TOAD: a numerical model for the 4MOST instrument

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ABSTRACT

TOAD, the "Top Of the Atmosphere to Detector" simulator, is a primary engineering tool that accompanies the development of the 4MOST instrument. The ultimate goal is to provide a detailed, end-to-end performance model of 4MOST by providing the detector image for an artificial target field with less then 5% error. TOAD will be able to create a realistic output for any reasonable input. The input can be anything, from point sources through extended sources, calibration lamps or stray-light, entering the system at virtually any point in a optical path. During the development of the 4MOST facility, the TOAD simulator will give invaluable insight into the interaction of various parts of the instrument and the impact of engineering design decisions on the system performance.

Keywords: TOAD, 4MOST, VISTA, numerical model, performance model, instrument simulation

1. INTRODUCTION

4MOST is a wide-field, high-multiplex spectroscopic survey facility under development for the VISTA telescope of the European Southern Observatory (ESO). Its main science drivers are in the fields of galactic archeology, highenergy physics, galaxy evolution and cosmology. 4MOST will in particular provide the spectroscopic complements to the large area surveys coming from space missions like Gaia, eROSITA and Euclid, and from ground-based facilities like VISTA, VST, DES, LSST and SKA. 4MOST features a 2.5 degree diameter field-of-view with ≈ 2400 fibres in the focal plane that are configured by a fibre positioner based on the tilting spine principle. The fibres feed two types of spectrographs; ≈ 1600 fibres go to two spectrographs with resolution R > 5000and ≈ 800 fibres to a spectrograph with R > 18000. Both types of spectrographs are fixed-configuration, threechannel spectrographs. 4MOST will have an unique operations concept in which 5 year public surveys from both the consortium and the ESO community will be combined and observed in parallel during each exposure, resulting in more than 25 million spectra of targets spread over a large fraction of the southern sky.

The **T**op of the **A**tmosphere to **D**etector (TOAD) instrument¹ simulator is a software, designed to provide detailed simulation of the 4MOST instrument, including the atmosphere. In this paper, we describe the inner structure of TOAD, as well as the requirements and restrictions that have lead to this approach. The simulator is far from being finished, but all the ground work is already available, details of what has been done and what is missing are described in the text below. The next section, Section 2 gives an overview over the motivation of developing TOAD, as well as the decisions made, based on the requirements and restrictions. Section 3 contains a description of the inner data representation of TOAD, which is key to understand how the individual physical parts of the optical paths can be simulated by channeling the data through the modules, described in Section 4. The Paper finishes with some outlook and acknowledgements, in Section 5

2. REQUIREMENTS AND DESIGN

During the development of the 4MOST instrument, a tool for systems engineering² is required, that can simulate the impact of design decisions on the behaviour of the instrument. For example the impact of the positioner accuracy, design of the calibration unit, optical performance of the atmospheric dispersion corrector, fibre length, spine tilt and many more. TOAD is the tool that can provide this functionality. Especially the combination of many different decisions can lead to unexpected results, which is why a simulation including all optical relevant

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properties of the instrument needs to be simulated. Additional to being a systems engineering tool, TOAD shall provide simulated detector images for early versions of the data reduction pipelines/data management system³ and it shall provide throughput curves that can be used by the throughput simulator.

The primary output of TOAD will be simulated detector images and any other information gathered within the simulated light path. The design goal is, that TOAD shall produce detector images with a target light per pixel illumination accuracy of 5%, measured in the real instrument for example with flat fields and other calibration targets. How we will test the achievement of the goal in detail is not decided yet.

There are also budget restrictions on TOAD that influence its design. Most noticeably, roughly 0.5 FTE per year until commissioning of the instrument are assigned for the development of the source code of TOAD. Additionally, other workpackages within 4MOST need to dedicate a small amount of resources to provide TOAD with information that are necessary to build the simulation. For example the spectrograph teams provide TOAD with PSF information generated with ZEMAX that are part of the model of the spectrographs within TOAD, see Section 4.6. An other example are the parameters and convolution functions, which are needed to model the fibres within TOAD.

As a consequence of the tight budgets, TOAD can not be arbitrarily complex. For example, TOAD can not be designed to be a ray-tracer due to its inherent complexity. Instead, TOAD is simulating the distribution of light on fixed locations within the optical train described in the next section. Also, it should run on a normal desktop computer system because developing source code for a distributed system like a computer cluster is too time consuming at this stage. TOAD should be able to adapt to the ongoing development of the 4MOST instrument, which means it should be possible to reflect alternative instrument designs. This flexibility is ensured by developing TOAD in a highly modular way, presented in Section 4.

There are no initial restrictions on the programming language or host operating system for TOAD. But given the restrictions above, especially the limited amount of labour, we settled with python on a Linux operation system. With the ability to use C-subroutines if necessary, python provides the required development flexibility that is needed for the development of TOAD. The source code will become open-source shortly after commissioning of 4MOST at which point a final release is issued.

3. TARGET LIGHT REPRESENTATION

TOAD is designed to simulate all light paths of the 4MOST instrument. In this paper, only the science light path is discussed but other light paths work in the same fashion. The science light path is simulated, considering one target at a time. The end product is a detector image in FITS format which can accumulate many targets that are added sequentially. Since a ray-tracing approach is too complex, the light is modelled as an intensity distribution on a plane (called light plane) that is perpendicular to the optical axis of the light path (see Subsection 3.1). This approach also puts certain restrictions on the effects that can be modelled with the simulator (discussed in Subsection 3.3).

TOAD is organised in modules (discussed in Section 4) with identical input and output data interfaces. The only exception is the interface between the spectrograph- and detector module where the expected photon values are converted into an array of pixels that cover the images of all fibres of one spectrograph. A light plane is passed through the modules and is altered by each module according to their optical effects. This design is very flexible, any module is easily exchangeable and it is easy to insert a light plane at any point in the light path.

3.1 Light Plane

A light plane can be seen as a cross section at a particular location in a light path, oriented perpendicular to the local light ray direction. For example at the focal surface of the telescope, at the surface of a optical fibre or in a plane right in front of the telescope. The data object it self consists of 3 principal elements, a spatial 2-dimensional distribution of light S, an angular 2-dimensional distribution of light A and the spectral representation of the light P. The spectrum is represented as a 1-dimensional array, where each resolution element is of arbitrary width, the represented spectral interval is not allowed to have any gaps.

The two 2-dimensional distributions S and A are represented as 2-dimensional arrays with square resolution elements. The scale of the elements change by passing through the modules, according to the optical properties



Figure 1. TOAD example light plane. Top left: spatial distribution of light. Top right: angular distribution of light. Bottom: spectrum, expressed in photons per resolution element length. The color sequence within the spatial distribution represents the wavelength dependent spatial offset vectors as indicated in the spectrum. This particular offset vectors and spectra have no particular meaning, their values are for demonstration purposes only.

of the modules, but the number of resolution elements remains constant. The light distributions S and A are modelled as proper probability distributions, which means, they individually integrate to 1. The value, stored in one resolution element s_{ij} of S represents the probability to find a photon in that area. Likewise, the value, stored in a resolution element a_{ij} of A represents the probability to find a photon in the solid angle, represented by a_{ij} . If for example a vignetting effect is introduced that changes the spatial distribution S, the lost light is reflected by reducing the number of photons in the spectrum P and the spatial distribution S is rescaled to become a probability distribution again.

For this to make sense, a resolution element p_i in the spectrum P must represent the expected number of photons within p_i . Being an expectation number means p_i can represent a floating point number of expected photons. To allow for spectral regions of interest or for a spectrum with constant resolution everywhere, the resolution elements of the spectrum P can have arbitrary length. The borders of the resolution elements are stored in a separate list with |P| + 1 elements.

Each spectral resolution element is accompanied with two further 2-dimensional offset vectors that can provide a flat offset to the spatial and angular light distribution. With these offset vectors, it is possible to model wavelength dependent location and angular offsets as long as they do not change the distribution of light. If necessary, a affine transformations instead of just location offsets can be defined, which would create more flexibility with wavelength dependent effects on S and A. Also currently, no polarization effects can be modelled with the given light plane model. It would be easy to add linear polarization, circular polarization would be more difficult but still possible.



Figure 2. The TOAD module structure. Orange boxes show data source modules; blue boxes indicate modules that take the light plane at the input and generates an output; yellow boxes are data sinks, which means they store the result to the hard drive or generate an image but have no exit within TOAD. Greyed out boxes indicate, that these modules are not implemented yet but might be implemented later.

See Figure 1 for an example light plane. This particular collection of images visualizes a light plane at the entrance surface of a fibre for a point source with 1.1 arc sec seeing and 8mm tilt of the fibre (see Section 4.4). The spectrum is a test spectrum without special meaning and the offset vectors visualized within the spatial distribution is generated artificially to visualize the concept. In this example, no offset vectors are associated with the angular distribution, which is why they are constant at (0,0).

3.2 Light Path Stacking

E.Schmalzl et al.⁴ used different colour modes for their instrument simulator: single spectra mode, multiple spectra mode and data cube mode. Within TOAD, we use something similar, but do not utilize different modes within the program it self. Any light path can be utilized with an arbitrary set of light planes $L = \{l_1, \ldots, l_n\}$. The light planes in L are completely independent, they might or might not overlap spectrally, they can be from the same target but also from different targets. At the end of a light path, at the level of the detector, the light of all light planes in L are summed up constructively.

With this method, it is possible to model different spectral sections of the same target. This is also useful to simulate the influence of the sky light independently of target light or to simulate the contribution of several targets that couple light into the same fibre in crowded fields. It is even possible to use one light plane for each spectral resolution element, forming a data cube at the cost of a lot of computation time. At this point it should be noted, that the computation time depends largely on the resolution of the spatial and angular distributions S and A, but almost not on the spectral resolution P for one light plane.

3.3 Assumptions and Limitations of the Approach

One major assumption with this way of simulating the light path is that spatial and angular distribution are independent. That assumption is valid only for small regions of the field of view of the telescope, which is why TOAD can only simulate one target at a time but not the entire field of view of the telescope at once. For a small region on the focal surface of the telescope, the angular distribution of light is identical for all points within that small region. At the same time, it can be assumed that the spatial light distribution is identical for a very narrow solid angle within a collimated section of the beam. So therefore, either the angular distribution must cover only a very narrow solid angle or the spatial distribution must be very localized. This restricts the effects, that can be modelled with the system. For example, it is only possible to introduce vignetting effects on focal surfaces and in collimated sections of the light beam, but not in arbitrary locations.

The simulator takes advantage of external software tools like ZEMAX to model the (localized) optical properties of parts of the instrument and to fill gaps where its own capabilities are limited. For example, the PSF, introduced by the atmosphere, telescope and wide field corrector can be regarded as constant near a specific location in the focal surface of the telescope and a narrow wavelength range. Likewise, the PSF of a spectrograph can be regarded as being constant for a narrow wavelength interval and a specific location at the slit. In such situations, the spatial distribution of light can be convolved with the PSF in order to account for effects, calculated using ZEMAX but unavailable for TOAD directly.

4. MODULES

The principle structure of the TOADs modules is visualized in Figure 2, the science light path is indicated as black arrows. Other modules (grey boxes) and light paths (grey paths) might be implemented later if needed. In the target generator, a light plane with all relevant information is created. Then, it is channelled through the virtual instrument until the light is integrated on the detector to create a detector image. Each module can be composed of further smaller modules internally, which might be useful for example to test the influence of different wide field corrector designs within the telescope optics. The light path may split along the way, as indicated by the various arms of the spectrographs.

4.1 Target Generator

The target generator is capable of generating light planes for a variety of targets. Depending on the physical extension of the target, the module is able to generate point sources (stars) and extended or diffuse sources (galaxies, nebulae, multi-star system). As a result of the target generator, a light plane is delivered, including the spatial distribution, angular distribution and spectrum. The generator module can load predefined spectra or generate artificial spectra like continuum sources or rake spectra, artificial arc lamp spectra and others. A stellar model to generate simulated star spectra is not planned, but with the capability of loading external spectra, this task can easily be accomplished by using an existing software. Overlapping targets, for instance two stars that are very close together, can not be simulated within one light plane object, instead light plane stacking (see Section 3.2) can be used.

In the top most row of distribution plots in Figure 3, the initial light distributions for a point source are presented. The light of the point source is distributed uniformly over the entire spatial region (units are meters), but since the light comes only from one direction, the angular distribution shows only a little dot (units are arc seconds).

4.2 Atmosphere

The atmosphere module projects the light plane from its edge to a plane surface just above the telescope, see Figure 3. The module it self is currently not fleshed out, but a detailed implementation is planned for the near future. The atmosphere is currently modelled by convolving the angular distribution of the target with a Gaussian function with the correct FWHM. This is only a place-holder solution, more accurate simulation involving other convolution functions like Moffat functions and a proper implementation of an atmosphere model, depending on seeing conditions, telescope pointing and atmosphere transmission curve and wavelength dependent atmospheric dispersion is planned. Chromatic aberrations can be modelled using the offset vectors, mentioned in Section 3.1, which introduce only a shift in the angular light distribution. An atmospheric emission model depending on telescope pointing, moon visibility and other parameters is also planned.

Consider again he light distributions in Figure 3. Due to the atmosphere, the dot-like angular light distribution is convolved with the seeing parameters.

4.3 Telescope

The telescope optics module contains the effects of VISTAS primary (M1) and secondary (M2) mirror as well as the wide field corrector (WFC) and the atmospheric dispersion corrector (ADC), as designed for 4MOST.¹ The two mirrors and the WFC are simulated as one unit, projecting the target light onto the focal surface. First, the central obstruction of M2 and the footprint of the M2 spider as well as the shape of M1 are applied to the spatial distribution of the light plane. Since a telescope maps angles to locations and vice versa, the angular distribution of the the light plane is mapped to the spatial distribution and the spatial distribution is mapped to the angular distribution. This creates the characteristic doughnut shape in the angular distribution and diffuse light distribution (due to atmospheric effects) on the spatial distribution on the focal surface.



Figure 3. Transition of a light plane between the target generator, and the telescope focal surface. The target generator module generates the first light plane. The atmosphere module projects the light plane to right above the telescope and the telescope module projects that light plane onto the focal surface of the telescope.

Since the angular distribution and spatial distribution are effectively swapped, one resolution element in the angular distribution before the telescope corresponds to one resolution element in the spatial distribution on the focal surface and vice versa. So the initial angular distribution of the light plane, generated in the target generator, must take the size of the target on the focal surface into account in order to generate meaningful data (the angular distribution of the target light plane in Figure 3 is magnified by a factor of 20 to make the point source visible). Also the optical properties of the telescope are taken into account on the spatial distribution of the light plane by convolving with the telescopes PSF. The PSF for the telescope and WFC/ADC unit is obtained from a ZEMAX model.

The ADC is optically included within the WFC, but for TOAD, it is modelled by introducing a wavelength dependent offset of the spatial light distribution on the focal surface that counteracts the dispersion of the atmosphere. Residual atmospheric effects will be a result of the atmospheric model and the ADC model because both effects do not exactly match. The WFC will also introduce a lateral colour effect, which will be modelled using the wavelength dependent offset vectors in the same way as for the ADC, for an example see the colour coded offset vectors within the spatial direction in Figure 1. The effects of the WFC and ADC can be verified using the ZEMAX software for a small collection of telescope conditions and field angles. Based on this separation within TOAD, the performance of the ADC can easily be estimated for a large series of field locations and telescope pointing which might be useful when considering alternative ADC designs.

It is indeed expected that the 4MOST instrument will generate residual chromatic effects. Current ZEMAX simulations show that the total effect can be 25 microns in the worst case between an object location for wavelength 400nm vs. 900nm on the focal surface of the telescope. For comparison, the fibre core diameter is 85 microns, which means the effect can have a significant impact on the final flux on the detector.

The transition between the atmosphere module output light plane and the telescope module output light plane is visible again on the left-hand side in Figure 3. The vignetting of the primary and secondary mirror shows up in the angular distribution while seeing induced fuzzy image is visible in the spatial distribution.

4.4 Positioner

The 4MOST positioner⁵ is based on the ECHIDNA tilting spine concept. The positioner module simulates all effects, related to positioning the fibre and projects the light plane from the focal surface of the telescope onto the surface of the fibre, see Figure 4. This includes a flat shift in the angular distribution as a result of fibre tilt,



Figure 4. Transition of the light plane between telescope focal surface, fibre surface and fibre exit. The telescope module projects the light plane onto the telescope focal surface, locally for one target. The positioner projects that light onto a light plane on the surface of the fibre, perpendicular to the fibre. The fibre module projects the light plane to the exit of the fibre.

a random shift in location due to positioning and alignment errors and the defocus effect, introduced because the fibre surface moves on a spherical surface. The resulting light plane is parallel to the fibre tip surface, which means the centre of the light plane corresponds to the centre of the fibre and the optical axis is perpendicular to the (tilted) fibre surface. The spines are $\approx 250mm$ long and have a patrol radius of 12mm. Between 0 position and maximum tilt of the spine, the fibre tip has a differential focus movement of $\approx 288\mu m$ (indicated as the fibre patrol surface in Figure 4). The defocus of the fibre will be modelled by convolving the spatial distribution with the angular distribution, magnified according to the distance of the fibre tip to the focal surface of the telescope.

The effect of the positioner module can be observed in the transition from the top to the middle row of light distributions in Figure 4. The defocus effect is not modelled yet, but the shift in the angular distribution is visible, as indicated by the tilted light plane surface on the right hand side of the image.

4.5 Fibre

Within the fibre module, several effects are modelled. The fibre aperture vignetting at the fibre input is a wavelength dependent throughput loss due to chromatic effects from the atmosphere and the telescope optics, discussed in Subsections 4.2 and 4.3. Since the chromatic effect is modelled with an offset vector in the spatial distribution of light, it is easy to cut a circular shape from the input distribution of light, taking the chromatic effect into account. The vignetting shape differences (elliptical instead of circular shapes) due to fibre tilt are not considered in the model because their estimated effect is too small. The surface of the fibre couples light into the fibre, depending on the angle between the fibre and the light beam due to Freshnel reflection. The effect is mainly a throughput loss, reflected in the angular distribution of the light (larger angles are coupled less effectively than small).

Focal ratio degradation (FRD) is a major contributor to light loss in multimode fibres, it broadens the angular distribution of light exiting the fibre and therefore creates a loss in throughput at the spectrograph collimator. FRD^6 is caused by numerous effects such as fibre termination-end effects at the input-end (positioner) and the output-end (spectrograph), the fibre connector can be an FRD source as well as tightly bending of the fibre. The fibre scrambles the light azimuthally in the angular distribution, which means that the light from one angle at the entrance is distributed uniformly over the surface of the corresponding solid angle at the exit, broadened by the FRD.



Figure 5. FRD convolution of the far field of a fibre with 0mm tilt (top) and a fibre with 12mm tilt (bottom). The images (from left to right) show: 2-dimensional angular distribution at the entrance of the fibre; average light intensity as a function of radius; average light intensity as a function of radius after convolution with the FRD model; 2-dimensional angular distribution at the exit of the fibre. All angle values are in degrees.

To account for the azimuthal scrambling, the angular distribution of light is integrated azimuthally as a function of radius from the origin of the angular distribution (circle-integration). The now 1-dimensional representation of the angular distribution is convolved with a (radius-dependent) function that models the various sources of FRD within the fibre. At the exit of the fibre, the light is distributed azimuthally again in order to form the new 2-dimensional angular distribution of the light. See Figure 5 for a visualization of two fibres, one with 0mm tilt and one with the maximum 12mm tilt. Due to the tilt of the fibre, the entrance light beam is broadened already as indicated in the figure, which introduces an effect similar to FRD at the exit. The function and its parameters for the FRD model are measured in the laboratory, described by D.M.Haynes.⁷ The used model is not entirely correct as the parameters of the FRD model depend on the angle. Due to a lack of laboratory measurements, we currently use only one set of parameters for the FRD convolution. A radius dependent FRD convolution function will be implemented as soon as we take measurements from a 4MOST fibre prototype and characterize the FRD parameters.

Until we have a better fibre model, we assume that the light will be perfectly scrambled in the spatial distribution. This is not entirely true, but the exit light spatial distribution does not (to first order) depend on the spatial distribution at the entrance, which means the exit spatial distribution is modelled to be uniform on the fibre core surface. Exit light distribution influences due to fibre bending and other effects might be modelled later, after we have build a suitable prototype.

4.6 Spectrograph

The 4MOST spectrographs are complex optical systems that can not be simulated directly in TOAD. An optimal dummy spectrograph was implemented using TOADs capabilities, but it does not take aberrations and non-perfect optical properties into account. The real spectrograph will be modelled, relying heavily on the ZEMAX software and macros to extract the information that is needed for TOAD. It is not planned to use ZEMAX as an external software package to render the spectrographs within TOAD like it is done in S.Barns.⁸ A macro is applied to the spectrographs ZEMAX models to generate all necessary information which are then stored in a data base that is loaded within TOAD.

The light path through the spectrograph is simulated per spectrograph arm individually. The light plane is copied for each arm and the relevant part of the spectrum is cut off due to the dichroic. Obviously, the different arms of a spectrograph are loaded with different parameters, but they are executed using the same program code since they are reasonably similar. A light plane is not feasible to model the output of the spectrograph since



Figure 6. Small section of the output of the detector module.

the light intensity on the detector is wavelength dependent. For each pixel of the detector the expected number of photons and their average wavelength are stored in an array, which is sufficient to model the detector (see Section 4.7).

From the ZEMAX model, a grid of 11×11 PSF density maps are created. That means, for 11 fibres and 11 wavelength values, a PSF map is generated by the ZEMAX macro. The location of the PSFs on the detector is used to create an position map to project the fibre output onto the CCD surface, depending on slit location and wavelength. The integrated light intensity within each PSF is used to generate a similar map for throughput due to vignetting and transmission loss within the glass. Since the PSF changes with wavelength and slit location, the PSF grid is interpolated in between the stored PSF spots. It is assumed that the difference between two neighbouring images is small enough to allow for such an interpolation. If the difference between two neighbouring PSFs is found to be too large, it is planned to sample the detector area with a tighter grid of PSFs. A scattered light model is not yet available for TOAD but it will be implemented in a similar manner as the PSF model of the spectrographs.

Before projecting the light of the light plane onto the detector surface, the optical parameters of the spectrograph are taken into account, primarily image demagnification. For a particular wavelength and slit location, it is now possible to create a fibre image on the detector surface. The location map determines the location of the image while the (interpolated) PSF and scattered light map are convolved with the fibre image. The location map also creates a connection between wavelength and the location on the detector. For each pixel of the detector in wavelength direction, a fibre image is created, using the centre of the pixel and the corresponding wavelength to generate the fibre image. The flux within the fibre image is determined by the integrated flux of the spectrum between the projected left and right edge of the pixel. This procedure is executed for each pixel in spectral direction, generating a series of overlapping fibre images that are summed up in above mentioned detector array. Due to the large amount of projections, this process can be quite time consuming and require the bulk of the computation time for one target.

If multiple targets are simulated, to generate a single detector image they are integrated at this point. That means, all targets add their expected photons to the same light array before the data is passed to the detector. This way it is possible to simulate the detector image of just one target, multiple targets that go through various fibres or even targets that couple light into the same fibre.

4.7 Detector

The detector module is converting the array of expected photons into expected electron detections and through a analogue/digital converter to produce a fits file. A small section of such an output is presented in Figure 6, using the example spectrum from Figure 1 and a dummy implementation of the spectrograph module. The light, conveniently placed into an array of values that correspond to the detector pixels, is transformed into electrons using the quantum efficiency of the detector. For the quantum efficiency, the wavelength of the photons is taken into account. Depending on the detector model, full well capacity, linearity, charge transfer efficiency and others can be considered. In the current model, there is no need for this detail but that might change in the future and it is easy to implement if needed.

If a realistic image is desired, noise factors have to be added using a noise generator and also photon noise has to be considered. The spectrograph model delivers the expectation value of the light intensity which can be directly used to generate Poisson distributed values. Also dark current and readout noise as well as bias values can easily be added if desired. The result can be stored as an image for analysing crosstalk, image quality or as FITZ file to be processed by data reduction and management software. FITS header parameters can be added according as required.

5. OUTLOOK AND ACKNOWLEDGMENTS

So far, most of the internal infrastructure of TOAD is available, but clearly still a lot of work has to be done, especially in completing the individual modules. Based on the current performance and planned development, TOAD is on a good track to provide data for an early throughput simulator and artificial detector images for an early data management and pipeline. TOAD will also be in a good position to give answers to many questions that might come up in the framework of systems engineering. Together with the 4MOST system, TOAD will grow and become procedurally more complex and will be adapted to the needs of 4MOST. Close to commissioning the instrument, TOAD will be released as an open source python package and may provide the basis for other fibre fed spectroscopic instrument simulators.

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