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The JWST/NIRSpec instrument performance simulator

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ABSTRACT

The future James Webb space telescope (JWST), developed jointly by the American, European and Canadian space agencies (NASA, ESA and CSA), is scheduled for launch in 2013. Among its instrument suite, the spectrograph NIRSpec will provide astronomers with multi-object, integral-field and classical slit spectrographic capabilities in the near-infrared (0.6-5.0 μm). NIRSpec is being built by EADS Astrium for ESA and it was quickly realized that given the complexity of the instrument, it was necessary to develop dedicated software for the modeling of its performances. In this context, the Centre de Recherche Astrophysique de Lyon (CRAL) is responsible of the development of the so-called NIRSpec instrument performance simulator (IPS) that will serve as a basis for early performance verification purposes; provide inputs and support for the verification and calibration campaigns, as well as for the development of the instrument calibration, target acquisition and data reduction procedures.

In this paper, we present the IPS software itself, emphasizing its capability to generate simulated NIRSpec detector exposures for the various modes of the instrument (multi-object, integral field unit, fixed slits) and for a large variety of situations (test, calibration, scientific observations...). We will also show simulations results.

Keywords: Astronomy, simulation, numerical model, spectroscopy, JWST, NIRSpec

1. INTRODUCTION TO THE JWST/NIRSPEC PROJECT

NASA and ESA - joined by the Canadian Space Agency (CSA) - have since 1996 collaborated on the definition of a successor to Hubble space telescope, the James Webb Space Telescope (JWST). JWST is a passively cooled, 6.5m aperture class telescope, optimized for diffraction limited performance in the near-infrared wavelength region (1 - 5 μm), but with extensions to either side into the visible (0.6 - 1 μm) and Mid-IR (5 - 28 μm) regions. To achieve the scientific program for the JWST mission, the observatory will be capable of high-resolution imaging and spectroscopy. The definition, procurement and commissioning of the near-infrared spectrograph (NIRSpec) is responsibility of ESA with hardware procured through European industry (EADS ASTRIUM).

1.1. Overview of the NIRSpec instrument

NIRSpec 4 is a near-infrared spectrograph that will allow astronomers to obtain the spectra of more than one hundred individual objects in one shot when used its multi-object spectrograph (MOS) mode. It will cover the wavelength range from 0.6 μm to 5.0 μm . The 9 square arc-minute scene on the sky will be re-imaged through the fore-optics on a micro-shutter array. This array is fully-addressable and allows to select the desired targets and then to obtain their spectra on the two 2048 \times 2048 HgCdTe detector arrays. The instrument will also be used in imaging mode with no dispersive element and all micro-shutters open.

In addition to these MOS and imaging modes, NIRSpec includes an integral field spectrograph mode (IFU) and a classical long-slit spectrograph mode. The 3 arcsec \times 3 arcsec field-of-view of the IFU mode is rearranged into thirty 0.1 arcsec \times 30 arcsec slices aligned into one pseudo-slit at the entrance of the NIRSpec spectrographic stage.

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Figure Fig. 1 provides an overview of the optical layout of the NIRSpec instrument behind the JWST optical telescope element (OTE). The two main image planes are the plane of the micro-shutter assembly (MSA) and the plane of the detector. When NIRSpec is used in its IFU mode, the additional IFU optical module is inserted at the location of the MSA plane (which corresponds to both the entrance and exit planes of the IFU).

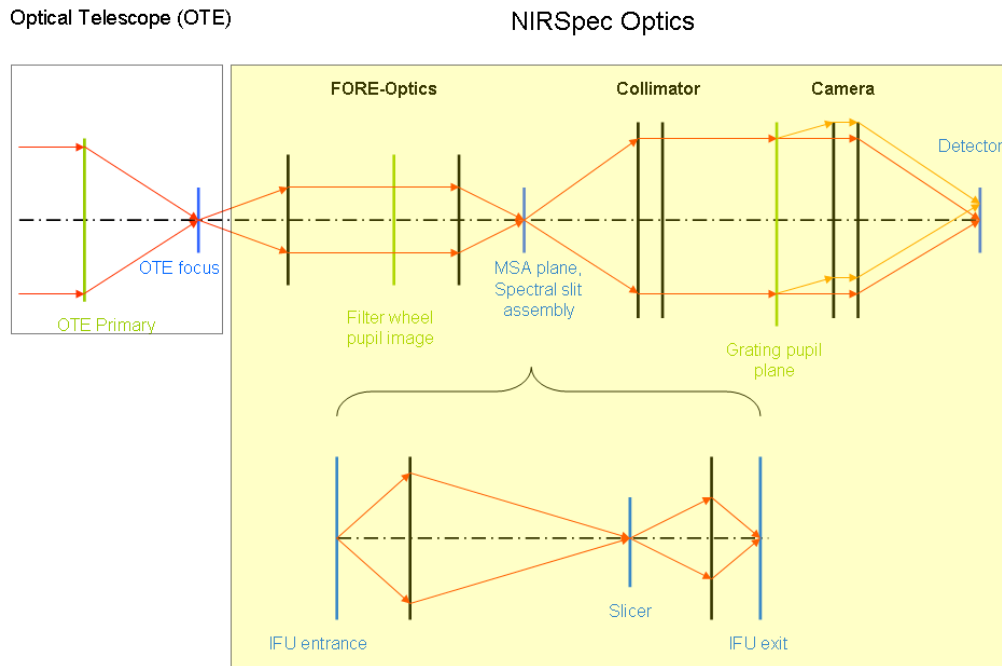


Fig. 1 : NIRSpec optical instrument concept.

1.2. Goals of the IPS

Early in the NIRSpec project, it was realized that given the complexity of the NIRSpec instrument, achieving better understanding of the instrument and of its performances required the development of a dedicated instrument performance simulator (IPS) .

This software is being developed by the Centre de Recherche Astrophysique de Lyon (CRAL 4) and is part of the NIRSpec electrical ground support equipment (EGSE). It is already used or will be used for a large variety of tasks:

- Provide inputs for performance-related trade-offs and for the early verification of the instrument performances.
- Provide inputs and support for the preparation and execution of the verification and calibration campaigns. In particular through the computation of simulated verification and calibration data.
- Provide inputs and support for the development of the instrument calibration, target acquisition and data reduction procedures (e.g. provide inputs for the development and tuning of the TA algorithms and for the verification of the NIRSpec quick-look, calibration and analysis software).

It is also becoming clear that the simulated exposures generated by the IPS will be important elements in the analyses that will demonstrate the compliance of NIRSpec with some key performance requirements.

Note that a second simulation software called hIPS is being developed in parallel by ESA [8].

2. IPS SOFTWARE DESCRIPTION

2.1. IPS software overview

The IPS must be capable of modeling the performances of the instrument in its imaging mode and in its three spectrographic modes: multi-object spectroscopy (MOS, using the micro-shutter array), slit spectroscopy (SLIT, using a set of 5 small slits) and integral field spectroscopy (IFU, using the IFU module). The following main functionalities are therefore being implanted:

- model the instrument optical performances (synthetic PSF computations)
- model the geometrical distortion maps between various stages of the instrument
- model the radiometric response of the instrument
- compute the absolute sensitivity of the instrument for point-like sources and for uniformly illuminated apertures (micro-shutters, fixed slits or IFU field of view)
- simulate calibration, scientific and tests exposures (detector outputs)

It is divided in seven main software components:

- a Fourier optics software which will be used to model the modes and configurations of the instrument (including its calibration and test configurations) and to produce synthetic PSF in the planes of the micro-shutter (MSA) and detector (FPA).
- a commercial optical design software (the ZEMAX software) that will be used to extract the information needed by the Fourier optics software from the optical design of the instrument
- a coordinate transform computation and fitting software, which will be used to parameterize modeled or measured distortion maps between key optical planes
- a radiometric response computation tool, which will include slit and diffraction losses when relevant
- an absolute sensitivity estimator
- an exposure simulator, which will be able to generate synthetic detector readouts for a limited number of astrophysical sources and for calibration and test sources
- an instrument model database, which will be used to ensure the traceability between a simulated element (PSF, exposure...) and the instrument model used to generate it.

These software components are accessible through a single application, with a common user interface. The IPS software and the associated instrument models are progressively updated when verification and calibration data either for sub-systems or for the instrument itself become available.

2.2. The IPS software environment and development constraints

The CRAL is to deliver to EADS Astrium the IPS software and a dedicated hardware. This hardware contains 8 processors and more than 1TB RAID-5 of hard disk drive storage. The IPS software is implemented in C++ for Linux using some open source libraries: GSL, Qt4, CCFits, CppUnit, and FFTW. The IPS computer operating system is a Red Hat 5. The Qemu machine emulator is used to run the Zemax raytracing software under WindowsXP. Data are stored in a database using SQLite library.

The IPS shall comply with industrial quality standards. This implies spending more time than usual to validate the UML design, to produce end user documentations, to review the code and to test the software. Moreover the IPS is coded and tested according to the industrial quality standards. A bug tracker system (Mantis) and versioning tool (SVN) was introduced early in the project. All these tools allowed our team (one project manager, one project assurance and 4 developers) to write 100 kSLOC* with a perfect traceability. In order to deliver early exposures to ASD, to check the implemented algorithms and to test the IPS software, a prototype has been developed in Python.

* 1kSLOC = 1000 Source Lines Of Code.

2.3. IPS software simulation workflow

In Figure Fig. 2, we have provided a simple sketch of the main IPS-2 workflow. We can distinguish in the grey box the operations that can only be executed by an expert user. The IPS software has two different types of users. The IPS standard user mode allows the user to produce simulation results from a given (already prepared) instrument model. The expert user mode allows the user create instrument models as well as to access every functionality available to the standard user.

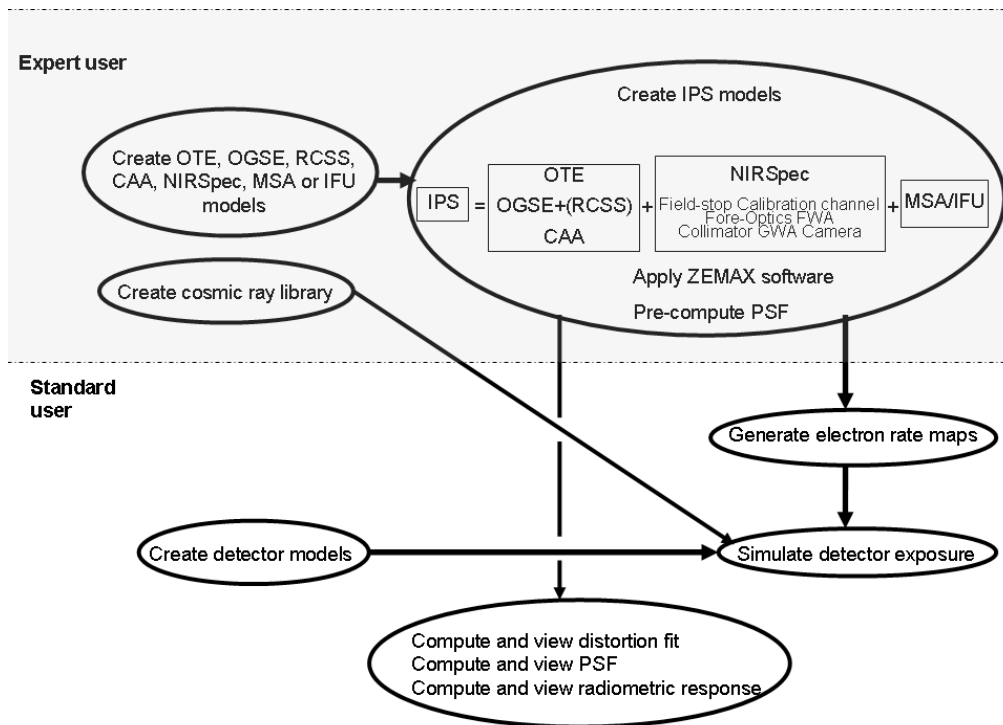


Fig. 2: Sketch providing an overview of the main IPS-2 workflow.

This flow shows that the simulation has been split in two steps, one corresponding to the computation of a map of the electron rates per pixel and a second one corresponding to the exposure simulation itself (with in between detector model preparation). This was done to try to decouple as much as possible the modelling of the detector and the observation parameters from the instrument modelling itself.

This allows:

- To give the standard user access to the detector model preparation (this is not the case for the remaining parts of the instrument) and to allow him to easily change key detector parameters like the dark current, the noise parameters...
- To generate multiple fake exposures with different detector and exposure parameters without having to restart a complete electron rate simulation.

In order to provide a good traceability of the inputs that are being used in a given model conducted using the IPS, the IPS software includes a dedicated database. The IPS software modules automatically store the model and simulation information in the database in a transparent way. The database is also used by the IPS software to provide the user with the existing lists of models and files available for given tasks.

2.4. The instrument model

Prior to any simulation, it is necessary to provide the IPS with all the information to create a model of the instrument (see grey area in Figure Fig. 2). This task is performed by an expert user and is divided in 4 steps.

During the step #1 of the model creation, the expert user enters the description of the various optical elements / modules present in the complete optical system. This step is long and tedious due to the huge number of elements that have to be entered. In order to limit the effort needed to create a model, the structure of the model is modular. The expert first creates models of optical sub-systems like the optical telescope (OTE), the integral field spectrograph (IFU), the micro-shutters array (MSA), the calibration assembly (CAA), the calibration light source (CLS) or NIRSpec itself (excluding the IFU, the MSA and the CAA) that are stored in the IPS database and made available to the expert users. The complete model of the system (which is associated to an input ZEMAX file and is called an IPS model) is then created by selecting the relevant optical subsystems. This way, it is possible to use the same NIRSpec model for different configurations, e.g. when creating a model OTE + NIRSpec + MSA (on sky observation, MOS mode) and when creating a model CAA + NIRSpec + IFU (calibration, IFU mode).

For most optical modules, the optical parameters, the throughput information, the coordinate transform (distortion) information, and the wave-front error (WFE) maps have to be entered. For optical parameters, WFE and distortion, the user is offered to let the IPS software automatically extract the information from the ZEMAX file or to provide its own information. For the throughput and the WFE it is possible to consider the global module or each optical element. The user can also describe all the masks, the field-stop, the gratings parameters ... This list illustrates the large number of parameters that have to be entered and the important options that are offered to the user allowing him to build models with very different levels of detail and input data from very different origins.

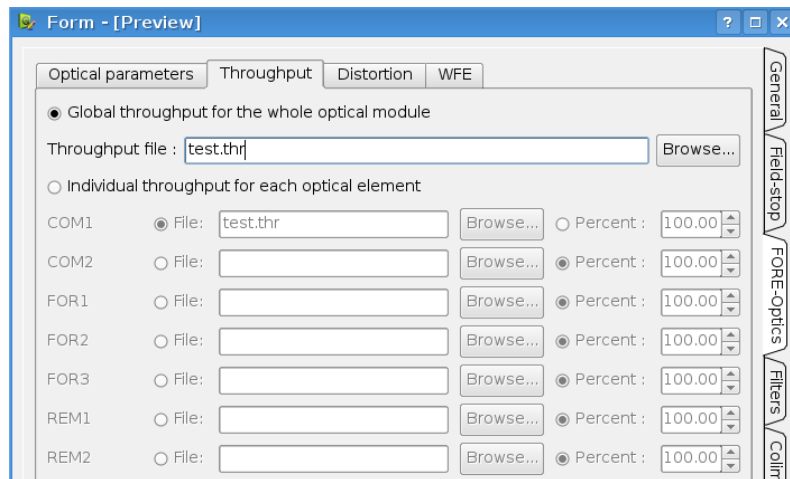


Fig. 3: Example of graphical interface for an optical module showing the four classical tabs for the optical parameters, the throughput, the distortion and the WFE

During step #2, ZEMAX macros are used to process the input ZEMAX file associated with an IPS model. Unfortunately, the ZEMAX COTS software can only be used under the Windows operating system while the IPS software is developed for a Linux environment. The problem of the communication between the two operating systems was solved by using the QEMU/Windows XP operating system and shared directories (SAMBA-based sharing) where input and output files for the specific ZEMAX macro are stored.

The step #3 consists mainly in retrieving the output files from step #2 (using the shared directories between the Linux and QEMU/Windows XP operating systems) and processing them into data suitable for the next steps of the simulations.

During this step #4, we take the opportunity to pre-compute as many elements as possible in order to minimize the time needed later on to perform a simulation. At the core of this step #4 we will therefore find the pre-computation of a library of PSF and of the radiometric response of the system.

At this stage, the IPS model is ready and can be used by standard and expert users to generate simulated exposures.

2.5. Coordinate transforms

A component of the IPS software simulates the distortion. Distortion corresponds to the departure from an equivalent ideal optical (paraxial) system. In NIRSpec, an analysis of the design distortion map has shown that it is possible to parameterize the distortion using a fifth degree 2D polynomial. This should be enough at this stage if coordinate transforms were achromatic. This is unfortunately not the case in some parts of NIRSpec (e.g. between the OTE image plane and the plane of the MSA due to the presence of the filters). The analysis has shown that using linearly wavelength dependant coefficients for the 2D polynomial was enough to describe the distortion. So, the distortion computation, using the coordinate transform ZEMAX files, consists in two successive fits: first the output image points are fitted as a function of space. The result is a bi-dimensional polynomial for each wavelength. Then these points are fitted as a function of the wavelength. The same operation is done for the reverse distortion, i.e. when going from the output plane to the input plane.

Figure Fig. 4 shows the IPS tool able to display the distortion map in a convenient way. On the left side, the distortion map displays the position of the point (in the plane of the MSA) both as computed for an equivalent paraxial system and as computed using the fit. On the right, the residual map displays the position of the points both as listed in the input file and as computed by the fit. This way, what appears on the screen is really an indicator of the quality of the fit. Note that most of the time the residuals are so small that they are barely visible.

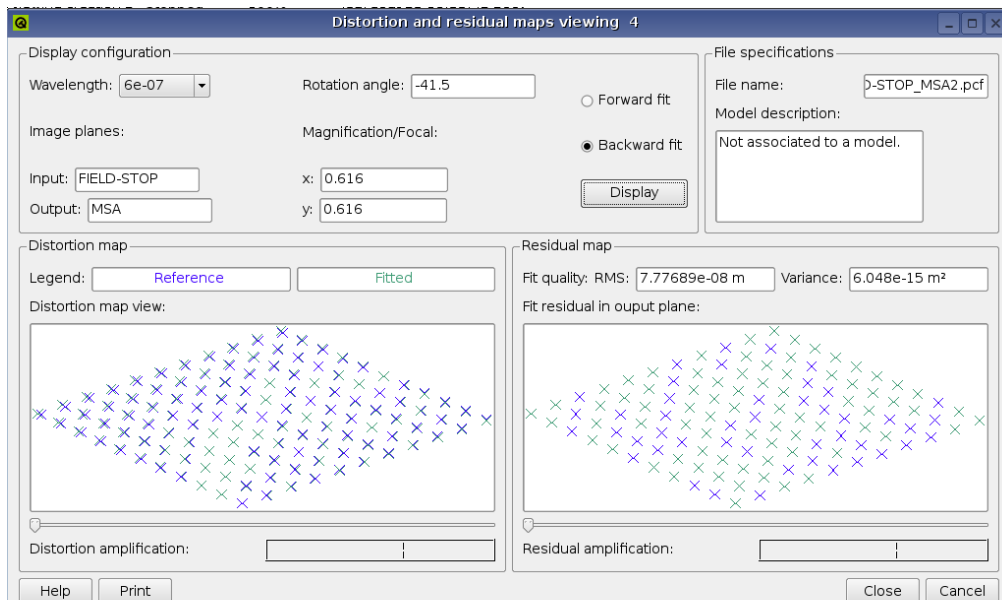


Fig. 4 : Snapshot of the distortion and residual maps viewing window.

The coordinate transforms will be used to model the position of an object in various planes of the NIRSpec instrument. The plots of the grids and the various field points in the grating wheel and the detector planes are shown in figure Fig. 5.

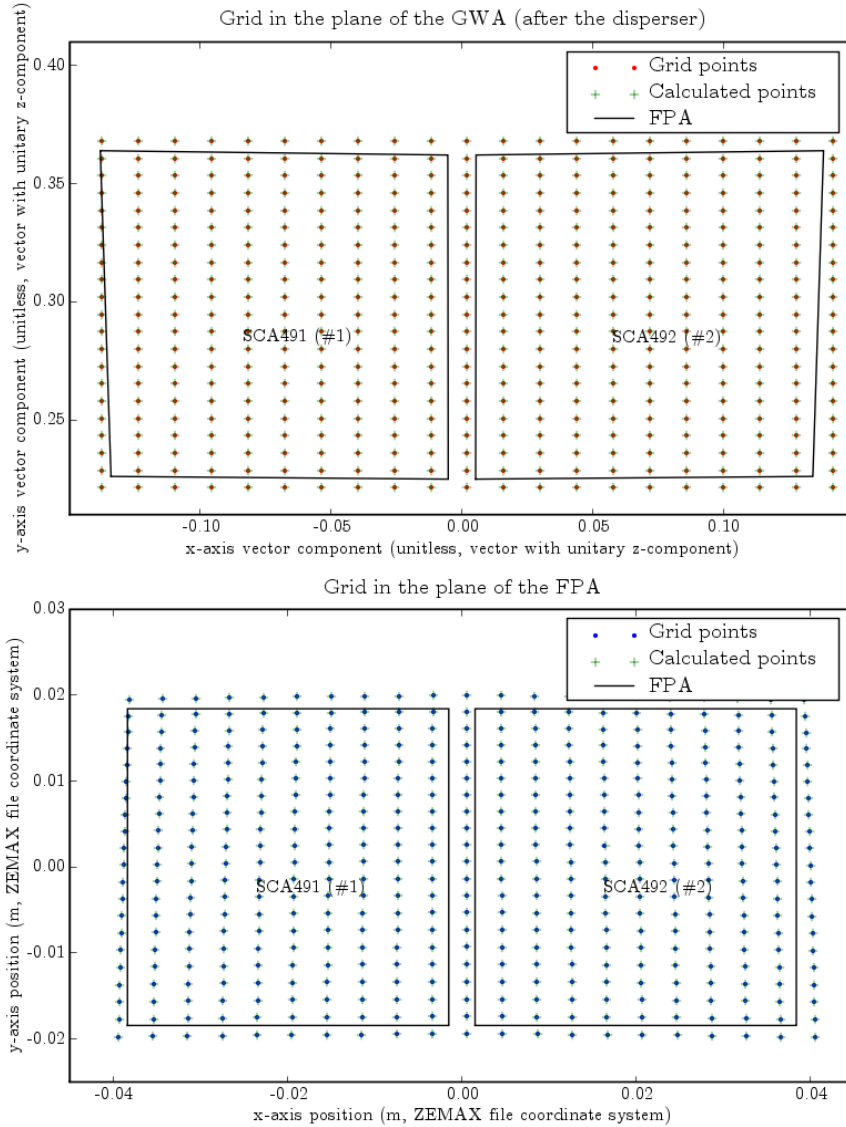


Fig. 5: Plot of the grids and FPA geometry in the plane of the GWA (after the disperser) and of the FPA.

2.6. Electron rate maps computation

Using an instrument model and a source file (which may in fact contain a collection of sources), the user can generate the associated electron rate maps. This step of the simulation is at the heart of the modeling of the instrument and it uses the PSF library, the modeled instrument response and the coordinate transforms to compute the electron rates for each pixel of the two SCAs.

The pre-computed database of PSF contains PSF of each “optical modules” suitable for conventional Fourier optics (i.e. straddled by conjugate planes) for given wavelengths between 0.6 and 5 μm . For example, in MOS mode, we have considered 3 optical modules: from the plane of the sky to the plane of the MSA (i.e. including the OTE and NIRSpc fore-optics); from the plane of the MSA to the plane of the dispersers (i.e. the collimator); and from the plane of the dispersers to the plane of FPA.

In a typical PSF calculation, we take the Fourier transform of the input complex amplitude (wavefront in the object plane) with scaling factors corresponding to the parameters of the optical module. The resulting complex amplitude (corresponding to the illumination in a pupil plane) is then multiplied by intensity and phase masks to account for the effects of diffraction (truncation of the beam by the intensity mask) and optical aberrations (phase mask that will introduce the wave-front errors of the optics). Last, we take the inverse Fourier transform of this truncated and distorted complex amplitude to compute the complex amplitude in the image plane 44.

In the case of coherent point's sources, the input complex amplitude must be propagated through the complex system. This coherent Fourier formalism based approach is repeated from image to pupil and from pupil to image plane along the optical train to compute the PSFs.

For non-coherent sources, non-coherent propagation will be used. In this case the intensity in the object plane will be used (we are not talking anymore of complex amplitude) and the corresponding intensity in the image plane will be computed by applying the relevant scaling factors and by convolving it with the PSF of the optical module. This is used for the simulation of extended sources 4.

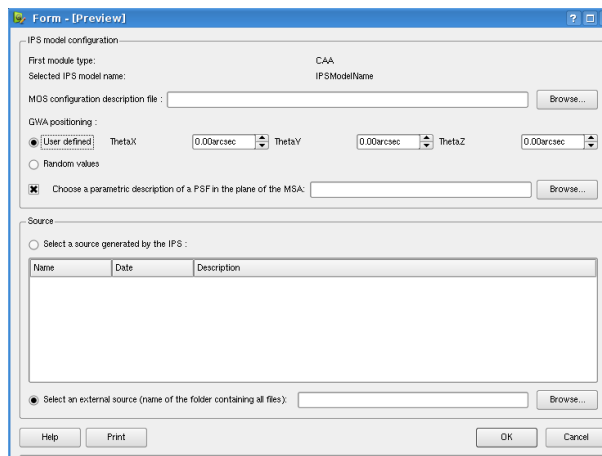


Fig. 6 : Screenshot of the electron rate map generation window (MOS mode).

2.7. Detector exposure simulations

2.7.1. Exposure computation overview

The NIRSpec detector is made of two Single Chip Arrays (SCA), each SCA being made of an array of 2048×2048 pixels. Note that all the pixels located in the four first and last rows and columns are reference pixels and are not sensitive to light.

The detector exposure simulations are generated from a map of the photon rates per pixel, for all the detector pixels of the two SCA, constructed or not by the IPS software.

We emphasize that these electron rates do include all “photon-generated” electrons, i.e. coming from light incident on the detectors, these electron rates do not include the dark current, the computation of these electron rates does take into account any intra-pixel sensitivity effect and does not take into account inter-pixel cross-talk.

The organization of an exposure with multiple integrations starts with a series of resets. Then a sequence of groups is obtained and each group is the average of separated frames. The key element to keep in mind during the construction of a NIRSpec exposure is that each frame is not independent of the previous ones. Each frame has therefore to be constructed using the previous frame as a starting point and by adding only the amount of electrons accumulated in the meantime (and the associated noise).

2.7.2. Exposure time computation

When computing the accumulated number of electrons for a pixel during a readout, one important parameter is the time elapsed since reset for this given pixel. This time is computed by adding readout and reset times.

The readout time is the time needed to read all the pixels including the overscanned ones. In full-frame mode (i.e. a complete SCA is read), four readout sequences are performed simultaneously using four different outputs, each of them spanning 512 rows and 2048 columns. In addition to this full-frame mode, the detector can also be read in a sub-array mode. This mode allows the user to define his own window format.

The reset time is the time needed to reset all the pixels depending on their position and the chosen reset mode. The default reset mode is the pixel-to-pixel reset mode, in which all pixels of a given output are reset individually and sequentially. The second reset mode is a row-by-row reset mode in which all the pixels in a given column are reset simultaneously and the columns are reset sequentially. The last reset mode corresponds to a full-frame reset in which all the detector pixels of a given output are reset simultaneously.

When a reset is performed, a common offset is applied to all the detector pixels. These random fluctuations of the offset are described by a Gaussian distribution with a sigma (in electrons) that will depend on the output.

2.7.3. Detector effects

The first step of the procedure is to compute the total electron rates for each detector pixel by adding the electron rate associated to the dark current (obtained from dark current maps provided on input to the program).

In order to simulate the inter-pixel cross-talk, a convolution is applied to the input electron rate maps. We will assume that the same convolution kernel is valid for all detector pixels.

When computing the accumulated charge for a pixel, it is necessary to take into account the non-linearity of the detector. This effect is represented by a function of the 2nd order, of the nominal electron rate and the number of accumulated electrons. When the number of accumulated electron is high it is necessary to introduce an asymptotic behavior.

Most of the detector pixels exhibiting anomalous behaviors can be classified into dead or hot pixels. The number of ADUs of these pixels will be set either to 0 (dead pixels) or to the saturation value (hot pixels) just after creating the frame (just after readout).

For the simulation of in-orbit exposures, it is also necessary to include a simulation of the impact of the cosmic rays on the exposures.

The detector exposure computation parameters in IPS are shown in figure Fig. 7, which represents screenshots of the Graphical User Interface (GUI) software.

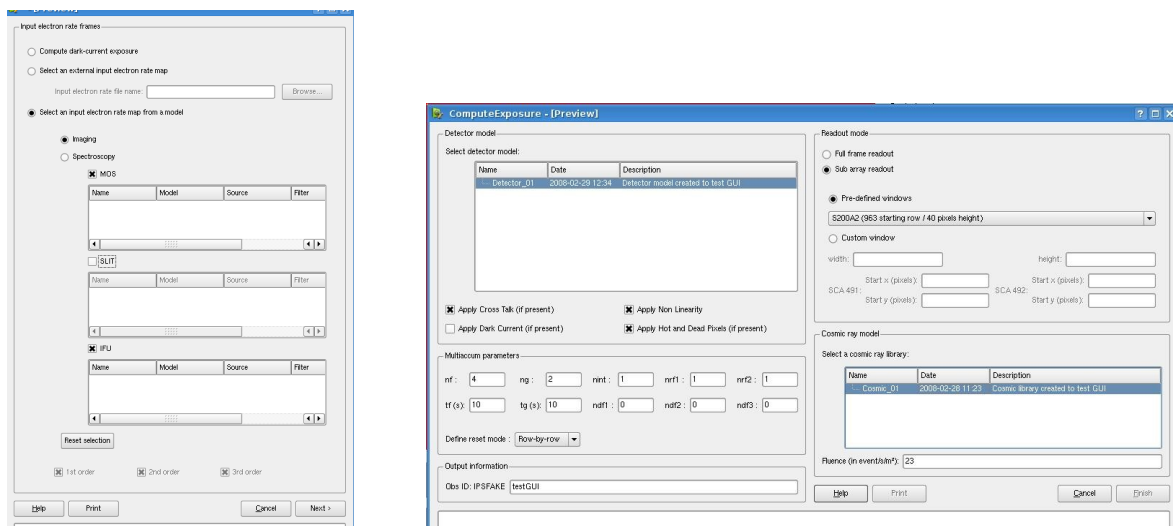


Fig. 7: GUI of detector exposure computation

3. EXAMPLES OF PRELIMINARY RESULTS

The first version of the IPS software, labeled IPS-1, has been developed specifically for the simulation of the development model (DM) of the NIRSpec instrument, in the test setup that will be used during the associated calibration and characterization campaign. The NIRSpec DM is optically representative up to the plane of the micro-shutter array (MSA) where the detector will be installed. In this configuration, the instrument is an imaging device.

The figures below are the result in log scale of a simulation with the IPS-1 software. The detector model used for this exposure computation reflects the expected performances of the engineering grade DM detectors. In particular, the simulation uses measured dark current rates. Effects like inter-pixel cross-talk, non-linearity, hot and dead pixels, dark current and cosmic rays are accounted for.

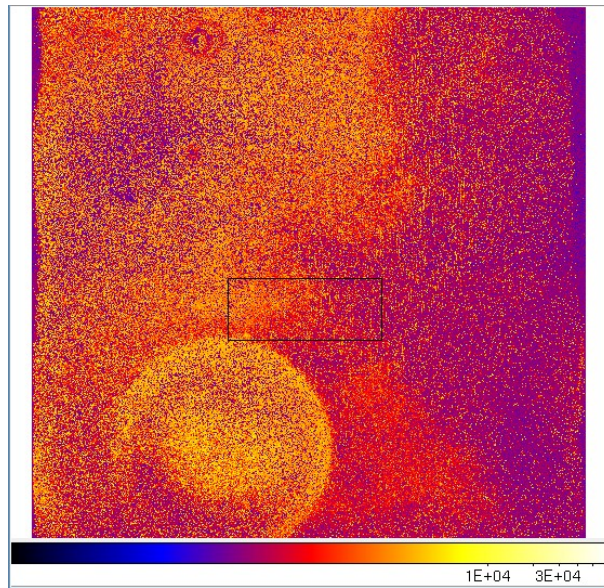


Fig. 8: Exposure simulation with DM detector (SCA491).

The figures Fig. 9 and Fig. 10 represent a zoom of the area in the previous exposure where two pinholes are located. The first map corresponds to the input, noiseless electron rate map (in log scale, peak electron rate of 100 electron per second and per pixel), while the second corresponds to the same area in the last frame of a simulated exposure. Note the extremely strong contribution of the dark current due to the fact that engineering grade detectors with degraded performances are used.

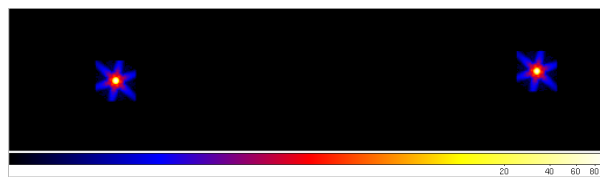


Fig. 9 : Zoom on pinholes in the electron rate map.

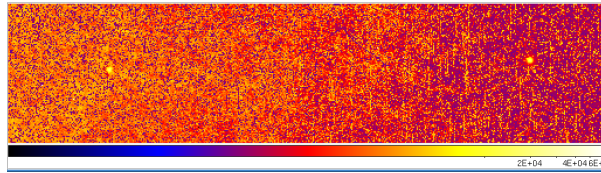


Fig. 10: Zoom on pinholes in the DM detector.

The version 2 of the IPS software, which will allow simulating the complete NIRSpec instrument in all its spectrographic configurations, is currently being developed (see next section). Although we not yet have simulation of spectra available, we show below an example of how the modeling of the coordinate transforms in the instrument can be used to compute the location of the spectra in the plane of the detectors.

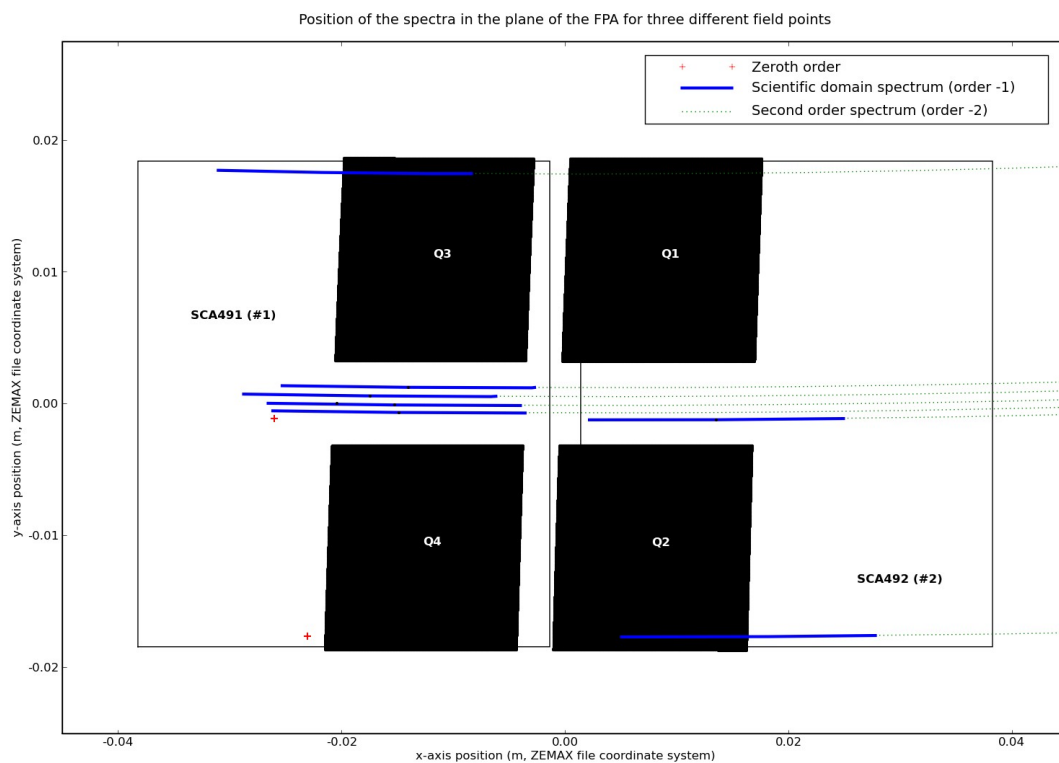


Figure 11: Plot showing the location of the a selection of spectra in the plane of the detectors, overlaid on the monochromatic projection of the MSA sub-arrays (Q1 to Q4).

The simulation has been performed using the design characteristics of the instrument in its so-called medium-resolution band-I configuration covering the 1.0-1.8 μm domain at a spectral resolution of approximately 1000. In this figure, several important elements are displayed:

- the geometry of the two 2048 \times 2048 detector arrays (labeled SCA 491 and SCA 492),
- the monochromatic image of the micro-shutter sub-arrays (labeled Q1 to Q4) through the NIRSpec spectrograph and in the detector plane,

- the location of the 0th, -1st and -2nd orders of spectra corresponding to two opposite corners of the NIRSpec field of view (bottom and top spectra),
- the location of the 0th, -1st and -2nd orders of spectra of the 5 NIRSpec slits (central spectra)

Note the presence of various different distortion effects that are responsible for the slight bending of the spectra or the important shear present in the images of the MSA sub-arrays.

4. SOFTWARE STATUS

The first version of the IPS software, labeled IPS-1, has been delivered to ASD in fall 2007. It has recently been updated to include a more accurate and complete modeling of the behavior of the detectors. It has been delivered with a database containing a dedicated model of the NIRSpec DM detectors. The models included in the IPS-1 database are being used by Astrium for the verification of the NIRSpec quick-look, calibration and analysis software [7].

The second version of the IPS software, labelled IPS-2, is dedicated to the modeling of the NIRSpec Flight Model Design. The software detailed design phase closed in February 2008 with successful critical design review (CDR). The IPS-2 software is now in its coding and testing phase and will be delivered to ASD toward the end of 2008. The detector and coordinate transform modules have been coded and tested, the Fourier optics module has been coded and is actually being tested, and the next step will be the implementation of the electron rate computation. Preliminary results with simulations of on-ground calibration exposures will be available before the summer break.

The last version of the IPS software will be labeled IPS-3 and will correspond to the as-built instrument. It will be delivered to ASD and ESA a few months after the end of the cryogenic tests of the instrument.

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