Chandra X-ray Center

Data Product Interface Document: mkgrmf LSF Input Data

Revision 1.0.0—04 Feb 2021

version	author
1.0.0	H. M. Günther
0.2.1	David S. Davis
0.1.2	David S. Davis
0.1.1	David S. Davis

To: Jonathan McDowell, SDS Group Leader
Janet DePonte Evans, DS Software Development Manager
Dale Graessele, CALDB manager

Document and Change Control Log			
Date	**Version**	**Section**	**Status**
19 Mar 2001	0.1.0	all	Initial Draft
23 Apr 2001	0.1.1	all	Format Changes
02 May 2001	0.1.2	all	Four columns added
21 Sep 2001	0.2.0	all	Revised
28 Dec 2001	0.2.1	all	Revised
15 Jan 2021	1.0.0	all	Bring definitions of functions in line with CIAO practice, add ACIS-I and HRC-I as detectors. Address Defocus.

Contents

1 Introduction **1**
1.1 Purpose . . . 1
1.2 Scope . . . 1

2 Applicable Documents **1**

3 Functional Description **1**
3.1 Data Content Summary . . . 1
3.2 Recipients and Utilization . . . 2
3.3 Pertinent Relationships with Other Interfaces . . . 2

4 Assumptions and Constraints **2**
4.1 Products Not Covered . . . 2
4.2 Substructure Definition and Format . . . 2

5 Access **2**
5.1 Access Tools; Input/Output Protocol . . . 2
5.2 Retrieval from the CALDB . . . 2

6 The File Structure for the Grating LSF Data **3**
6.1 File Names . . . 3
6.2 Column Descriptions . . . 3
6.2.1 Comments on the Columns . . . 3
6.3 Allowed Functional Forms . . . 4
6.4 Normalization of components . . . 5
6.5 Size Estimates . . . 5

7 FITS Header Templates **5**
7.1 Content description and observation component . . . 5
7.2 CALDB keywords . . . 6

1 Introduction

This document describes the interface to be employed in accessing the PSF Library products, according to the requirements stipulated in Applicable Document 3.

1.1 Purpose

The purpose of this document is to define the input data for the Line Spread Function (generically referring to LSF) Library to be used in Level 2 processing for the grating RMF generator (mkgrmf).

1.2 Scope

This interface shall apply to all Grating specific LSF data products used by the tool `mkgrmf` and distributed to the CXC Data Archive during the course of the Chandra mission.

2 Applicable Documents

The Applicable Documents required for background and detail on grating products are as follows:

1. AXAF Data Products Guide:
   `https://cxc.cfa.harvard.edu/ciao/data_products_guide/`

2. AXAF Coordinate Systems:
   `https://cxc.cfa.harvard.edu/ciao/manuals.html` (see section General - Chandra Coordinate Systems)

3. ASC AMO-2400 (SE03):
   ASC Data System Requirements (ASC.302.93.0008)

4. ASC AMO-2401 (DS01)
   ASC Data System Software Design (ASC.500.93.0006)

5. HEASARC FITS Standards:
   `https://heasarc.gsfc.nasa.gov/docs/heasarc/ofwg/ofwg_recomm.html`

6. ASC FITS File Designers' Guide:
   `https://cxc.cfa.harvard.edu/contrib/arots/fits/ascfits.ps`

7. HEASARC FITS CALDB Standards:
   `https://heasarc.gsfc.nasa.gov/docs/heasarc/caldb/caldb_doc.html`

8. AXAF CALDB Architecture
   `https://cxc.cfa.harvard.edu/caldb/index.html`

3 Functional Description

3.1 Data Content Summary

All Grating LSF Library files shall consist of data files conforming to the FITS format (Applicable Document 5). These files contain header keyword entries and binary table (BINTABLE) extensions. These files will contain a primary header, possibly null, followed by a set of binary tables as described in Applicable Document 6. In addition, these files will conform to the HEASARC CALDB conventions (Applicable Document 7) and have CONTENT, EXTNAME, and HDUCLASS keywords that conform to Applicable Document 8.

3.2 Recipients and Utilization

The primary recipients, via distribution from the archive, of the LSF Library are Chandra observers, who will utilize these data products for scientific data analysis. The CXC may also make use of specific LSF Library data products for instrument calibration, instrument and/or spacecraft monitoring and trends analysis, and validation and verification of the Level 0, Level 1, and Level 1.5 software and of the data products themselves.

3.3 Pertinent Relationships with Other Interfaces

Changes to the definition of CXC FITS, as described in Applicable Documents 6, may affect the format of the PSF data products described in the current document.

4 Assumptions and Constraints

It is assumed that these products are placed into an exportable calibration database (CALDB) for users.

4.1 Products Not Covered

PSF products that are used for maintenance and diagnostic purposes (those that are not supplied to the user for scientific data analysis), or which are generic AXAF Level 2 products, are not currently included within the interface defined by this document.

4.2 Substructure Definition and Format

The header components for the primary header and all binary table extensions are defined and listed in the Applicable Documents. In general, the column or row numbers in the example FITS headers are arbirary unless otherwise indicated. It is the column name and its attributes that specify the requirment. Additional columns not specified here may be added to the file also long as they do not violate the interface. Software used to process the data can ignore the additional columns, copy them to the output file, or optional use them for data processing. Likewise, HDU order is arbitrary, except for the primary HDU which must be first. HDUs are intended to be referenced by name, not position.

5 Access

5.1 Access Tools; Input/Output Protocol

Since LSF Library products obey the formatting rules described in Applicable Documents 6, they may be accessed by any software that conforms to those standards, including all versions of the FITSIO libraries that support the BINTABLE extension. In addition, since they adhere to HEASARC standards (Applicable Document 5), LSF data product files are compatible with the input/output routines that constitute the CXC data interface.

5.2 Retrieval from the CALDB

The LSF input data isassumed to be placed in the CALDB, and the CALDB specification determines keywords and other pertinent information required for this purpose (Applicable Document 8 and any subsequent updates). To help read the FITS file headers though, a few informational remarks are in order:

- For the HRC, the DETNAM is set to either HRC-I or HRC-S. On the other hand, for ACIS, the DETNAM is not one of the columns that the CALDB uses. Instead, the SIM_Z values is used to distinguish between ACIS-S and ACIS-I.
- LSFs calculated with different settings of RAND_TG can be stored in different files with different applicable keywords, such that the correct version can be retried from the CALDB by the user.

6 The File Structure for the Grating LSF Data

This section describes the LSF parameter library which is a FITS file containing the LSF fit parameters for the Chandra gratings. Each file will contain the parameters for one grating type. The * in the table below denotes the ASC principal HDU.

HDU	HDU Type	EXTNAME	EXTVER	CONTENT	HDUCLAS1	HDUCLAS3	Description
0	NULL	...	...	...	...	...	...
1 (*)	BINTABLE	MEG	1	LSF_PARAM	RESPONSE	LSF	LSF coefficients

Table 1: File structure for the table with the LSF fit coefficients

6.1 File Names

The filename convention shall be

$$\{det\}\{grat\}\{order\}D\{date\}lsfparmN\{version\}.fits$$

where $\{det\}$ is one *aciss*, *hrcs*, *acisi*, or *hrci* and $\{grat\}$ is one of *leg*, *meg*, or *heg*. $\{order\}$ gives the diffraction order of the grating. Negative orders are prefixed with "-"; positive orders have no sign, i.e. "-1" and "1" are the negative and positive first diffraction order, respectively. $\{date\}$ follows the date convention in Applicable Document 6.

As an example the lsf file for the HRC-S using the LETG grating should be of the form `hrcsleg1D1999-07-22lsfparmN0000.fits` while the file for the MEG using ACIS-S should be `acissmeg1D1999-07-22lsfparmN0001.fits`.

6.2 Column Descriptions

Multiple parameter sets are allowed for 8 and 9. So for instance, LSFs descrbied by two Gaussian components will have columns named GAUSS1_PARM and GAUSS2_PARM. Also, n is the number of wavelengths, m is 3×n, and k is 3×n×NUM_WIDTHS.

6.2.1 Comments on the Columns

The `NUM_WIDTH` column give the number of widths for which the LSF was extracted and tabulated. In the current incarnation this value is three for the MEG and HEG files. For the LETG only one width is currently implemented.

The `WIDTH` column gives the width, in degrees, of the extraction region used to extract the LSF data. The next column gives the number of wavelengths at which the LSF is tabluated. Currently these must be the same for each extraction width and are assumed to be in angstroms. The columns `TG_LAM_LO` and `TG_LAM_HI` give that lower and upper wavelength of the box that was used to extract the LSF data. The `LAMBDA` column gives the wavelength of the peak position of the LSF.

The encircled energy fraction is tablulated in the `EE_FRAC` column. The vector column containing the EE_FRAC is a 2-dimensional vector with the ee_frac for each wavelength as a vector and additional rows are for the ee_frac for each different width as defined above. This means that the dimensionality of the vector will be num_lambdas × num_widths.

The columns for the fit parameters shall be a matrix of n×j×k where n is the number of parameters and their order is

1. gauss_parms(0,j,k) = Gaussian amplitude,
2. gauss_parms(1,j,k) = Gaussian σ in Å,
3. gauss_parms(2,j,k) = peak position in Å.

#	TTYPE	TUNIT	TFORM	TLMIN	TLMAX	Comment
1	NUM_WIDTHS		I	0	TBD	Number of Extraction Widths
2	WIDTH	Degrees	3E	0	TBD	Extraction Width
3	NUM_LAMBDAS		J	0	TBD	Number of wavelength points
4	TG_LAM_LO	Angstroms	nD	0.0	TBD	Low wavelength of the extraction region
5	TG_LAM_HI	Angstroms	nD	0.0	TBD	High wavelength of the extraction region
6	LAMBDAS	Angstroms	nD	0.0	TBD	Input Photon Wavelength
7	EE_FRACS	N/A	mD	0.0	1.0	Encircled Energy fraction
8	GAUSS*i*_PARMS	N/A	kE	N/A	N/A	vector containing Gaussian parameters
9	LORENTZ*i*_PARMS	N/A	kE	N/A	N/A	vector containing Lorentzian parameters
10	THETA_MIN	degrees	E	0	N/A	min off-axis angle
11	THETA_MAX	degrees	E	0	N/A	max off-axis angle for which this is valid
12	PHI_MIN	degrees	E	0	N/A	min azimuthal angle for which this is valid
13	PHI_MAX	degrees	E	0	N/A	max azimuthal angle for which this is valid
14	SIM_X_MIN	mm	E	-9	+10	minimum SIM_X (focus) for which this is valid
15	SIM_X_MAX	mm	E	-9	+10	maximum SIM_X (focus) for which this is valid

Table 2: Binary table with the LSF fit coefficients

The number of elements is given by j and the maximum value of j is NUM_LAMBDAS. The number of widths is given by k. The function parameters at a given j must be for the wavelength range TG_LAM_LO(j) and TG_LAM_HI(j) and the maximum value of j is given by NUM_WIDTHS.

For the Lorenzian parameters the order of the parameters in the matrix shall be

1. lorentzian_parms(0,j,k) = Lorentzian amplitude,
2. lorentzian_parms(1,j,k) = Lorentzian FWHM in Å,
3. lorentzian_parms(2,j,k) = peak position in Å,

with the j, k obeying the convention for the Gaussian parameters above.

6.3 Allowed Functional Forms

The functional forms that are allowed for the LSF in mkgrmf are currently a Gaussian and a Lorentzian.

$$G(r) = \frac{A}{\sqrt{2\pi\sigma^2}} e^{\frac{-(r-r_0)^2}{2\sigma^2}} \tag{1}$$

where A is the amplitude, σ is the Gaussian width in angstroms and r_0 is the peak of this component of the LSF.

$$L(r) = \frac{A}{2\pi} \frac{FWHM}{(r-r_0)^2 + \left(\frac{FWHM}{2}\right)^2)} \tag{2}$$

where A is the amplitude, r_0 is the peak position of the Lorenztian component in questions, which need not be the same any of the other compoments, and $FWHM$ is the full width of the line profile at half the maximum.

6.4 Normalization of components

All Gaussian and Lorentzian components have an ampitude defined in their parameters. However, the total normalization of each RMF is given by the `EE_FRACS` column. That means that for LSFs defined by just a single component, the given component amplitude is arbitrary. For LSFs with multiple components the amplitude of each component only matters in a relative sense: After adding up all LSF components, the LSF is normalized such that the sum over all channels is the number given in the `EE_FRACS` column. If, for example, all amplitudes A are doubled but the `EE_FRACS` values is constant, the resulting LSF does not change.

6.5 Size Estimates

The ASC primary extension of each file will have 15-20 columns to describe the LSF parameters at each energy (depending on how many components are used). The vector columns are real floating point numbers so the size of the file can be estimated by the number of entries $\times$ 11 (the number of vector columns). So for a typical MEG LSF file with $\sim$2500 entries the size of the data area should be 30-50 MB.

7 FITS Header Templates

The following header sections are examples, based on the ASC FITS file specification and the format of CALDB v4. The following header sections have been taken from the ASC FITS file specifications. The example FITS headers given here are examples only, the column numbers, axis numbers, and keyword values are *not* necessarily those in the LSF data files.

7.1 Content description and observation component

```
CREATOR = 'makelsftable.py'    / Version 1.0 by H. Moritz Guenther
DATE    = '2004-03-19T21:55:51' / file creation date (YYYY-MM-DDThh:mm:ss UTC)
CONTENT = 'CDB_LEG_LSFPARM'    /
HDUCLASS= 'ASC     '           /
HDUCLAS1= 'PARAMETERS'         /
HDUCLAS2= 'PSF     '           /
HDUCLAS3= 'LSF     '           /
TELESCOP= 'CHANDRA '           /
FILTER  = 'NONE    '           /
GRATING = 'LETG    '           /
GRATTYPE= 'LEG     '           /
TG_M    =                    1 /
ORDER   =                    1 /
SHELL   = '1111    '           /
RAND_TG =              0.00000 /
DETNAM  = 'ACIS-S  '           /
INSTRUME= 'ACIS    '           /
CCLS0001= 'CPF     '           /
CDTP0001= 'DATA    '           /
CCNM0001= 'LSFPARM '           /
CVSD0001= '1999-07-22T00:00:00' /
CVST0001= '00:00:00'           /
CDES0001= 'LEG line spread function, input for mkgrmf' /
```

7.2 CALDB keywords

```
CBD10001= 'ORDER(1)'
CBD20001= 'RAND_TG(0.0)'
CBD30001= 'SHELL(1111)'
CBD40001= 'SIM_Z(-206.8000030518:-174.1999969482)mm'
CBO10001= 'GRATING(LETG)'
CBO20001= 'GRATTYPE(LEG)'
CBO30001= 'TG_M(1) '
FDLT0001= 0.0000000000000E+00 / Calibration fidelity or precision
CAL_QUAL= 0 / Calibration quality 0-5 integer
```