Grating Response Matrices for XSPEC ...and Beyond.

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1 Introduction

An important phase of AXAF calibration at XRCF involves the use of the HXDS detectors with the transmission gratings in place. Since the MST uses XSPEC for fitting the spectra, it would be beneficial if a grating response could be incorporated into the XSPEC response. These notes provide a definition of such a response and also generalize it to accomodate imaging detectors. The extra dimensionality needed is not within the current scope of XSPEC.

An important reference, which these notes draw upon, is Chapter 2 of the "XSPEC User's Guide" available fromthe High Energy Astrophysics Science Archive Research Center (HEASARC) at Goddard Space Flight Center.

"XSPEC: An X-Ray Spectral Fitting Package, User's Guide for version 9", `http://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/u_manual.html`

An acronym list is given in Appendix A.

2 The Basic Response

X-ray telescopes transform the incident spectrum, $s(\lambda, t, \alpha, \delta)$, where λ is the photon wavelength, t the arrival time, and (α, δ) are the angular coordinates of the photon on the sky, into a distribution of counts on a detector, $c(p, t, r)$, where p is the signal from a pulse-height amplifier (PHA), t is the time, and $\vec{r}$ is the reported position on the detector.

I prefer to use wavelength (λ) instead of the "traditional" X-ray astronomy dimension of energy (E) because the gratings disperse linearly in wavelength.

If we consider for the moment an observation with a spectroscopic detector (integrated over a specific time interval and over a sky region) without the use of diffraction gratings, this transformation can be written as

$$c(p) = \int_0^\infty R(p, \lambda)\, s(\lambda)\, d\lambda. \qquad (1)$$

The quantity, $R(p, \lambda)$, represents the instrumental efficiency (including the mirror and any filters) and redistribution from wavelength into PHA — the *response*. These three terms, c, R, and s, can also be represented as discrete quantities (see the XSPEC manual, Chapter 2) and binned into vectors and matrices; the equvalent matrix equation can be written as

$$c = R\, s, \qquad (2)$$

where c and s are vectors — the former is the *pulse-height spectrum*, and the latter is the *model spectrum* — and R is the two-dimensional *response matrix*. These are *binned* (a.k.a. integrated, discrete) forms of the differential (a.k.a. continuous) distributions. The matrix form is a notational convenience; each element of c is given by the summation

$$c_p = \sum_{\lambda} R_{p\lambda} s_{\lambda}, \tag{3}$$

where the subscripts refer to their corresponding binned indices.

This is the form familiar in data analysis for most X-ray observatories to date, such as *ROSAT*, *ASCA*, and *Einstein*. Software such as *PROS* or *XSPEC* solve this equation for $s(\lambda)$ through iterative forward folding techniques, since it cannot be directly inverted due to the form of R.

3 Response with a Grating

A diffraction grating in the beam adds another redistribution, that of photon wavelength into angle and ultimately position, r, on the detector. Though we have a high resolution spectrum in the spatial domain, we still need PH discrimination, if possible, in order to order-sort. We can express the transformation from incident spectrum to counts as

$$c(p,r) = \int_0^{\infty} R(p,\lambda,r)\, s(\lambda)\, d\lambda. \tag{4}$$

For a particular spatial region centered at r_0 and of extent Δr, such as a bin defined by a slit or pinhole aperture in conjunction with an HXDS SSD or FPC detector, we integrate over the spatial bin to obtain a PH spectrum:

$$c(p;r_0,\Delta r) = \int_{\Delta r} c(p,r)\, dr = \int_0^{\infty} \left\{ \int_{\Delta r} R(p,\lambda,r)\, dr \right\} s(\lambda)\, d\lambda. \tag{5}$$

The term inside the "{}" is our response to be cast as a matrix. It can be factored into two independent terms, one for the detector and one for the grating:

$$R(p,\lambda,r) = D(p,\lambda) \int_{\Delta r} G(r,\lambda) dr, \tag{6}$$

where D is the detector's response and G is the grating's response. (Actually, the "detector" part also contains the mirror efficiency and should be written $D(p,\lambda) \rightarrow A(\lambda,\theta,\phi)D(p,\lambda)$, but for simplicity, the mirror response is left implicit.)

We can write the components of the desired response in discrete form as

$$R_{p\lambda;r_0\Delta r} = D_{p\lambda} \sum_{\Delta r} G_{r\lambda}. \tag{7}$$

The resulting spectrum of PH counts is then given by

$$c_{p;r_0\Delta r} = \sum_\lambda \left\{ D_{p\lambda} \sum_{\Delta r} G_{r\lambda} \right\} s_\lambda. \qquad (8)$$

The general form for the two-dimensional distribution of PH with position is

$$c_{pr} = \sum_\lambda D_{p\lambda} G_{r\lambda} s_\lambda. \qquad (9)$$

Spatial Information The primary purpose of the diffraction gratings is to turn a spectrum into a spatial distribution. Hence, grating data are typically not taken at a single position in the spectrum. (A notable exception is the measurement of a known bright line, for example, for the efficiency or effective area measurements with large apertures and the FPC or SSD.) If the detector is not an imaging detector, an "image" is derived by performing a stepped scan along the spectrum. If the detector is an imaging detector, we obtain counts at many different positions simultaneously. In addition, different sources may have very different spectral energy distributions, and different detectors may have very different quantum efficiencies and spectral resolutions. Thus, we need to be able to *simultaneously* model the PH and spatial distributions in order to properly assess off-band contribution from overlapping orders. HXDS slit scans may have up to 20 observations per line. For imaging detectors, we would probably choose about as many spatial bins to isolate a line or continuum region. Thus, we wish to fit about 20 PH spectra (c_p) with 20 distinct response matrices and one unique input spectrum. The BND responses (up to 7), also need to be fit with the same input model spectrum but with independent normalization. XSPEC does allow such simultaneous fitting, ***but its performance needs to be evaluated for a large number of observed spectra and responses*** and in a ***non-interactive mode!***

XSPEC's performance needs to be evaluated for a large number of observed spectra and responses in a non-interactive mode.

Some simplying approximations can probably be made. For a known model profile, we may be able to determine the model parameters from many fewer bins. Since the region in $\Delta\lambda$ is small, the response changes very slowly over the region (if there are no edges in any of the overlapping orders) and a mean response and slope may suffic to characterize the response.

3.1 Matrix Definitions and Examples

I will define the various quantities in more detail here. Only brief descriptions of already common items such as mirror effective area and detector response matrices will be given, since more detailed definitions of these are available elsewhere. Most attention will be given to the grating response.

Binning As mentioned previously, the matrices and vectors are discrete representations of continuous functions — they are *binned* quantities. For example, to obtain a spectral model vector, we define wavelength bins and integrate the continuous model over the wavelength range of each wavelength bin to obtain the array element:

$$s_j = \int_{\lambda_j}^{\lambda_j+\Delta\lambda_j} s(\lambda) d\lambda, \tag{10}$$

where I have now explicitly labeled the subscript on s with a j to emphasize the discrete nature. The units of $s(\lambda)$ are photons $\mathrm{cm}^{-2}\,\mathrm{s}^{-1}\,\text{Å}^{-1}$, and of s_j are photons $\mathrm{cm}^{-2}\,\mathrm{s}^{-1}\,\mathrm{bin}^{-1}$. Analogous integration is applied to the PH and position efficiency functions (or tables).

Mirror Response, A_λ The mirror response is commonly known as the *effective area*, since it is given in area units of cm^2. It is simply a vector, a_λ giving the bin-integrated area as a function of wavelength. Less simply, the mirror area is a function of off-axis angle and azimuth (vignetting) and solid-angle (encircled-energy).

Mirror response is known as an Auxiliary Response File, or ARF, in XSPEC.

Mirror Scattering, $\Theta_{r\lambda}$ We can represent mirror scattering, or point-spread-function (PSF), as a two-dimensional matrix, if we only consider scattering in one dimension and assume a certain acceptance function in the cross-dispersion direction. (This will be important in later definition of the grating response.) We will consider the mirror scattering matrix to be a function of wavelength and scattering angle and so it is a matrix. Each column represents a wavelength bin, and the profile down each column is the probability of deviation by a given angle vs that angle (or position, r, at some focal distance) at that wavelength. The direction we will be interested in that of the dispersion, hence the use of r for the spatial coordinate (which is proportional to the more fundamental angular coordinate).

There is no XSPEC equivalent to Θ. Instead, the mirror scattering profile is integrated into the detector response.

Detector Response, $D_{p\lambda}$ The detector response is a two-dimensional quantity (hence a matrix) describing the probability of detection and redistribution of an input photon in wavelength bin λ into pulse-height bin p. If we let the columns represent input wavelengths, then the sum of elements in any column is the QE at that wavelength, while the value vs PH bin is the line-response function (related to the spectral resolution). The units are counts photon^{-1}. If the detector response is combined with the mirror response by multiplying each column of D by the corresponding wavelength bin of A, then performing a matrix multiplication of this onto the spectrum vector acts as a convolution and transforms the wavelength spectrum into a counts spectrum (if we are not using a grating). Note that this makes assumptions about a spatial (α, δ) region and detection region $(\Delta\vec{r})$.

The detector response matrix is known in XSPEC as a Response Matrix File, or RMF.

In practice, the detector response matrix is factored into a normalized redistribution probability, $\mathcal{D}_{p\lambda}$, and the normalization, or QE, ϵ_λ; $D_{p\lambda}$ is obtained by multiplying each column of $\mathcal{D}$ by the corresponding element (λ index) of ϵ.

In XSPEC, the combination of detector and mirror responses is known as an "rsp" file, or the "response".

For a solid-state detector such as a CCD, the detector response matrix is strongly diagonal, but not necessarily sparse. CCD's have escape peaks, low energy tails, fluorescence, and other effects which fill in the matrix with low-level values. For the BND FPC detectors, the resolution is lower and the diagonal band is broader. For HRC or HSI, there is little or no PH resolution, so the matrix is nearly singular (rows identical).

Grating Response The grating response is the new structure. It defines the diffraction efficiency and spatial redistribution.

Efficiency The efficiency is a function of wavelength and diffraction order, as well as many other parameters, such as the bar geometry, material, and support material. Efficiency is not necessarily symmetric with respect to positive and negative orders. It is a major calibration effort to measure and model this efficiency as accurately as possible.

Programs in IDL and C, exist for calculating efficiency.

Position The position redistribution is described by the grating equation,

$$
\begin{aligned}
m\lambda &= P(\sin\theta_d + \sin\theta_i) && (11)\\
&\approx P\sin\theta_d && (12)\\
&\approx (P/X_{\mathrm{Rowland}})r, && (13)
\end{aligned}
$$

where m is the diffraction order (an integer), λ the photon wavelength, P the grating mean period, θ_d the diffraction angle, θ_i the photon angle of incidence onto the facet, X_{Rowland} the Rowland diameter (or grating node to detector distance), and r the diffraction distance at a distance equal to X_{Rowland}. (This is the one-dimensional form of the diffraction in the dispersion direction. A full 3-D formulation also incorporates other terms, such as the grating bar direction and all tilts.) The positional blur, or resolution, is defined by the grating period distribution within and between facets (LSF) and by the mirror blur (PSF) in the dispersion direction. The grating PSF is independent of wavelength. (Other grating terms also apply, but the period distribution is a major term in the budget.)

For a detailed 3-D formulation of grating coordinates, see the memos by J. Davis for the forward transformation (in draft), and by D. Huenemoerder for the inverse transformation ("AXAF Transmission Grating Diffraction Coordinates", D. Huenemoerder, 2 April, 1996).

The Grating Matrix A grating response matrix can be defined which is analogous in form to the detector response matrix. Columns represent wavelength bins, but the rows are now position bins instead of PH bins. The matrix is comprised of many narrow bands, one for each order, and progressively steeper for higher orders. The matrix is also very sparse. Matrix multiplication of this onto a spectrum model vector tranforms the spectrum into counts versus position, but with the counts at each position originating from many orders coming from different wavelengths in the spectrum.

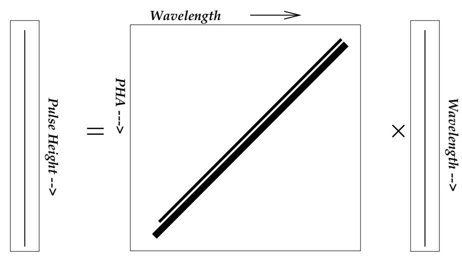
The grating response could be factored into normalized redistribution and efficiency terms as the detector response is. However, this is of less practical use for the grating response because the efficiency is no longer a single vector, but a unique function for each order.

We can incorporate one dimension of the mirror PSF into this array. Each column of the array must be convolved with the corresponding column of the mirror scattering matrix in the same direction. The mirror term is energy dependent.

4 Graphical Examples

It is helpful to view the transformations in tableaus of the matrices and their operations. It should be remembered that matrix notation is shorthand for summations, and that matrices can be represented as a collection of vectors. The size will be discussed in the next section.

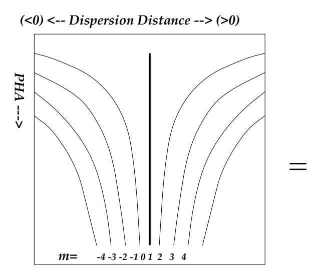
Without a grating, we have the usual non-dispersive spectrometer relation described by equation 2. It can be diagrammed as



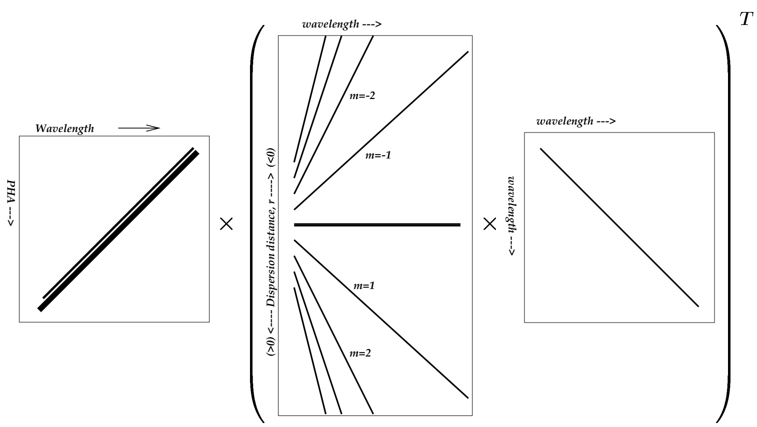
$$c_p = \quad R_{p\lambda} \quad \times s_\lambda .$$

The matrices are arranged in the standard mathematical way with the origin in the upper left corner (or top if a vector). Matrix multiplication goes across the row of the left operand and down the columns of the right operand.

We can write a matrix equation for the case with the grating if we express the spectrum as a diagonal matrix. This is a mathematical artifice which allows us to use a series of matrix multiplications to transform into a two-dimensional space of PH and position.



$$c_{p\lambda} =$$



$$D_{p\lambda} \times \left(G_{r\lambda'} \times S_{\lambda'\lambda}\right)^T .$$

This matrix equation is the equivalent of equation 9. The result on the left-hand-side is a schematic of what one would observe with a grating and an imaging spectroscopic detector. Each hyperboloidal band represents an order; $r = 0$ is at the center, and near it in either direction are small wavelengths with higher energy and hence greater PH values than at large r. (The bands would, of course, have a width in the vertical direction proportional to the detector PH resolution.) A non-spectroscopic detector such as HRC would observe this distribution collapsed along the PHA direction onto the r-axis — orders overlap in position. Conversely, the projection along the other axis would yield a low-resolution PH spectrum.

A small-aperture detector would sample some small range in r and yield a PH-spectrum over that range; that is what equation 8 represents.

$$c_{p;r_0\Delta r} = \sum_{\lambda} \left\{ D_{p\lambda} \sum_{\Delta r} G_{r\lambda} \right\} s_{\lambda} \quad (8)$$

This treatment of the response is not directly amenable to use in XSPEC, since we have coupled the spectrum to the grating response — in effect as far as XSPEC is concerned, we have altered the model. In order to simultaneously fit the same model spectrum to both focal-plane and BND detectors, these must be decoupled. It can be shown through the rules of matrix multiplication that the operations in this tableau are exactly identical to the summation shown in equation 9.

$$c_{pr} = \sum_{\lambda} D_{p\lambda} G_{r\lambda} s_{\lambda} \quad (9)$$

5 Issues: Cross-dispersion spatial information

All the proceding discussion has ignored the spatial distribution in the cross-dispersion direction. This distribution comes from several sources: the mirror PSF, grating astigmatism, finite facet size effects, facet mis-alignments, LETG support structure cross-dispersion, for examples. These cannot be ignored. But if they can be calibrated, they can be integrated in the responses, such that the response represents some observation "aperture" in the cross dispersion direction (or aperture function, to allow the size to change with position). When response matrices are generated, the generating function must integrate over some cross-dispersion aperture (and duly record the parameters in a header).

6 Issues: Optimized Gridding for Model Spectra

In order to accurately model the higher diffraction orders of a predicted spectrum, the input model spectrum must have sufficient resolution to properly represent detector sampling. A grid which matches the first order spectrum will be undersampled in higher orders. A short wavelength bin in third order will be three times the width. We would like that width to match the detector pixel size (or oversample it by some small factor).

If the grid were set to match the highest order to be considered, then the input spectrum would have a very large number of grid points. This is unnecessary, since much of the spectrum is diffracted to distances greater than the length of the detector. I describe a grid which has increasingly finer resolution at progressively shorter wavelengths. The grid spacing is discontinuous at boundaries where the next higher order will fall off the detector.

Gridding can be done as follows:

- From L to $L/2$, (where L is the approximate length of the spectrum on the detector as measured from the zero-order location) grid at the first order resolution (essentially the detector pixel size, possibly oversampled a bit).

Offset pointing will require some deviation from the typical array size.

- From $L/2$ to $L/3$, grid at half the first order bin-size.
- From $L/3$ to $L/4$, grid at one-third the first order bin-size.
- ... From $L/(M-1)$ to L/M, grid at $1/(M-1)$ the first order bin-size.

In general, let n_m be the number of grid points for order m, and n be the number of grid points required to span from $\lambda = 0$ (the zero-order centroid) to L at the first order resolution. Then,

$$n_m = nm \left\{ \frac{1}{m} - \frac{1}{m+1} \right\} = \frac{n}{m+1}.$$

Thus the total number of grid-points required is:

$$N = n \sum_{m=1}^{M} \frac{1}{m+1} = n \left\{ \Psi(2+M) - 1 + \gamma \right\},$$

where $\Psi(x)$ is the digamma function, γ is Euler's constant, and M is the maximum order to be considered for optimum gridding.

This is a diverging but slowly increasing function. For M of 10, 20, and 30, N is $2.0n$, $2.6n$, and $3.0n$, respectively. (If the spectrum were gridded at the highest resolution required, N would scale directly with M.)

Given some reasonable M (such as 30 for LETGS), the minimum wavelength grid point calculated as outlined above will still be above the minimum needed for model spectra. As a reasonable compromise, the grid step from that for $m = M$ to the lowest wavelength of the model can be constant at the finest resolution.

This gridding scheme strongly ties the discrete model spectra binning to the instrumental configuration and the maximum orders to be considered. For example, LETGS gridding will be different from HETGS due to the different detector lengths, grating periods, and pixel sizes. (HEG and MEG can both use an MEG grid which equally samples or slightly oversamples the optimal HEG grid.)

6.1 Examples

I have an IDL procedure, `wave_grid.pro`, which constructs vectors of bin centers and bin sizes for use in model generation. The usage, which illustrates the parameters, is as follows:

```
wave_grid, WavMin, Len, PixSize, OverSampl, TG_Period,
X_Rowland, MaxOrd, WavCtr, WavBinSize
```

Input variables:

WavMin: Minimum wavelength for output array, in Angstroms.

Len: Approximate length of detector array, from zero-order to outer limit, in mm.

PixSize: Pixel size of the array in mm (not necessarily a resolution element.

OverSampl: Amount of oversampling of pixels of size PixSize (e.g., if dithering gives half-pixel resolution, then specify OverSampl of 2); value is factor to divide PixSize by. (If coordinates are already oversampled, then specify value of 1.)

TG_Period: Period of the diffraction grating, in Angstroms.

X_Rowland: Rowland diameter of the grating in mm. (canonically 8635 mm, but larger at XRCF — about 8800 mm)

MaxOrd: Maximum order to consider.

Output variables:

WavCtr: Array of bin central wavelengths (in Angstroms).

WavBinSize: Array of bin full widths, corresponding to the WavCtr bins (in Angstroms).

For AXAF TGS, typical parameters are shown in the table.

Table 1: TGS model spectra gridding parameters

Parameter	LETGS	HETGS
WavMin	1.0	1.0
Len	160.	80.
PixSize	0.024	0.024
OverSampl	1	1
TG_Period	9921	4000
X_Rowland	8635	8635
MaxOrd	25	12
WavCtr length:	24,512	9,256

For some applications, it may be advantageous to consider only a small portion of a spectrum, say around some lines of interest.

However, the model must consider not only the region of interest, but the corresponding wavelength regions which when diffracted into higher orders will overlap the region of interest. I have another IDL function, `sub_wave_grid`, which will take an optimized broad-band grid and return indices for the overlapping chunks. When orders overlap, it concatenates the regions together. This chunky grid can be used to construct a chunky, optimally gridded spectral model of the region of interest which will include the overlapping orders. It's call is:

```
chunks=sub_wave_grid(WavReg, MaxOrd, WavCtr, WavBinSize).
```

`WavReg` is a two-element vector specifying the minimum and maximum wavelengths of interest, and the other parameters are as described above. The result, `chunks`, is a 2-D array of dimensions two by number-of-chunks giving the minimum and maximum array indices of `WavCtr` for each chunk.

Utility of `sub_wave_grid`, however, is questionable. Simulated zero-order pulse-height spectra cannot be properly interpreted. Array-size savings are not large. Chunk-gridding for LETGS 125-135 Å, for example, gives a 9926-element grid, which is less than a factor of three smaller. For HETGS 18-23 Å (O VII and O VIII lines), gives less than a factor of two.

6.2 Relevance to XSPEC

XSPEC regrids model spectra in accordance to the response matrix. If a model were defined and a simultaneous fit performed on both the focal-plane detection of a grating observation and the BND low-resolution monitor, the same spectrum could be used. The BND response matrix would specify a coarse gridding, and the focal plane an optimized gridding.

7 Issues: ACIS, HRC observations

The high spatial resolution of ACIS-S and HRC-S present new challenges to fitting and analysis of grating spectra. In effect, each spatial bin requires a new response matrix, if done in the XSPEC model. However, equation 9 is straightforward. We need a fitting engine which can handle this two-dimensional distribution.

$$c_{pr} = \sum_{\lambda} D_{p\lambda} G_{r\lambda} s_{\lambda} \tag{9}$$

8 Issues: Quick and Dirty Gratings Reponses for XSPEC

For many planning and simulation purposes, it is not necessary to have the full PHA-spatial event distribution. Instead, we can define first order or many-order response matrices which could be used in XSPEC to simulate HETGS or LETGS spectra. XSPEC need not know that the output bins defined by the matrix represent spatial position instead of PHA. Grating and mirror effects could be incorporated to simulate the spectral resolution (but not properly for each order of overlapping orders). The detector QE could be treated as an additional "ARF" and multiply the mirror "ARF".

Suitable normalizations would allow the same 4-shell mirror area file defined for typical imaging observations to be used with each grating area (MEG needs only HRMA shells 1 and 3, HEG 4 and 6). For example, the MEG first-order efficiency would be scaled by $(A_1 + A_3)/(A_1 + A_3 + A_4 + A_6)$, where A_n is the effective area of HRMA shell n.

The set of files needed would be:

- HEG first order ("RMF")
- MEG first order ("RMF")
- LEG first order ("RMF")
- LEG all orders ("RMF")
- HRMA area ("ARF")
- ACIS QE ("ARF")
- HRC QE ("ARF")
- ACIS QE and resolution ("RMF") (for "traditional" use)
- HEG+MEG zeroth order ("ARF")
- LEG zeroth order ("ARF")

The HEG, MEG, and LEG "RMF" files would be constructed by combining the mirror and grating line profile with the grating efficiency as outlined in Section 3.1, but for selected orders only: $m = +1$ for MEG and HEG, $m = 0$ for HEG, MEG, and combined HEG and MEG (since they overlap spatially with all HRMA shutters open), $m = +1$ for LEG, and $m = 1, 2, ..m_{max}$ for LEG. FTOOLS allow RMF and ARF files to be multiplied into an RSP file, so any desired combination for grating and detector can be constructed (within the basic set).

A Acronym List

Acronym	Definition
ADU	Analog-to-Digital Unit
ASCA	Advanced Satellite for Cosmology and Astrophysics
ARF	Auxiliary Response File (typically QE(E))
AXAF	Advanced X-Ray Astronomical Facility
BND	Beam Normalization Detector
CCD	Charge Coupled Device
FPC	Flow Proportional Counter
HRC	High Resolution Camera
HSI	High Speed Imager
HRMA	High Resolution Mirror Assembly
HXDS	HRMA X-Ray Detector System
LSF	Line Spread Function
MST	Mission Support Team
PH	Pulse Height
PHA	Pulse Height Analyzer
PROS	Post-Reduction Offline System
PSF	Point Spread Function
QE	Quantum Efficiency
RMF	Response Matrix File (typically normalized redistribution matrix)
RSP	ReSPonse file (typically RMF time ARF)
SSD	Solid State Detector
TGS	Transmission Grating Spectrometer
XRCF	X-Ray Calibration Facility
XSPEC	X-ray spectroscopy software (a mnemonic masquerading as an acronym)

B Document History

Original version: 9-11 March 1996

Update: 28 March 96 Incorporated substantial comments from D. Dewey and H. Marshall.