PDRs4all: NIRSpec simulation of integral field unit spectroscopy of the Orion Bar photodissociation region

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ABSTRACT

The James Webb Space Telescope (JWST) was launched on December 25 2021. This document presents a simulation of the Near Infrared Spectrograph (NIRSpec) observations of the Orion Bar which will be performed as part of the Early Release Sciences (ERS) program “PDRs4all”. The methodology to produce this data relies on the use of a direct forward model of the instrument applied to a synthetic scene of the Orion Bar, coupled to format matching in order to deliver data in JWST-pipeline data format. The resulting 3D cube for one order is provided publicly, and is compatible with tools developed by the STScI (e.g. Cubeviz) and with the science enabling products developed by the PDRs4all team. This cube can be used as a template observation for proposers who would like to apply for NIRSpec observations of extended sources with JWST.

1. INTRODUCTION

The James Webb Space Telescope (Gardner et al. 2006, JWST) is a space telescope developed jointly by NASA, European Space Agency (ESA) and Canadian Space Agency (CSA). This telescope, launched on December 25, 2021, has four main scientific focuses: “The End of the Dark Ages: First Light and Reionization”; “The Assembly of Galaxies”; “The Birth of Stars and Protoplanetary Systems”; and “Planetary Systems and the Origins of Life”. Thirteen Early Release Science (ERS) programs have been selected to demonstrate the scientific capabilities of JWST, to provide public data to the community, to educate and inform the community regarding JWST’s capabilities. This paper is part of this effort in the context of the ERS program “PDRs4all: Radiative feedback from massive stars”1 (ID1288) which focuses on observations of the Orion Nebula (Berné et al. 2022). This 40-hour program will make use of three instruments aboard JWST, and will dedicate about 12.71 hours to spectroscopy of the Orion Bar with the Near Infrared Spectrograph (NIRSpec, Bagnasco et al. 2007). The NIRSpec instrument (Bagnasco et al. 2007) is one of the four JWST instruments. There are four observing modes of NIRSpec and we are specifically interested in the imaging spectroscopy with the Integral Field Unit (IFU)3. The IFU mode has 9 disperser-filter combinations that span a total wavelength range of 0.6μm to 5.3μm, and provide three levels of resolving power4. As part of the PDRs4all ERS project, 6 NIRSpec observations are planned with 3 disperser-filter combinations covering wavelengths between 0.97μm and 5.27μm with a nominal resolving power of 2,700. Each exposure will have one integration and each integration will consist of 5 groups with 4 dithers giving a total integration time of 257.68s. The footprints of these NIRSpec observations post-process the pipeline output and to test the ecosystem of analysis tools developed for JWST data2. The paper is organised as follows: Section 2 gives an overview of the NIRSpec instrument. In Section 3, we present how we simulate the NIRSpec image following Guilloteau et al. (2020), and make it compatible with the NIRSpec output pipeline format.

2. NIRSPEC SPECTROSCOPY OF THE ORION BAR

The Near Infrared Spectrograph (NIRSpec, Bagnasco et al. 2007) is one of the four JWST instruments. There are four observing modes of NIRSpec and we are specifically interested in the imaging spectroscopy with the Integral Field Unit (IFU)3. The IFU mode has 9 disperser-filter combinations that span a total wavelength range of 0.6μm to 5.3μm, and provide three levels of resolving power4. As part of the PDRs4all ERS project, 6 NIRSpec observations are planned with 3 disperser-filter combinations covering wavelengths between 0.97μm and 5.27μm with a nominal resolving power of 2,700. Each exposure will have one integration and each integration will consist of 5 groups with 4 dithers giving a total integration time of 257.68s. The footprints of these NIRSpec observations

1 http://pdrs4all.org
2 https://jwst-docs.stsci.edu/jwst-post-pipeline-data-analysis
3 For more information: https://jwst-docs.stsci.edu/jwst-near-infrared-spectrograph
4 More information on IFU mode: https://jwst-docs.stsci.edu/jwst-near-infrared-spectrograph/nirspec-observing-modes/nirspec-ifu-spectroscopy
Canin et al.

Figure 1. NIRSpec field of view for the PDRs4all project as specified in the ERS 1288 APT file, with HST-WFC3 (Kimble et al. 2008) with the F656N filter (6.56\(\mu\)m) image of the Orion star forming region in background. Blue regions: NIRSpec footprints corresponding to planned observations. Red cross: position of the target at the coordinates R.A. = 5:35:20.4749, dec. = -5:25:10.45.

Figure 2. Zoom-in on the NIRSpec field of view from Fig. 1. Blue: NIRSpec footprints corresponding to planned observations. Black: field of view of the simulation. Green: adopted field of view for the NIRSpec simulated cube.

as specified in the Astronomer’s Proposal Tool (APT\textsuperscript{5}) positioned over the Orion Bar are shown in Fig. 1.

3. SIMULATION

3.1. Motivation and strategy

Creating NIRSpec simulations is useful to test JWST analysis tools developed by the PDRs4all team (Berné et al. 2022) or by other teams including those of the STScI (e.g. Cubeviz, Jones et al. 2019). These simulations are also useful to obtain an idea of the quality (in terms of SNR) and richness of the data for a given integration time, ahead of observations. However, performing such simulations is challenging. There exists an instrument simulator (Piquéras et al. 2010), however simulating a full 3D NIRSpec cube (i.e. two spatial dimensions and one spectral dimension) with realistic spatial and spectral textures using this tool is very computationally intensive. As part of a project to develop algorithms to perform data-fusion between NIRSpec and NIRCam, these authors have created a forward mathematical model of the NIRSpec instrument. They applied this forward model to a 3 dimensional input synthetic scene of the Orion Bar to create realistic NIRSpec simulations over the 1\(\mu\)m to 2.35\(\mu\)m wavelength range. As part of the PDRs4all project, a larger wavelength range is expected to be observed (0.97\(\mu\)m to 5.2\(\mu\)m) with NIRSpec. In addition, Guilloteau et al. (2020) did not implement any tools to write out the cubes in the JWST pipeline format. In this paper, we present how we have extended the method of Guilloteau et al. (2020). To obtain a NIRSpec IFU simulated cube, we apply the direct model of Guilloteau et al. (2020) on the Orion Bar synthetic scene including the 0.97\(\mu\)m to 5.2\(\mu\)m range, and from this simulation we extract a cube with precisely the properties of the JWST-NIRSpec pipeline. We thus produce a realistic simulated IFU NIRSpec cube in the stage 3 format of the JWST-NIRSpec pipeline.

3.2. Choice of region to be simulated

Fig. 1 presents an overview of the footprints of the NIRSpec IFU observations planned in September 2022 on the Orion Bar as part of PDRs4all. They span a cut across the Orion Bar, performed with a mosaic strategy (see Berné et al. 2022). Fig. 2 is a zoomed-in version of Fig 1 which includes additional information on the fields of view of the simulations. The black square shows the region over which we apply the direct model of Guilloteau et al. (2020) to the synthetic scene of the Orion Bar presented by the same authors. The green square in Fig. 2 corresponds to the field of view we adopted in the simulation of this paper. It is a 3 \(\times\) 3\(\prime\) square (corresponding to NIRSpec IFU) centered on coordinates R.A. = 5:35:20.2570, dec. = -5:25:04.612. The orientation angle is \(\frac{5}{2}\pi\) rad. It overlaps with the planned mosaic, however we have centered it on one of the Proplys, simply to help for coordinate calibration. We have only simulated one dither and one pointing. However, in principle, the method presented in this paper could be extended to simulate mosaics.

3.3. Direct model of NIRSpec

\textsuperscript{5} https://jwst-docs.stsci.edu/jwst-astronomers-proposal-tool-overview
3.3.1. General principles of the model

We follow and complement the formalism and notations of Guilloteau et al. (2020) to describe the forward mathematical model of NIRSpec that we will use. We use a synthetic scene of the Orion Bar $C_1$, which is a 3D cube sized $(12032 \times 300 \times 300)$, where 12032 is the number of spatial elements, and 300 $\times$ 300 the number of spatial elements. To compute this cube we define $X$, which is a vectorized version of $C_1$, sized $(12032 \times 90000)$, and computed with the matrix product:

$$X = HA,$$

where $H$ is a matrix of elementary spectra sized $(12032 \times 4)$ and $A$ is a matrix with the weight of the spectra spatially sized $(4 \times 90000)$. $Y_h$, the hyperspectral NIRSpec image of size $(12032 \times 8649)$, is simulated using:

$$\bar{Y}_h = L_h \mathcal{H}(X)S + N,$$

where $L_h$ is the NIRSpec throughput in a diagonal matrix, $\mathcal{H}(\cdot)$ is a spatial convolution with the JWST and NIRSpec point spread functions, which depends on wavelength and $S$ is a downsampling operator corresponding to the spatial sampling of the NIRSpec instrument and $N$ is the simulated noise (see details in Guilloteau et al. 2020). $Y_h$ is then reshaped in a $(12032 \times 93 \times 93)$ 3D cube, $C_s$. Finally, $C_s$ is cropped to the spatial dimensions of NIRSpec simulation, i.e. $(12032 \times 30 \times 30)$ to obtain the final NIRSpec simulated cube $C_f$. For each filter set, one cube $C_f$ is obtained, $C_{G140H/F100LP}$, $C_{G235H/F170LP}$ and $C_{G395H/F290LP}$.

3.3.2. Contents of model matrices

**Matrices A, S, N** — These matrices are computed in the same fashion as in Guilloteau et al. (2020).

**Matrix H** — This matrix contains the 4 elementary spectra which have been created as part of the PDRs4all project. The initial version of these 4 spectra was presented in Guilloteau et al. (2020), however an updated version of these spectra is described in Berné et al. (2022). Here we use the former version of $H$. The total wavelength range is 0.7$\mu$m $-$ 5.2$\mu$m for 12032 spectral points.

**Matrix L_h** — This matrix is a diagonal matrix where the diagonal corresponds to the throughput of NIRSpec. Pandea (Pontoppidan et al. 2016), a Python package developed at STScI, is used. These package calculates the throughputs of the four JWST instruments. For NIRSpec, several inputs are needed: the mode, the disperser, the filter, the readout pattern, the number of integration and the number of groups. All this information is available in the ERS APT proposal (ID 1288, ‘PDRs4all’). Pandea also needs the wavelengths table on which to calculate the throughputs. In our case, the mode is IFU, the readout pattern is nrsrapid, there is 1 integration and 5 groups. The observations are planned with the following disperser-filter combinations: $G140H/F100LP$, $G235H/F170LP$ and $G395H/F290LP$. So, 3 different curves are obtained depending on the dispersers/filters. These curves correspond to the diagonal of the matrix, so there are 3 matrices. The code to calculate these throughputs is presented in Listing A.1. Fig. 7 presents the curves obtained for each disperser-filter combination and only for those used in the ERS program.

**Operator $\mathcal{H}(\cdot)$** — The operator $\mathcal{H}(\cdot)$ is a convolution with point spread functions (PSFs), stored in a matrix we call $G$. $G$ has 4 dimensions and stores the fast Fourier transform (fft) of the NIRSpec PSFs. The two first dimensions are the spatial dimensions of the PSF. The third dimension is the spectral dimension and the last one is for the real part and the imaginary part of the NIRSpec PSF fft.

First, we calculate the NIRSpec PSF with weebpsf (Perrin et al. 2014), a Python package from the STScI. This package allows to calculate the PSF of NIRSpec for each spectral point. Then, the fft of the PSFs cubes are calculated and saved in fits files. They are assembled to form one unique cube with all the wavelengths in the matrix $G$. The code to calculate the PSF with weebpsf is presented in Listing A.2. Fig. 3 shows two examples of NIRSpec PSF obtained after the fft.

3.3.3. Format matching

Here we consider the case of the G140H/F100LP filter. We create a file in the stage 3 format of the pipeline, i.e. an _s3d file in fits format. This file includes data and metadata. The data is comprised of several extensions. Extension 1 is the primary data, we use $C_{G140H/F100LP}$. 

**Figure 3.** Real part of the NIRSpec fft PSF at 0.99$\mu$m and 2.38$\mu$m.
cube interpolated on the spectral grid of the NIRSpec simulated cube for filter G140H/F100LP provided by the STScI. Extension 2 is the error, here we use an error of 10% of G^{G140H/F100LP}. Extension 3 is the data quality array coded on 32 bits. For instance, 0 means that there are no problems with the pixel while a value of 513 (2^9 + 2^9) corresponds to a bad pixel (2^10) outside the science area of detector (2^9). Here we use a cube with dimensions of C^{G140H/F100LP} with all elements set to 0 corresponding to good pixels only, since the simulation does not contain bad pixels or pixels with issues.

The metadata is composed of two fits headers, a primary header and a header for extension 1 of the data (primary image). We create these headers by making a copy of the header provided by STScI for NIRSpec IFU simulated observations. The primary header contains the information related to the program such as the name of the mission, program, PI, etc. This header is common to all instruments, we replace the relevant information with that from the header created for our ERS program using the pipeline for NIRCam simulations (Canin et al. 2021). In addition, information related to the target and the exposure is replaced manually using the information found in the APT proposal. In the image header, the information relative to the WCS parameters is replaced manually with the coordinates (CRVAL1, CRVAL2) = (83.8343959, −5.4179437) at the reference point (CRPIX1, CRPIX2) = (15, 15). An extract of the image header is presented in Fig. 8.

The file corresponding to this simulation can be downloaded at (Canin et al. 2022). The same approach allows to compute the NIRSpec IFU files for the other filter sets (i.e. G235H/F170LP and G395H/F290LP), provided one has the template format for these filters, which is not the case at the time we publish this document.

Figure 5. Spectra extracted from the Cf NIRSpec simulated cubes, corresponding to filters G140H/F100LP, G235H/F170LP and G395H/F290LP.

Figure 6. Image taken from the final NIRSpec simulated cube Cf at 2.12µm. The green region corresponds to the one on which the spectra in Fig. 5 were calculated.

4. RESULTS

Fig. 4 presents the contents of the Cs cube for two wavelengths, 0.97µm and 2.87µm. Fig. 5 presents the spectra of the three Cf cubes extracted in the green circle region in Fig. 6 which presents an image of the final simulated cube Cf, at 2.12µm. This cube can be downloaded at this link.
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NIRSpec IFU data set at https://www.stsci.edu/jwst/science-planning/proposal-planning-toolbox/simulated-data

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6 NIRSpec IFU data set at https://www.stsci.edu/jwst/science-planning/proposal-planning-toolbox/simulated-data
APPENDIX

A. LISTINGS

A.1. Command to calculate the throughputs

```python
obsmode = {'instrument': 'nirspec', 'mode': 'ifu', 'disperser': 'g140h', 'filter': 'f100lp'}

detector = {'readout_pattern': 'nrsrapid', 'nint': 1, 'ngroup': 5}

conf = {'instrument': obsmode, 'detector': detector}
i = pandeia.engine.instrument_factory.InstrumentFactory(config=conf)
pce = i.get_total_eff(tabwave)
```

A.2. Command to calculate the NIRSpec PSF

```python
nrs = webbpsf.NIRSpec()
nrs.image_mask = None # No MSA for IFU mode
wl = tabwave[start:end] # Cropped cube
cube = nrs.calc_datacube(wavelengths=wl, fov_pixels=fov_pixels)
```

B. FIGURES

**Figure 7.** a. All the NIRSpec throughputs depending of the disperser-filter combination; b. The NIRSpec throughputs of the disperser-filters used in the ERS.
Figure 8. Extract from the image header of the final NIRSpec simulated cube $C_T$. 

```
PDRs4all: JWST NIRSpec simulation

XTENSION = 'IMAGE' / Image extension
BITPIX = -64 / array data type
NAXIS = 3 / number of array dimensions
NAXIS1 = 30
NAXIS2 = 30
NAXIS3 = 3945
PCOUNT = 0 / number of parameters
GCOUNT = 1 / number of groups
EXTNAME = 'SCI' / extension name
SPEC_TYPE = 'EXTENDED' / Source type used for calibration
BUNIT = 'MJy/sr' / physical units of the array values

Photometry information
PHOTMJD = 2454517026.1522 / Flux density (MJy/steradian) producing 1 cps
PHOTUJ = 1 / Flux density (uJy/arcsec2) producing 1 cps
PIXAR Jr = 2.35840007004737E-13 / Nominal pixel area in steradians
PIXAR Jr = 0.0100000002908233 / Nominal pixel area in arcsec^2

Information about the coordinates in the file
RADESYS = 'J2K' / Name of the coordinate reference frame

WCS parameters
WCSAXES = 3 / number of World Coordinate System axes
CRPIX1 = 15 / axis 1 coordinate of the reference pixel
CRPIX2 = 15 / axis 2 coordinate of the reference pixel
CRPIX3 = 1.0 / axis 3 coordinate of the reference pixel
CRVAL1 = 0.83343959 / first axis value at the reference pixel
CRVAL2 = 0.01419457 / second axis value at the reference pixel
CRVAL3 = 0.9665214562468713 / third axis value at the reference pixel
CTYPE1 = 'RA---TAN' / first axis coordinate type
CTYPE2 = 'DEC---TAN' / second axis coordinate type
CTYPE3 = 'WCSC' / third axis coordinate type
CUNIT1 = 'deg' / first axis units
CUNIT2 = 'deg' / second axis units
CUNIT3 = 'arcsec' / third axis units
CDDL = 2.77777777777777E-05 / first axis increment per pixel
CDDEL2 = 2.77777777777777E-05 / second axis increment per pixel
CDDEL3 = 2.00000000000000E-06 / third axis increment per pixel
PC1_1 = 0.9404007750381200 / Linear transformation matrix element
PC1_2 = 0.1736401776669308 / Linear transformation matrix element
PC1_3 = 0 / Linear transformation matrix element
PC2_1 = 0.1736401776669308 / Linear transformation matrix element
PC2_2 = 0.9404007750381200 / Linear transformation matrix element
PC2_3 = 0 / Linear transformation matrix element
PC3_1 = 0 / Linear transformation matrix element
PC3_2 = 0 / Linear transformation matrix element
PC3_3 = 1 / Linear transformation matrix element
```