METIS Science Simulation during FDR

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History

v0.1 orginal draft 4.Feb.2020
v0.2 include comments by DSP: Wolfram Freudling, Lodovico Coccato, and Valentin Ivanov,
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1. Introduction

This document provides a list of METIS Science Simulation that needs to be achieved during the FDR phase of the project. The document has the focus on the science needs. We refer to ESO-044156 and do not discuss specifications of the technical and engineering issues such as compliances to DICD standards, DFS keywords, use of data product standards, data format, and restrictions in the pipeline developments.

The overall deliverable specifications of the dataflow for ESO observatories are specified in ESO-03761. In Sect. 4.6 of that document the ESO needs for simulated instrument data are detailed. Specifics of such needs for METIS are described in the Statement of Work for the Construction of METIS (ESO-257874). The specification for the METIS Science simulations during the FDR phase can be summarised as follows:

- There shall be at least one simulation data set for each observation strategy (instrument mode). The simulated raw data shall match the instrument design and the expected properties of the observations as they are specified at FDR.

- For each instrument mode, one such science case shall be simulated. The data format of every intermediate product and final science reduced data product shall be demonstrated.

- The simulated raw data shall match the instrument design and the expected properties of the observations as they are specified at the FDR. In particular both the raw and products shall have realistic noise properties and include the most important systematic errors caused by instrumental features (artefacts).

- The DFS shall be tested with simulated data using as reference the ETC specifications and design as they are available at FDR.

Following the above the Consortium and ESO agreed during the Consortium meeting #10, held in Feb. 2020 at ESO, that the METIS simulated data have to satisfy two areas:

A. Performance demonstrator: Presentation of a science case to demonstrate the ultimate performance of METIS. Example: a simulation whether METIS can detect an Earth-like planet around eps-Eridani. This simulation is important to demonstrate the excellent scientific performance of METIS. However, it might require thousands of images and it is not expected to provide the entire set of raw data for this case. Instead, a careful run of the METIS instrument simulator, resulting in a final image that presents this METIS Science Case is sufficient.
B. Use cases for a representative science observation, e.g. of a moderately bright source. Here, all aspects of the observation should be considered, incl. target acquisition, AO control look, instrument configuration, filter settings, slit configurations, derotator and ADC settings, as well as chopping/nodding or dithering strategies. Similarly, the calibration observations for that particular observations need to be specified, and the resulting raw data frames need to be simulated. Those

raw data will be used to (i) assess the realistic implementation of an observation and the associated wall-clock time (i.e., overheads), and (ii) provide the representative dataset, which is to be run through the data pipeline.

The Top-Level Requirements for ELT-MIDIR (ESO-204695) provides a list of Science Cases. The advances in mid infrared astronomy in general and of the METIS project during its PDR phase resulted in a comprehensive description of updated METIS science cases (ESO-331117). We take this update and present in the Section 2 and subsections a science case for each instrument observing mode that is suggested for detailed simulation in either of both areas A and B. Whenever during the development, a different science case appears that seems more attractive or timely than the one proposed here it can be taken as a replacement. Such a change requires mutual agreement between the Consortium and ESO's Project Scientist.

We also provide in Section 3 some suggestions for strategic improvements and additions of the science simulator that shall strengthen the validity of the FDR science case simulation. For this we summarize the development plan of the METIS science simulator (simMETIS) and discuss necessary improvements for the FDR version of it. This includes a realistic noise modelling where estimates of the various systematic noise components are treated as well as a modelling of the METIS adopted observing strategy (chopping and nodding) for the raw data. Unfortunately, during PDR there was no data simulator available for long-slit spectroscopy so that this missing-part of simMETIS appears most pressing during the upgrade. This FDR version of simMETIS shall be applied when simulating the science cases of Section 2. For each science case we add a simulation of standard star observation that can be taken to simulate PSF subtraction or telluric corrections. Simulating the observation of a star seems most trivial and therefore we recommend that they will cover area B ("Use Case") of the simulated data delivery.

2. Science Simulation

We present science cases suited for data simulation using simMETIS for each observing mode. METIS observing modes are presented in the operational concept description (ESO-331092) and are shown in the Table 2-1 below. In total 10 instrument modes are defined at PDR for METIS. Please, note that band Q will likely no longer be offered.

Table 2-1: METIS instrument modes

Science Observing Mode	Instrument Configuration						Code
	Sub-Syst.	Band	IFS Setting	HCI Mask	PT	FT	
Direct Imaging	IMG	L,M	N/A	N/A	•	•	IMG_LM
	IMG	N,Q	N/A	N/A	•	•	IMG_NQ
High Contrast Imaging	IMG	L,M	N/A	RAVC/CVC	•		IMG_LM_(RA/C)VC
			N/A	APP	•		IMG_LM_APP
			N/A	CLC	•		IMG_LM_CLC
	IMG	N	N/A	CVC	•		IMG_N_CVC
			N/A	CLC	•		IMG_N_CLC
Longslit spectroscopy	IMG	L,M	N/A	N/A		•	SPEC_LM
	IMG	N	N/A	N/A		•	SPEC_N_LOW
IFU spectroscopy	LMS	L,M	full IFU field	N/A	•	•	IFU_nominal
	LMS	L,M	spectral IFU Δλ~300nm	N/A	•	•	IFU_extended
IFU+HCI spectroscopy	LMS	L,M	full IFU field	APP	•		IFU_nominal_APP
				RAVC/CVC	•		IFU_nominal_(RA/C)VC
				CLC	•		IFU_nominal_CLC
	LMS	L,M	spectral IFU Δλ~300nm	APP	•		IFU_extended_APP
				RAVC/CVC	•		IFU_extended_(RA/C)VC
				CLC	•		IFU_extended_CLC

1 Direct L, M, N band imaging

As performance demonstrator of the direct imaging observing mode, we continue modelling the proto-planetary disks and planet formation science case. The scientific rationale, the input model, and the predicted METIS image is presented in the METIS science cases document at PDR (ESO-331117) and shown here in Fig.1. The disk structure is computed by a hydrodynamical code assuming a 1 Jupiter mass planet separated by 40 AU form the star. The planet opens a gap and the spiral structure.

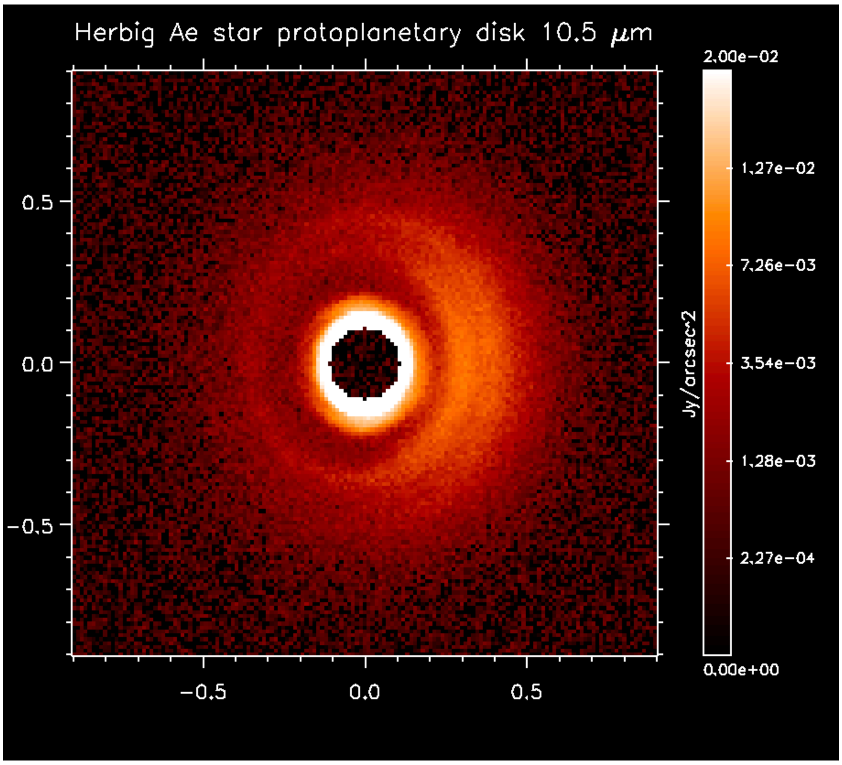

Figure **Error! No sequence specified.**: *N band METIS simulated observation of a Herbig star protoplanetary disk at a distance of 140pc. Axis units are arcseconds.*

Update the METIS PDR simulations with the improved instrument simulator outlined in Sect. 3 Repeat the simulation choosing a broad band L, M, and N band filter for a 1h chopping and nodding observing sequence. Repeat the same set-up of the simulation using a standard star. Repeat the simulations changing the size of the source shown in Fig. 1 (3 times and 0.5 times) to test the capabilities of the sky-background removal for extended objects.

2 High contrast extended source imaging

As performance demonstrator of the high contrast imaging on an extended source, we continue modelling the debris disk and exozodiacal light science case. The scientific rationale, the input model, and the predicted METIS image is presented in the METIS science cases document at PDR (ESO-331117) and shown here in Fig.2.

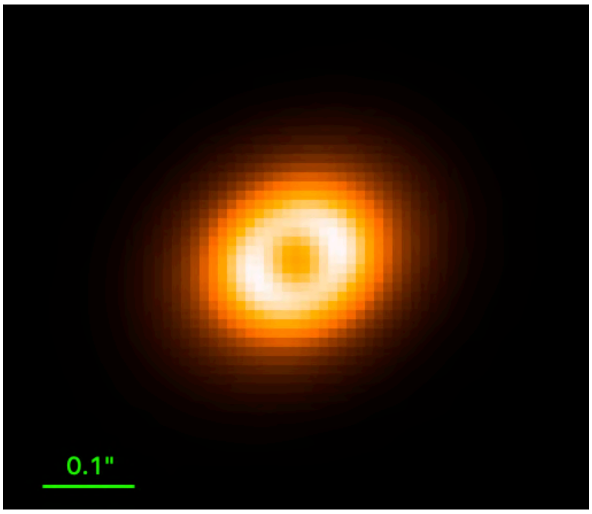

Figure 2:N band METIS simulated image of the debris disk of eta CrV.

Update the METIS PDR simulations with the improved instrument simulator outlined in Sect. 3 Repeat the simulation choosing a broad band M and N band filter for a 1h chopping and nodding observing sequence. Adopt in the simulation the different coronagraphic masks and for three different observing conditions. Repeat the same set-up of the simulation using a standard star. Likely in the M band a source extension will not be detected.

3 High contrast point source imaging

As performance demonstrator of the high contrast imaging on a companion, we continue modelling the potential planet in the habitable zone of αCen. The scientific rationale, the input model, and the predicted METIS image is presented in the METIS science cases document at PDR (ESO-331117) and shown here in Fig.2.

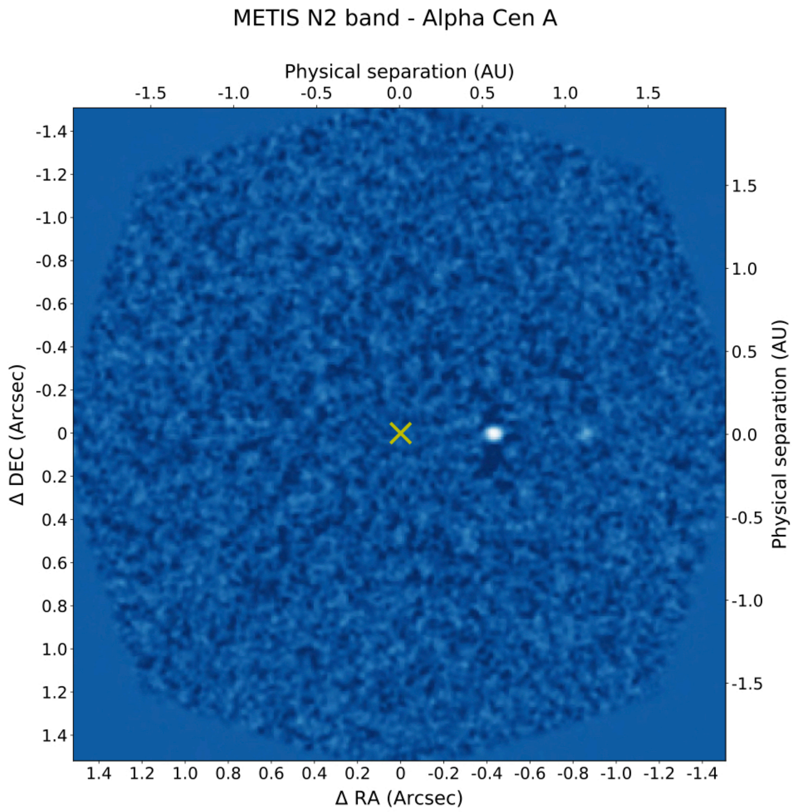

Figure 3:N2 band METIS simulated image of the Earth-like planets at 0.55 and 1.1 AU of αCen.

Update the METIS PDR simulations with the improved instrument simulator outlined in Sect. 3 Repeat the simulation choosing the N2 band filter for a 10h chopping and nodding observing sequence. It would be worth comparing the simulation for the L band. At that wavelength the scattering light of the Earth like planet needs to be added to its thermal emission.

Adopt in the simulation the best suited coronagraphic mask and the observing condition flagged as “good”. Repeat the same set-up of the simulation using a standard star. Take particular care in modeling the background, centering, and other striking systematic errors (e.g. Sect.3). For testing the computing capacities at the DFS of ESO it would be useful that the full set of raw data, this is area B “Use Case” of Sect. 1, will be delivered to ESO.
It would be worth comparing the simulation for the L band. At that wavelength the scattering light of the Earth like planet needs to be added to its thermal emission.

4 Long-slit L,M band spectroscopy

As performance demonstrator of the Long-slit L, M band spectroscopy

I suggest taking the CRIRES data of 8P/Tuttle. The scientific rationale, the CRIRES data is presented in the METIS science cases document at PDR (ESO-331117) and shown here in Fig.4. Unfortunately, at PDR simMETIS was not ready for this mode. Therefore, when simMETIS is able to do end-to-end FDR simulation one shall consider taking a different input data set/model.

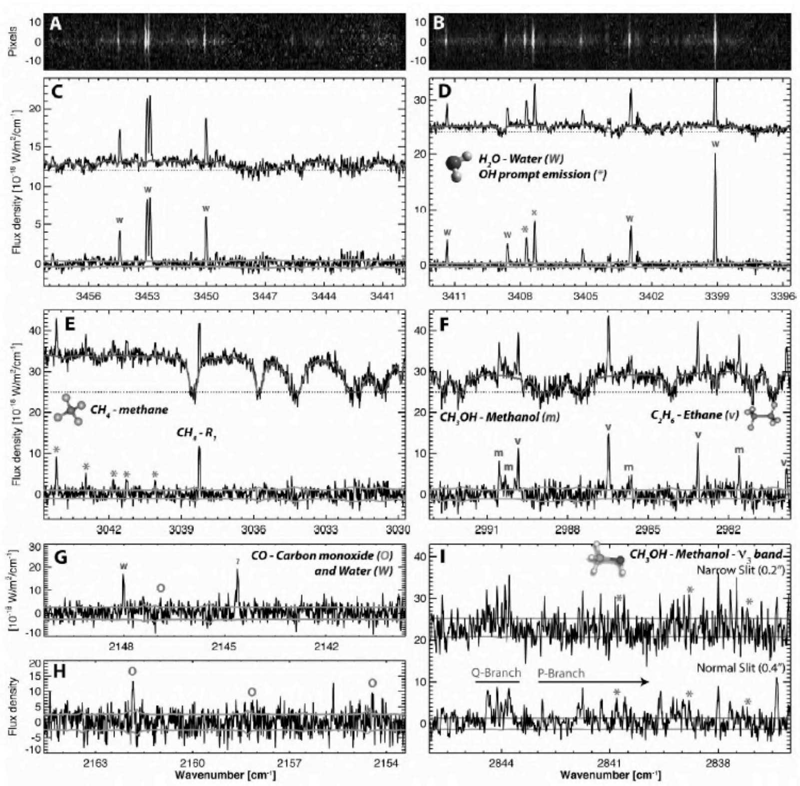

Figure 4: CRIRSE spectra of 8P/Tuttle. Upper panel 2D spectrum followed by 1d spectra in the annotated bands.

Perform a METIS simulation using the instrument simulator outlined in Sect. 3 for the long-slit L,M band mode. Do this for the science target and a reference star that is observed at slightly different airmass and ambient condition than adopted for the science simulation. This will allow testing the impact of residual telluric corrections using the standard approach which is dividing the science by the telluric. METIS is also investigating the performance applying a telluric correction in the L, M band by atmospheric models. Both methods of telluric corrections shall be applied to the science observations and the residuals compared.

5 N band spectroscopy

As performance demonstrator of the N band (low resolution) spectroscopy
One may use the Spitzer spectrum of 3C249.1 demonstrating the silicate emission band. The scientific rationale and the data (see Fig. 5) and model is presented by Siebenmorgen et al. (2004). Unfortunately, at PDR simMETIS was not ready for this mode.

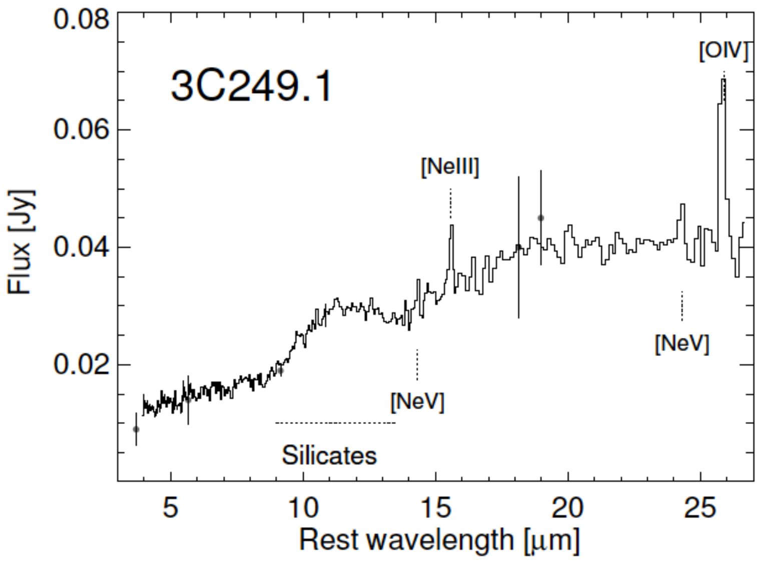

Figure 5: Spitzer spectrum of 3C249.1

Perform METIS simulations using the instrument simulator outlined in Sect. 3 for the low-resolution N band. Do this for the science target and a reference star that is observed at slightly different airmass and ambient condition than adopted for the science simulation. This will allow testing the impact of residual telluric corrections using the standard approach which is dividing the science by the telluric. METIS is also investigating the performance applying a telluric correction in the N band by atmospheric models. However, at present such an approach which seems to work well at shorter wavelengths shows limited success in the N band.

6 IFU spectroscopy

As performance demonstrator of the IFU, we continue modelling the imprint of Jupiter mass planets planet in disks of Herbig Ae/Be stars. The scientific rationale, the input model, and the predicted METIS image is presented in the METIS science cases document at PDR (ESO-331117) and shown here in Fig.6.
The simulation already considered a static PSF of the segmented mirror.

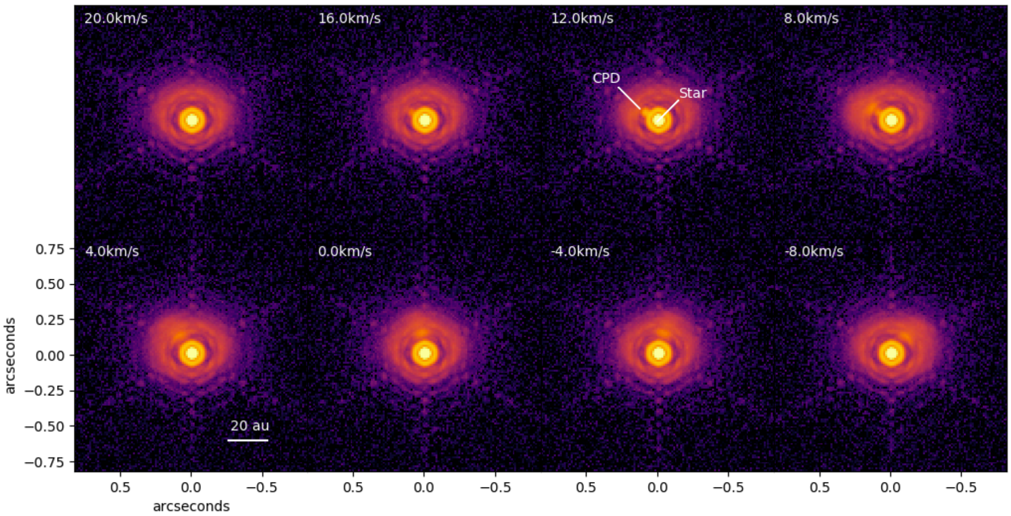

Figure 6: METIS simulated IFU 4.7μm channel map of the CO v (1-0) band in the HD100546 disk.

Update the METIS PDR simulations with the improved instrument simulator outlined in Sect. 3 Repeat the simulation with the same observing parameters as done during PDR. Pay attention if the circumplanetary disks remains detectable when considering the time variation of the segmented PSF. Repeat the same set-up of the simulation using a standard star.

7 High contrast IFU spectroscopy

As performance demonstrator of the high contrast IFU spectroscopy we continue modelling the detection and characterisation of an Earth like planet around Proxima b. The scientific rationale, the input model, and the predicted METIS image is presented in the METIS science cases document at PDR (ESO-331117) and shown here in Fig.7.

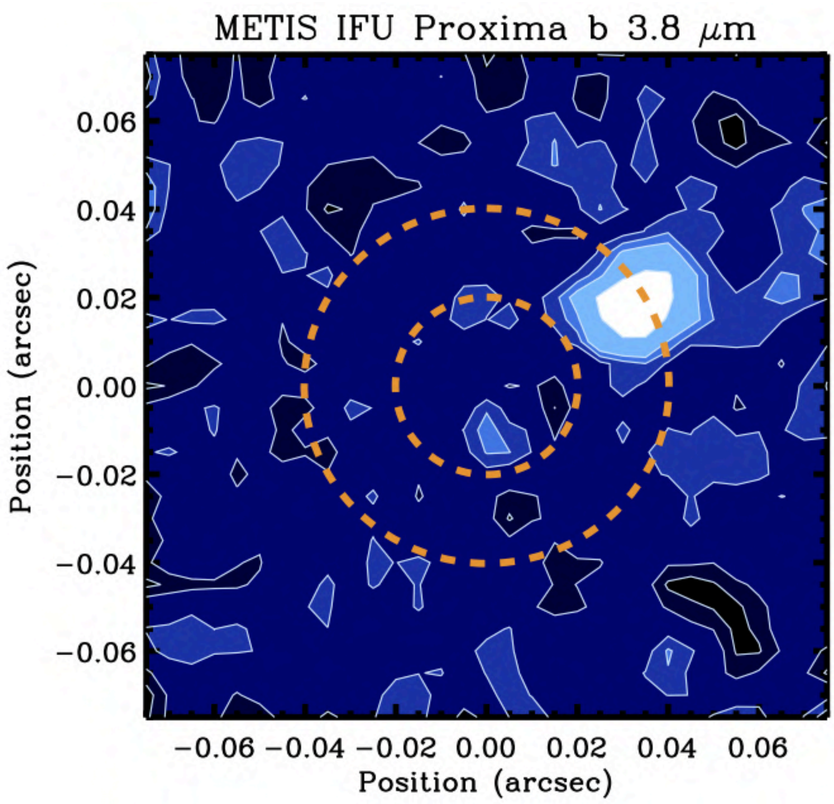

Figure 7: METIS simulated IFU 3.8 μm high contrast image of an Earth like planet in the Proxima b system.

Update the METIS PDR simulations with the improved instrument simulator outlined in Sect. 3 Repeat the simulation with the same observing parameters as done during PDR. Test the outcome of the simulation applying different coronagraphs. Test the impact of imperfect centering of the star behind the mask. Repeat the same set-up of the simulation using a standard star. For testing the computing capacities at the DFS of ESO it would be useful that the full set of raw 3D data cube for this 10h observation, this is area B "Use Case" of Sect. 1, will be delivered to ESO.

8 High contrast IFU extended mode spectroscopy

The combination of high contrast and high resolution IFU spectroscopy with extended mode coverage is outlined in the METIS science cases document at PDR (ESO-331117). It is applied to simulate a hot Jupiter τ Bootis b. In Fig.8 we show the simulation of the cross-correlation signal between model and planet spectrum as presented at PDR. The method has been tested on real data using CRIRES (Snellen et al. 2014).

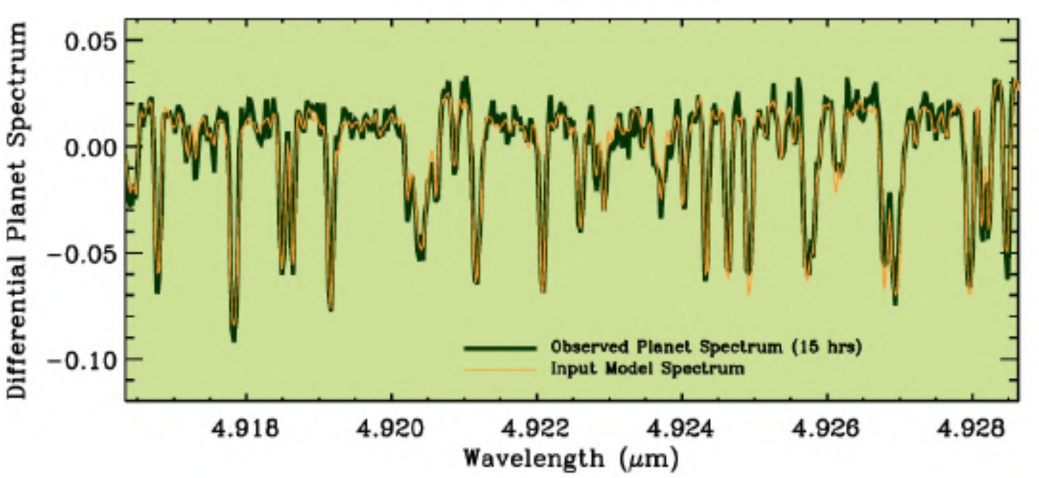

Figure 8: METIS simulated high contrast IFU extended mode observations of the hot Jupiter τ Bootis b. The figure compares the planet and model input spectra in the 4.7 – 5 µm region is shown.

Update the METIS PDR simulations with the improved instrument simulator outlined in Sect. 3 Repeat the simulation with the same observing parameters as done during PDR.

3. Instrument data simulator

3.1 SimMETIS status

The METIS instrument data simulator of the PDR release is called SimMETIS v0.2 and is described in ESO-331078. During PDR the focus was set on simulating images with correct detector counts and realistic statistical noise properties, useful for scientists to judge the expected capabilities of METIS. The simulator includes functionality to simulate the spectrophotometry of the L and M band high-resolution integral field spectrograph (LMS). So far, the simulator supports only two observing modes: direct imaging and IFU spectroscopy. Systematic errors and instrumental artefacts were not included but are required to be implemented during FDR as outlined in Section 1. For IFU spectroscopy the geometry of the spectral layout on the detectors was ignored, so that only perfectly rectified spectral data cubes were computed.

3.2 SimMETIS developments

The development plan presented by the Consortium at PDR (ESO-331078) stated that during SimMETIS will be upgraded to include:

a. Emissivity of the entrance window and warm elements of the telescope pupil.
b. Detector noise features and cosmetics.
c. Support L, M and N band low resolution spectroscopy.
d. Distortion and spectral curvatures for L, M and N slit and IFU spectroscopy.
e. For long-slit spectroscopy frames including atmospheric dispersion by the fixed ADC.
f. Time resolved PSF computations for high contrast imaging.
g. Production raw data.

During Consortium Meeting 10 the DFS work package stated that in addition for SimMETIS:

a. The development plan for PSF reconstruction is accepted.
b. Enhanced detector specific background subtraction schemes will be implemented.
c. A flat fielding procedure, persistence, and error propagation of the detector noise model will be implemented.
d. LSS order layout and in particular the time variability of that layout will be implemented.

3 Systematic errors

There are known and expected systematic errors while, observing with the combined observing system: the METIS instrument, the ELT, and the ambient atmosphere. Ignoring these systematic effects will result in false claims and wrong predictions of the achievable performance of METIS science observations. Following the definition of the DFS development most of these degrading effects were ignored in the data simulator at PDR During FDR it is required for all ELT instrument to include and to the extent possible the major limitations in science observations that are caused by systematic effects (Section 1). For some cases there are model predictions of the systematic errors while for others some best guess of a non-zero systematic noise component need to be added so that the data simulator becomes more realistic. This procedure is also followed by the ELT first light instruments MICADO and HARMONY and will be followed by METIS. Below we provide a list of some of the most striking systematic errors that are known from experience with the VLT instrumentation or form the lessons learnt by other observatories:

Atmosphere:

Consider variations of atmosphere (good, medium, bad conditions).
In particular for spectroscopy:

i. Telluric corrections: estimate the achievable spectral fidelity and the usefulness of atmospheric models.
ii. Consider errors, uncertainties and (time) instabilities of the wavelength solution/calibration.
iii. Consider time variations of the sky conditions (both continuum and lines) between different nodded/chopped exposures.

Telescope:

i. Background corrections: Include estimates of the variations of non-uniform background of the ELT while applying chopping and nodding.
ii. Estimate residuals of background subtraction while chopping/nodding is performed on a non-uniform sky (crowded fields).
iii. Include temporal variations of the PSF (typical scale for VISIR is ~100msec).
iv. Consider PSFs of different qualities as delivered by the telescope. This includes PSFs resulting from observations with significant changes in the seeing and/or AO performance during the observation.
v. Include telescope alignment in the simulations as source of systematic error.

Detectors:

i. Cross talk correction by coupling matrix as done for SPHERE.
ii. Non-linearity correction, conversion of ADU to e-.
iii. Persistence (likely not applicable to GeoSnapp).
iv. Bad pixels (hot/dead), channel crossing (which resulted in detector ghosts when using the Aquarius).
v. Read out noise and detector gain, bias, dark variations.
vi. Add pattern noise, e.g., odd-even column effect, which is quite common for NIR and MIR detectors.

Distortions

i. Insert results of ray tracing to establish a distortion matrix
ii. Test 2d image reconstruction schemes of a 3d IFU data cube by including wavelength dependent scattering effects for oversampled spaxels.

iii. Predict image quality losses of the IFU e.g. elongations of PSF observed by MUSE. For example insert best guess estimates derived by ray-tracing.

Ghosts:

Include treatment of optical ghosts (predictions of ghost may be derived by ray-tracing).

Filter

Include transmission profiles and variations of shifts that might be caused by filter tilts (possibly such effects are small for METIS). If the beam is not parallel, filter transmission variation may be important.

ADC

i. Include uncertainties in the atmospheric dispersion model.
ii. Provide estimates introduced by using the static ADC used by METIS.

WCU

i. Include wavelength shifts effects caused by the different light path of the arc lines of the Warm Calibration Unit and the science target.

High contrast imaging:

a. Apply different ADI techniques and verify results by inserting spurious planets into the raw data. Starting point of inseeting an ADI technique could be http://laurent.mugnier.free.fr/publis/Mugnier-JOSAA-09.pdf or others.)

b. Test procedure of the achievable contrast versus theoretical predicted contrast: Insert fake point sources (“planets”) at different brightness and separation from the star (already presented at PDR).

c. Include effects of non-common path aberrations (NCPA).

d. Treatment of speckles in the high contrast imaging case.

e. Include imperfect centering of the coronagraphic masks. For estimating the amplitude and time variations of the jitter while centering the source on the coronagraph one may inspect the NERA data.

f. Include intra-pixel sensitivity variations: This might be important for the direct imaging science case of exo-planet as done by e.g. Sakar et al. (2020, https://arxiv.org/abs/2002.03739).

g.
   i. Low wind effect (“Mickey Mouse” observed by SPHERE, Milli et al 2018)
   ii. Wind driven halo (“Butterfly effect”)
   iii. Wind vibrations, as studied for Subaru telescope, Lozi et al., arXiv:1809.08296

3.4 Essential FDR data simulations

For the data simulation of the science cases presented at FDR the following is considered to be essential:

- SimMETIS will be upgraded following the development plan presented at PDR and including the proposed upgrades at CM10 as listed in the previous section.

- SimMETIS instrument parameters and noise model will be updated to reflect the FDR design and error budget (noise model) of the instrument.

- SimMETIS will consider a realistic representation of the ELT PSF considering significant time variations of the PSF.

- SimMETIS will simulate raw data including the chopping and nodding observing concept.

- SimMETIS will include step-by-step a more realistic description of systematic errors for which some of them are listed in Section 3.3.

- SimMETIS will be able to provide all the needed RAW files to test the pipeline performances (e.g., BIAS, FLATS, RAW SCIENCE), in particular with respect to background subtraction, telluric correction, and wavelength calibration (for point-like or extended objects, and for faint or bright sources).