Chandra PSF Library

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1. INTRODUCTION

The Chandra X-Ray Observatory (Chandra) produces sharper images then any other X-ray telescope to date and therefore provides an opportunity for high-angular and spectral resolution studies of X-ray sources. Crucial to these studies is the knowledge of the characteristics of the Point Spread Functions (PSFs).

A standard set of simulated Chandra PSFs covering the field of view of the detectors is available to the users for data analysis via the standard PSF library files. In addition to these standard PSF libraries, the user may construct their own library files as long as the FITS HDUs and PSF images conform to the general structure (described later in this document).

The standard PSF library files consist of two dimensional simulated monochromatic PSF images "postage stamps" (energies ranging from 0.277 keV to 8.6 keV), stored in multi-dimensional FITS images (hypercubes) with azimuth and elevation steps (in telescope fixed system) of either 1 arcminute or 5 arcminutes. The user can extract the desired PSF model image from a library file by interpolating within the energy and off-axis angle grids, using the Chandra Interactive Analysis of Observations package (CIAO) tool **mkpsf**. The usage of the current PSFs libraries for a detailed spatial/spectral analysis has limitations mainly due to the coarse energy and spatial grids, especially for large off-axis angles. We highlight some of the limitations and caveats at the end of this document.

In the following we describe how are the PSF models generated and the design and content of the Chandra PSF library files.

2. CHANDRA PSFs

The Chandra high-angular resolution is mainly a result of the innovative design of this observatory, including the guidance systems, the mirror assembly (High Resolution Mirror Assembly, or HRMA), and the science instruments. The detectors' pixel size and resolution are well matched to capture the sharp images formed by the mirrors and to provide information about the incoming X-rays: their number, position, energy and time of arrival. The current spreading of the point source images due to residual aspect is well below detectors' pixel sizes (0.49200 arcsecond for ACIS-I and ACIS-S, and 0.13175 arcsecond for HRC-I and HRC-S).

The shape and size of the HRMA PSFs vary significantly with source location in the telescope field of view (FOV), as well as with the spectral energy distribution of the source. Figure 1 shows the 85% encircled energy diameter as a function of off-axis angle and energy. Because of the Wolter Type I design, the image quality is best in a small area centered about the optical axis. In fact, the mirrors were designed to produce images with better than one arc-second resolution; in particular to concentrate better than 85% of the energy at 0.277 keV within a 1" diameter. This is why a substantial pre- and post-launch effort was directed at creating a faithful model of the HRMA's mechanical and optical systems (Jerius at al 2000, Proc. SPIE 4012; http://asc.harvard.edu/cal/Hrma/hrma/psf).

The simulated Chandra PSFs used in the standard PSF library files are generated in two steps:

- (1) ray files are generated using SAOsac, a ray-trace code which models the interaction of photons (rays) passing through the HRMA (Jerius et al 2000).
- (2) PSF model images are made by projecting these rays to the detector surface and then creating images with pixel sizes smaller than the pixel sizes of the detectors.

We note that the choice of providing PSF images (rays projected on detectors' planes) to the user rather then ray files was based mainly on the fact that the size of the individual ray files (e.g. 14 Mb *per* ray file for a 10⁵ photons simulation) is much larger than that of the images (e.g. 0.2 Mb *per* image).

The software used to generate the rays for the PSF images in the current version of CIAO CALDB 2.0 standard libraries is the trace-shellz3 driver script, and several other SAOsac routines. This software includes the multi-layer reflectivity and uses the HRMA model configuration orbit_XRCF+tilts_02. This HRMA model includes the following major changes when compared to the model configuration orbit_HDOS+HATS+XRCF_scat-970220_03 used to generate the previous set of PSF library files (released with CIAO 1.0):

- a new set of mirror surface scattering coefficients
- a new set of optical constants, derived from synchrotron results including a contamination layer on the witness flats
 - modeling of the optics' surfaces as multi-layers
 - inclusion of an extra tilt in mirror shell 6, as determined from testing at the XRCF

Figure 2 shows examples of the HRC-I PSF variation as a function of off-axis angle.

The improved HRMA model allows a better definition of the morphology of the PSFs as a function of off-axis angle and energy, a better estimate of the encircled energy, as well as a better understanding of HRMA induced distortions in the images of the observed

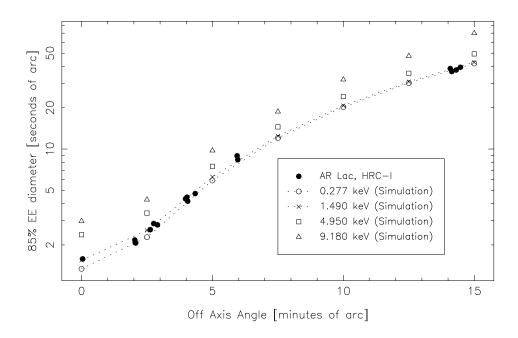


Fig. 1.— Observed and simulated 85% encircled energy diameters from Jerius et al 2000 .

sources. This is important for more accurate detection of the sources, and it will preclude misidentification of PSF-related structures as structures intrinsic to observed source. However, the calibration of the HRMA PSF, especially the wings) is an ongoing effort (see for example: http://asc.harvard.edu/cal/Hrma/hrma/psf).

Depending of the desired signal-to-noise in the individual PSFs, the number of rays used in the raytracing of the PSFs can vary. For efficiency reasons, the raytraces do not normally discard rays which may have been absorbed by the optics; instead rays are assigned weights which are the product of the reflection probabilities at each optical surface. The weight of the ray at the focal plane is thus the total probability that it would have reached it. We use the weights to normalize the individual PSF images, and they are included in the PSF library files (note: the current version of mkpsf does not include an option of directly retrieving the weights. The option will be added in a later release).

We describe in the following section the general design of the PSF library and the content of the standard set of PSF library files.

3. CIAO PSF LIBRARY

3.1. General PSF Library Definition and Format

The PSF library general format is summarized in Table 1:

The HDUs in PSF data FITS files		
HDU	Type	Description
Primary array	1	hypercube
IMAGE extension	2	SUMRCTS image (optional)
BINARY table	3	Irregular coordinate definitions (as many as needed; optional)

Table 1: Single hypercube self-contained PS F

HDU type 1 – **the PSF image:** - These are n-dimensional images, hypercubes primary array) that extend along a minimum of five coordinates. The known coordinate axes are:

1 - spatial x-direction of the PSF image (PSFX)

m - spatial y-direction of the PSF image (PSFY)

X - spatial x-direction offset coordinate (DETX)

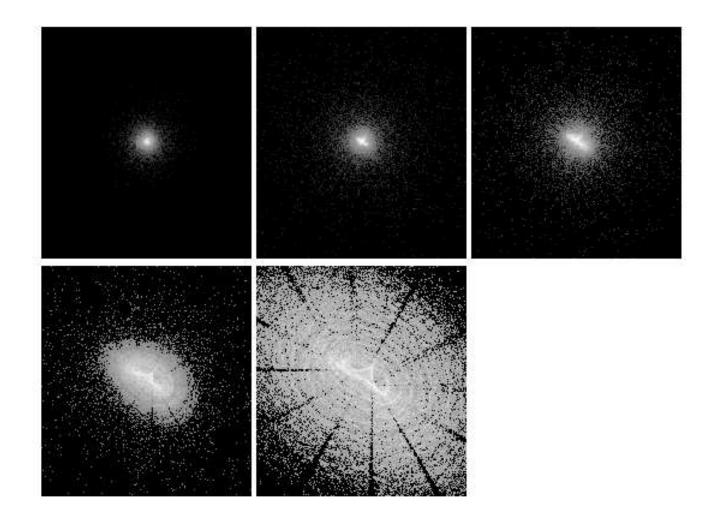


Fig. 2.— Examples of simulated PSFs for the HRC-I instrument at 1.4967 keV as a function of off-axis angles (log display); clockwise from the top off-axis angles: 0 (on axis), 1.5', 3', 6', and 12'. The size of the FOV is about 0.5'.

Y - spatial y-direction offset coordinate (DETY)

E - energy (ENERG)

f - defocus (DEFOCUS)

Every image is required to have the following axes: (l, m, E, X, Y, f)

Each coordinate may be regularly sampled, in which case the sample points are defined by the usual CTYPEi, etc., keywords; or irregularly, in which case the sample points are defined in a table extension (in the same file).

Each coordinate has to have one or more pixels, but one is expressly allowed. If there is only one point along any of the required axes, the axis still needs to be present and its coordinate value are defined in the usual way (CTYPEi, etc.). The coordinate axes (most notably the spatial ones) have several aliases defined in the header. The headers of these images contain the required Caldb keywords. These images have SUMRCTS=1.0.

HDU type 2 – the irregularly sampled coordinate definition table s: - These are binary tables which allow an unambiguous translation of "bins" or "pixels" to physical coordinates (e.g., energy, defocus).

HDU type 3 − SUMRCTS image: - The SUMRCTS images contain the information on how many photons (weights) are there per individual PSF data in the PSF hypercubes. These images match the PSF hypercubes exactly, except that the l and m axes are missing. The image pixels indicate the number of counts used for each 2-D PSF image. The SUMRCTS images are kept in IMAGE extensions.

3.2. Standard 2D-PSF Library Structure and Content

For each instrument configuration (ACIS-I, ACIS-S, HRC-I, and HRC-S), there are four standard library files (F1, F2, F3, F4) for the 2D_PSF library. These PSF library files are comprehensive, covering the entire FOV or a section of the FOV in a regular grid. The HDU for each of those files contains the self-contained PSF data, as a single hypercube (6-D; NAXIS=6) with image extension containing information on the number of photons (weights) needed for normalization of the PSF models, and one or more binary tables containing irregular coordinate definitions.

The PSF models incorporated in the PSF 2-D library hypercubes are single size arrays (images) on a fixed, regular grid. The initial number of rays for these simulations was approximately 10⁵. They do not contain spreading due to aspect or detector related spreading and effects. The following parameters were used for calculating the coordinate values in the HDU:

- ACIS-I and ACIS-S chip scale: 0.024 mm and 0.49200 arcsecond;
- HRC-I and HRC-S chip scale: 0.0064294 mm 0.13175 arcsecond. (note: the actual resolution, an "effective pixel size" for HRC can be obtained by convolving with a gaussian with sigma of 1.5 HRC pixels).

The PSF model images are made using the nominal aim-point and the nominal SIM-Z position for each detector. Currently, the standard libraries contain PSF models calculated for one defocus position (defocus=0) and 5 energies (0.277 keV, 1.4967 keV, 4.51 keV, 6.4 keV, 8.6 keV).

When designing the standard library we had to make a compromise between the need for fine spatial and spectral resolution in the PSF grids, and the need for a reasonable file size of each individual library hypercube delivered to the user; The size-limit of each individual hypercube was chosen so the user can copy the file on their own disk, and use it for data analysis in CIAO. The size-limits of the PSF "post stamp" images (e.g. 512x512 pixels) were chosen so they could contain a large fraction of the PSF, including at large off-axis angles. In fact, the large size of the individual PSF "post stamp" image files was a limiting factor on how many can be incorporated in the standard PSF library files, and still provide a useful off-axis angle and energy sampling of the PSFs, and at the same time cover a reasonable FOV.

Four libraries for each instrument are delivered with the CIAO CALDB 2.0. The naming convention for PSF files is as follows:

[detector][date(year_month_day)][2dpsf][n(standard psf library id number)][N*].

e.g.: acisi1998-11-052dpsf2N0002.fits

is a 2-dimensional PSF library for ACIS-I configuration valid for data (calibration and flight) obtained since 5 Nov 1998. The standard reference id number of this library file is 2 (library file F2).

Two of the four PSF library files distributed with CIAO (F2 and F4) are shown schematically (NOT TO SCALE) in Figures 3-6. We note that the F2 library for HRC-I (see Figure 5) covers an area -25 arcmin to +25 arcmin in azimuth, and -25 to +25 arcmin in elevation. The images outside the detector FOV contain zeros. They are not used in the interpolation using the mkpsf tool.

In the following we summarize the content of the standard 2-D PSF library files for different instrument configurations. For analysis, we suggest to use the library files No. 1 (F1) if the off-axis angle of the source is within the library field of view. For larger off-axis angles please use library file F2 with caution because of the coarse grid for interpolation.

ACIS-I Configuration Libraries

The center of the coordinate system is the ACIS-I aimpoint, which is at x=4096.5, y=4096.5 in DETECTOR coordinates (i.e. relative to the mirror), and at 0,0 in azimuth and elevation.

File 1 (F1):

256x256 pixels images for currently only one defocus position (0), 5 energies, and 21x21 off-axis angles defined by the elevations:

elevation (-10, -9, -8, -7, -6, -5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10) arcminutes

azimuth (-10, -9, -8, -7, -6, -5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10) arcminutes

Pixel size: 6 μ m

File Size: 580 Mb

File 2 (F2):

512x512 pixels images for one defocus position, 5 energies, and off-axis angles defined by the following elevations and azimuths:

elevation (-25, -20, -15, -10, -5, 0, 5, 10) arcminutes

azimuth (-10, -5, 0, 5, 10) arcminutes

Pixel size: 12 μ m

File Size: 204 Mb.

File 3 (F3)

512x512 pixels images for one defocus position, 5 energies, and 13x13 off-axis angles defined by the following elevations and azimuths:

elevation (-6,-5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6) arcminutes

azimuth (-6,-5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6) arcminutes

Pixel size: 2 μ m

File Size: 890 Mb.

File 4 (F4)

512x512 pixels images for one defocus positions, 5 energies, and 3x3 off-axis angles defined by the following SAOSAC elevations and azimuths in arcminutes:

elevation (-1, 0, 1) arcminutes

azimuth (-1, 0, 1) arcminutes

Pixel size: 1μ m

File Size 46 Mb for 1 defocus position.

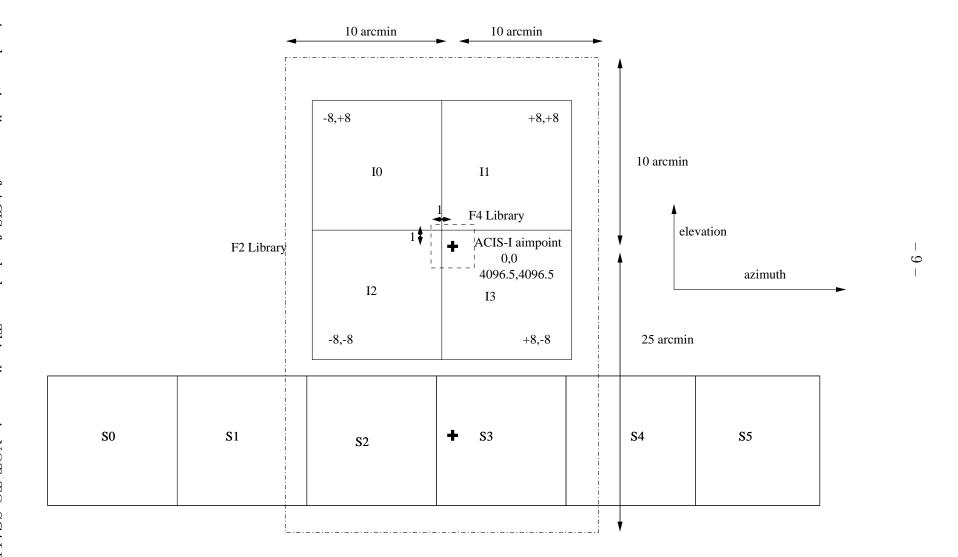


Table 3: ACIS-S Standard Library files

The center of the coordinate system is the ACIS-S aimpoint is at x=4096.5, y=4096.5 in DETECTOR coordinates at 0,0 in azimuth and elevation.

File 1 (F1):

256x256 pixels images for currently only one defocus position, 5 energies, and 21x11 off-axis angles defined by the elevations:

elevation (-5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5) arcminutes

azimuth (-10, -9, -8, -7, -6, -5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10) arcminutes

Pixel size: 6 μ m

File Size 580 Mb

File 2 (F2):

512x512 pixels images for one defocus position, 5 energies, and off-axis angles defined by the following elevations and azimuths:

elevation (-5, 0, 5) arcminutes

azimuth (-25, -20, -15, -10, -5, 0, 5, 10, 15, 20, 25) arcminutes

Pixel size: 12μ m

File Size 170 Mb.

File 3 (F3):

512x512 pixels images for one defocus position, 5 energies, and 13x13 off-axis angles defined by the following elevations and azimuths:

elevation (-6,-5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6) arcminutes

azimuth (-6,-5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6) arcminutes

Pixel size: 2 μ m

File size 890 Mb.

File 4 (F4):

512x512 pixels images for one defocus positions, 5 energies, and 3x3 off-axis angles defined by the elevations and azimuths:

elevation (-1, 0, 1) arcminutes

azimuth (-1, 0, 1) arcminutes

Pixel size: 1μ m

File Size 46 Mb for 1 defocus position.

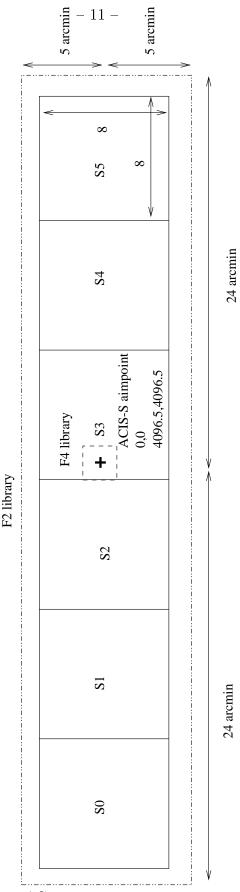


Fig. 4.— A schematic diagram of ACIS-S chips. This diagram is NOT TO SCALE!! The aimpoint is marked with a cross. The pixel size is 0.02400 mm, corresponding to 0.49 arcsec.

HRC-I Standard Library files

The center of the coordinate system is the HRC-I aimpoint at x=16384.5, y=16384.5 in DETECTOR coordinates (0,0 in azimuth and elevation).

File 1 (F1):

256x256 pixels images for currently only one defocus position (0), 5 energies, and 21x21 off-axis angles defined by the elevations:

 $elevation \; (\textbf{-}10,\, \textbf{-}9,\, \textbf{-}8,\, \textbf{-}7,\, \textbf{-}6,\, \textbf{-}5,\, \textbf{-}4,\, \textbf{-}3,\, \textbf{-}2,\, \textbf{-}1,\, 0,\, 1,\, 2,\, 3,\, 4,\, 5,\, 6,\, 7,\, 8,\, 9,\, 10) \; arcminutes$

azimuth (-10, -9, -8, -7, -6, -5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10) arcminutes

Pixel size: 6 μ m

File Size 580 Mb

File 2 (F2):

512x512 pixels images for one defocus position, 5 energies, and off-axis angles defined by the following elevations and azimuths:

elevation (-25, -20, -15, -10, -5, 0, 5, 10, 15, 20, 25) arcminutes

azimuth (-25, -20, -15, -10, -5, 0, 5, 10, 15, 20, 25) arcminutes

Pixel size: 12μ m

File Size 620 Mb.

File 3 (F3):

512x512 pixels images for one defocus position, 5 energies, and 13x13 off-axis angles defined by the following SAOSAC elevations and azimuths in arcminutes:

elevation (-6,-5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6) arcminutes

azimuth (-6,-5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6) arcminutes

Pixel size: 2 μ m

File Size 890 Mb

File 4 (F4):

512x512 pixels images for one defocus positions, 5 energies, and 3x3 off-axis angles defined by the following elevations and azimuths:

elevation (-1, 0, 1) arcminutes

azimuth (-1, 0, 1) arcminutes

Pixel size: 1μ m

File Size 46 Mb.

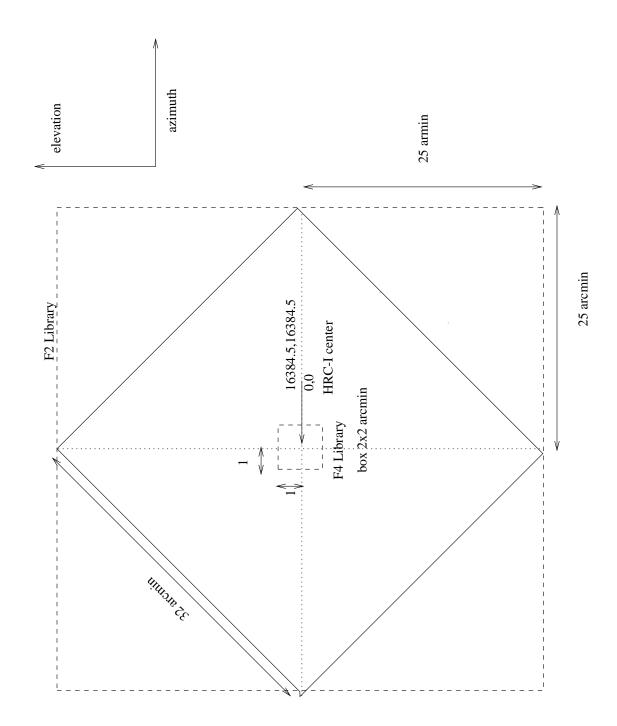


Fig. 5.— A schematic diagram of HRC-I detector. This diagram is NOT TO SCALE!! The aimpoint is marked with a cross. The pixel size is 0.006429 mm, corresponding to 0.13175 arcsec.

HRC-S Standard Library files

The center of the coordinate system is the HRC-S aimpoint, which is at x=32768.5, y=32768.5 in DETECTOR coordinates, and at 0,0 in azimuth and elevation.

File 1 (F1):

256x256 pixels images for currently only one defocus position (0), 5 energies, and 21x21 off-axis angles defined by the elevations:

elevation (-5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5) arcminutes

azimuth (-10, -9, -8, -7, -6, -5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10) arcminutes

Pixel size: 6 μ m

File Size 300Mb

File 2 (F2):

512x512 pixels images for one defocus position, 5 energies, and off-axis angles defined by the following elevations and azimuths:

elevation (-5, 0, 5) arcminutes

azimuth (-30, -25, -20, -15, -10, -5, 0, 5, 10, 15, 20, 25, 30) arcminutes

Pixel size: 12μ m

File Size 200 Mb.

File 3 (F3):

512x512 pixels images for one defocus position, 5 energies, and 13x13 off-axis angles defined by the following elevations and azimuths:

elevation (-6,-5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6) arcminutes

azimuth (-6,-5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5, 6) arcminutes

Pixel size: 2μ m

File Size 890 Mb.

File 4 (F4):

512x512 pixels images for one defocus positions, 5 energies, and 3x3 off-axis angles defined by the following SAOSAC elevations and azimuths in arcminutes:

elevation (-1, 0, 1) arcminutes

azimuth (-1, 0, 1) arcminutes

Pixel size: 1μ m

File Size 46 Mb.

Fig. 6.— A schematic diagram of HRC-S detectors. This diagram is NOT TO SCALE!! The aimpoint is marked with a cross. The pixel size is 0.006429 mm, corresponding to 0.13175 arcsec.

4. CAVEATS

The PSF library is not derived directly from calibration data, but rather through the SAOSAC ray-tracing routine, with inputs specifying the current Chandra HRMA model. The version of the model configuration is "orbit_XRCF+tilts_02". This model seems to replicate the low-energy core and wings of the on-axis PSF well. High energy (greater than 2keV) comparisons of the wings are not yet sufficiently mature enough to draw conclusions (see http://asc.harvard.edu/cal/Hrma/hrma/psf). Also, the detailed comparisons of the simulated off axis PSF to observations are not complete; we believe that in general the PSF matches, but specifics are not yet available.

The standard PSF libraries can be used to view the general distortions and structure of the HRMA PSFs, and the variations as a function of off-axis (angle and energy. The variation can be significant even for small off-axis angles. They are by no means the "exact" PSFs needed for detailed analysis or for deconvolution. The current PSFs will help estimate the size of the PSF and provide information on how the PSF shape changes as a function of off-axis angles and energy. This would help avoid misidentification of PSF-related structures as structures intrinsic to the observed source.

The PSF library grids are very coarse (azimuth and elevation angular off-sets of 1' or 5', only 5 energies, and only one defocus position). Therefore, the user needs to interpolate in these grids to get a PSF for the off-axis angle and the energies (spectrum) of the observed source.

The PSF library grids are very coarse (azimuth and elevation angular off-sets of 1' or 5', only 5 energies, and only one defocus position). Therefore, the user needs to interpolate in these grids to get a PSF for the off-axis angle and the energies (spectrum) of the observed source. If the current linear spatial/spectral interpolation incorporated in the **mkpsf** tool is not satisfactory to the user for their analysis, users can use their own interpolation scheme after extracting the PSF models in detector coordinates from the four grid locations closest to the location of the source, and at the five standard energies.

At this time the mkpsf tool cannot access the weight information in the PSF library hypercubes. Our plan is to make this option available in the next CIAO release. The current standard library files do not contain the error information due to uncertainties in the parameters of the models used to produce the PSF images. We plan to address this and other issues in the future, and to produce updated PSF libraries based on the on-orbit calibration information.