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Preliminary design of the HARMONI science software

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ABSTRACT

This paper introduces the science software of HARMONI. The Instrument Numerical Model simulates the instrument from the optical point of view and provides synthetic exposures simulating detector readouts from data-cubes containing astrophysical scenes. The Data Reduction Software converts raw-data frames into a fully calibrated, scientifically usable data cube. We present the functionalities and the preliminary design of this software, describe some of the methods and algorithms used and highlight the challenges that we will have to face.

Keywords: Astronomy, ELT, HARMONI, science software, instrument model, data reduction, integral field spectrograph

1. INTRODUCTION: THE HARMONI INSTRUMENT

HARMONI, or the High Angular Resolution Monolithic Optical and Near-infrared Integral field spectrograph [1], is a visible and near-infrared integral field spectrometer (0.47 to 2.45 μm), producing more than 30,000 spectra in a single exposure, with a wide range of spatial pixel (spaxel) scales and spectral resolving powers (see Table 1 for the full design specifications). It is one of the first-light instruments for the European Extremely Large Telescope (E-ELT). Thanks to the enormous 39-meter main mirror of the E-ELT, HARMONI will be used to explore galaxies in the early Universe, study the constituents of the local Universe and characterize exoplanets in great detail.

HARMONI is a combination of optical systems for real-time atmospheric correction (SCAO and LTAO) and an integral field spectrograph placed in a cryogenic environment. The cryostat interfaces with the instrument rotator and the AO systems. Within the cryostat, the light is first scaled by the pre-optics sub-system to be suitable for input to the IFU (Integral Field Unit) sub-system. Then, the IFU sub-system splits the field of view into 4 pseudo-linear output pseudo-slits (Figure 1). Finally, the spectrograph subsystem disperses the light coming from these pseudo-slits to produce a two-dimensional spectroscopic image (Figure 2).

A Calibration Unit (CU) system reproduces the exit pupil of the telescope. It provides uniform white and arc light illumination at the telescope focal plane and over the complete HARMONI field of view. The CU system will also include a set of calibration masks that can be inserted in the telescope focal plane.

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Table 1. Current design parameters for HARMONI

Wavelength range	0.47 to 2.45 μm
Spatial scales (FoV)	4 mas (0.86arcsec x 0.61 arcsec) 10 mas (2.14arcsec x 1.52 arcsec) 20 mas (4.28 arcsec x 3.04 arcsec) 60 x 30 mas (9.12 arcsec x 6.42 arcsec)
Spectral resolution (and waveband)	3500 (V + R; Iz + J; H + K) 7500 (Iz, J, H, K) 20000 (half of each NIR band)
Temperature	140 K 40 K detectors
Detectors	Teledyne HgCdTe 4k x 4k for NIR 4k x 4k CCD for visible
Throughput	Target ≥ 30 per cent average
AO modes	SCAO, LTAO, seeing-limited

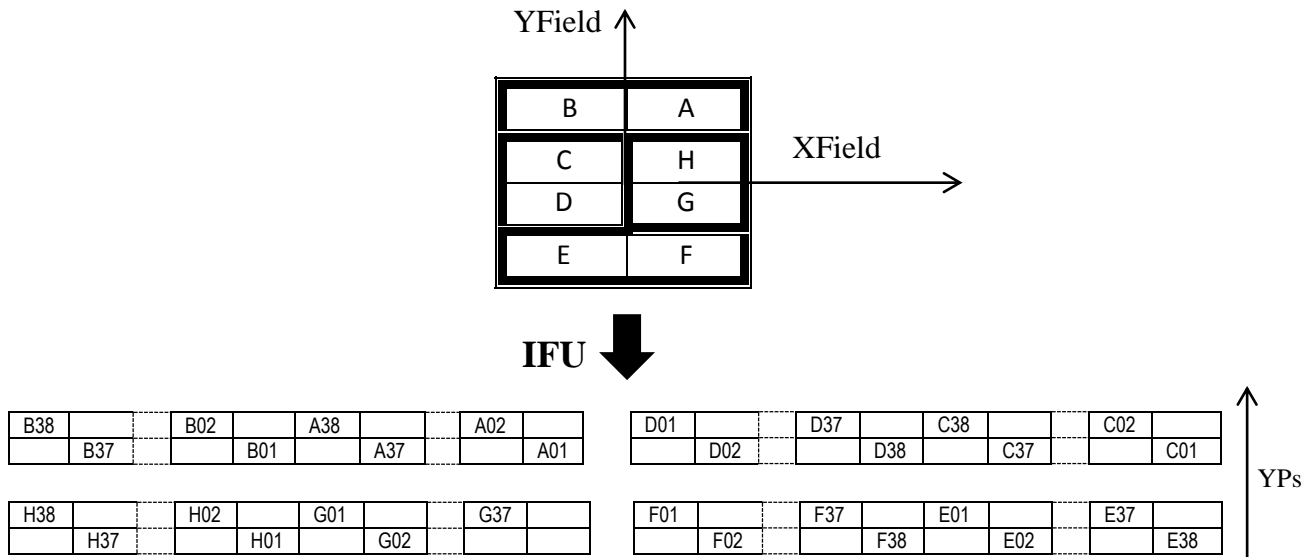


Figure 1. IFU sub-system

On the top, the scheme shows how the field splitter divides the field in 8 relays paths named from A to H. Each sub-field is then divided by a slicer system into 38 slits. The bold lines group the two fields feeding one spectrograph. On the bottom, are plotted the 4 pseudo slits (one per spectrograph) produced by the 4 pairs of paths (pair AB, CD, EF, GH) [2]. The view is oriented looking towards the telescope (Zfiled), YField is the direction of the slices, YPs is the direction of the dispersion.

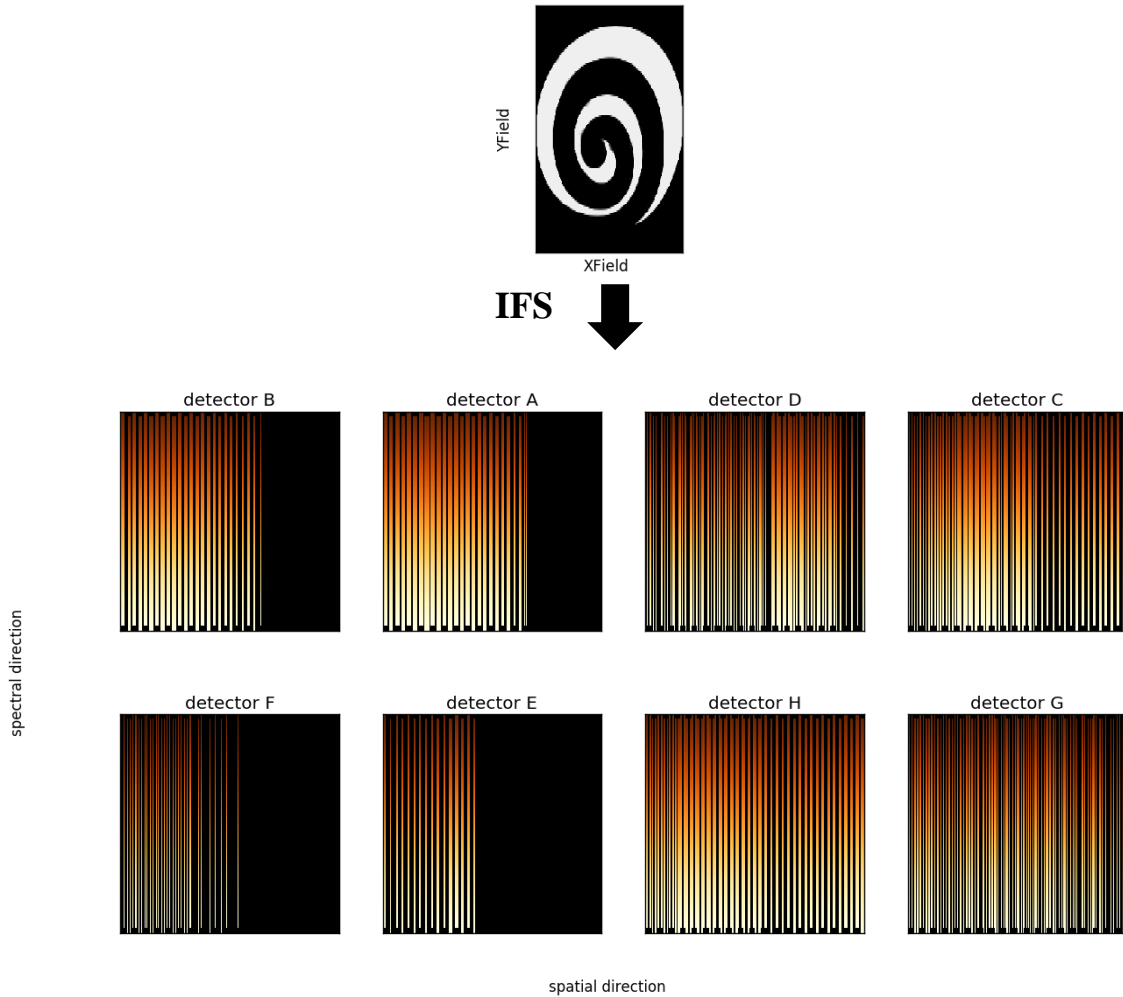


Figure 2. These pictures show the location of the spectra on the 8 detectors of HARMONI given a field at the entrance of the integral field spectrograph (IFS).

2. SCIENCE SOFTWARE

In the HARMONI project, the Science Software includes different tools as the Data Reduction Software, the Instrument Numerical Model, the end-to-end Simulator HSIM, the Exposure Time Calculator and the Observer Support Software. This paper focus on the tools CRAL is responsible for, which are:

- the Instrument Numerical Model (INM), which mimics the optical behavior of the full instrument (from the Telescope to the detectors) and provides mock data as distributed by the detector control software,
- the Data Reduction Software (DRS), which goal is to remove entirely the instrumental signature from raw data frames, correct the data from the environment effects (e. g. atmospheric refraction, sky background) and convert the data into astrophysical units. It includes tools for data quality monitoring, for fast image reconstruction and for the combination of single reduced frames into a final data set. Other tasks beyond the instrument-related data reduction steps are not addressed.

The end-to-end simulator HARMONI [3] provides simulated observations by replacing both the instrument and the data reduction software in a single simulation. By using different assumptions (as the homogeneity of the point spread function in all the field of view for example), simulations are done in a much shorter timescale, which is suitable to test science cases. Combining the INM and the DRS results in a more realistic simulation but at the price of a greater complexity and a longer timescale. There are thus complementary tools.

In order to code, test, and deploy the science software with a perfect traceability, we will use early in the project a GitLab forge [4]. Gitlab is a free software which provides, amongst other things, Git repository management, code reviews and issue tracking.

3. THE HARMONI INM

3.1 The need for an end-to-end instrument simulator

An instrument numerical simulator (or model) is a software which reproduces the light path throughout the instrument. It replaces the instrument while being built, creating from astrophysical scenes raw data similar to those produced by the detectors in the future instrument.

The new generation of super-telescopes and associated instrumentation projects enter such ambitious scales and complexity of design, that it is becoming imperative to develop sophisticated models for these instruments. These models are a tool to understand the instrument, to help on performance-related trade-offs or to provide early validation of specification before the on-sky commissioning. They are also essential to provide synthetic detector readouts for the development of various software (integration tools, data reduction pipeline, data analysis tools) and for the science preparation.

3.2 Principle of the simulator

In a nutshell our HARMONI instrument simulator takes in input astrophysical data (x, y, wavelength) representing the observed area on the sky. It propagates them using the optical principles through the atmosphere, the telescope and the whole instrument up to the detectors where the various steps of the conversion from photons into computer data are simulated. For one observation it produces the same FITS files as will produced the real instrument.

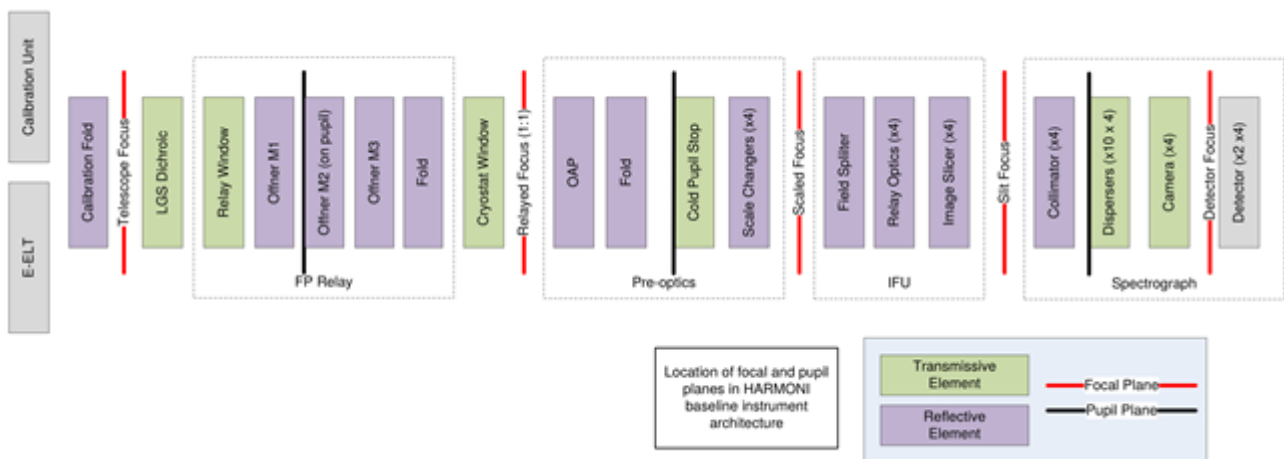


Figure 3. End-to-end optical path with major items and focal pupil planes

The architecture of the simulator is presented in Figure 4. Following the path of the photons traveling from the stars to the detectors they first goes through the atmosphere. We do not directly simulate the atmosphere in our simulator, but

instead use the results of dedicated simulations which also include the corrections done by the adaptive optics. The photons then travel through the telescope and through the instrument, and then reach the detectors which convert the photons into electrons and then into computer data. To simulate the light propagation from the sky to the detectors, we split our optical schematics into optical modules (see Figure 3): atmosphere and adaptive optics, telescope, FP relay, pre-optics, IFU, spectrograph. There are multiple instances of several modules, for instance there are 304 different IFU modules as the instrument is based on 4 slicers of 76 slices. For each of these optical modules simulating the light propagation consists in answering the following questions:

- **How is the light spread?** This is done by convolving the data at the input of a module by its Point Spread Function (PSF). The PSF is usually the result of Fourier optics computation taking into account the optical aberrations, the wave-front errors and the diffraction effects. In practice the PSF is variable both as a function of wavelength and position within the field-of-view, so we must use shift-variant blur techniques to model the variation of the PSF [5].
- **Where goes the light?** This is done by applying the rules of geometrical optics. They are usually provided directly by ZEMAX software or by a separate model for the dispersers.
- **How many photons reach the output plane?** The effects of the transmission and efficiency of the instrument are taken into account as weighting curves.

It should be noted that having chosen the convolution approach, we do not propagate a wave-front through the instrument, and thus all the sources arriving to the instrument are considered non-coherent. This is clearly an approximation for point source objects (e.g. stars), but we assume that for significantly long exposures (at least a few seconds), the atmosphere breaks the coherency of the light. In any case propagating a wave-front would mean that we first need to do a propagation for every instantaneous phase mask of the atmosphere during the exposure which would require a huge amount of computation time. In addition it would also mean that the input data cube should contain only independent object (for instance all the stars in a galaxy) and that they shall be propagated one by one through the instrument.

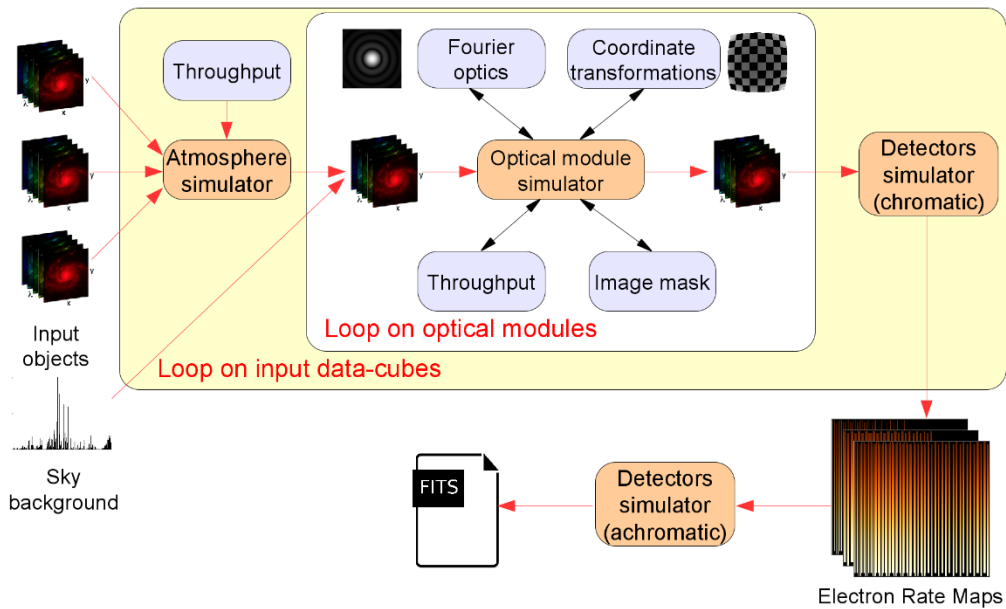


Figure 4. Principle of the simulation

The input astrophysical data is actually composed of a set of data-cubes, each of them corresponding to a subset of the observed field of view both spatially and spectrally. Each of these data-cubes might use a different spatial and spectral sampling to better suit the data it contains. This way a diffuse source with little spatial structure will be represented by a cube with a coarse spatial sampling. It will be propagated throughout the instrument with this sampling up to the moment it has to be increased to correctly simulate an optical effect, for instance reaching the sharp edge of an optics. This greatly reduces the computation time provided the input data is appropriately sampled. In turn, this makes the parallelization trivial, each small data-cube can be propagated independently and its contribution summed at the detector level. It should be noted that the separation of the input astrophysical data into small data-cubes can be done in various ways. One can for instance split the spectra into a continuum and the emission lines. Alternatively each small data-cube can correspond to an astrophysical object, which usually matches the output of astrophysical simulation. In practice a mix of both methods is usually chosen.

The same principle is used to simulate calibration exposures. The input data-cubes instead contain the spectra of calibration lamps and the shape of calibration masks, and atmosphere simulator is skipped.

Both the telescope and the instrument are designed using the ZEMAX software [6]. Instead of extracting the design from this software and also to avoid reinventing the wheel, we will use it for computations that it is good at. We use the ZEMAX Programming Language (ZPL) to extract the relevant data: the coordinate transformations and the wave front error maps.

3.3 Fourier optics software module

According to the Fourier optics concept [7], assuming that we are in far-field Fraunhofer diffraction regime, we can compute the complex amplitude between conjugate planes (e.g. between the exit pupil plane and the exit image plane of an optical system, see Figure 3) by using a Fourier transform. This requires building an equivalent paraxial optical system. Using the ZEMAX software with the ZPL language, we can build such a system for each optical module and extract the corresponding data: the focal lengths, the pupil mask and the map of the wave-front errors. Note that the wave-front maps in such an equivalent system are chromatic.

As we have chosen the convolution approach, we use Fourier optics to compute the PSF of an optical module, for a given wavelength and a given position in the field-of-view. To propagate an input data-cube through a module we need to know the PSF at multiple locations and wavelengths. Many instrument simulators [8] [9] pre-compute a database of highly sampled PSFs, which are later interpolated both in location and wavelength. However PSFs can only be accurately interpolated with a very big database, as the size and the shape of the PSFs tends to vary a lot, especially as a function of the wavelength due to the diffraction.

For the HARMONI simulator we have chosen to compute the PSFs needed for each convolution “on the fly” using a database of wave-front error maps (the ones extracted from ZEMAX). The wave-front error maps still have to be interpolated, but as they vary much more smoothly, a sparser database can be used. By using zero-padding techniques and by adding a linear phase to the wave-front error maps to control the decentering, it becomes possible to compute a PSF with a given sampling, at any spatial and spectral point of an optical module. When the PSF sampling is chosen to match the one of each input data-cube, the convolution can therefore be done without any preliminary interpolation or resampling. As a result this method is faster than the one using a database of PSFs, and also requires less disk space.

3.4 Coordinate transformation parameterization

The goal of the coordinate transformations is to build a model able to compute the location of the chief ray through the whole instrument. We extract the information from ZEMAX using the ZPL language, by scanning the field of view and the range of HARMONI wavelength and use ray tracing to create coordinate transformation maps between key optical planes. These coordinate transformations are then fitted into a 3D polynomial.

The parameterization of the coordinate transformations allow us to compute very quickly (i.e. using a few multiplications and additions) the chief ray through the whole instrument for a given input point in the field of view. It also gives us the possibility to directly apply the coordinate transformations of an optical module to a data-cube by first computing the non-regular output grid corresponding to a regular input grid, and then resampling the input data-cube onto a regular grid. The corresponding intensity modulation can be computed by using the Jacobian determinant of the polynomial.

The dispersers are modeled from the coordinate transformations point of view using the grating equation.

3.5 Atmosphere, adaptive optics and telescope simulation

For ground-based instruments it is essential to simulate the various effects of the atmosphere, at least the most important ones. Our goal is to simulate the atmospheric effects in a way which is realistic and compatible with the resolution of the instrument, not to model these effects in a very precise manner. The numerical model takes into account the following effects: atmospheric turbulence coupled with the adaptive optics of the instrument, atmospheric refraction, sky, and telescope.

Introducing the atmosphere turbulence is usually complex and could lead to huge computation times, thus not compatible with the use of an instrument simulator, in the context of software development or scientific exposure preparation. In addition, the simulation of these effects is usually out of scope of an instrument simulator, as it is often done by different people in dedicated simulations, from which only the final results are available. In our case these simulations are done by the HARMONI adaptive optics team [10], and include both the atmosphere and the adaptive optics. They have developed an IDL software which provides the power spectral density as a function of various parameters (AO mode, turbulence, position with the FoV, NGS and LGS distance, etc.). Using a map of the static wave-front aberrations, it is possible to obtain the corresponding PSFs, which can then be used by our simulator.

The effects of atmospheric refraction are well known and several authors [11] [12] have extensively discussed them. As the refractive index of air is somewhat larger than one, the light coming from outside the earth atmosphere is refracted towards zenith. This affects the position of objects in the sky in two ways, depending on the wavelength and on the airmass. In turn this affects the raw exposures with three different effects:

- Usually, the guide probe is sensitive to a given wavelength which is generally different from instrument wavelength range. This introduces a chromatic differential refraction between the guiding wavelength and the extreme wavelengths of the instrument.
- As the exposure spans over time, the airmass changes during the course of the exposure, leading to a degradation of the PSF.
- The airmass is not constant over the field-of-view, which leads to a field differential refraction. However this effect is negligible in the HARMONI case as the field-of-view is small.

The first effect is modeled using coordinate transformations derived from the Fillipenko [12] equations and applying them to each of the the input cubes. The second effect is applied by convolving each of the input cubes by the PSF corresponding to the variation of the refraction during the exposure, which depends on the wavelength. When the detectors are used with multiple non-destructive readouts the full simulation from the sky to the detector has to be done for each successive readout.

The sky effects are modeled using the ESO Skycalc sky model [13] for both emission and transmission. The emission part is simulated using an additional input cube with low spatial resolution, and propagated through the simulator like any other input cube. The transmission part is integrated in the throughput.

Finally we also model the telescope thermal emission as a grey-body whereby a thermal blackbody curve for the given site temperature is multiplied by a constant emissivity.

3.6 Detector modeling

HARMONI observes in both the visible and the near-infrared. It uses 4k x 4k CCDs for the visible range, and 4k x 4k HgCdTe detectors for the near infrared. Their simulation is split into two different parts. The chromatic part deals with photons as an input and produces an electron-rate map as an output. The non-chromatic part deals with electrons and converts them into ADU. The non-chromatic part of the simulation is an order of magnitude faster than the chromatic part, as it deals with a much smaller amount of data. The separation in two different parts allows the user to change most of the detector properties and redo only the second part of the simulation.

The effects modeled in the chromatic part of the simulation include the sampling by the detector matrix, the intra-pixel sensitivity (for the NIR), the quantum efficiency and the charge diffusion (for the visible). The non-chromatic part of the simulation adds the following effects: hot and dark pixels, dark current, shot noise, cross-talk, non-linearity, blooming, saturation, charge transfer efficiency (for the visible), read-out noise, and conversion into ADU for the various readout

modes. Finally the last step adds the effects of the cosmic rays, based on libraries of cosmic rays (one for visible, one for the NIR) gained from the dark exposures of similar detectors.

3.7 Software environment

An instrument simulator is a computation intensive program which requires multi-threaded code to run in reasonable time and fined-grained memory control to work on computers with limited memory. Despite the above constraints we have chosen to develop it in the Python language, using the Numpy, Scipy and Astropy libraries. This greatly simplifies the development of the simulator by providing high level I/O, signal processing and astronomical related functions, while doing the same for instance in C would require either re-implementing many standard algorithm or using many different libraries. Given the timescale of an E-ELT project, we will develop our code directly in Python 3, as Python 2 will be obsolete when the instrument will be on sky. We then plan to profile our code to identify the parts which would benefit from being implemented in a lower level language. These parts will then be implemented in C, using OpenMP for the parallelization and vectorization. In addition we will use the Matplotlib library for visualizing intermediate data during development.

4. THE HARMONI DRS

The goal of the DRS is to transform the raw CCD-based data of HARMONI into a data-cube corrected from the instrumental signature and from the environment effects. Moreover, it includes tools for data quality monitoring, for fast image reconstruction and for the combination of single reduced frames into a final data set. The science analysis tasks are not considered.

4.1 The ESO context and the software environment

As any other ESO data reduction software, the DRS of HARMONI will be split into data-reduction tasks (known as "recipes"). These recipes could be executed manually, can be triggered by the pipeline, or run through the ESO standard data-reduction framework (Reflex [14]). These recipes shall be developed with ESO-CPL (The Common Pipeline Library), an ESO toolkit containing a set of ISO-C libraries offering high-level I/O routines to load and play with exposure data and a variety of general-purpose image and signal processing functions [15]. ESO also offers HDRL, the High Level Data Reduction Library, which provides several common astronomical data reduction algorithms for data reduction pipelines [16].

Obviously, the HARMONI DRS shall comply with ESO deliverable quality standards. Thus the delivery includes all documentation associated to the development, design and tests of the data reduction software and of course the all end user documentations. Mock data, some of them created by the INM, are also required at different stages of the project in order to test the recipes.

4.2 Data reduction philosophy

Input/output

The HARMONI DRS will receive as input raw detector exposures for science and calibration data and will create as output the following data:

- 3D data cube,
- associated variance cube (as FITS extension),
- quality control (QC) parameters and performance monitoring values.

Detector preprocessing

A HARMONI raw exposure will consist in a single FITS file with multiple extensions, usually one extension per detector (visible and near-infrared). It cannot be used as such and a preprocessing step must be performed in order to obtain an electron rate map per detector. At this stage, some key detector artifacts are removed: gain correction, non-linearity correction, cosmic ray rejection, bias, dark and flat-field correction...

Moreover, for the NIR detectors when using the up-to-ramp readout mode (default mode), a raw FITS extension will contain a sequence of frames coming from successive non-destructive readouts of the detector [17]. For each detector pixel, one can obtain from the sequence of frame a 1D curve, the slope of which corresponds to the cumulative number of counts as a function of time. Repeating this operation for each detector pixel will yield an electron rate map.

At the end of the preprocessing step, for each pixel, we will get the electron rate value (with the detector effects removed), the status (the data quality) and the variance (the pixel statistic).

Calibrations recipes

The calibration unit for HARMONI is currently under development; nevertheless one can assume that the lamps shall be defined to have the required flux to keep the exposure time to a minimum, the arc lamps shall provide the required density of lines for relevant wavelength calibration, and the set of masks must be chosen at best to allow different purposes calibrations (e.g. trace spectra, geometric transformation).

In the end, the HARMONI calibration unit will provide data for the following measurements:

- flat field exposures to monitor the instrument throughput,
- spectra of arc lamps to determine the wavelength solution of the instrument,
- pinhole observations to trace the location of the spectra on the detector,
- a set of standard stars exposures to create a flux response curve and telluric correction/calibrations.

The HARMONI DRS will include the classical routines to analyze these calibration data, derive corrections and apply it to the raw data.

Basic reduction

This step, which removes the signature of each IFU, is the core of the data reduction. It uses the results of the calibration recipes to associate each detector pixel with a position on the sky, a wavelength, a flux value and a variance value. In order to establish this association, tracing, geometrical transformation and wavelength calibration are applied on the pixel coordinates; a possible flux calibration may be applied to the pixel values.

Environment effects correction

The next steps of the data reduction are the atmospheric refraction correction and sky subtraction, and contrary to the previous reduction steps they make use of all pixel values over the entire HARMONI field-of-view. Atmospheric refraction is quite significant for HARMONI due to the small field-of-view and will be challenging as we will be limited by our knowledge of the physical parameters in the atmosphere at the time of observation. Accurate sky subtraction will be critical, in particular for faint astrophysical sources, as the sky brightness dominates the signal to be measured and has strong fluctuations in time and spatial location in the near-infrared. Several sky subtraction techniques are currently under study for HARMONI: most of them rely on the use of a fraction of the field-of-view to estimate the sky contribution over the entire field:

- Physical model: unlike the sky emission continuum, which combines very different contributions difficult to model (moon light, zodiacal light, scattering, thermal emission), sky emission lines have a well-known physical origin, occur at specific wavelengths and according to precise line ratios. Provided one can accurately model the

Line Spread Function (LSF) of the instrument at each spatial location/fiber it is possible to accurately subtract sky emission lines. [18]

- Empirical estimate: sky emission in the continuum can be estimated from the closest spatial pixels not covered by astrophysical sources [19].
- PCA (Principal Component Analysis) sky subtraction (e.g. [20], [21]): the aforementioned techniques are limited in the accuracy of the physical model and/or the instrument calibrations, such as the knowledge of the LSF, slice-to-slice flat field and scatter light, or wavelength calibration. PCA techniques intend to recover from these limitations by analyzing and subtracting sky subtraction residuals from science data. The risk behind PCA techniques is the potential subtraction of science signal mistakenly taken for sky subtraction residuals.

A single interpolation to create the final data-cube

We propose to follow a reduction approach similar to the pipelines for 2nd generation VLT instruments (KMOS [22] or MUSE [23]) and reconstruct the 3D data cube from the electron rate maps in a single interpolation step. One of the features of the DRS is to propagate errors through all reduction steps and to minimize the introduction of correlated noise components in the data. If more than one interpolation is done, pixels and their errors become entangled across several pixels, so that error estimates become less meaningful. In addition, each interpolation step can also propagate artifacts.

That is why the final data-cube for an exposure will be created by re-sampling the output pixels, (flux, quality flag and variance) onto a suitable regular output grid. Combination of different exposures, for mosaicked or dithered fields can be achieved by appending or merging all data before the final interpolation.

Fast image reconstruction

The HARMONI instrument having no imaging capability, a tool will be necessary to create the image of the field of view from raw spectra for a quick look check. This capability shall be kept short in time since it may be used also to assess the telescope pointing before observing.

5. SOFTWARE STATUS AND PLAN

The HARMONI project is now in design phase. The aim is to have an instrument simulator ready for the PDR in fall 2017. We are now in the early phase of its design, testing new methods using the MUSE optical parameters because those from the design of HARMONI are not available yet.

We also reviewed the science software top level specification, the input and output format and the E-ELT Generation software standards. From the specifications, we will derive the layout of DRS recipes and write the associated technical documentation (including the development plan). We will also participate in the design discussions of the calibration unit which is under investigation.

The next three years will be dedicated to the design and prototyping of the DRS. The tracing, the geometrical transformation and the sky subtraction are critical and we plan to develop prototypes of these challenging reduction steps. All these methods will highly benefit from the knowledge gained from the instrument model.

The implementation and test phase will then produce the full off-line DRS pipeline able to reduce the data right from the outset. The commissioning runs and the science verification program will fully benefit from it.

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