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How to Piece Together Diffracted Grating Arms for AXAF Flight Data

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Abstract. The Advanced X-ray Astrophysics Facility's (AXAF) High and Low energy transmission gratings (HETG, LETG) data require new tools and data structures to support x-ray dispersive spectroscopy. AXAF grating data files may be a hundred megabytes (MB) in size, however, they will typically only be a few MB. We are writing data analysis software which can efficiently process the data quickly and accurately into wavelengths, orders and diffraction angles for each event. Here we describe the analysis procedure as well as some of the technical constraints we had to overcome in order to process the tasks efficiently.

1. Data Processing

1.1. Standard ACIS/HRC Event Processing

Initial data processing applies transformations from detector to sky coordinates for each photon in the data set. However, with grating data, additional event processing must be performed before data analysis can commence.

1.2. Select Zero Order Sources/Find Observed Target

In order to find where the dispersed photons lie, the center of the zero order source position on the sky must be determined, since this is the origin of the spectral coordinates. Source detection must not be fooled by emission lines located away from the center of the field; several methods exist to discriminate bright emission lines from zero order sources. Primarily, emission lines have a small variance in the PHA (energy) spectrum, while zero order has a large variance since it encompasses all of the source energies. Alternatively, the PSF (Point Spread Function) can be used instead of PHA, to weed out emission lines. Once zero order source positions are found, the target source is identified by matching the sky positions with an observation target list.

1.3. Identify Spectrum Parts Geometrically

Grating data events may be categorized by their part of the spectrum. This is done by creating mask regions for each grating part and by checking every photon for inclusion within the mask regions. For the HETG grating data, the relevant parts for each source are: zero order, MEG photons, HEG photons, and background photons. Regions are defined as rectangles in diffraction coordinates, in which the zero order is the origin, and one axis is parallel to the spectrum (dispersion direction), and the other perpendicular to it (cross-dispersion direction). The width of the rectangle is calculated using the effective PSF (mirror psf, Rowland geometry astigmatism, instrument de-focus, and aspect). These regions are translated into sky coordinates using each zero order source position, and by rotating the region by the grating angle (known) plus the mean observed telescope roll angle. Any event inside the rectangle is then assigned to that part of the spectrum (HEG or MEG, or LEG). Zero order photons are assigned by being within some radius of the zero order centroid. Each photon is tagged with one or more source ID's as well as grating part(s), depending on the number of regions into which it falls (overlaps).

1.4. Compute Linear Diffraction Coordinates

To calculate the diffraction angle (r) of a photon, work needs to be done in the geometric system in which the photon was diffracted. The sky coordinates, which are referenced to the telescope mirror node and therefore independent of the grating reference node, are only useful for the imaging of zero order and the filtering of grating arm photons. Grating diffraction coordinates are referenced to the grating assembly node. Reverting back to the original chip coordinates (chip number, chip position, grating node and zero order position) allows grating diffraction coordinates to be calculated for each time interval.

1.5. Compute "first order" Wavelengths

Now that diffraction angles have been determined parallel to the dispersion angle, the basic grating equation, $m\lambda = Pr$, can be applied to determine $m\lambda$ for each photon. Here, m is the integral diffraction order, P is the known mean period of the set of gratings (MEG, HEG, LEG), and r is the diffraction angle.

1.6. Resolve Orders (ACIS only)

The ACIS detector provides moderate spectral resolution via a pulse-height (PHA, or PI) for every photon. This resolution is enough to determine, with high confidence, what the spectral order is at any r or $m\lambda$, since only integral multiples are allowed at any given position (grating equation, diagram below). Order sorting is also useful for photons in overlapping mask regions. These events can be resolved as belonging to one arm/source versus another through order sorting. Since the HRC detector has no energy resolution, a method has yet to be determined for resolving orders or any overlapping regions in data taken by this instrument. The grating equation is used to calculate an estimate of the grating order (m_est), using physical constants and previously calculated values: $m_{est} = Pr(PI)/hc$. Here, hc is a physical constant; PI is the "Pulse Invariant" energy from the CCD; r is the calculated diffraction angle; and, P is the known grating period.

The ACIS instrument response determines the distribution of PI. This information permits the calculation of an allowed range of m for each photon. If m_est is within this range, then the grating order is equal to the rounded value of m_est. Otherwise, the order is unresolved. For ACIS overlap regions, order is calculated for each region. If the order can be uniquely identified as belonging to a single region then it is resolved. Otherwise, the order is left as unresolved.

1.7. Bin into 1D spectra

Now that the data are complete with identifiers for the part of the spectrum, diffraction angles, orders, wavelengths, and counts spectra vs λ can be created. These spectra are used for further data analysis (i.e., emission line identification and flux analysis).

2. Software Solutions

Processing grating data comprised of multiple sources is a non-trivial task. Many design tradeoffs were considered in attempting to create efficient and effective analysis software. This section identifies some of the considerations taken into account when designing the gratings software.

The possibility that parts of different sources may overlap imposes a great challenge to the data analysis software. All overlapping regions need to be identified and the software must be able to decompose these regions into the component source parts. While standard IRAF region software can easily support overlapping regions of a few sources via region algebra, a mechanism is still necessary for keeping track of the source parts in a given overlap region. As the total number of regions (including overlaps) has an exponential growth (5 to the n for HETG), this method is impractical when dealing with several sources. For instance, the worst case scenario for 10 HETG sources is over 9.5 million source parts and overlap combinations to track. Realistic scenarios may contain approximately 10 sources, but these sources will typically be more spread out (i.e., Orion Trapezium).

To circumvent this problem, the software has been designed to maintain tables for all of the parts of each source (resulting in 5n tables for HETG). Photons are checked for inclusion in each table and source bits are set to indicate the sources and parts to which the photon may belong. Since the geometry of the regions being utilized is limited to circles and rectangles, the tables simply contain sky coordinate range boundaries. To save memory, the axis spanning the minimum distance for any given source part is offset to zero and utilized as the index. For cases where the instrument roll angle equals 45 degrees, the index axis is arbitrarily chosen as neither of the axes provides an advantage.

3. Future Challenges

AXAF data fields may contain multiple sources. In order to be able to detect, mask out, coordinate transform, and order sort all these sources correctly is quite a challenge. We have made the software flexible for the users to be able to specify source specific characteristics/mask widths and response matrices. We hope that these extra features will allow severely crowded fields to be scientifically analyzed in the same context as more common single source fields.

For more details on the AXAF grating flight processing software, see:
http://space.mit.edu/ASC/analysis/L1.5_overview/L15.html

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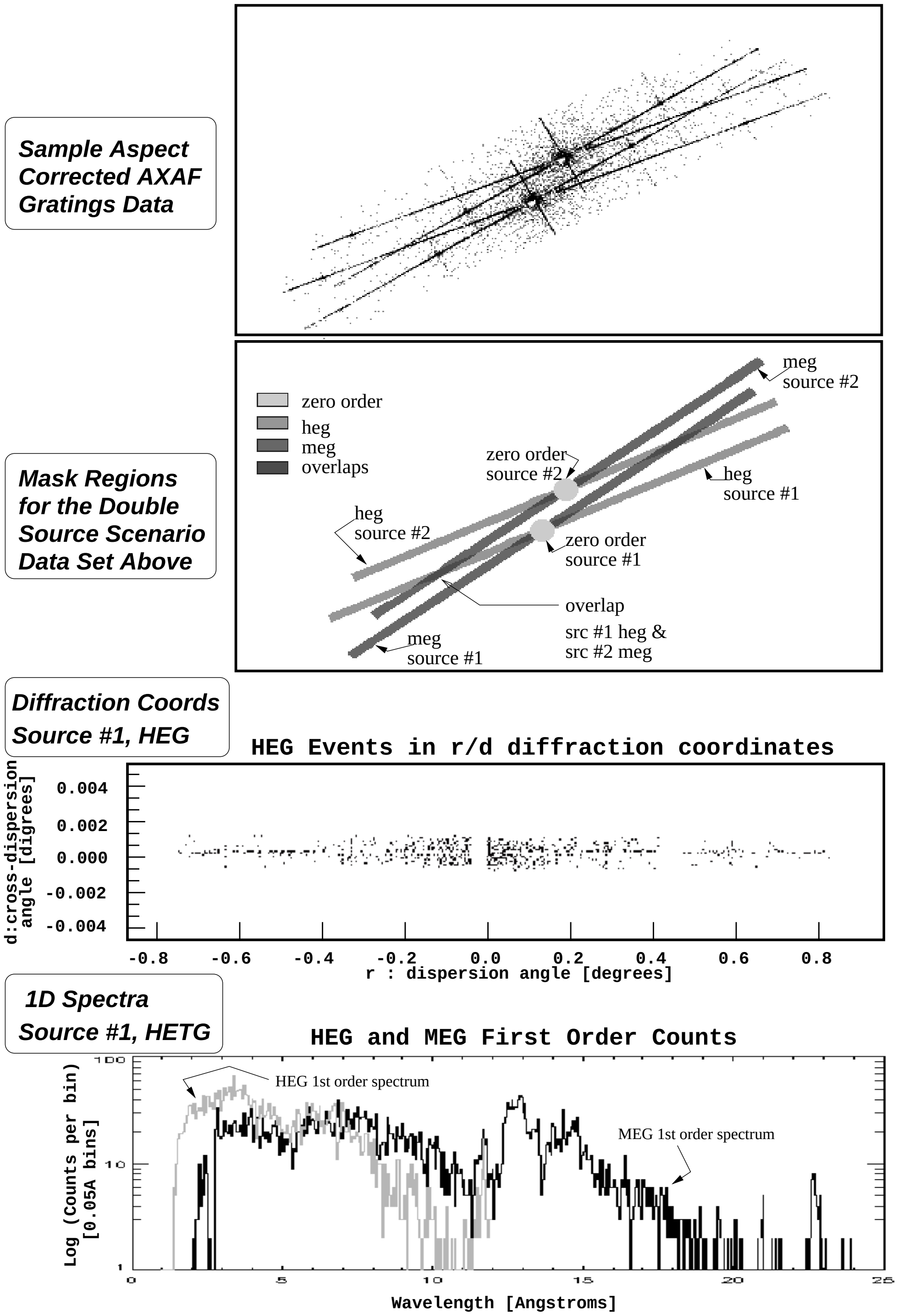

Figure 1. Cumulative look at the Processing Steps using Mock Data