TECHNICAL REPORT

Title: Features of the Software Tool Used to Define Observations with the NIRSpec Microshutter Array (MSA)

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1 Abstract

This document describes necessary and highly desirable features of the software tool that JWST observers will use to define observations with the microshutter array (MSA) in the Near Infrared Spectrograph (NIRSpec). Observers will use the tool to choose which MSA shutters to open and where to point the telescope in order to obtain simultaneous spectra of dozens of targets. Visualizing the MSA is complicated because individual shutters are small compared to the full field of view of NIRSpec. The tool must be simple enough that a novice observer can learn to specify a basic observation, yet powerful enough that an experienced observer can specify a complex observation.

In this document, we briefly summarize relevant characteristics of the NIRSpec instrument. We then describe core capabilities of the software tool that will be needed to use the NIRSpec MSA. We describe in decreasing order of priority additional features of the software tool that are highly desirable from the standpoint of usability and scientific optimization. We describe the typical sequence of activities an observer will perform when defining an MSA observation, highlighting input data the observer must provide. We explain conceptually how to specify an MSA configuration as a list of apertures and give a specific example. We describe conceptually the creation of an initial MSA configuration, based on an input catalog of possible targets. We present a list of algorithms that the tool could implement to automatically select the optimal subset of possible targets that should be observed. We describe conceptually various user interface and diagnostic output options, evaluating their cost and value. Finally, we discuss the interface between the observation definition tool and the data analysis pipeline.

We identify certain design philosophies that we believe will yield a more effective tool. The basic user interface must be as simple as possible to improve usability and to contain user support costs. Given the complexity of observations with the MSA, very extensive

usability testing is needed during the design process to validate proposed interfaces. Finally, the core capabilities of the VTT must be significantly enhanced or redesigned to support the graphical interface envisioned for the MSA tool.

2 Introduction

2.1 Instrument Overview

The Near-Infrared Spectrograph (NIRSpec) on the James Webb Space Telescope (JWST) has a micro-shutter array (MSA) to select targets for multi-object spectroscopy. The MSA consists of four separate quadrants, each with 365 shutters along the dispersion axis (x-axis) and 171 shutters along the spatial axis (y-axis), for a grand total of 251,600 shutters. The shutter pitch is approximately 0.26” along the dispersion axis and 0.51” along the spatial axis, projected onto the sky. The clear aperture of an open shutter is approximately 0.20” x 0.45”, projected onto the sky. The framework that separates shutters along both axes is approximately 0.06” wide, projected onto the sky. Geometric distortion between the sky and the MSA is predicted to be nearly linear, so that targets remain in their apertures (<1 mas of differential shift across the field of view), even for relatively large dithers (20 arcsec).[1]

A magnet sweeps across the back[2] of the MSA (facing the detector) to push all operable shutter doors open towards front of the MSA (facing the sky). Electrostatic force holds each shutter open until it is electronically released. Shutter release will be synchronized with a return sweep of the magnet to damp the spring action of the shutter, which would otherwise cause the shutter to pass through the closed position and strike the light shield. After the forward sweep, all operable shutters will be open, allowing imaging activities such as target acquisition, slitless spectroscopy, and calibration. After the reverse sweep, shutters may be closed to form apertures, allowing multi-object spectroscopy. A few percent of the shutters may be inoperable, i.e. permanently open or closed. The set of inoperable shutters is expected to grow over the course of the mission.

One or more shutters may be opened to create an aperture that is used to observe one point or extended source in the 3.6’ x 3.4’ field-of-view (FOV) of NIRSpec. Many sources can be observed simultaneously by using an MSA configuration with many apertures distributed over the FOV. Each aperture containing a source produces a spectrum that runs along the dispersion axis (x-axis). When using a NIRSpec grating, two apertures in the same MSA row will typically produce two spectra that overlap. However, prism spectra are short enough that the two spectra may not overlap, if enough shutters separate the two apertures. Observers may chose to open multiple shutters per MSA row, if the overlapping spectra contain isolated emission lines with no underlying continuum.

Shutter throughput is a function of wavelength, source extent, and source location in the shutter. For point sources, aperture throughput can drop by a factor of three from a position at the center of an aperture to a position under the MSA framework between that separates shutters. Absolute flux calibration requirements are satisfied only in the central

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[1] Based on polynomial coefficients in “Characterization of the optical distortion of NIRSpec” by Xavier Gnata and Pierre Ferriut (CRAL-PJT-NIRS-TN-200505-04).

[2] During MSA fabrication, the terms “front side” and “back side” have meanings that are opposite to our usage of “front” and “back” in this memo. From an operational nomenclature perspective, incoming light encounters the front of the MSA before the back.

region of a shutter, known as the *acceptance zone*. The size of the acceptance zone depends on wavelength and hence dispersing element. Acceptance zone size also depends on whether the target is a point source or an extended source.

2.2 MSA Tool Purpose and Use

NIRSpec observers will use the MSA tool to select a subset of available targets in the field-of-view, specify the corresponding MSA configuration, and provide metadata that will be used by the data analysis pipeline. Calibration scientists and engineers will use the same tool to plan calibration and engineering visits. The tool should be an integrated component of the more general program definition tool, used by investigators to specify visits in an observing program.

We describe here a typical session with a strawman MSA tool that implements all the required and highly desirable features advocated in this document. Later in this document we distinguish between these two types of features. The observer specifies a tentative telescope orientation and a NIRSpec pointing, expressed as the desired right ascension and declination of a fiducial point on the MSA near the center of the field-of-view. The tool displays an image of the region with an overlay showing the boundaries of the four MSA quadrants and the fiducial point. Individual shutters are much too small to visualize in an image of the entire field of view.

The observer provides a catalog of potential targets with extremely precise (<10 mas) relative coordinates. Targets may be segregated into a limited number of priority bins. The tool automatically selects the largest subset of targets located in acceptance zones with non-overlapping spectra, taking target priority into account. If desired, the observer can use the tool to search for a better solution by perturbing the pointing or exploring a range of orientations. Perturbing the pointing moves targets in or out of the acceptance zone. Adjusting the orientation changes whether spectra of particular targets overlap. Once a target set is selected, the entire pattern of open shutters may be shifted by an integer number of shutters along the spatial or spectral axes to avoid bad shutters or bad detector pixels. After the tool has selected a subset of targets, the user may edit the target list by hand, adding or rejecting targets from the catalog.

The tool creates an MSA configuration with one aperture for each target in the list. Initially, all apertures have the same shape, but the user can alter individual apertures using an integrated GUI or a text editor. The tool warns the observer about targets that are outside the acceptance zone, apertures that produce overlapping spectra, and apertures that contain permanently closed shutters.

To aid the data analysis pipeline, the MSA tool automatically assigns a purpose (target or background) to each shutter and attempts to associate a set of background shutters with each target. The user can manually alter the purpose of each shutter and the associations.

3 Data Provided by the Observer

3.1 Catalog Files

The MSA tool will read and write *catalog* files that contain data for potential science targets or potential acquisition targets. Catalog files will contain ecliptic coordinates (right ascension and declination) for every potential target. We assume that equinox J2000 will be used commonly throughout the lifetime of JWST, so all input and output coordinates in catalog files will be equinox J2000. Observers may use external tools to precess coordinates prior to constructing an input catalog file, if necessary. Coordinates will be specified in the ICRS reference frame, which is used by version 2 of the Guide Star Catalog (GSC2). We assume that targets with significant parallax (> 5 mas) or proper motion (> 5 mas/yr) will not be dense enough on the sky to warrant multi-object spectroscopy. Thus, catalog files will assume zero parallax and proper motion. The MSA planning tool will not provide support for moving targets.

Catalog files may contain optional data for each potential target. The observer may assign each potential target a *priority* to guide target selection algorithms. Priorities are integers between 1 and 9, where a lower value indicates a higher priority. A default priority of 1 is assumed for all targets that do not have an assigned priority. Some of the target selection algorithms proposed below consider target priority when selecting targets to observe.

Some MSA fields-of-view will contain so many targets that multiple MSA configurations will be required to observe all the targets. In this case, the observer may segregate a target list into *target sets*, each containing a subset of the full target list for a particular field-of-view. Each potential target may be assigned to a target set by the observer or by target selection algorithms in the tool. Each valid target set has an integer label between 1 and 9. Potential targets that do not have an assigned target set are assumed to be in target set 1. Target selection algorithms will ignore objects in target set 0. Thus, observers may use target set 0 to exclude targets from consideration without deleting them from a catalog.

3.2 NIRSpec Pointing and Telescope Orientation

NIRSpec pointing and telescope orientation must be specified before the MSA can be projected onto sky coordinates. The MSA tool expresses pointing and orient in terms of the MSA, rather than the observatory. NIRSpec pointing is specified as the ecliptic coordinates of a *fiducial point* near the center of the MSA field-of-view. The user need not know the offset between the MSA fiducial point and other reference points in the JWST field-of-view. Telescope orientation is expressed in terms of an MSA *projection angle*, which is the angle (measured North through East) between the MSA spatial axis (+y-axis) and the declination axis. For example, a projection angle of 45 degrees means the spatial axis of the MSA points northeast, when projected onto the sky. The tool will automatically translate between MSA projection angle and telescope orient.

The tool will calculate the initial MSA pointing and projection angle from data in the main proposal, if available. In the main proposal, the orient may be constrained to a particular range or set of ranges, without being uniquely specified. The tool will convert orient constraints into MSA projection angle constraints and vice versa. If MSA pointing is unspecified, the tool will set telescope pointing to the mean of target coordinates in the target list, if specified. If position angle ranges are specified, the tool will set the projection angle to the midpoint of the first position angle range. If no position angle values or constraints are specified, the tool will set the position angle to North.

The user can manually enter a new MSA pointing or a new MSA projection angle or range. Users may have the ability to interactively adjust the MSA pointing and projection angle, perhaps via a graphical interface. Algorithms for automatically selecting targets may also reset the MSA pointing and projection angle.

3.3 Image Data

To improve visualization of target placement in MSA shutters, the user may provide image data in a FITS file. The world coordinate system in the header of the FITS file must specify the mapping between pixels to ecliptic coordinates. Ideally, the tool will allow users to add targets to a target list by measuring the position of objects in the image. This capability may be shared with other JWST tools.

4 Apertures

Observers who want to do multi-object spectroscopy must specify in advance which MSA shutters to leave open during an exposure. Observers will usually specify an MSA configuration as a list of rectangular *apertures*, each consisting of one or more shutters. Each aperture must be fully contained in a single quadrant. Apertures may overlap, but the data analysis pipeline may not be able to process spectra obtained with overlapping apertures. For example, an observer might be able to disentangle overlapping emission line spectra of multiple sources, using the known rest wavelengths of strong lines and additional constraints on velocity, whereas a generic pipeline would only be able to return the composite spectrum and a wavelength scale for each aperture. Observers should be strongly encouraged to provide reduced data to the archive, whenever they choose to use an observing strategy that the pipeline cannot process fully.

A default aperture will consist of one target shutter flanked by a pair of background shutters, aligned along the spatial axis. Advanced users may change the formal location and size of the rectangular aperture, and they may specify for each shutter in the aperture one of three allowed combinations of shutter state (open or closed) and purpose (target or background):

- Open shutter containing the (possibly extended) target
- Open shutter containing background
- Closed shutter

The observatory only needs shutter state to perform the observation, but the data analysis pipeline also needs shutter purpose to process the data automatically. Shutter state and purpose should be stored in a human readable and editable format.

Appendix 1 gives one of many possible nomenclatures for specifying apertures. The actual nomenclature will be determined during the detailed development process, which will include extensive usability testing.

5 Specifying an MSA Configuration

Users may specify an MSA configuration explicitly in an MSA configuration file or implicitly via a catalog of potential targets, NIRSpec pointing, and telescope orientation. The latter two parameters define the NIRSpec field of view. Typically, an observer will begin by using the tool to map target coordinates into an initial MSA configuration (§ 5.1), which can be saved in an MSA configuration file. Observers may edit or construct manually an MSA configuration file (§ 5.2) and then use the tool to validate the result. The tool should also allow users to adjust an MSA specification via a graphical interface (§ 5.3), though this highly desirable capability is not mandatory. In the remainder of this section, we describe these different options for specifying an MSA configuration.

5.1 Target List, Pointing, and Orientation

Given a NIRSpec pointing and telescope orientation, each set of target coordinates (α,δ) on the sky maps to a particular location (x,y) in the MSA focal plane. NIRSpec requirements dictate that distortion of sky coordinates projected onto the MSA shall be described adequately by a two-dimensional 5th order polynomial. The MSA tool must know and apply this distortion transformation when mapping coordinates on the sky to location on the MSA.

Users may implicitly specify an MSA configuration by providing target coordinates in a target data file and specifying separately the pointing and orientation of NIRSpec. The tool will map each target to an MSA shutter, but in the simplest case does no filtering of the target list (see target selection algorithms in § 6). For every target in the field of view, a target shutter will be opened, regardless of where the target is located in the shutter. Targets outside the four MSA quadrants will generate warnings.

Users define the field of view by specifying the coordinates of a reference point near the center of the MSA and the telescope orientation. Users may change interactively the desired NIRSpec pointing and telescope orient, thereby altering the set of open shutters corresponding to the list of targets.

By default, the tool opens one background shutter above and one background shutter below each target shutter to record background immediately adjacent to the target. This default aperture is adequate for most unresolved or slightly extended sources. Using only one background shutter above and below each target limits the probability that apertures will overlap or that background shutters will contain an extraneous source.

Advanced users may change the default number of background shutters (0-5) above and below each target shutter and the default number of target shutters (0-5), used when the tool automatically creates apertures for selected targets. This flexibility enables users to create most of the aperture types[3] beyond the default that they are likely to need, without having to understand the nomenclature used to specify apertures. Very advanced users may specify an arbitrary aperture template to serve as the default.

Diagnostics will warn the user about apertures that overlap or are affected by inoperable shutters. The basic user may respond by adjusting manually the requested pointing, orientation, and target list. Advanced users may also edit manually individual aperture specifications in the MSA configuration file (§ 5.2), but this requires an understanding of the underlying nomenclature. If possible, the tool should also allow observers to specify target and background shutters interactively (§ 5.3).

5.2 MSA Configuration File

To extend the basic capability described in § 5.1, advanced users need the ability to specify explicitly set the state (open or closed) and purpose (target or background) of individual shutters, independent of target location. The most fundamental method of specifying an MSA configuration is to edit directly the MSA configuration file, which should be in a format that is relatively easy to parse and edit. The tool should use a common nomenclature in printed diagnostics and MSA configuration files. Advanced users may specify MSA configurations as a list of rectangular apertures, a bitmap, or a

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[3] For example, ‘T’, ‘bBb’, ‘bbTbb’, ‘btTtb’, ‘bbtTtbb’ in the strawman nomenclature of Appendix 1.

replicated pattern. Basic users will prefer a graphical interface for editing MSA configurations (§ 5.3), but the ability to edit an MSA configuration file is more fundamental.

Users may specify a default state for all shutters and then alter the state of shutters in rectangular apertures, as described in § 4. Observers will typically need only one rectangular aperture per target, but observers may use an aperture list to construct an arbitrary MSA configuration. Due to bandwidth limitations of the protocol that will be used on the 1553 bus, transferring an aperture list from the ISIM computer to the MSS electronics will be much faster than sending a bitmap representation of the states of all MSA shutters.

The MSA tool must report output<-(diagnostics) and warnings for each proposed aperture. Diagnostics must include:

- NIRSpec pointing
- Telescope orientation
- Aperture identifier
- Aperture description (state and purpose of each shutter in the aperture)
- Target identifier (e.g., number and name)
- Target location on the MSA (expressed in shutter coordinates, Appendix 1.2)

Warnings must include:

- Apertures that cannot be formed because of a permanently closed shutter
- Apertures that are bordered by a permanently open shutter
- Apertures that overlap each other
- Apertures that contain a target outside the acceptance zone
- An aperture with target and background shutters in the same row

For point sources in sparse fields, a text-based interface would be adequate. For crowded fields or for targets that fill a significant fraction of the field of view, correctly specifying background regions requires a graphical interface. Separate analysis tools exist to generate automatically a catalog with the coordinates of every detectable source in an image, but these tools do not automatically identify background regions.

Advanced users may specify the state of every MSA shutter, using a binary bitmap with one bit per shutter, independent of the presence or location of sources. Appendix 2.1 describes one of many possible implementations.

Calibration scientists and instrument engineers will be able to specify or select a pattern of open and closed shutters that repeats across each MSA quadrant (e.g., a checkerboard or stripes). Using an aperture list would be a cumbersome way to specify some patterns. Patterns will be used for calibration and engineering activities (e.g., to map the geometric distortion between the MSA and the detector). Appendix 2.2 gives one of many possible pattern nomenclatures. A less flexible, but adequate alternative would be to provide a menu of a few predefined patterns. The actual nomenclature will be determined during the detailed development process.

5.3 Interactively Set Shutter State

Basic users will prefer to use an interactive graphical interface to set the state (open or closed) and purpose (target or background) of individual shutters. The tool will show graphically any failed shutters and issue will issue a warning if the requested state is not possible because a particular shutter is permanently open or closed. The user will not be able to select an individual shutter in a display of the entire MSA because of the large range in size scales, so the interface will have to provide a zoom window that magnifies a region of interest on the MSA. The region of interest may be specified explicitly by a quadrant label and shutter indexes or implicitly by selecting a target of interest from the target list. Pan buttons may allow the user to shift the set of shutters visible in the zoom window.

In its crudest form, the zoom window would only show the boundaries of shutters in the region of interest and the acceptance zone within each shutter. If the user has provided a target list, then the zoom window would also indicate nominal target locations projected onto the shutters. If the user has provided an image of the region, then the tool could also display the relevant portion of the image in the zoom window. Users could also use an interactive zoom window to manually indicate coordinates for new targets.

6 Optimizing Target Selection

Choosing which MSA shutters to open is straightforward, once the observer has specified exactly which targets to observe. The more difficult problem is selecting which subset of potential science targets should be observed, when only a subset may be observed in a single exposure. In this section we consider target selection algorithms of increasing sophistication that approach the optimal observing strategy for a given list of potential targets. In general, the capabilities we describe are cumulative, so that the basic features described first should still be available, even if more sophisticated algorithms are also implemented.

6.1 "Acceptance zone" Filtering

This algorithm selects from a target set every target located inside the *acceptance zone* of an operable shutter, regardless of whether the corresponding apertures overlap. The acceptance zone is the central area of a shutter, where a target must be located to achieve the desired flux calibration accuracy. The size of the acceptance zone size depends on the longest wavelength of interest, which the user must specify. Advanced users may adjust the size of the acceptance zone by changing either the desired flux calibration accuracy (default: 10%) or the source extent in mas (default: point source). Setting the desired flux calibration accuracy to a very large value (e.g., 999%) expands the acceptance zone to the full area of each shutter.

An aperture will be created for every target in the acceptance zone of an operable shutter with adjacent shutters for recording background. By default, the tool opens one shutter above and one shutter below each target to record background adjacent to the target. Advanced users may alter this behavior, as described in section 4.2. The tool will reject any target with a background region that extends off the edge of a quadrant.

The tool warns the user about overlapping apertures, which can affect data quality. Apertures overlap if they share at least one MSA row in common, except that two apertures per row are possible when using the prism, which produces relatively short spectra. Two prism apertures do not overlap if they are in different MSA quadrants and the column index quadrant A or B is less than the column index in quadrant C or D. The user corrects overlapping spectra by indicating manually which targets to delete from the current target set or which background shutters to close. If the user adjusts the field of view enough that targets move out of their acceptance zones, then the user will generally need to begin again with the original target list.

The tool provides a simple way for users to put all targets outside acceptance zones into a new target set. This feature enables the user to observe as many targets as possible in the first target set and then as many of the remaining targets as possible in a second target set and so on.

6.2 Automatically Avoid Overlapping Apertures

As a refinement of the acceptance zone filtering algorithm, the tool should automatically pare down the set of selected targets until there are no overlapping apertures, as defined in the previous section. There are an enormous number of pared target lists that satisfy the non-overlapping aperture constraint, including poor solutions such as a pared target list with only one target. Additional constraints are needed to define the algorithm.

Generally, observers want to maximize the number of high priority targets, filling in remaining gaps with lower priority targets. Rigorously maximizing the number of targets with non-overlapping apertures is computationally very difficult, so the tool will use a heuristic algorithm. For example, the tool could order by increasing spatial coordinate y the highest priority targets returned by the sweet-spot algorithm in section 5.1. The tool could then work sequentially through this list, selecting the first available target with a new aperture that does not overlap any existing apertures and skipping targets with new apertures that overlap an existing aperture. The tool would then repeat the process for targets with progressively lower priority. We suspect that this heuristic algorithm will achieve close to the maximum number of non-overlapping apertures without the computational difficulty of the rigorous solution.

6.3 Automatically Select Spatial and Spectral Offsets

As a further refinement of the algorithm described in section 5.2, the tool could step through small offsets in x and y, maximizing the total number of high priority targets in acceptance zones with non-overlapping apertures. The tool would have a default step size (1/10 the shutter pitch) and number of steps (10) along each axis, but advanced users could modify these parameters. For each offset of the field of view, the tool would perform the analysis described 5.2, obtaining the total number of high priority targets. The tool would select the x and y offsets with the maximum number of high priority targets, using total number of targets as a secondary criterion. After selecting the best sub-aperture offset, a subsequent optimization step would consider shifting the field of view by an integer number of shutters to avoid broken shutters and to minimize the impact of gaps between MSA quadrants.

6.4 Choose the Best Orient

As a further refinement of the algorithm described in section 5.3, the tool could step through the specified range of orients, maximizing the total number of high priority targets in acceptance zones with non-overlapping apertures. The tool would have a default step size (1 degree), but advanced users could modify these parameters. For each step in orient, the tool would perform the analysis described 5.3, obtaining the total number of high priority targets. The tool would select the orient with the maximum number of high priority targets, using total number of targets as a secondary criterion. If target coordinates are available, orients should also be expressed as the range of allowed observing dates.

7 Target Acquisition and Dither Patterns

Observers will specify acquisition target information (e.g., coordinates on the sky) using the same syntax (and ideally the same software module) as the program definition tool used by all JWST investigators. The MSA tool will generate an error if any of the acquisition targets are located close to the edge or outside of the four MSA quadrants. The tool will generate a warning if any of the targets are near a permanently closed shutter. We assume that the exact phasing of the acquisition targets with the grid structure of the MSA has a negligible effect on pointing precision, so observers will not evaluate or tune this phasing.

A target set will generally include targets distributed uniformly across the acceptance zone of the open shutters. If the geometric distortion of the sky projected onto the MSA is highly nonlinear, then large dithers will cause the targets to spread out of the acceptance zone. This appears not to be an issue for NIRSpec. For a 20 arcsec dither, the differential change in target spacing across the full field of view is currently expected to be less than 1 mas. A target set should remain in the acceptance zone, even for large dithers.

8 Output from the Tool

8.1 Feasibility Diagnostics

When practical, the tool should check that each hypothetical observation is feasible. Most of these feasibility tests will be common to all instrument modes, suggesting that code to perform these tests should be modular. Each time the MSA pointing, MSA projection angle, or observing date is specified, the tool should check that the requested values do not violate JWST pointing and orient constraints. If ranges are specified for these parameters, feasibility will be assessed throughout the range. The tool will also check whether guide stars are available for each requested pointing and orient.

8.2 MSA Configuration File

Users may command the MSA tool to save a valid MSA configuration and all associated data in an MSA configuration file. Valid MSA configurations may have warnings, but no errors. MSA observers will use the general-purpose program definition tool to associate one or more MSA configuration file with each visit description.

Observers can command the MSA tool to read an MSA configuration and all associated data from MSA configuration file. Although investigators may begin defining an MSA observation from scratch using a catalog file (§ 3.1), all necessary data from the catalog file will be copied into the MSA configuration file, so that the original catalog file is no longer necessary to read, edit, and submit an MSA configuration file.

An MSA configuration file will contain all of the information needed by the observatory to configure the MSA for one observation. The primary data are the state of each shutter, commonly expressed as a list of apertures. MSA configurations are usually tied to a given NIRSpec pointing and telescope orientation, so these data will also be recorded in the file. Pointing and orientation will not be constrained for some configurations (e.g. slitless spectroscopy or internal calibration). Each file will contain only one configuration, but a given file may be associated with multiple exposures or multiple visits.

An MSA configuration file will contain all of the configuration metadata needed by the data analysis pipeline to process the data. The primary data are the coordinates and predicted location of each target on the MSA and the purpose (target or background) of each open shutter. Purpose may not be defined for some configurations. In principle, the metadata could be stored in a separate file, but we advocate bundling together all information about an MSA configuration in a single file.

An MSA configuration file will contain data input by the user and data derived by the tool. For example, the user inputs target coordinates, and the tool calculates the corresponding location on the MSA. Input and derived data should be clearly distinguished in an MSA configuration file, for example by storing them in separate fields. A user may edit the input fields with an external editor, in which case the derived data become invalid.

9 Interface with the Data Analysis Pipeline

Generally, each aperture will be confined to a single column, but occasionally apertures may span multiple columns, e.g. for sources that are extended along the dispersion axis. Adjacent shutters in the same row produce spectra that overlap almost completely, so the data analysis pipeline will produce a single extracted spectrum for all adjacent shutters in an MSA row. An aperture row spanning multiple columns should contain either target shutters or background shutters, but not both, so that the pipeline can categorize the extracted spectrum for that row as either target or background.

The pipeline will create separate extracted spectra for each row in each aperture. Each row of each aperture will yield either an extracted target spectrum or an extracted background spectrum. The pipeline will subtract background from an extracted target spectrum, if the extracted target spectrum can be associated with extracted background spectra. The pipeline obtains these associations from metadata provided by the observer or possibly archive users. If the metadata are invalid or do not exist, the pipeline may attempt to determine these associations automatically.

Automatically determining associations between target and background regions can be difficult in some cases, so the MSA tool should allow observers to specify associations manually. For example, an observation of a large spiral galaxy might target bright knots in the galaxy and subtract from each knot a mean background based on several shutters around the periphery. The tool should capture the intent of the observer during program specification, rather than making the data analysis pipeline guess later. However, the MSA tool should also be simple to use for standard observations, so the tool should create associations automatically for standard observing scenarios.

If an aperture specification contains both target and background shutters (e.g., the first example in § A1.3), then by default the data analysis pipeline will associate all the background shutters in that aperture with each target shutter in that same aperture. This is the standard use case for fields with many isolated sources. If an MSA quadrant contains one or more apertures without target shutters (e.g., the second example in § A1.3), then by default the pipeline will associate all shutters in the pure background apertures with each target shutter in an aperture without background shutters. This is the standard use case for fields that are very crowded or contain very extended sources. A single MSA configuration may contain both types of automatic associations.

The user may specify an MSA configuration with open shutters that cannot be associated automatically, for example when an aperture without a background shutter occurs in an MSA quadrant with no pure background apertures. In such cases, the tool warns the user that an automatic association is not possible, but allows the configuration, and the data analysis pipeline may not produce background-subtracted spectra for the affected target shutters. If an investigator uses a bitmap (see § 5.2), rather than an aperture list, to specify an MSA configuration, the tool may not be able to associate automatically background and target shutters. When a calibration scientist or engineers uses a pattern (see § 5.2), the data analysis pipeline will process the two-dimensional images, but not extract spectra.

Appendix 1 Aperture Nomenclature – An Example

To help clarify some of the abstract concepts discussed above, this appendix provides a specific example of nomenclature that the tool could use to represent apertures in an MSA configuration. This example is not meant to specify low-level requirements. The actual nomenclature used to represent apertures will be determined during the detailed design process, which will include extensive usability testing.

A1.1 Shutter Codes – An Example

Table 1 provides one of many possible systems of *shutter codes*, which could provide a succinct method of specifying the purpose of each shutter in an aperture. Distinct codes indicate whether an open shutter contains the target (‘t’) or background (‘b’) or whether the shutter should be closed (‘c’). The shutter code is capitalized for the one shutter in each aperture that contains the position on the MSA corresponding to the target coordinates. The tool and the data analysis pipeline need to know where each aperture is located and which shutters to open. The data analysis pipeline also needs to know whether each open shutter should be processed as target data or background. Observers do not have to understand shutter codes, if they adopt the default apertures returned by the tool or if they use a graphical interface to modify default apertures.

Table 1: Shutter Codes

State	Codes	Shutter Purpose
Open	t or T	Target
Open	b or B	Background
Closed	c or C	Occulted target

A *shutter code sequence* implicitly defines aperture size and explicitly specifies the state (open or closed) and purpose (target or background) of every shutter in the aperture. The sequence also indicates via capitalization which shutter contains the target coordinates. Table 2 gives a few examples of plausible shutter code sequences. The ‘bcTcb’ sequence may reduce contamination in background shutters by closing shutters immediately adjacent to the target. The ‘bbttCttbb’ sequence enables spectroscopy of faint extended emission around a bright central source by blocking direct light from the central source. We emphasize that observers do not need to understand shutter code sequences, if they adopt the default apertures returned by the tool or if they use a graphical interface to modify the default apertures.

Table 2: Examples of Shutter Code Sequences

Shutter Code Sequence	Type of Aperture
bTb	Default aperture
bTbbb	Extended background on one side
bB	Isolated 1x2 background region
bbtTtbb	Extended source covering 3 apertures
bcTcb	Reduced contamination in background shutters
bbttCttbb	Extended emission around a bright source

A1.2 Target Location on the MSA – An Example

Given a NIRSpec pointing and telescope orientation, each set of target coordinates (α,δ) maps to a particular location in the MSA focal plane. NIRSpec requirements dictate that distortion of sky coordinates projected onto the MSA shall be described adequately by a two-dimensional 5th order polynomial. This section describes one of many possible nomenclatures for specifying target location on the MSA. Target location on the MSA could be expressed as a quadrant label ('A', 'B', 'C', or 'D') and a decimal location (x,y) in that quadrant, expressed in terms of shutter indexes. Decimal locations (x,y) take integer values at the center of each shutter, so that rounding a decimal location gives the integer indexes of the shutter containing that location. Indexes begin at 1, not 0, in the center of the lower left pixel.

Figure 1 shows one of many possible ways to label quadrants and index shutters within each MSA quadrant. The x axis (dispersion) and y axis (spatial) form a right-handed coordinate system. Adjacent shutters in the same row produce overlapping spectra, whereas adjacent shutters in the same column produce parallel spectra. When two shutters in the same row produce overlapping spectra, each element of the composite spectrum contains longer-wavelength light from the shutter on the left (smaller shutter index, smaller value of x) and shorter-wavelength light from the shutter on the right (larger shutter index, larger value of x). Conceptually, wavelength increases to the right in the figure, though the actual projection onto the MSA, disperser, or detector depends on the number of reflections and viewing direction.

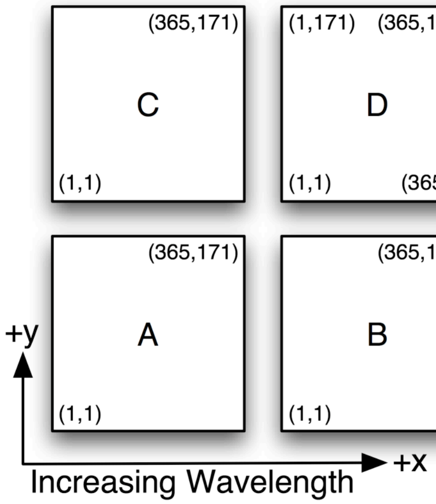

Figure 1: Quadrant labels, coordinate axes, and shutter indexes.

A1.3 Aperture Nomenclature – An Example

This section describes one of many possible nomenclatures for specifying apertures in an MSA configuration file. Aperture configurations could consist of a shutter code sequence (§ A1.1), an '@' separator, and the target coordinates mapped onto the MSA (§ A1.2). For example, 'bTb@A213.36,106.92' denotes a standard aperture in column 213 of quadrant A, with the target in row 107 and background shutters in rows 106 and 108. As a second example, 'T@C182.51,84.49' denotes an isolated target in column 183 and row 84 of quadrant C, while 'Bbb,bbb@C302.19,2.36' denotes an isolated 3x2 background aperture in columns 302-304 and rows 2-3 of quadrant C.

Shutter code sequences define the location and purpose of shutters in an aperture, relative to the location of the target on the MSA. This makes it relatively simple to see the effect of dithers, since only one coordinate pair per aperture needs to be modified.

Appendix 2 Alternate MSA Representations

A2.1 Bitmap Representation – An Example

Advanced users may specify the state of every MSA shutter, using a binary bitmap with one bit per shutter, independent of the presence or location of sources.

This section describes one of many possible nomenclatures for specifying bitmaps. The bit order in a bitmap could correspond to the sequence of shutters starting with column 1 and row 1 in quadrant A and cycling through all columns and then all rows and then all quadrants. A bit value of 0 indicates a closed shutter, and a bit value of 1 indicates an open shutter. Users will not compress the bitmap.

A2.2 Replicated Pattern – An Example

Advanced users may specify a pattern of open and closed shutters in a rectangular cell, which will be replicated across each MSA quadrant. Cell replication begins at row 1 and column 1 in the bottom left corner of each quadrant and proceeds with a regular spacing towards higher row and column index. Replicated cells are truncated at the top and right edges of each quadrant, if necessary. Only instrument engineers and calibration scientists will specify patterns.

This section describes one of many possible nomenclatures for specifying patterns. Pattern specifications could begin with “P” and then list shutter states (+ for open, - for closed) left to right (increasing column index) within each row and then bottom to top (increasing row index), with a comma separator between rows. For example, “P+” opens all shutters, “P+-” creates vertical stripes along the spatial axis, “P+,-” creates horizontal stripes along the dispersion axis, and “P+-,-+” creates a checkerboard. All of these examples have an open shutter in the bottom-left corner of each quadrant, but parity may be reversed.

Appendix 3 Formal Use Cases for a Typical Visit

A3.1 Using a Tool with Only Required Capabilities

Investigators use the MSA Planning Tool (MPT) in its most basic form to define MSA configurations for NIRSpec MSA observations.

Use Case Number: PPS-UC-TBD
Use Case Name: Bare-bones MPT use-case
Objective: Use the MPT to define an MSA configuration.
Primary Actor: Investigators
Preconditions:

- Investigator has a proposal/program open in APT and has a NIRSpec MSA observation selected.
- Investigator has a list of prioritized targets of interest in the field in the proper format for input to the MPT.

Trigger Event: N/A
Main Success Scenario:

1) The investigator selects the MPT from the APT toolbar and uses it to read in the user-supplied list of targets of interest.
2) The MPT obtains the initial pointing (RA and DEC of the NIRSpec aperture fiducial) and orientation from the attributes of the selected observation in APT, if available. Otherwise the MPT calculates the initial pointing as the centroid of the supplied target list and selects a nominal orientation for the pointing.
    a) The investigator optionally requests that the APT check for the availability of guide stars at this pointing and orientation. This step could also be performed prior to starting the MPT in order to verify the feasibility of the observation.
3) The investigator instructs the MPT to calculate the MSA configuration.
    a) By default, the MPT uses an aperture of one background shutter above and below the target shutter (bTb).
        i) The investigator has the option of specifying a different default aperture to use.
    b) The MPT opens an aperture for each target in the target list.
    c) The MPT generates a recommended MSA configuration and saves it to a file.
    d) The MPT generates diagnostics for: targets that do not fall in one of the four MSA quadrants, targets that are in a quadrant but not in a acceptance zone, overlapping apertures, and targets affected by inoperable shutters.

4) The investigator reviews the recommended MSA configuration.
   a) The investigator has the option of reviewing the configuration in a text file format or viewing the configuration graphically.
   b) The MSA configuration can optionally be displayed as an overlay on a FITS image.
5) The investigator may iterate this process (2-4) by changing the pointing or orient and calculating a new MSA configuration. Parameters that the investigator may change are:
   a) Add/delete targets.
   b) Change target priorities.
   c) Change the orientation.
   d) Change the pointing.
   e) Change the default aperture shape.
   f) Modify the shape of individual apertures by editing the MSA configuration file.
6) The investigator saves the MSA configuration.
   a) The MSA configuration is saved to a file and associated with the selected observation.
   b) The pointing and orientation information is updated for the selected observation in the proposal.

Post conditions:

- An MSA configuration file is generated and associated with an observation.

Notes and Assumptions:

- The resulting MSA configuration file can be edited using a text editor.
- As a final step prior to accepting the MSA configuration the investigator should verify the availability of guide stars for the observation given the new pointing and orientation.