

The SOXS Data-Reduction Pipeline

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ABSTRACT

The Son-Of-X-shooter (SOXS) is a dual arm spectrograph (UV-VIS & NIR) and Acquisition Camera (AC) due to be mounted on the European Southern Observatory (ESO) 3.6m New Technology Telescope (NTT) in La Silla.

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Designed to simultaneously cover the optical and NIR wavelength range from 350-2050 nm, the instrument will be dedicated to the study of transient and variable events with many Target of Opportunity requests expected.

The goal of the SOXS Data Reduction pipeline is to use calibration data to remove all instrument signatures from the SOXS scientific data frames for each of the supported instrument modes, convert this data into physical units and deliver them with their associated error bars to the ESO Science Archive Facility (SAF) as Phase 3 compliant science data products, all within 30 minutes. The primary reduced product will be a detrended, wavelength and flux calibrated, telluric corrected 1D spectrum with UV-VIS + NIR arms stitched together. The pipeline will also generate Quality Control (QC) metrics to monitor telescope, instrument and detector health.

The pipeline is written in Python 3 and has been built with an agile development philosophy that includes adaptive planning and evolutionary development. The pipeline is to be used by the SOXS consortium and the general user community that may want to perform tailored processing of SOXS data. Test driven development has been used throughout the build using ‘extreme’ mock data. We aim for the pipeline to be easy to install and extensively and clearly documented.

Keywords: SOXS, Pipeline, Data Reduction, Spectroscopy, Imaging

1. INTRODUCTION

The SOXS (Son Of X-Shooter) instrument is a new medium resolution spectrograph ($R \simeq 4500$) capable of simultaneously observing 350-2000nm (U- to H-band) to a limiting magnitude of $R \sim 20$ (3600sec, S/N ~ 10). It shall be hosted at the Nasmyth focus of the NTT at La Silla Observatory, Chile (see¹ for an overview). This paper describes the design of the SOXS data-reduction pipeline and data-products it shall generate and is part of a series of contributions¹⁻¹⁴ describing the current development status of the SOXS subsystems.

Section 2 gives details about the individual instruments that the SOXS pipeline shall receive data from. Section 3 details the various observation modes SOXS will be able to operate in and the products the pipeline is expected to generate for each of those modes. In Section 4 we propose how we will automate much of the data-reductions for SOXS, followed by how users in will be able to interact with the pipeline on their own machines in Section 5, the development environment we are using in Section 6 and finally giving an overview of the architecture of the pipeline code-base in Section 7.

2. THREE SOXS DETECTORS

SOXS will host three instruments; the UV-VIS and NIR spectrographs and the AC. Figure 1 shows how these instruments are to be mounted on the NTT’s Nasmyth focus rotator-flange. The SOXS pipeline will be capable of reducing the pixel-data collected by each of these instruments as well as outputting Quality Control metrics used to monitor the health of each unit.

2.1 UV-VIS Spectrograph

The UV-VIS spectrograph³ employs 4 ion-etched transmission gratings in the first order ($m = 1$) to record spectra in the 350-850nm wavelength range (providing a 50nm overlap with the NIR arm for cross-calibration). The spectral band is split into four poly-chromatic channels and sent to their specific grating. The spectral format of these four quasi-orders will be linear as shown in Figure 2. The main characteristics of the UV-VIS spectrograph and the e2V CCD44-82 detector¹⁰ can be found in Table 1.

2.2 NIR Spectrograph

The SOXS NIR spectrograph¹⁴ is a cross-dispersed echelle that employs the ‘4C’ (Collimator Correction of Camera Chromatism) to obtain spectra in 800-2000nm wavelength range in 15 orders (providing a 50nm overlap with the UV-VIS arm for cross-calibration). Unlike the UV-VIS spectrograph the NIR orders display a curvature as evidenced by the spectral format of the NIR orders shown in Figure 3.

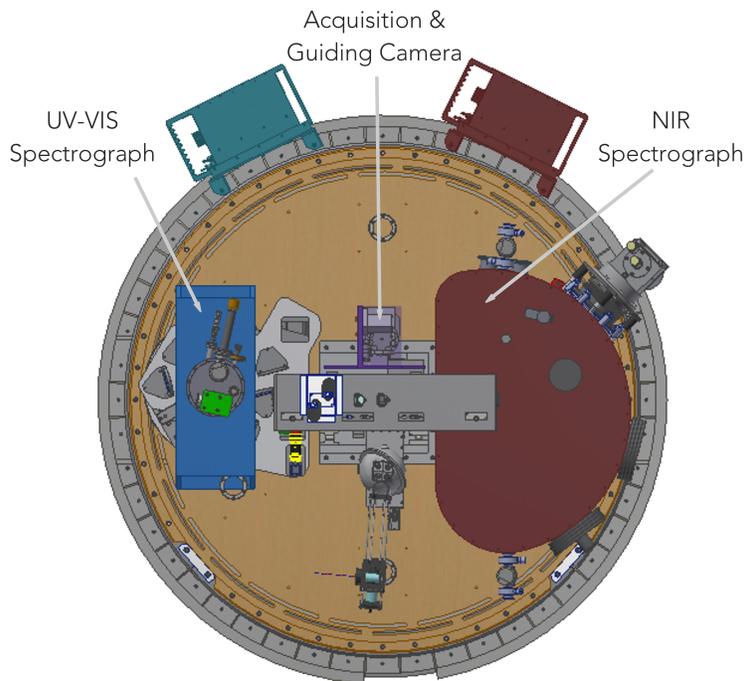


Figure 1. A face-on view of SOXS on the NTT nasmyth-focus rotator flange.

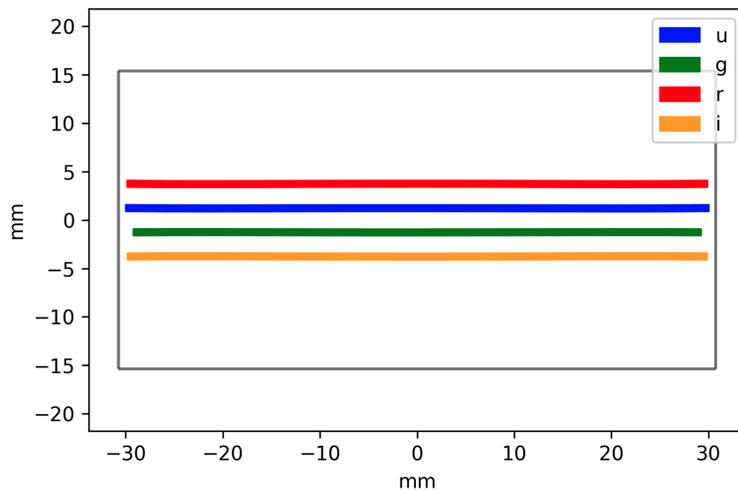


Figure 2. The four quasi-orders of the SOXS UV-VIS spectral format realised on the UV-VIS detector plain.

2.3 Acquisition Camera

The Acquisition Camera⁸ with a $3.5' \times 3.5'$ FOV will also allow for science-grade multi-band photometry.

The primary use of the acquisition camera is to acquire spectral targets and centre them on the slits. In addition, the camera's $3.5' \times 3.5'$ FOV and 0.205 arcsec/px scale will also allow for science-grade multi-band photometry. Observers will be able to select from 7 filters; the LSST u, g, r, i, z, y set and Johnson V .

Table 1. Characteristics of the SOXS UV-VIS Spectrograph & CCD.

Detector	e2V CCD44-82
Pixel-Size	15 μm
Array-Size	2048 \times 4096px; 30.7 \times 61.4mm
Array-Scale	0.28 arcsec/px
Peak Signal	200,000 e^- /px
Gain	Slow: $0.6 \pm 0.1 e^-/\text{ADU}$ Fast: $2 \pm 0.2 e^-/\text{ADU}$
Read noise (rms)	Slow: $< 3e^-$ Fast: $< 8 e^-$
Dark current @ 153K	$< 0.00001 e^-/\text{s}/\text{px}$
Resolution (R)	3500-7000 ($\simeq 4500$ mean)
Wavelength Range	350-850nm
Slit Widths	0.5, 1.0, 1.5, 5.0 arcsec
Slit Length	12 arcsec
Grating Blaze Angle	41 $^\circ$
Orders (quasi)	4

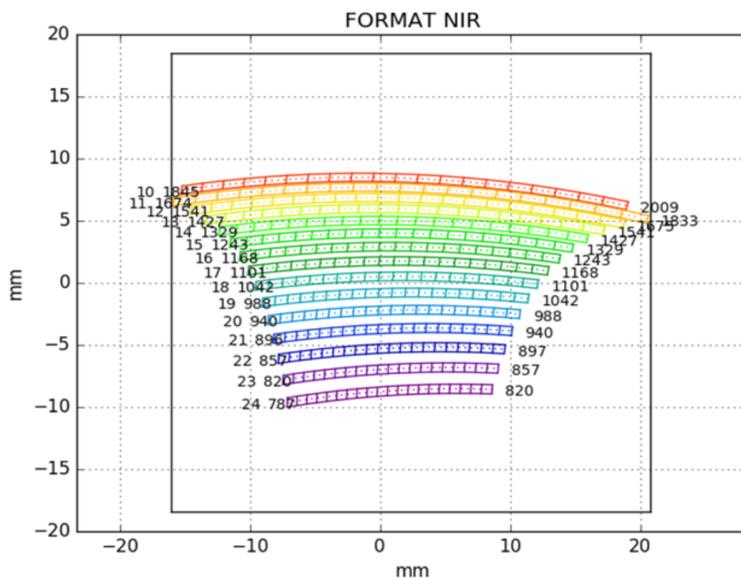


Figure 3. The 15 orders of the SOXS NIR spectral format realised on the NIR array plain

3. OBSERVATION MODES AND PIPELINE DATA-PRODUCTS

The challenge faced by any pixel-based data reduction pipeline is to identify and remove (or minimise) all sources of noise from the raw data so as to be able to best extract the scientific information contained on the frames. Alongside the standard detrending stages of calibration needed to remove instrument signatures (bias, dark-removal and flat-field correcting), the pipeline will calculate and apply accurate wavelength- and flux-calibration solutions to the spectra. For observations taken in the standard stare-mode it must also solve the notoriously difficult problem of removing the unwanted signal of diffuse light scattered in the earth's atmosphere (the *sky-background*). Finally, the pipeline must provided the means to extract the object spectra from the 2D image

Table 2. Characteristics of the SOXS NIR Spectrograph & Detector Array

Detector	Teledyne H2RG
Pixel-Size	18 μm
Array-Size	2048 \times 2048px
Array-Scale	0.25 arcsec/px
Read noise (rms)	Double correlated: $<20 e^-$ 16 Fowler pairs $<7 e^-$
Dark current @ 40K	$<0.005 e^-/s/px$
Resolution (R)	$\simeq 5000$ (1 arcsec slit)
Wavelength Range	800-2000 nm
Slit Widths	0.5, 1.0, 1.5, 5.0 arcsec
Slit Length	12 arcsec
Grating Blaze Angle	44 $^\circ$
Detector Operating Temp	40K
Spectrograph Operating Temp	150K
Orders	15

Table 3. Characteristics of the SOXS AC.

Camera	Andor iKon M934
Detector	BEX2-DD
Pixel-Size	13 μm
Array-Size	1024 \times 1024; 13.3 \times 13.3mm
Peak Signal	130000 e^-/px
Dark Current @ 173 K	0.00012 $e^-/s/px$
Read noise (rms)	2.9 e^-
Filters	u, g, r, i, z, y, V

frames in a manner that maximises the signal-to-noise of the data; otherwise known as *optimal-extraction*.

SOXS will be able to operate in 6 different spectroscopic observation modes:

1. **Stare-mode.** Standard ‘point-and-shoot’ observation.
2. **Stare-mode, synchronised.** Standard ‘point-and-shoot’ observations where the mid-point of the UV-VIS and NIR exposures are matched.
3. **Nodding-mode.** The telescope ‘nods’ between two-positions along the slit throughout exposure, allowing for on-the-fly sky background removal.
4. **Fixed sky-offset mode.** This mode is for extended objects where not enough uncontaminated sky-background is seen within the 12'' slit to allow for measurement and removal.
5. **Generic sky-offset mode.** User defined pattern of telescope offsets.
6. **Mapping-mode.** Used to ‘map’ an object or location.

Together with these spectroscopic modes, an imaging observation mode will also be available via the AC. The pipeline will be able to reduced data from this imaging-mode alongside the first 3 spectroscopic modes in a completely automated fashion (see Section 4).

Table 4 details each of the final data-products the pipeline shall produce. These products shall meet ESO’s Phase III data-products standards and are uploaded and archived on the ESO SAF¹⁵ for dissemination to data owners.

Table 4. Final data-products generated by the SOXS pipeline.

Product	Description
1D Source Spectra	1D spectra in FITS binary table format, one for each arm. Each FITS spectrum file will contain 4 extensions: <ol style="list-style-type: none"> 1. Wavelength- and flux-calibrated spectra with absolute flux correction via scaling to acquisition image source photometry, 2. an additional spectrum with correction for telluric absorption via MOLECFIT, 3. the variance array and 4. the sky-background spectra.
1D Merged Source Spectrum	1D UV-VIS & NIR merged spectrum in FITS binary table format with PDF visualisation. This spectrum will be rebinned to a common pixel scale for each arm. This spectrum file will also have the same 4 extensions described above.
2D Source Spectra	A 2D FITS image for each spectral arm containing wavelength and flux calibrated spectra (no other corrections applied) allowing users to perform source extraction with their tool of choice. Note that rectification of the curved orders in the NIR introduces a source of correlated noise not present in extractions performed on the unstraightened orders as done by the pipeline.
Acquisition Camera Images	<i>ugrizy</i> astrometrically and photometrically (<i>griz</i> only) calibrated to Refcat2 ¹⁶

4. AUTOMATED DATA-REDUCTION AND DATA FLOW

The pipeline is being designed to reduce all SOXS data to ESO Phase III standards ‘out-of-the-box’ with the aim of reducing most of the SOXS data and delivering the final-products to the ESO SAF without the need for human-interaction. The pipeline will run automatically on all point-source targets above an AB magnitude of $r = 19$ (with the stretch goal of $r = 20$). Below this magnitude, the pipeline will *attempt* to run automatically but it may require some user interaction to optimise object extraction. The pipeline may also struggle to provide an optimal absolute flux calibration and/or source extraction for sources with in crowded fields or with complex backgrounds.

The current design for the flow of data from the telescope to the archive is as follows:

1. Data is acquired by NTT & SOXS on the summit at La Silla, Chile.
2. Raw data is transferred within 10 minutes to the ESO SAF (Garching, Germany).
3. Raw data is downloaded from the SAF to the SOXS Data Reduction And Wellness Reporter (DRAWER) cluster in Belfast, UK.
4. Data is reduced on the cluster by the SOXS pipeline and streamed back to the SAF where it can be accessed by data rights owners.

Our goal is to populate the ESO SAF with the fully reduced data products within 30 min of the raw exposures appearing in the ESO SAF (15 min stretch goal). This is possible thanks to the fixed format of SOXS (apart from the exchangeable slit) allowing calibration frames to be prepared ahead-of-time before science data reductions.

Access to the ‘open stream’ method of shipping reduced data immediately to the ESO SAF will initially require the ESO Quality Control Group to review and verify a moderately sized collection of SOXS-pipeline reduced data. Once the quality and content of the data produced by the pipeline has met with ESO Phase III standards, we will then be allowed to upload data-products to the archive without further need of passing through a gatekeeper.

5. PIPELINE USAGE

As stated in Section 4, the SOXS pipeline will be designed to reduce most SOXS data in a non-interactive, automated fashion. However, users will be able to download and install the pipeline on their own machines and drive the pipeline to reduce the data to their own preferences. We foresee that the pipeline functionality will be accessible via at least two user-interfaces; a Command-Line Interface (CLI) and via ESO’s Reflex GUI.

The CLI being developed has a syntax similar to ESO’s Common Pipeline Library (CPL) interface *Esorex*.¹⁷ Each recipe can be called with an individual command and takes as input a set-of-files (SOF) list containing the required file input (raw data, static calibration products, etc.) and the path to a settings file containing the parameter values for the recipes such as sigma-clipping thresholds, polynomial orders for fitting, etc.

Usage:

```
soxspipe init
soxspipe mbias <inputFrames> [-s <pathToSettingsFile>]
soxspipe mdark <inputFrames> [-s <pathToSettingsFile>]
soxspipe mflat <inputFrames> [-s <pathToSettingsFile>]
soxspipe disp_sol <inputFrames> [-s <pathToSettingsFile>]
soxspipe order_centres <inputFrames> [-s <pathToSettingsFile>]
```

Options:

<code>init</code>	setup the soxspipe settings file for the first time
<code>mbias</code>	the master bias recipe
<code>mdark</code>	the master dark recipe
<code>mflat</code>	the master flat recipe
<code>disp_sol</code>	the disp solution recipe
<code>order_centres</code>	the order centres recipe
<code>inputFrames</code>	path to a directory of frames or a set-of-files file
<code>-h, --help</code>	show this help message

The most recent version of ESO’s *ESOReflex*¹⁸ GUI now includes a Python based plugin API that shall allow us to integrate the SOXS pipeline into this data-reduction control and visualisation tool (see Figure 4). Those experienced with the X-Shooter data reductions will be familiar with this tool and should easily transition to reducing SOXS data with the same tool. *ESOReflex* integration will be included in the final version of the pipeline, released after the SOXS’s Preliminary Acceptance Chile (PAC).

6. DEVELOPMENT ENVIRONMENT

At this current point in time the astronomical community have overwhelmingly adopted Python as their scripting language of choice and there a plethora of well maintained, mature python packages to help with basic data-reduction routines not to mention visualisation, user-interaction and data manipulation. To this end we have opted to develop the SOXS pipeline in Python 3.

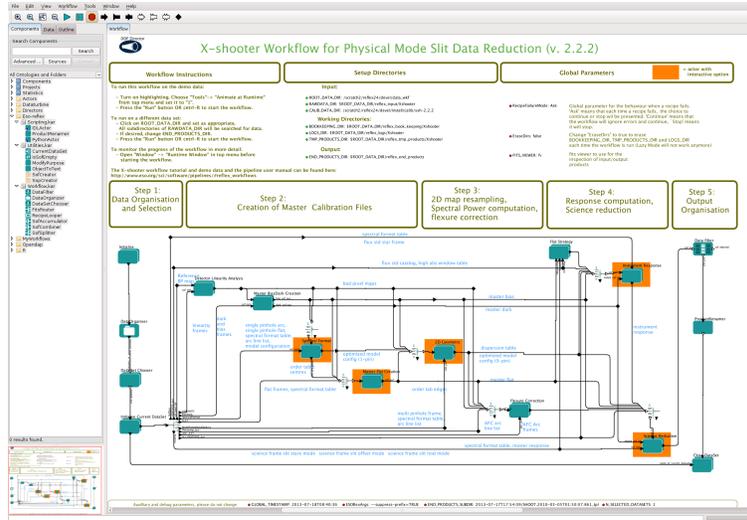


Figure 4. The ESO Reflex environment for X-shooter.¹⁸

The pipeline is being built with in agile development philosophy that includes adaptive planning and evolutionary development. As with any project, one of the greatest risks is knowledge loss due to a team member leaving the before project completion. To mitigate this risk we employ pair-programming techniques throughout to share knowledge, both explicit and tacit, between two developers. In times of travel bans and remote working a JupyterHub server with Python based notebooks and shared screens within video conferencing tools have been invaluable to execute these techniques.

We aim for the pipeline to be easy to install and extensively and clearly documented. Installing the pipeline is as simple as running the command:

```
pip install soxspipe
```

Pipeline documentation is being written in parallel with the code in docstrings and stand-alone markup files. A push of new code to github triggers a new build of the documentation on readthedocs* using the back-end sphinx documentation engine.

6.1 Test Driven Development

To verify the pipeline is not only able to reduce a typical data-set but also data that is far from ideal we are using test driven development throughout the build using ‘extreme’ mock data. This data helps push the pipeline to the limits of it capabilities and allows us to develop for possible edge-case scenarios that the pipeline will experience in real-time production.

This mock data is generated via the SOXS End-to-End (E2E) simulator⁵ which is able to synthesise 2D images that take into account the main optical behaviour of the system (grating dispersion, sampling, PSF, noises and position of various resolution elements coming from full ray-tracing). An example of the mock data is reported in Figures 5 and 6.

In particular, the plan is to generate mock data by varying different observing conditions in terms of source magnitude (faint or bright continuum), sky-brightness and calibration frames so as to provide a full suite of stress tests for point-like sources down to the limit magnitude considered for SOXS.

The E2E model will be also able to provide synthetic simulated frames produced by the acquisition camera with the same aim to test the data flow of the reduction chain for the photometry performed with the AC.

*readthedocs <https://soxspipe.readthedocs.io/>

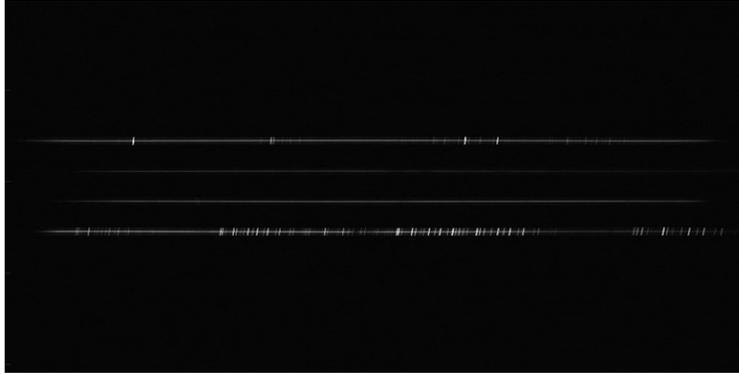


Figure 5. Simulated UV-VIS spectral image of a GOV star ($V = 18$) object and different tilts on the slit for each pseudo-order. Seeing $0.87''$, slit $1''$, exposure 1800s.

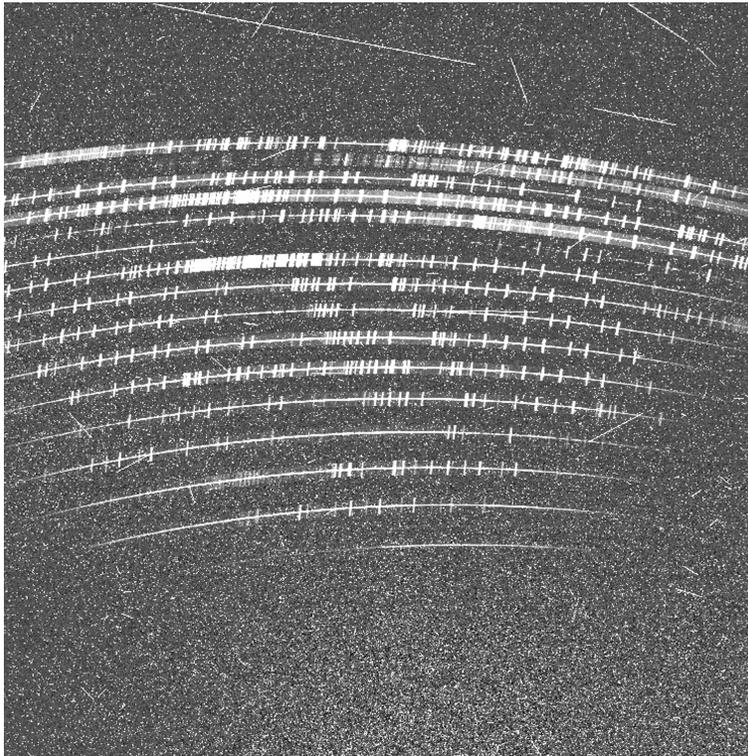


Figure 6. Full NIR arm displaying a synthetic image of black body at 5800 K at $V = 16$ mag point-source. Seeing $1''$, slit $1''$, 300 sec exposure.

Code is version controlled with git, hosted on github[†] and linked to a Jenkins Continuous Integration/Continuous Deployment server via webhooks. A push of new code to any branch in the github pipeline repository triggers a new ‘build’ of the code where all unit-tests are ran. If all tests pass then the branch is merged into its parent branch (which in turn triggers a new testing of the parent branch). If the master branch being tested and all tests pass then a new dot release version of the code is shipped to PyPI[‡] for deployment.

[†]github <https://github.com/thespacedoctor/soxspipe>

[‡]pypi <https://pypi.org/project/soxspipe/>

7. PIPELINE ARCHITECTURE

The SOXS pipeline borrows the informative concept of ‘recipes’ employed by ESO’s CPL to define the modular components of the pipeline. These recipes can be strung together to create an end-to-end workflow that takes as input the raw and calibration frames from the instrument and telescope and processes them all the way through to fully reduced, calibrated, ESO Phase III compliant science products.

We also employ the term ‘utilities’ to define reusable functions designed to be called from multiple recipes. Recipes are named with the prefix ‘soxs’ (e.g. `soxs_mbais`) followed by a succinct description of the recipe.

Table 5. Index of SOXS Pipeline Recipes.

Recipe	Reduction Stage
<code>soxs_data_organiser</code>	pre-processing
<code>soxs_lingain</code>	calibration
<code>soxs_img_mflat</code>	calibration
<code>soxs_mbias</code>	calibration
<code>soxs_mdark</code>	calibration
<code>soxs_disp_solution</code>	rectification
<code>soxs_order_centres</code>	rectification
<code>soxs_spatial_solution</code>	rectification
<code>soxs_spec_mflat</code>	rectification
<code>soxs_straighten</code>	rectification
<code>soxs_line_check</code>	rectification
<code>soxs_nod</code>	sky-subtraction
<code>soxs_stare</code>	sky-subtraction
<code>soxs_offset</code>	sky-subtraction
<code>soxs_extract</code>	extraction+
<code>soxs_response</code>	extraction+
<code>soxs_merge</code>	extraction+
<code>soxs_astro_phot</code>	extraction+

The reduction cascade of SOXS pipeline for spectroscopic data is reported in Figure 7 while the cascade associated to acquisition camera imaging reduction is depicted in Figure 8.

In particular, the association maps in Figures 7 and 8 show how spectral and imaging data cascade flow through the SOXS pipeline. The input data, calibration products required and the output frames are shown for each pipeline recipe implemented in the pipeline. Each of the vertical lines in the map depict a raw data frame, the specific recipe to applied to that frame and the data product(s) output by that recipe. Horizontal lines show how those output data products are used by subsequent pipeline recipes. Time loosely proceeds from left-to-right (recipe order) and from top-to-bottom (recipe processing steps) on the map. To the right of the grey dashed line in 7 there are input calibration products generated from a separate pipeline processing cascade.

The recipes required to reduce spectroscopic data from raw frames to 1D flux calibrated spectra are:

- `soxs_lingain`: Identify pixels that respond to varying levels of flux in a different way compared to the typical pixel.
- `soxs_mbias`: Used to create Master Bias frame and the first guess of bad pixels on the detectors.

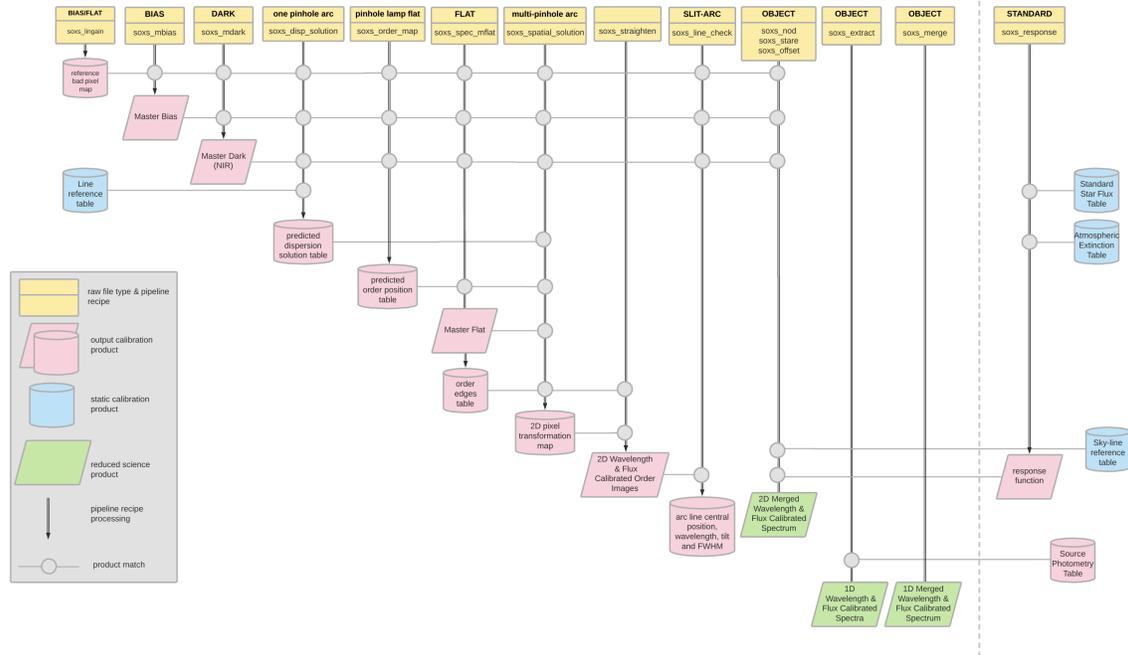


Figure 7. The SOXS Spectroscopic Data Reduction Cascade

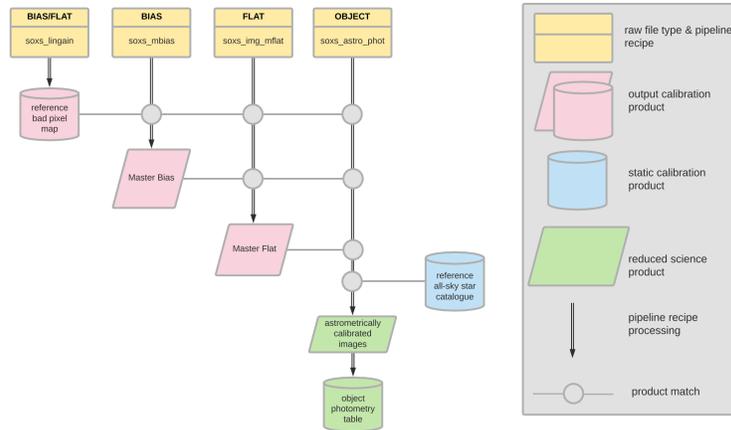


Figure 8. SOXS Imaging Data Reduction Cascade

- **soxs_mdark**: Remove the mean dark current from images and identify all hot or cold pixels.
- **soxs_disp_solution**: Generate first guess of the instruments spectral format and dispersion solutions and central trace positions for each order. Results from this recipe are shown in Figure 9.
- **soxs_order_centres**: This recipe, starting from the traces first approximated in the **soxs_disp_solution** accurately measures the central trace of each order. An example of the output of the recipe and its achieved performance is reported in Figure 10.
- **soxs_spec_mflat**: The recipe generates master flat-field frames, flag hot and dead pixels. The spatial extension of the orders is also measured at this stage. Figure 11 depicts results obtained against X-shooter NIR arm data.
- **soxs_spatial_solution**: This recipe estimates the spatial- *and* dispersion-solutions to generate a 2D map used later to translate curved order images into a linear (λ , s) space. The recipe is similar in logic to

`soxs_disp_solution` but it also samples along the slit in the cross-dispersion direction (i.e. Y-axis) by using the multi-pinhole slit frames illuminated by the arc lamp.

- `soxs_straighten`: This recipe uses the 2D map (modeled via polynomials) computed in `soxs_spatial_solution` to straighten (rectify) the curve order images and merge them together. Users will be able (if they wish) to perform source extraction on these rectified frames via the pipeline or using their own extraction routines.
- `soxs_nod`, `soxs_stare`, `soxs_offset`: These recipes are in charge of extracting the spectra in counts (order by order) and, in the case of stare mode, produce a model of the sky spectrum to be subtracted before extraction of the science pixels.
- `soxs_response`: Starting from observation of standard stars, this recipe computes the efficiency curve and response curve of SOXS to flux calibrate spectra for each order.
- `soxs_merge`: The orders extracted and flux calibrated in the previous step are merged together in order to obtain a unique, rectified and calibrated 1D spectra of the source (with sky subtraction).

8. CONCLUSIONS

SOXS is expected to be delivered to Chile (La Silla) in mid 2022 and offered to the community for the GTO and regular proposals from ESO by the end 2022. To meet this goal, we designed an agile framework of development based on Python 3 to develop a robust pipeline that can be used both automatically and interactively by supporting standard Esoreflex workflow.

In the paper, we presented the current status of the pipeline by especially focusing on the design architecture and development environment that foresee the use of current state-of-the-art technologies in the context of software development frameworks. At the moment of writing of this manuscript, the team is almost on schedule for delivering the pipeline by end 2021 where first tests of SOXS will take place in Europe. The adoption of agile framework, presented in Section 6 and the use of Python 3 greatly helped on meeting the time constraint while assuring high quality of the written software in terms of maintainability, readability and robustness.

ACKNOWLEDGMENTS

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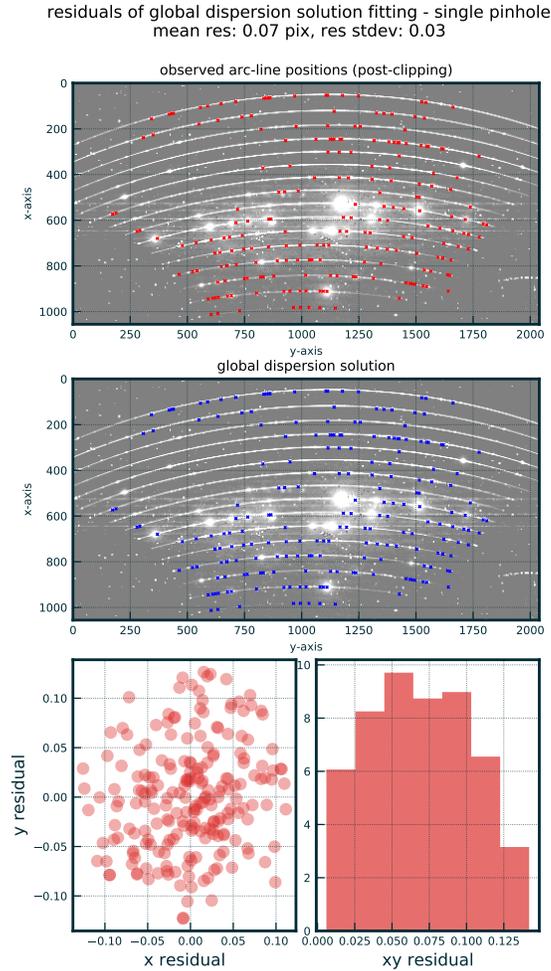


Figure 9. `soxs_disp_solution` recipe output. Top panel - Identified lines against a raw frame single pinhole illuminated by calibration lamp. Central panel - Survived spectral lines after sigma clipping and iteration on the global fit. Bottom panel: residuals (in px)

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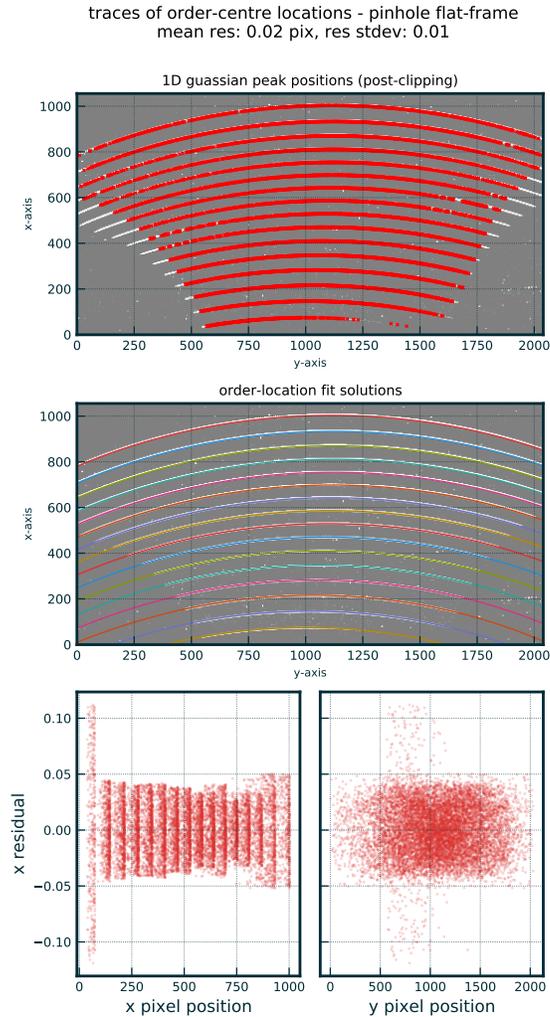


Figure 10. `soxs_order_centres` recipe output. Top panel - Fitted position of orders on the raw single-pinhole image. Central panel - Global fit obtained by interpolating red points of top panel. Bottom panel: residuals (in px)

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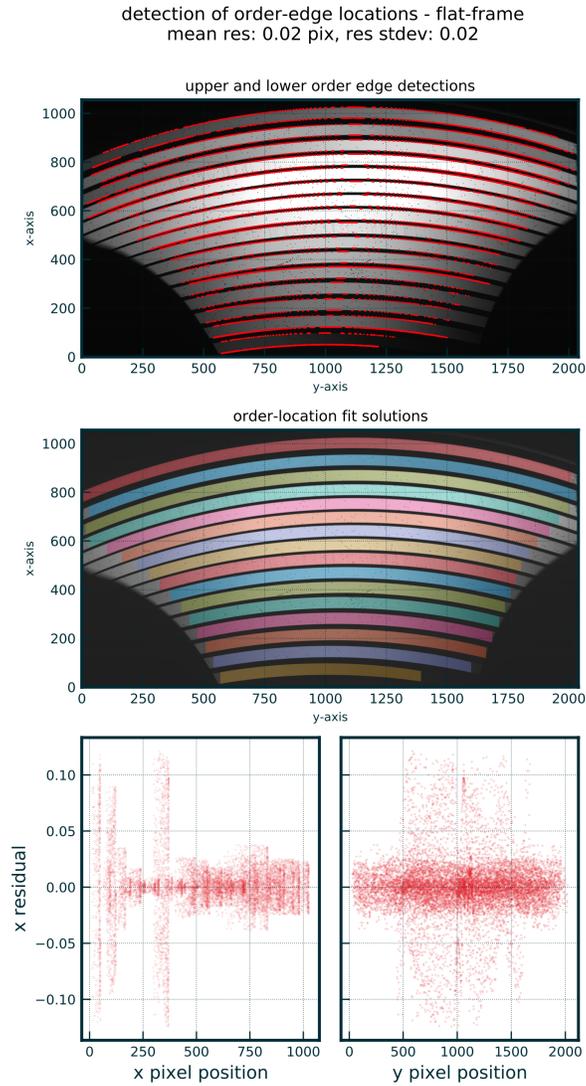


Figure 11. `soxs_mflat` recipe output. Top, Central and bottom panel are similar to Figure 10

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