved:	W.Freudling		
	Name	Date	Signature
Released:	M. Sterzik		
	Name	Date	Signature

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Change record

Issue/Rev.	Date	Section/Parag. affected	Reason/Initiation/Documents/Remarks
1.0	15/11/2013	All	First public release
6.1.3	03/06/2020	All	Update to Reflex 2.10
6.1.6	20/05/2021	All	Public release 6.1.6
6.1.8	19/05/2022	All	Public release 6.1.8
6.6.2	05/22/2026	All	Public release 6.6.2

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1 Introduction to `Esoreflex`

This document is a tutorial designed to enable the user to to reduce his/her data with the ESO pipeline run under an user-friendly environment, called `EsoReflex`, concentrating on high-level issues such as data reduction quality and signal-to-noise (S/N) optimisation.

`EsoReflex` is the ESO Recipe Flexible Execution Workbench, an environment to run ESO VLT pipelines which employs a workflow engine to provide a real-time visual representation of a data reduction cascade, called a workflow, which can be easily understood by most astronomers. The basic philosophy and concepts of Reflex have been discussed by Freudling et al. (2013A&A...559A..96F). Please reference this article if you use Reflex in a scientific publication.

Reflex and the data reduction workflows have been developed by ESO and instrument consortia and they are fully supported. If you have any issue, please have a look to https://support.eso.org to see if this has been reported before or open a ticket for further support.

A workflow accepts science and calibration data, as downloaded from the archive using the CalSelector tool[1] (with associated raw calibrations) and organises them into DataSets, where each DataSet contains one science object observation (possibly consisting of several science files) and all associated raw and static calibrations required for a successful data reduction. The data organisation process is fully automatic, which is a major time-saving feature provided by the software. The DataSets selected by the user for reduction are fed to the workflow which executes the relevant pipeline recipes (or stages) in the correct order. Full control of the various recipe parameters is available within the workflow, and the workflow deals automatically with optional recipe inputs via built-in conditional branches. Additionally, the workflow stores the reduced final data products in a logically organised directory structure employing user-configurable file names.

This tutorial deals with the reduction of FLAMES-UVES observations only via the FLAMES-UVES workflow. The user is referred to the FLAMES-UVES web page (http://www.eso.org/sci/facilities/paranal/instruments/flames/) for more information on the instrument itself, and the FLAMES-UVES pipeline user manual for the details of the pipeline recipes (http://www.eso.org/sci/software/pipelines/).

The workflow uses association rules known to work with files downloaded from the ESO archive with the CalSelector tool (from year 2003 onwards). For datasets where the data were directly delivered to the PI (e.g. in DVDs) see 7.

[1] *https://www.eso.org/sci/archive/calselectorInfo.html*

2 Software Installation

`Esoreflex` and the workflows can be installed in different ways: via package repositories, via the `install_esoreflex` script or manually installing the software tar files.

The recommended way is to use the package repositories if your operating system is supported. The pipelines and Reflex can be installed from the ESO `macports` repositories that support macOS platforms, the and the `rpm/yum` repositories that support Fedora and CentOS platforms. For any other operating system it is recommended to use the `install_esoreflex` script.

The installation from package repository requires administrative privileges (typically granted via sudo), as it installs files in system-wide directories under the control of the package manager. If you want a local installation, or you do not have sudo privileges, or if you want to manage different installations on different directories, then use the `install_esoreflex` script. Note that the script installation requires that your system fulfill several software prerequisites, which might also need sudo privileges.

Please note that in case of major or minor (affecting the first two digit numbers) Reflex upgrades, the user should erase the `$HOME/KeplerData`, `$HOME/.kepler` directories if present, to prevent possible aborts (i.e. a hard crash) of the `esoreflex` process.

2.1 Installing `Esoreflex` workflows via `macports`

This method is supported for the macOS operating system. It is assumed that macports (*https://www.macports.org*) is installed. Please read the full documentation at *https://www.eso.org/sci/software/pipelines/installation/macports.html*, which also describes the versions of macOS that are currently supported.

2.2 Installing `Esoreflex` workflows via `rpm/yum/dnf`

This method is supported for Fedora and CentOS platforms and requires sudo rights. Please read the full documentation at *https://www.eso.org/sci/software/pipelines/installation/rpm.html*, which also describes the versions of Fedora and CentOS that are currently supported.

2.3 Installing `Esoreflex` workflows via `install_esoreflex`

This method is recommended for operating systems other than those indicated above, or if the user has no sudo rights. Software dependencies are not fulfilled by the installation script, therefore the user has to install all the prerequisites before running the installation script.

The software pre-requisites for `Reflex 2.11.5` may be found at:
https://www.eso.org/sci/software/pipelines/reflex_workflows

To install the `Reflex 2.11.5` software and demo data, please follow these instructions:

1. From any directory, download the installation script:

```
wget https://eso.org/sci/software/pipelines/install_esoreflex
```

2. Make the installation script executable:

```
chmod u+x install_esoreflex
```

3. Execute the installation script:

```
./install_esoreflex
```

   and the script will ask you to specify three directories: the download directory `<download_dir>`, the software installation directory `<install_dir>`, and the directory to be used to store the demo data `<data_dir>`. If you do not specify these directories, then the installation script will create them in the current directory with default names.

4. Follow all the script instructions; you will be asked whether to use your Internet connection (recommended: yes), the pipelines and demo-datasets to install (note that the installation will remove all previously installed pipelines that are found in the same installation directory).

5. To start `Reflex`, issue the command:

```
<install_dir>/bin/esoreflex
```

   It may also be desirable to set up an alias command for starting the `Reflex` software, using the shell command `alias`. Alternatively, the `PATH` variable can be updated to contain the `<install_dir>/bin` directory.

2.4 Demo Data

Together with the pipeline you will also receive a demo data set, that allows you to run the `Reflex FALES-UVES` workflow without any changes in parameters. This way you have a data set to experiment with before you start to work on your own data. The demo data for FLAMES-UVES includes example data for the workflow.

Note that you will need a minimum of ∼3.9 GB, ∼0.6 GB and ∼6.8 GB of free disk space for the directories `<download_dir>`, `<install_dir>` and `<data_dir>`, respectively. The FLAMES-UVES demo data have been retrieved with the CalSelector tool[2].

[2] *http://www.eso.org/sci/archive/calselectorInfo.html*

3 Quick Start: Reducing The Demo Data

For the user who is keen on starting reductions without being distracted by detailed documentation, we describe the steps to be performed to reduce the science data provided in the UVES demo data set supplied with the `esoreflex 2.11.5` release. By following these steps, the user should have enough information to perform a reduction of his/her own data without any further reading:

1. First, type:

   ```
   esoreflex -l
   ```

   If the `esoreflex` executable is not in your path, then you have to provide the command with the executable full path `<install_dir>/bin/esoreflex -l` . For convenience, we will drop the reference to `<install_dir>`. A list with the available `esoreflex` workflows will appear, showing the workflow names and their full path.

2. Open the UVES Echelle by typing:

   ```
   esoreflex uves&
   ```

   Alternatively, you can type only the command `esoreflex` the empty canvas will appear (Figure 3.1) and you can select the workflow to open by clicking on `File -> Open File`. Note that the loaded workflow will appear in a new window. The UVES Echelle workflow is shown in Figure 3.2.

3. To aid in the visual tracking of the reduction cascade, it is advisable to use component (or actor) highlighting. Click on `Tools -> Animate at Runtime`, enter the number of milliseconds representing the animation interval (100 ms is recommended), and click `OK`.

4. Change directories set-up. Under "Setup Directories" in the workflow canvas there are seven parameters that specify important directories (green dots).

   By default, the `ROOT_DATA_DIR`, which specifies the working directory within which the other directories are organised. is set to your `$HOME/reflex_data` directory. All the temporary and final products of the reduction will be organized under sub-directories of `ROOT_DATA_DIR`, therefore make sure this parameter points to a location where there is enough disk space. To change `ROOT_DATA_DIR`, double click on it and a pop-up window will appear allowing you to modify the directory string, which you may either edit directly, or use the `Browse` button to select the directory from a file browser. When you have finished, click `OK` to save your changes.

   Changing the value of `RAW_DATA_DIR` is the only necessary modification if you want to process data other than the demo data

5. Click the  button to start the workflow

6. The workflow will highlight the `Data Organiser` actor which recursively scans the raw data directory (specified by the parameter `RAW_DATA_DIR` under "Setup Directories" in the workflow canvas) and constructs the datasets. Note that the raw and static calibration data must be present either

in `RAW_DATA_DIR` or in `CALIB_DATA_DIR`, otherwise datasets may be incomplete and cannot be processed. However, if the same reference file was downloaded twice to different places this creates a problem as `esoreflex` cannot decide which one to use.

7. The `Data Set Chooser` actor will be highlighted next and will display a "Select Datasets" window (see Figure 3.3) that lists the datasets along with the values of a selection of useful header keywords[3]. The first column consists of a set of tick boxes which allow the user to select the datasets to be processed. By default all complete datasets which have not yet been reduced will be selected. A full description of the options offered by the `Data Set Chooser` will be presented in Section 6.3.2.

8. Click the `Continue` button and watch the progress of the workflow by following the red highlighting of the actors. A window will show which dataset is currently being processed.

9. Once the reduction of all datasets has finished, a pop-up window called *Product Explorer* will appear, showing the datasets which have been reduced together with the list of final products. This actor allows the user to inspect the final data products, as well as to search and inspect the input data used to create any of the products of the workflow. Figure 3.4 shows the Product Explorer window. A full description of the *Product Explorer* will be presented in Section 6.3.3.

10. After the workflow has finished, all the products from all the datasets can be found in a directory under `END_PRODUCTS_DIR` named after the workflow start timestamp. Further subdirectories will be found with the name of each dataset.

Well done! You have successfully completed the quick start section and you should be able to use this knowledge to reduce your own data. However, there are many interesting features of `Reflex` and the UVES workflow that merit a look at the rest of this tutorial.

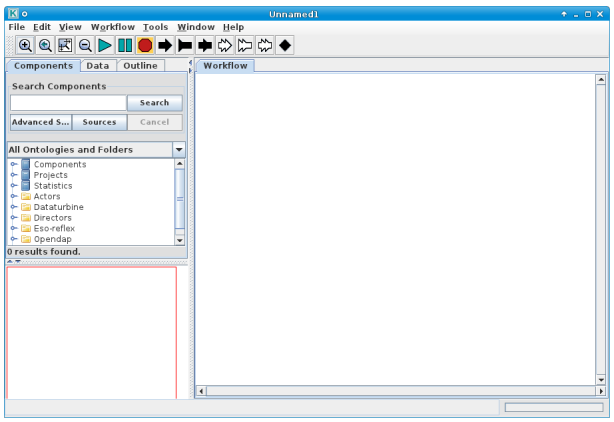


Figure 3.1: *The empty* `Reflex` *canvas.*

[3]The keywords listed can be changed by double clicking on the `DataOrganiser` Actor and editing the list of keywords in the second line of the pop-up window. Alternatively, instead of double-clicking, you can press the right mouse button on the `DataOrganiser` Actor and select `Configure Actor` to visualize the pop-up window.

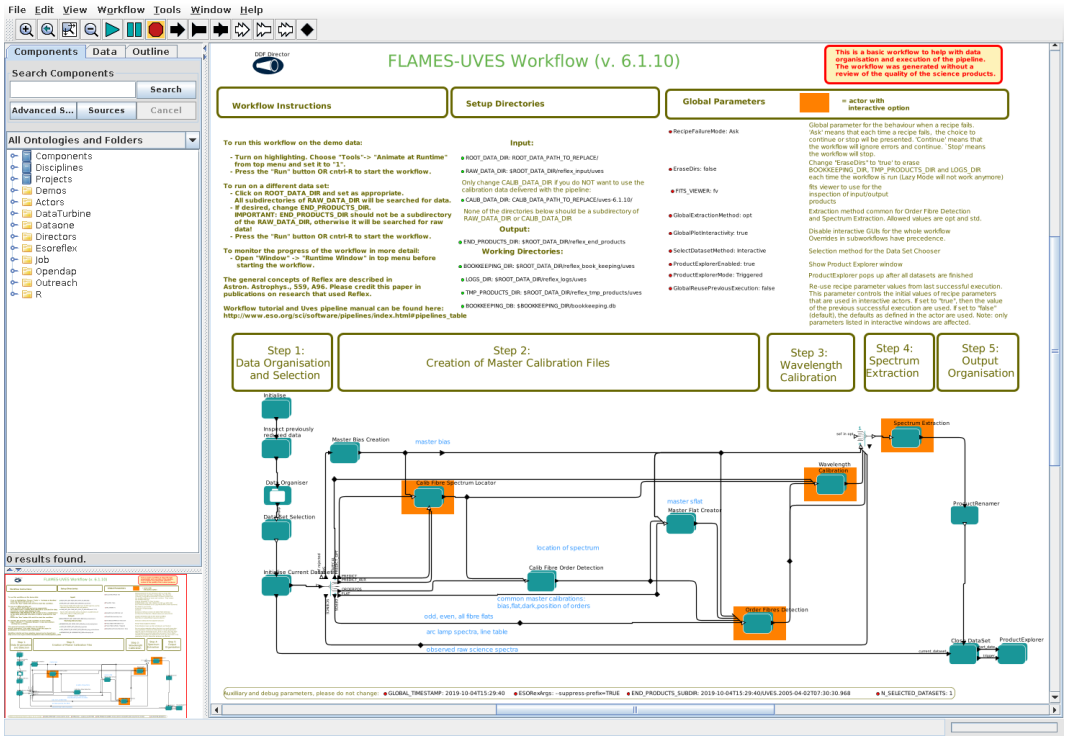


Figure 3.2: *FLAMES-UVES workflow general layout.*

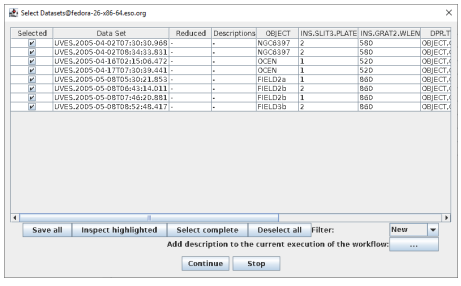


Figure 3.3: *The "Select Datasets" pop-up window.*

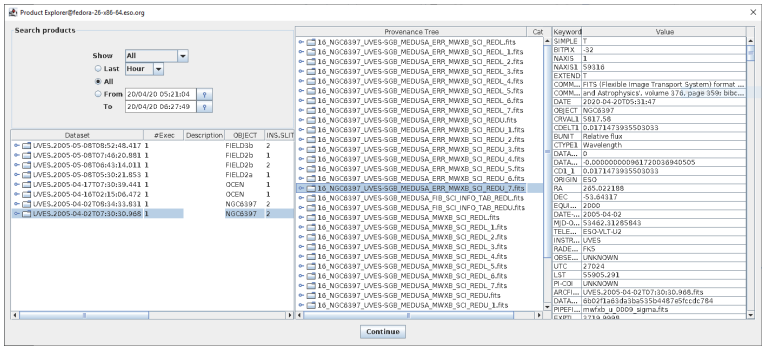


Figure 3.4: *The Product Explorer shows all datasets reduced in previous executions together with the full reduction chain for all the pipeline products.*

4 About the main `esoreflex` canvas

4.1 Saving And Loading Workflows

In the course of your data reductions, it is likely that you will customise the workflow for various data sets, even if this simply consists of editing the `ROOT_DATA_DIR` to a different value for each data set. Whenever you modify a workflow in any way, you have the option of saving the modified version to an `XML` file using `File -> Export As` (which will also open a new workflow canvas corresponding to the saved file). The saved workflow may be opened in subsequent `esoreflex` sessions using `File -> Open`. Saving the workflow in the default Kepler format (.kar) is only advised if you do not plan to use the workflow with another computer.

4.2 Buttons

At the top of the `esoreflex` canvas are a set of buttons which have the following functions:

-  - Zoom in.
-  - Reset the zoom to 100%.
-  - Zoom the workflow to fit the current window size (Recommended).
-  - Zoom out.
-  - Run (or resume) the workflow.
-  - Pause the workflow execution.
-  - Stop the workflow execution.

The remainder of the buttons (not shown here) are not relevant to the workflow execution.

4.3 Workflow States

A workflow may only be in one of three states: executing, paused, or stopped. These states are indicated by the yellow highlighting of the , , and  buttons, respectively. A workflow is executed by clicking the  button. Subsequently the workflow and any running pipeline recipe may be stopped immediately by clicking the  button, or the workflow may be paused by clicking the  button which will allow the current actor/recipe to finish execution before the workflow is actually paused. After pausing, the workflow may be resumed by clicking the  button again.

5 The UVES Workflow

The UVES workflow canvas is organised into a number of areas. From top-left to top-right you will find general workflow instructions, directory parameters, and global parameters. In the middle row you will find five boxes describing the workflow general processing steps in order from left to right, and below this the workflow actors themselves are organised following the workflow general steps.

5.1 Workflow Canvas Parameters

The workflow canvas displays a number of parameters that may be set by the user. Under "Setup Directories" the user is only required to set the `RAW_DATA_DIR` to the working directory for the dataset(s) to be reduced, which, by default, is set to the directory containing the demo data. The `RAW_DATA_DIR` is recursively scanned by the `Data Organiser` actor for input raw data. The directory `CALIB_DATA_DIR`, which is by default within the pipeline installation directory, is also scanned by the `Data Organiser` actor to find any static calibrations that may be missing in your dataset(s). If required, the user may edit the directories `BOOKKEEPING_DIR`, `LOGS_DIR`, `TMP_PRODUCTS_DIR`, and `END_PRODUCTS_DIR`, which correspond to the directories where book-keeping files, logs, temporary products and end products are stored, respectively (see the Reflex User Manual for further details; Forchì (2012)).

There is a mode of the `Data Organiser` that skips the built-in data organisation and uses instead the data organisation provided by the CalSelector tool. To use this mode, click on `Use CalSelector associations` in the `Data Organiser` properties and make sure that the input data directory contains the XML file downloaded with the CalSelector archive request (note that this does not work for all instrument workflows).

Under the "Global Parameters" area of the workflow canvas, the user may set the `FITS_VIEWER` parameter to the command used for running his/her favourite application for inspecting FITS files. Currently this is set by default to `fv`, but other applications, such as `ds9`, `skycat` and `gaia` for example, may be useful for inspecting image data. Note that it is recommended to specify the full path to the visualization application (an alias will not work).

By default the `EraseDirs` parameter is set to `false`, which means that no directories are cleaned before executing the workflow, and the recipe actors will work in Lazy Mode (see Section 5.2.4), reusing the previous pipeline recipe outputs if input files and parameters are the same as for the previous execution, which saves considerable processing time. Sometimes it is desirable to set the `EraseDirs` parameter to `true`, which forces the workflow to recursively delete the contents of the directories specified by `BOOKKEEPING_DIR`, `LOGS_DIR`, and `TMP_PRODUCTS_DIR`. This is useful for keeping disk space usage to a minimum and will force the workflow to fully re-reduce the data each time the workflow is run.

The parameter `RecipeFailureMode` controls the behaviour in case that a recipe fails. If set to `Continue`, the workflow will trigger the next recipes as usual, but without the output of the failing recipe, which in most of the cases will lead to further failures of other recipes without the user actually being aware of it. This mode might be useful for unattended processing of large number of datasets. If set to `Ask`, a pop-up window will ask whether the workflow should stop or continue. This is the default. Alternatively, the `Stop` mode will stop the workflow execution immediately.

The parameter `GlobalPlotInteractivity` controls whether the interactive windows will appear for those windows which are *enabled* by default. The possible values are `true, false`. Take into account that some

windows are disabled in the default configuration and therefore are not affected by this parameter.

The parameter `GlobalReusePreviousExecution` controls the initial values of recipe parameters that are used in interactive actors. The possible values are `true, false: false` (the default) will use the parameter defaults defined in the actor, `true` will instead cause the values of the previous successful execution to be used. Note that this only applies to parameters listed in the actor: some recipe parameters may not be listed, and for those the value will always be as defined by the recipe itself, regardless of the value of `GlobalReusePreviousExecution`.

The parameter `ProductExplorerMode` controls whether the `ProductExplorer` actor will show its window or not. The possible values are `Enabled`, `Triggered`, and `Disabled`. `Enabled` opens the ProductExplorer GUI at the end of the reduction of each individual dataset. `Triggered` (default and recommended) opens the ProductExplorer GUI when all the selected datasets have been reduced. `Disabled` does not display the ProductExplorer GUI.

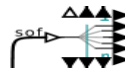
5.2 Workflow Actors

5.2.1 Simple Actors

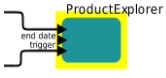
Simple actors have workflow symbols that consist of a single (rather than multiple) green-blue rectangle. They may also have an icon within the rectangle to aid in their identification. The following actors are simple actors:

- 

- The `DataOrganiser` actor.
- 

- The `DataSetChooser` actor (inside a composite actor).
- 

- The `FitsRouter` actor Redirects files according to their categories.
- 

- The `ProductRenamer` actor.
- 

- The `ProductExplorer` actor (inside a composite actor).

Access to the parameters for a simple actor is achieved by right-clicking on the actor and selecting `Configure Actor`. This will open an "Edit parameters" window. Note that the `Product Renamer` actor is a jython script (Java implementation of the Python interpreter) meant to be customised by the user (by double-clicking on it).

5.2.2 Composite Actors

Composite Actors have workflow symbols that consist of multiply-layered green-blue rectangles. They generally do not have a logo within the rectangle. A Composite Actor represents a combination of more Simple or Composite Actors which hides over-complexity from the user in the top-level workflow.

Composite Actors may also be expanded for inspection. To do this, right-click on the actor and select `Open Actor`, which will expand the Composite Actor components in a new `Reflex` canvas window. If the Composite Actor corresponds to a pipeline recipe, then the corresponding `RecipeExecuter` actor will be present as a Simple Actor, and its parameters are accessible as for any other Simple Actor. Alternatively you may still find Composite Actors, on which you need to repeat the first step to access the `Recipe Executer`.

5.2.3 Recipe Execution within Composite Actors

The FLAMES-UVES workflow contains Composite Actors to run pipeline recipes. This is in the most simple case due to the `SoF Splitter`/`SoF Accumulator`[4], which allow to process calibration data from different setting within one given DataSet (e.g. lamp frames taken with different preoptics/band-filters). More complex Composite Actors contain several actors (e.g. `Recipe Executer`).

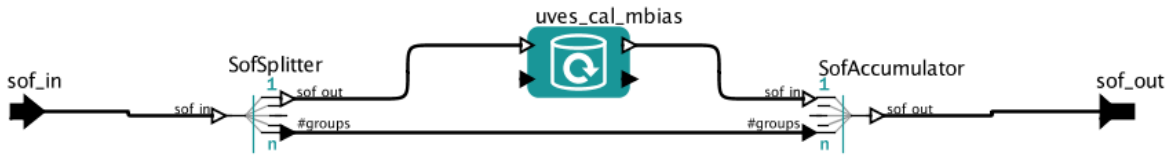


Figure 5.1: *This is the window you get when you choose* `Open Actor` *for the Composite Actor* `Master Bias Creation`. *This is the most simple case for a Composite Actor. Using* `Configure Actor` *on* `uves_cal_bias_1` *gives you Fig. 5.2.*

The central elements of any Reflex workflow are the `RecipeExecuter` actors that actually run the recipes. One basic way to embed a `RecipeExecuter` in a workflow is shown in Fig 5.1, which is the most simple version of a Composite Actor. The `RecipeExecuter` is preceded by an `SofSplitter`, and followed by an `SofAccumulator`. The function of the `SofSplitter` is to investigate the incoming SoFs, sort them by "purpose", and create separate SoFs for each purpose. The `RecipeExecuter` then processes each of the SoFs independently (unless they are actually the same files). Finally, the `SofAccumulator` packs all the results into a single output SoF. The direct relation between the `SofSplitter` and `SofAccumulator` is used to communicate the number of different SoFs created by the `SofSplitter`. A workflow will only work as intended if the purpose of all the files a recipe needs as input is identical. The only exception to this rule is that a purpose can also be "default". In this case, the file is included in any output SoF created by the `SoFsplitter` and `SofAccumulator`.

[4]SoF stands for Set of Files, which is an ASCII file containing the name (and path) of each input file and its category (e.g. `BIAS`).

The reason for this scheme is best explained by an example. For a complex DataSet, the `Data Organiser` might have selected a large number of individual raw biases. The different biases are to be used to calibrate different frames, e.g. the science frames and the standard star frames. The `Data Organiser` determines and records this "purpose" of each bias, and this information is included in the DataSet and each SoF created from this DataSet. The `FitsRouter` directs all raw biases to the calibration Composite Actor. The `SofSplitter` then creates SoFs, one for the biases to be used for the science frames, and (probably) separate ones for the biases to be used for the standard star observations. The calibration recipe creates one master bias (and other products) for each SoF, and the `SofAccumulator` then creates a SoF that contains all the products.

A `RecipeExecuter` actor is used in the workflow to run a single FLAMES-UVES pipeline recipe (e.g: in the `Master Bias Creation` actor the recipe `uves_cal_mbias` is executed). In order to configure the `RecipeExecuters`, one has to first use `Open Actor` to get to the level of the recipe executors (see Fig. 5.1).

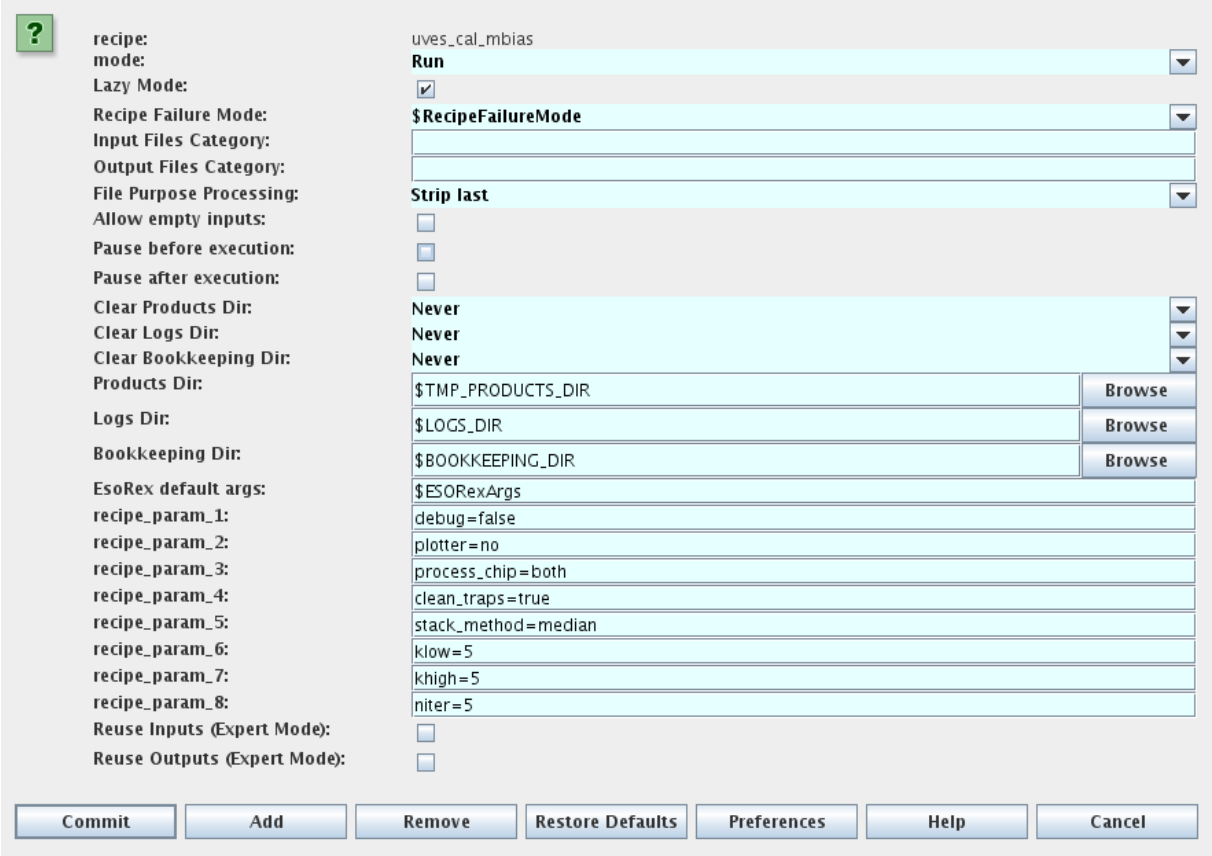


Figure 5.2: *The "Edit parameters" window for a typical* `RecipeExecuter` *actor, the* `uves_cal_mbias` *actor which runs the* `uves_cal_mbias` *pipeline recipe.*

In Figure 5.2 we show the "Edit parameters" window for a typical `RecipeExecuter` actor, which can be displayed by right-clicking on the actor and selecting `Configure Actor`. In the following we describe in more detail the function of some of the parameters for a `RecipeExecuter` actor:

- The "recipe" parameter states the FLAMES-UVES pipeline recipe which will be executed.

- The "mode" parameter has a pull-down menu allowing the user to specify the execution mode of the actor. The available options are:
  - `Run`: The pipeline recipe will be executed, possibly in Lazy mode (see Section 5.2.4). This option is the default option.
  - `Skip`: The pipeline recipe is not executed, and the actor inputs are passed to the actor outputs.
  - `Disabled`: The pipeline recipe is not executed, and the actor inputs are not passed to the actor outputs.
- The "Lazy Mode" parameter has a tick-box (selected by default) which indicates whether the `RecipeExecuter` actor will run in Lazy mode or not. A full description of Lazy mode is provided in Sect. 5.2.4.
- The "Recipe Failure Mode" parameter has a pull-down menu allowing the user to specify the behaviour of the actor if the pipeline recipe fails. The available options are:
  - `Stop`: The actor issues an error message and the workflow stops.
  - `Continue`: The actor creates an empty output and the workflow continues.
  - `Ask`: The actor displays a pop-up window and asks the user whether he/she wants to continue or stop the workflow. This option is the default option.
- The set of parameters which start with "recipe param" and end with a number or a string correspond to the parameters of the relevant FLAMES-UVES pipeline recipe. By default in the `RecipeExecuter` actor, the pipeline recipe parameters are set to their pipeline default values. If you need to change the default parameter value for any pipeline recipe, then this is where you should edit the value. For more information on the FLAMES-UVES pipeline recipe parameters, the user should refer to the FLAMES-UVES pipeline user manual (Modigliani et al. 2013[5]).

The description of the remainder of the `RecipeExecuter` actor parameters are outside the scope of this tutorial, and the interested user is referred to the Reflex User Manual for further details (Forchì 2012). Any changes that you make in the "Edit parameters" window must be saved in the workflow by clicking the `Commit` button when you have finished to take effect. If you want to reuse the parameters you have to save the workflow with the saved parameters.

5.2.4 Lazy Mode

By default, all `RecipeExecuter` actors in a pipeline workflow are "Lazy Mode" enabled. This means that when the workflow attempts to execute such an actor, the actor will check whether the relevant pipeline recipe has already been executed with the same input files and with the same recipe parameters. If this is the case, then the actor will not execute the pipeline recipe, and instead it will simply broadcast the previously generated products to the output port. The purpose of the Lazy Mode is therefore to minimise any reprocessing of data by avoiding data re-reduction where it is not necessary.

One should note that the actor's Lazy Mode depends on the contents of the directory specified by the parameter `BOOKKEEPING_DIR` and the relevant FITS file checksums. Any modification to the directory contents and/or

[5] Available at *https://ftp.eso.org/pub/dfs/pipelines/instruments/uves/uves-fibre-pipeline-manual-6.6.2.pdf*

Table 5.1: The FLAMES-UVES pipeline actors and their contents

actor	recipe	description
Master Bias Creation	`uves_cal_mbias`	create master bias
Calib Fibre Spectrum Locator	`flames_cal_predict`	create fibre line and order guess tables
calib Fibre Order Detection	`flames_cal_orderpos`	determine fiber order trace
Master Flat Creator	`flames_cal_mkmaster`	create master flat
Order Fibre Detection	`flames_cal_prep_sff_ofpos`	determine all fibre order traces
Wavelength Calibration	`flames_cal_wavecal`	determines wavelength solution
Spectrum Extraction	`flames_obs_scired`	reduces science data

the file checksums will cause the corresponding actor to run the pipeline recipe again when executed, thereby re-reducing the input data.

The re-reduction of data at each execution may sometimes be desirable. To force a re-reduction of data for any single `RecipeExecuter` actor in the workflow, right-click the actor, select `Configure Actor`, and uncheck the Lazy mode parameter tick-box in the "Edit parameters" window that is displayed. For many workflows the `RecipeExecuter` actors are actually found inside the composite actors in the top level workflow. To access such embedded `RecipeExecuter` actors you will first need to open the sub-workflow by right-clicking on the composite actor and then selecting `Open Actor`.

To force the re-reduction of all data in a workflow (i.e. to disable Lazy mode for the whole workflow), you must uncheck the Lazy mode for every single `RecipeExecuter` actor in the entire workflow. It is also possible to change the name of the bookkeeping directory, instead of modifying any of the Lazy mode parameters. This will also force a re-reduction of the given dataset(s). A new reduction will start (with the lazy mode still enabled), but the results of previous reduction will not be reused. Alternatively, if there is no need to keep any of the previously reduced data, one can simply set the `EraseDirs` parameter under the "Global Parameters" area of the workflow canvas to `true`. This will then remove all previous results that are stored in the bookkeeping, temporary, and log directories before processing the input data, in effect, starting a new clean data reduction and re-processing every input dataset. *Note: The option* `EraseDirs = true` *does not work in* `esoreflex` *version 2.9.x and causes the workflow to crash.*

6 Reducing your own data

In this section we describe how to reduce your own data set.

First, we suggest the reader to familiarize with the workflow by reducing the demo dataset first (Section 3), but it is not a requirement.

6.1 The `esoreflex` command

We list here some options associated to the `esoreflex` command. We recommend to try them to familiarize with the system. In the following, we assume the `esoreflex` executable is in your path; if not you have to provide the full path `<install_dir>/bin/esoreflex`

To see the available options of the `esoreflex` command type:

```
esoreflex -h
```

The output is the following.

```
-h | -help              print this help message and exit.
-v | -version           show installed Reflex version and pipelines and exit.
-l | -list-workflows    list available installed workflows and from
                        ~/KeplerData/workflows.
-n | -non-interactive   enable non-interactive features.
-e | -explore           run only the Product Explorer in this workflow
-p <workflow> | -list-parameters <workflow>
                        lists the available parameters for the given
                        workflow.
-config <file>          allows to specify a custom esoreflex.rc configuration
                        file.
-create-config <file>   if <file> is TRUE then a new configuration file is
                        created in ~/.esoreflex/esoreflex.rc. Alternatively
                        a configuration file name can be given to write to.
                        Any existing file is backed up to a file with a '.bak'
                        extension, or '.bakN' where N is an integer.
-debug                  prints the environment and actual Reflex launch
                        command used.
```

6.2 Launching the workflow

We list here the recommended way to reduce your own datasets. Steps 1 and 2 are optional and one can start from step 3.

1. Type: `esoreflex -n <parameters>` UVES Echelle to launch the workflow non interactively and reduce all the datasets with default parameters.

<parameters> allows you to specify the workflow parameters, such as the location of your raw data and the final destination of the products.

For example, type (in a single command line):

```
esoreflex -n
  -RAW_DATA_DIR /home/user/my_raw_data
  -ROOT_DATA_DIR /home/user/my_reduction
  -END_PRODUCTS_DIR $ROOT_DATA_DIR/reflex_end_products
  uves
```

to reduce the complete datasets that are present in the directory /home/user/my_raw_data and that were not reduced before. Final products will be saved in /home/user/my_reduction/reflex_end_products, while book keeping, temporary products, and logs will be saved in sub-directories of /home/user/my_reduction/. If the reduction of a dataset fails, the reduction continues to the next dataset. It can take some time, depending on the number of datasets present in the input directory. For a full list of workflow parameters type esoreflex -p UVES Echelle. Note that this command lists only the parameters, but does not launch the workflow.

Once the reduction is completed, one can proceed with optimizing the results with the next steps.

2. Type:

   ```
   esoreflex -e uves
   ```

   to launch the Product Explorer. The Product Explorer allows you to inspect the data products already reduced by the UVES Echelle esoreflex workflow. Only products associated with the workflow default bookkeeping database are shown. To visualize products associated to given bookkeeping database, pass the full path via the BOOKKEEPING_DB parameter:

   ```
   esoreflex -e BOOKKEEPING_DB <database_path> uves
   ```

   to point the product explorer to a given <database_path>, e.g., /home/username/reflex/reflex_bookkeeping/test.db

   The Product Explorer allows you to inspect the products while the reduction is running. Press the button Refresh to update the content of the Product Explorer. This step can be launched in parallel to step 1.

   A full description of the Product Explorer will be given in Section 6.3.3

3. Type:

   ```
   esoreflex uves &
   ```

   to launch the UVES Echelle esoreflex workflow. The UVES Echelle workflow window will appear (Fig. 3.2). Please configure the set-up directories ROOT_DATA_DIR, RAW_DATA_DIR, and other workflow parameters as needed. Just double-click on them, edit the content, and press OK. Remember to specify the same <database_path> as for the Product Explorer, if it has been opened at step #2, to synchronize the two processes.

4. (Recommended, but not mandatory) On the main esoreflex menu set Tools –> Animate at Runtime to 1 in order to highlight in red active actors during execution.

5. Press the button  to start the workflow. First, the workflow will highlight and execute the Initialise actor, which among other things will clear any previous reductions if required by the user (see Section 5.1).

Secondly, if set, the workflow will open the Product Explorer, allowing the user to inspect previously reduced datasets (see Section 6.3.3 for how to configure this option).

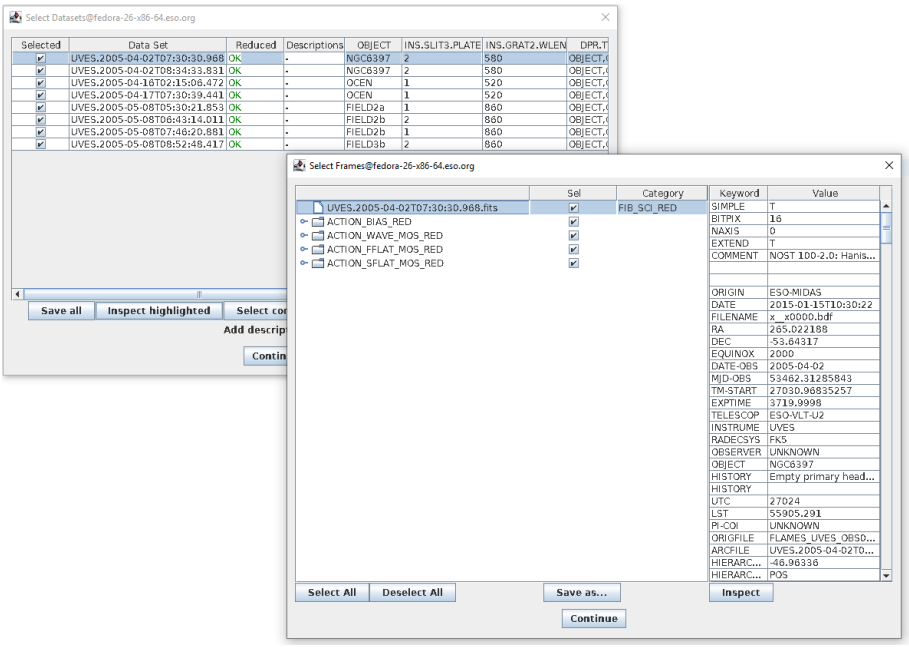


Figure 6.1: *The "Select Frames" window with a single file from the current Data Set highlighted in blue, and the corresponding FITS header displayed in the text box on the right. Hidden partially behind the "Select Frames" window is the "Select DataSets" window with the currently selected DataSet highlighted in blue.*

6.3 Workflow Steps

6.3.1 Data Organisation And Selection

The `DataOrganiser` (DO) is the first crucial component of a Reflex workflow. The DO takes as input `RAW_DATA_DIR` and `CALIB_DATA_DIR` and it detects, classifies, and organises the files in these directories and any subdirectories. The output of the DO is a list of "DataSets". A DataSet is a special Set of Files (SoF). A DataSet contains one or several science (or calibration) files that should be processed together, and all files needed to process these data. This includes any calibration files, and in turn files that are needed to process these calibrations. Note that different DataSets might overlap, i.e. some files might be included in more than one DataSet (e.g., common calibration files).

A DataSet lists three different pieces of information for each of its files, namely 1) the file name (including the path), 2) the file category, and 3) a string that is called the "purpose" of the file. The DO uses the OCA[6] rules to find the files to include in a DataSet, as well as their categories and purposes. The file cate-

[6]OCA stands for OrganisationClassificationAssociation and refers to rules, which allow to classify the raw data according to the contents of the header keywords, organise them in appropriate groups for processing, and associate the required calibration data for

gory identifies different types of files, and it is derived by information in the header of the file itself. A category could for example be RAW_CALIBRATION_1, RAW_CALIBRATION_2 or RAW_SCIENCE, depending on the instrument. The purpose of a file identifies the reason why a file is included in a DataSet. The syntax is action_1/action_2/action_3/ ... /action_n, where each action_i describes an intended processing step for this file (for example, creation of a MASTER_CALIBRATION_1 or a MASTER_CALIBRATION_2). The actions are defined in the OCA rules and contain the recipe together with all file categories required to execute it (and predicted products in case of calibration data). For example, a workflow might include two actions action_1 and action_2. The former creates MASTER_CALIBRATION_1 from RAW_CALIBRATION_1, and the later creates a MASTER_CALIBRATION_2 from RAW_CALIBRATION_2. The action_2 action needs RAW_CALIBRATION_2 frames and the MASTER_CALIBRATION_1 as input. In this case, these RAW_CALIBRATION_1 files will have the purpose action_1/action_2. The same DataSet might also include RAW_CALIBRATION_1 with a different purpose; irrespective of their purpose the file category for all these biases will be RAW_CALIBRATION_1.

The Datasets created via the DataOrganiser will be displayed in the DataSet Chooser. Here the users have the possibility to inspect the various datasets and decide which one to reduce. By default, DataSets that have not been reduced before are highlighted for reduction. Click either Continue in order to continue with the workflow reduction, or Stop in order to stop the workflow. A full description of the DataSet Chooser is presented in Section 6.3.2.

Once the Continue is pressed, the workflow starts to reduce the first selected DataSet. Files are broadcasted according to their purpose to the relevant actors for processing.

The categories and purposes of raw files are set by the DO, whereas the categories and purpose of products generated by recipes are set by the RecipeExecuter. The file categories are used by the FitsRouter to send files to particular processing steps or branches of the workflow (see below). The purpose is used by the SofSplitter and SofAccumulator to generate input SoFs for the RecipeExecuter. The SofSplitter and SofAccumulator accept several SoFs as simultaneous input. The SofAccumulator creates a single output SoF from the inputs, whereas the SofSplitter creates a separate output SoF for each purpose.

6.3.2 DataSetChooser

The DataSetChooser displays the DataSets available in the “Select Data Sets” window, activating vertical and horizontal scroll bars if necessary (Fig. 3.3).

Some properties of the DataSets are displayed: the name, the number of files, a flag indicating if it has been successfully reduced (a green OK), if the reduction attempts have failed or were aborted (a red FAILED), or if it is a new dataset (a black "-"). The column "Descriptions" lists user-provided descriptions (see below), other columns indicate the instrument set-up and a link to the night log.

Sometimes you will want to reduce a subset of these DataSets rather than all DataSets, and for this you may individually select (or de-select) DataSets for processing using the tick boxes in the first column, and the buttons

processing. They can be found in the directory <install_dir>/share/esopipes/<pipeline-version>/reflex/, carrying the extension .oca. The variable <install_dir> depends on the operative system and installation procedure. For installation through rpm: <install_dir>=/usr; for installation through macport <install_dir>=/opt/local; for installation through the installation script install_esoreflex it depends on the path specified during installation, e.g. <install_dir>=<specified_path>/install

Deselect All and Select Complete at the bottom, or configure the "Filter" field at the bottom left. Available filter options are: "New" (datasets not previously reduced will be selected), "Reduced" (datasets previously reduced will be selected), "All" (all datasets will be selected), and "Failed" (dataset with a failed or aborted reduction will be selected).

You may also highlight a single DataSet in blue by clicking on the relevant line. If you subsequently click on Inspect Highlighted, then a "Select Frames" window will appear that lists the set of files that make up the highlighted DataSet including the full filename[7], the file category (derived from the FITS header), and a selection tick box in the right column. The tick boxes allow you to edit the set of files in the DataSet which is useful if it is known that a certain calibration frame is of poor quality (e.g: a poor raw flat-field frame). The list of files in the DataSet may also be saved to disk as an ASCII file by clicking on Save As and using the file browser that appears.

By clicking on the line corresponding to a particular file in the "Select Frames" window, the file will be highlighted in blue, and the file FITS header will be displayed in the text box on the right, allowing a quick inspection of useful header keywords. If you then click on Inspect, the workflow will open the file in the selected FITS viewer application defined by the workflow parameter FITS_VIEWER.

To exit from the "Select Frames" window, click Continue.

To add a description of the reduction, press the button ... associated with the field "Add description to the current execution of the workflow" at the bottom right of the Select Dataset Window; a pop-up window will appear. Enter the desired description (e.g. "My first reduction attempt") and then press OK. In this way, all the datasets reduced in this execution, will be flagged with the input description. Description flags can be visualized in the SelectFrames window and in the ProductExplorer, and they can be used to identify different reduction strategies.

To exit from the "Select DataSets" window, click either Continue in order to continue with the workflow reduction, or Stop in order to stop the workflow.

6.3.3 The ProductExplorer

The ProductExplorer is an interactive component in the esoreflex workflow whose main purpose is to list the final products with the associated reduction tree for each dataset and for each reduction attempt (see Fig. 3.4).

Configuring the ProductExplorer

You can configure the ProductExplorer GUI to appear after or before the data reduction. In the latter case you can inspect products as reduction goes on.

1. To display the ProductExplorer GUI at the end of the datareduction:

- Click on the global parameter "ProductExplorerMode" before starting the data reduction. A configuration window will appear allowing you to set the execution mode of the Product Explorer. Valid options are:
  - "Triggered" (default). This option opens the ProductExplorer GUI when all the selected datasets have been reduced.

[7] keep the mouse pointer on the file name to visualize the full path name.

  - "Enabled". This option opens the ProductExplorer GUI at the end of the reduction of each individual dataset.
  - “Disable”. This option does not display the ProductExplorer GUI.

- Press the  button to start the workflow.

2. To display the ProductExplorer GUI “before” starting the data reduction:

- double click on the composite Actor "Inspect previously reduced data". A configuration window will appear. Set to "Yes" the field "Inspect previously reduced data (Yes/No)". Modify the field "Continue reduction after having inspected the previously reduced data? (Continue/Stop/Ask)". "Continue" will continue the workflow and trigger the DataOrganizer. "Stop" will stop the workflow; "Ask" will prompt another window deferring the decision whether continuing or not the reduction after having closed the Product Explorer.

- Press the  button to start the workflow. Now the ProductExplorer GUI will appear before starting the data organization and reduction.

Exploring the data reduction products

The left window of the ProductExplorer GUI shows the executions for all the datasets (see Fig. 3.4). Once you click on a dataset, you get the list of reduction attemps. Green and red flags identify successfull or unsucessfull reductions. Each reduction is linked to the “Description” tag assigned in the “Select Dataset” window.

1. To identify the desired reduction run via the “Description” tag, proceed as follows:

- Click on the symbol at the left of the dataset name. The full list of reduction attempts for that dataset will be listed. The column Exec indicates if the reduction was succesful (green flag: "OK") or not (red flag: "Failed").

- Click on the entries in the field "Description" to visualize the description you have entered associated to that dataset on the Select Dataset window when reducing the data.

- Identify the desired reduction run. All the products are listed in the central window, and they are organized following the data reduction cascade.

You can narrow down the range of datasets to search by configuring the field "Show" at the top-left side of the ProductExplorer (options are: "All", "Successful", "Unsuccessful"), and specifying the time range (Last, all, From-to).

2. To inspect the desired file, proceed as follows:

- Navigate through the data reduction cascade in the ProductExplorer by clicking on the files.

- Select the file to be inspected and click with the mouse right-hand button. The available options are:
  - Options available always:
    - Copy full path. It copies the full name of the file onto the clipboard. Shift+Ctr+v to past it into a terminal.
    - Inspect Generic. It opens the file with the FITS viewer selected in the main workflow canvas.
    - Inspect with. It opens the file with an executable that can be specified (you have to provide the full path to the executable).
  - Options available for files in the `TMP_PRODUCTS_DIR` directory only:
    - command line. Copy of the environment configuration and recipe call used to generate that file.
    - Xterm. It opens an Xterm at the directory containing the file.
  - Options available for products associated to interactive windows only:
    - Display pipeline results. It opens the interactive windows associated to the recipe call that generated the file. Note that this is for visualization purposes only; the recipe parameters cannot be changed and the recipe cannot be re-run from this window.

6.3.4 Recipe execution

Once the datasets to be reduced are selected, press the `Continue` button on the dataset organised window to proceed with the data reduction. The workflow will automatically execute the pipeline recipes and construct the `.sof` files to feed the pipeline recipes with. Each sof file will be saved in the `BOOKKEPING_DIR` directory (and subdirectory within it), depending on the recipe it is associated to and the execution time. The pipeline parameters can be changed as shown in figure 5.2.

6.3.5 Final products

Once a dataset is reduced (i.e. when the `flames_obs_scired` recipe is terminated), a window containing the list of science product pops up. Each file can be inspected with the selected fits viewer. Final science products will be stored in the `END_PRODUCTS_DIR`, and sorted by execution time and dataset identifier (i.e. the name of the science frame the dataset is for). Default names for the science products are: `<TARG name>_ERR_MWXB_SCI_<CHIP>.fits`, `<TARG name>_FIB_SCI_INFO_TAB_<CHIP>.fits`, `<TARG name>_MWXB_SCI_<CHIP>.fits` (where `<CHIP>` may be REDL or REDU). We refer the user to the FLAMES-UVES pipeline manual for the description of these files.

By default, the products are not corrected for heliocentric nor barycentric velocity. Their values are however stored in the header: keyword `HIERARCH ESO DRS BARYCORR` holds the barycentric correction value and `HIERARCH ESO DRS HELICORR` holds the heliocentric. In order to velocity correct the products, set the recipe parameter **velocity_correction** to "barycentric" or "heliocentric" (default is "none") from within the interactive GUI of the `Spectrum Extraction` actor, in the `Recipe Parameters` panel to the right, under the `general` tab. Afterwards you will need to click `Re-run Recipe`.

Note that the application of the correction implies an adjustment of the wavelength values. Therefore if you wish to combine the spectra of the same target, you must interpolate the spectra to a common wavelength range.

7 Troubleshooting

In this section we describe some of the problems that may occur when reducing the FLAMES-UVES with the ESOrex pipeline. For a more comprehensive description we refer the user to the FLAMES-UVES user manual (`http://www.eso.org/sci/software/pipelines/`).

1. **Should I change the CALIB_DATA_DIR configuration?**

   This directory is setup automatically to point to the calibration database provided with the pipeline and in principle shouldn't be changed. However, if static calibration data are present in the RAWDATA_DIR (e.g. calibrations are downloaded from the archive, or copied from ESO-DVD distribution), then you might have to set this directory equal to RAWDATA_DIR (otherwise an obsolete static calibration file may be selected instead of the most appropriate one).

2. **Spectrum extraction failing with error "Keyword ESO TEL GEOLAT does not exist"** From time to time the reduction of science frames may fail indicating that "Keyword ESO TEL GEOLAT does not exist". This keyword is required to measure heliocentric velocity correction. The user should make sure the input data have proper FITS header, in particular contains the keywords "RA", "DEC", "ESO TEL GEOLAT", "ESO TEL GEOLAT","UTC", "MJD-OBS".

3. **Spectrum extraction failing with error "Input data do not match: Spectrum contains 12 orders, but line table absolute order numbering is 70 - 60" while reduction 860 setting data.** This problem is due to the fact that the wavelength calibration has switched off the generation of a solution for some fibre beacuse has not found the minimum number of searched liunes (minimum set to 1000). In this case we recommend the user to set the parameter **minlines** of flames_cal_wavecal to 600 (or less), and repeat the flames_cal_wavecal and flames_obs_scired steps.

4. **Not good spectrum extraction quality** We are aware that the science reduction on platforms where the compiler is clang (for example MacOSX) may be not good. We recommend the user to install and compile the kit using the GNU compiler (gcc).

8 Frequently Asked Questions

- **The error window fills the whole screen - how can I get to the `Continue`/`Stop` buttons?**

  Press the Alt key together with your left mouse button to move the window upwards and to the left. At the bottom the `Continue`/`Stop` buttons will be visible. This bug is known but could not yet be fixed.

- **I tried to `Open` (or `Configure`) an `Actor` while the workflow is running and now it does not react any more. What should I do?**

  This is a limitation of the underlying Kepler engine. The only way out is to kill the workflow externally. If you want to change anything while a workflow is running you first need to pause it.

- **After a successful reduction of a data set, I changed this data set in some way (e.g. modified or removed some files, or changed the rules of the Data Organizer). When I restart Reflex, the Data Set Chooser correctly displays my new data set, but marks it as "reduced ok", even though it was never reduced before. What does this mean?**

  The labels in the column "Reduced" of the Data Set Chooser mark each dataset with "OK", "Failed" or "-". These labels indicate whether a data set has previously successfully been reduced at least once, all previous reductions failed, or a reduction has never been tried respectively. Data sets are identified by their name, which is derived from the first science file within the data set. As long as the data set name is preserved (i.e. the first science file in a data set has not changed), the Data Organizer will consider it to be the same data set. The Data Organizer recognizes any previous reductions of data sets it considers to be the same as the current one, and labels the current data set with "OK" if any of them was successful, even if the previously reduced data set differs from the current one.

  Note that the Product Explorer will list all the previous reductions of a particular data set only at the end of the reduction. This list might include successful and/or unsuccessful reduction runs with different parameters, or in your case with different input files. The important fact is that these are all reductions of data sets with the same first raw science file. By browsing through all reductions of a particular raw science file, the users can choose the one they want to use.

- **Where are my intermediate pipeline products?** Intermediate pipeline products are stored in the directory `<TMP_PRODUCTS_DIR>` (defined on the workflow canvas, under Setup Directories) and organised further in directories by pipeline recipe.

- **Can I use different sets of bias frames to calibrate my flat frames and science data?** Yes. In fact this is what is currently implemented in the workflow(s). Each file in a DataSet has a purpose attached to it (Forchì (2012)). It is this purpose that is used by the workflow to send the correct set of bias frames to the recipes for flat frame combination and science frame reduction, which may or may not be the same set of bias frames in each case.

- **Can I run `Reflex` from the command line?** Yes, use the command:

  ```
  esoreflex -n <workflow_path>/<workflow>.xml
  ```

  The -n option will set all the different options for Kepler and the workflows to avoid opening any GUI elements (including pipeline interactive windows).

  It is possible to specify workflow variables (those that appear in the workflow canvas) in the command line. For instance, the raw data directory can be set with this command:

```
esoreflex -n -RAW_DATA_DIR <raw_data_path> \
             <workflow_path>/<workflow>.xml
```

You can see all the command line options with the command `esoreflex -h`.

Note that this mode is not fully supported, and the user should be aware that the path to the workflow must be absolute and even if no GUI elements are shown, it still requires a connection to the window manager.

- **How can I add new actors to an existing workflow?** You can drag and drop the actors in the menu on the left of the `Reflex` canvas. Under `Eso-reflex -> Workflow` you may find all the actors relevant for pipeline workflows, with the exception of the recipe executer. This actor must be manually instantiated using `Tools -> Instantiate Component`. Fill in the "Class name" field with `org.eso.RecipeExecuter` and in the pop-up window choose the required recipe from the pull-down menu. To connect the ports of the actor, click on the source port, holding down the left mouse button, and release the mouse button over the destination port. Please consult the Reflex User Manual (Forchì (2012)) for more information.

- **How can I broadcast a result to different subsequent actors?** If the output port is a multi-port (filled in white), then you may have several relations from the port. However, if the port is a single port (filled in black), then you may use the black diamond from the toolbar. Make a relation from the output port to the diamond. Then make relations from the input ports to the diamond. Please note that you cannot click to start a relation from the diamond itself. Please consult the Reflex User Manual (Forchì (2012)) for more information.

- **How can I manually run the recipes executed by Reflex?** If a user wants to re-run a recipe on the command line he/she has to go to the appropriate reflex_book_keeping directory, which is generally reflex_book_keeping/<workflow>/<recipe_name>_<number> There, subdirectories exist with the time stamp of the recipe execution (e.g. 2013-01-25T12:33:53.926/). If the user wants to re-execute the most recent processing he/she should go to the `latest` directory and then execute the script `cmdline.sh`. Alternatively, to use a customized `esorex` command the user can execute

```
ESOREX_CONFIG="INSTALL_DIR/etc/esorex.rc"
PATH_TO/esorex --recipe-config=<recipe>.rc <recipe> data.sof
```

where INSTALL_DIR is the directory where Reflex and the pipelines were installed.

If a user wants to re-execute on the command line a recipe that used a specific raw frame, the way to find the proper data.sof in the bookkeeping directory is via `grep <raw_file> */data.sof`. Afterwards the procedure is the same as before.

If a recipe is re-executed with the command explained above, the products will appear in the directory from which the recipe is called, and not in the reflex_tmp_products or reflex_end_products directory, and they will not be renamed. This does not happen if you use the `cmdline.sh` script.

- **If I enter "-" into an empty integer parameter of an interactive window it is automatically completed to "-1". Why?**

  The parameters are validated for correctness according to their type (e.g. string, integer, float). In the case of an integer or float parameter "-" alone is considered an invalid input and is therefore automatically completed to "-1". This is part of the validation of input done by the WxPython library.

- **Can I reuse the bookkeeping directory created by previous versions of the pipeline?**

  In general no. In principle, it could be reused if no major changes were made to the pipeline. However there are situations in which a previously created bookkeeping directory will cause problems due to pipeline versions incompatibility. This is especially true if the parameters of the pipeline recipes have changed. In that case, please remove the bookkeeping directory completely.

- **How to insert negative values into a textbox?**

  Due to a bug in wxPython, the GUI might appear to freeze when attempting to enter a negative number in a parameter's value textbox. This can be worked around by navigating away to a different control in the GUI with a mouse click, and then navigating back to the original textbox. Once focus is back on the original textbox the contents should be selected and it should be possible to replace it with a valid value, by typing it in and pressing the enter key.

- **I've updated my Reflex installation and when I run esoreflex the process aborts. How can I fix this problem?**

  As indicated in Section 2, in case of major or minor (affecting the first two digit numbers) Reflex upgrades, the user should erase the `$HOME/KeplerData`, `$HOME/.kepler` directories if present, to prevent possible aborts (i.e. a hard crash) of the esoreflex process.

- **How can include my analysis scripts and algorithms into the workflow?**

  EsoReflex is capable of executing any user-provided script, if properly interfaced. The most convenient way to do it is through the Python actor. Please consult the tutorial on how to insert Python scripts into a workflow available here: `www.eso.org/sci/data-processing/Python_and_esoreflex.pdf`

Forchì V., 2012, Reflex User Manual, VLT-MAN-ESO-19000-5037, Issue 0.7, *https://ftp.eso.org/pub/dfs/reflex/ReflexUserManual-3.1.pdf* 15, 19, 29, 30

FLAMES-UVES Pipeline User Manual, VLT-MAN-ESO-19500-3016, Issue 6.6.2 19