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ATHENA X-IFU RMF with extended Line Spread Function

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History		
Version	*Date*	*Observation*
1.0	May 14th, 2021	First Issue

Distribution	

List of acronyms

X-IFU	X-Ray Integral Field Unit
SXS	Soft X-ray Spectrometer
RMF	Redistribution Matrix File
ARF	Ancillary Response File
LSF	Line Spread Function
TES	Transition Edge Sensor
FWHM	Full Width Half Maximum
HR	High Resolution
LR	Low Resolution

Reference documents

[1] D. Barret, "The ATHENA X-ray Integral Field Unit (X-IFU)", Proc. SPIE, 106991G (2018) https://doi.org/10.1117/12.2312409

[2] M. E. Eckart et al., "Extended line spread function of TES microcalorimeters with Au/Bi absorbers", IEEE Transactions on Applied Superconductivity, Vol. 29, Issue 5 (2019)

[3] M. E. Eckart et al., "Ground calibration of the Astro-H (Hitomi) soft x-ray spectrometer", Journal of Astronomical Telescopes, Instruments, and Systems, Volume 4, id. 021406 (2018) https://doi.org/10.1117/1.JATIS.4.2.021406

[4] F. Pajot, "X-IFU Calibration Plan", XIFU-PL-XCAT-180626-IRAP, ref. 1.3 (2019)

[5] E. Cucchetti et al., "Testing the X-IFU calibration requirements: an example for quantum efficiency and energy resolution", Proc. SPIE 106994O (2018) https://doi.org/10.1117/12.2312188

[6] E. Cucchetti et al., "Energy scale calibration and drift correction of the X-IFU", Proc. SPIE 106994M (2018) https://doi.org/10.1117/12.2312170

[7] P. Peille et al., "The performance of the ATHENA X-ray Integral Field Unit", Proc. SPIE 106994K (2018) https://doi.org/10.1117/12.2313720

[8] M. E. Eckart, "XCaT–TN–005: X-IFU LSF Equation based on Astro-H LSF Measurements", v1.4, 2018

[9] M.E. Eckart, "XCaT–TN–NNN: X-IFU LSF parameter estimates for science simulations based on Astro-H SXS measurements and preliminary X-IFU measurements", v0.1, 2020

[10] E. Miller et al., "Analysis Techniques using Large RMFs", XRISM Science Team Meeting presentation

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1. INTRODUCTION

The present document describes the current implementation of the extended LSF model in the Athena X-IFU RMF and its usage for X-ray data analysis.
The ATHENA X-Ray Integral Field Unit (X-IFU) is an array of 3840 molybdenum-gold (Mo/Au) Transition Edge Sensors (TES), providing an unprecedented spatially resolved high resolution spectroscopy. Each TES pixel is coupled with an electro-plated absorbed composed by 1.7μm of gold and 4.2μm of bismuth (Au/Bi), with a pitch of 249 μm. The TES array composes an hexagonal field of view of 5 arcminutes equivalent diameter.

The instrument energy performance can be summarized as follows [1]:

- energy range = 0.2 - 12 keV
- energy resolution = 2.5 eV (FWHM) up to 7 keV, then smoothly decreasing down to 2.7 eV at 10 keV.

2. THE EXTENDED LSF MODEL

The energy dispersion in micro-calorimeters shows low-level non-Gaussian broadening terms that must be characterized. These terms depend on the composition of the X-ray absorber, the detailed x-ray absorption physics, the device thermalization processes, and the incident X-ray energy [2].
From ground calibration of the HITOMI Soft X-ray Spectrometer (SXS) [3] and preliminary measurements obtained with Mo/Au transition-edge sensors (TESs) with overhanging electroplated Au/Bi absorbers [2], a first model of the extended Line Spread Function for X-IFU has been provided in [8, 9] to be included in the RMF for science simulations and eventually drive the LSF calibration requirements [4].
The core of the LSF for a given pixel is Gaussian at every energy while a small fraction of events are redistributed to lower energies due to several energy loss mechanisms, giving rise to the "extended LSF".

The new release of the X-IFU RMF comprises:

- the core LSF, i.e. the Gaussian main peak already present in the nominal X-IFU RMF. This component is present at every energy and it depends on the detector and system noise, hence it requires both ground and in-orbit calibration [4, 7]. In the nominal RMF, 92 channels are assigned to each incident energy. Several types of energy dispersion configurations have been defined so far for the production of the nominal RMF [5, 6, 7]:
    - *Nominal*:
        - 2.5 eV (FWHM) from 0.05 keV to 7 keV;
        - a linearly increased energy dispersion from 7 to 12 keV, with a value ranging from 2.5 to 4.8 eV;
    - *Optimal* and *Optimal with margins*:
        - the energy resolution is described by a polynomial for the full energy range
    - *10eV*:
        - a constant energy dispersion of 10 eV (FWHM) is applied to the full energy range

- the extended LSF, composed by:
    - the exponential shoulder/tail caused by long-lived surface state excitations occurring preferentially near the surface of the absorber with energy loss decay scale of 6 eV, contributing to a fraction of energy losses that decreases linearly from 8% at 0 keV to 2% at 4 keV, and then remains constant at 2% above 4 keV [8, 9];
    - the electron loss continuum caused by scattering of photoelectrons out of the absorber with a roughly constant flux per unit energy.
    - *X-ray escape peaks induced by x-ray fluorescence photons that may escape from the absorber instead of being thermalized;*
    - *Si X-ray fluorescence lines of the detector frame.*

The current release of the X-IFU RMF with the extended LSF model does not include the presence of escape and fluorescence lines. The new model, given by the sum of the core and the extended (exponential and continuum energy losses) components, is shown in Fig. 1.

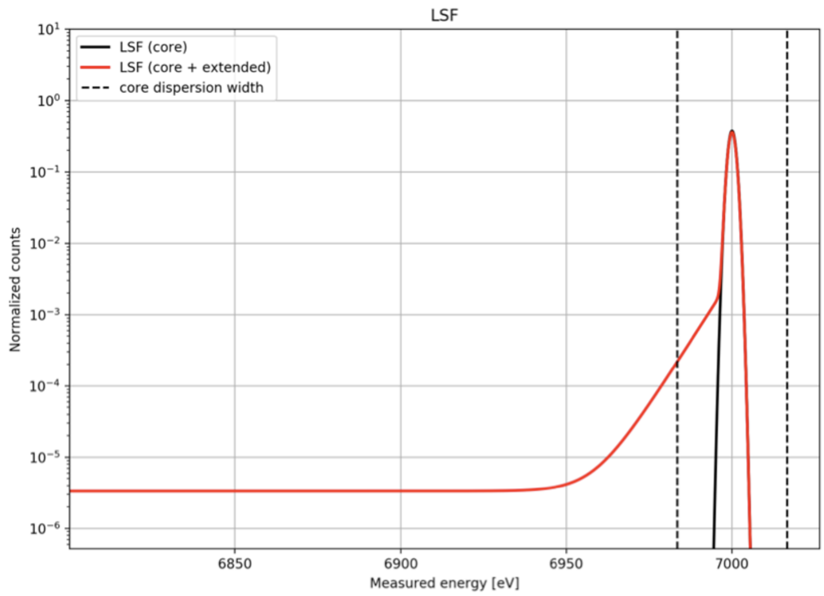

Fig. 1: Nominal core LSF (black line) and full (extended plus core) LSF (red line) for an incident energy of 7 keV. The dashed lines refer to the energy width of the channels associated with the incident energy in the nominal RMF.

3. IMPLEMENTATION IN THE X-IFU RMF

If the full LSF model is implemented in the RMF (Fig. 2, left panel), the size of the RMF FITS file is larger than 3 GB (24 MB is the size of the nominal RMF). Reducing the size of the RMF is mandatory to keep the computational time of the X-ray data analysis feasible. A solution already adopted by the HITOMI and XRISM teams [10] is splitting the model into two components (Fig. 2, right panel), the High Resolution (HR) model composed by the gaussian (core) and exponential tail, and the Low Resolution (LR) model, constituted by the continuum emission with a reduced resolution of the model energies:

- high resolution (HR): gaussian and exponential tail with same resolution as the nominal RMF and a low energy cut of the exponential tail (10^{-8} of the probability distribution);
- low resolution (LR): only continuum emission with same channel resolution but a lower resolution of the model energy.

The energy dispersion for the core component - the gaussian - is set to *Nominal*.

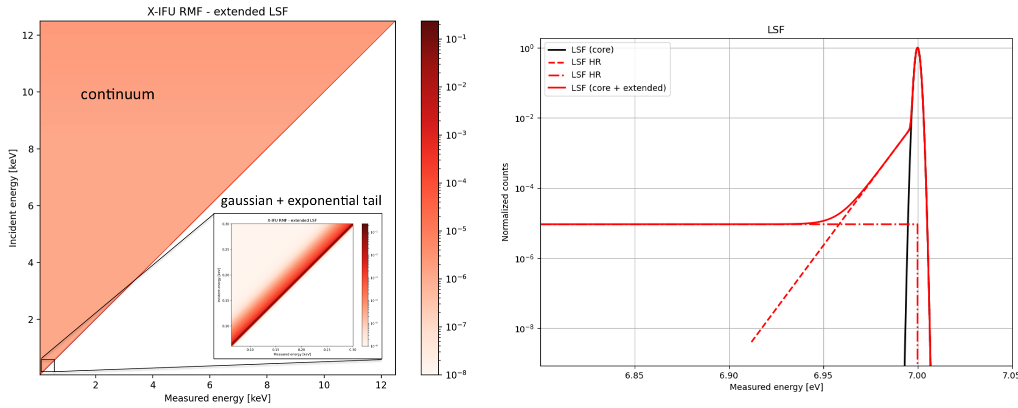

Fig. 2: Energy redistribution matrix with the inclusion of the extended LSF component (left panel) and LSF model with the separation of the HR (dashed red line) and the LR (dot-dashed line) components (right panel).

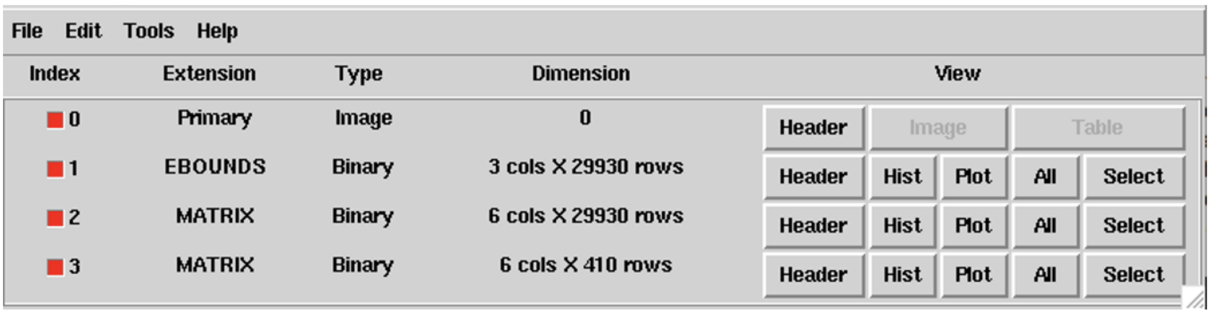

Fig. 3: New data format of the RMF FITS file with three extensions (the energy bounds, the HR and the LR components of the LSF).

The total probability of the distribution (HR + LR) is 1. While the current release of the extended LSF only reduces the number of model energies, the number of channels could also be reduced by the use of grouping in *Xspec*. Both RMF components are stored in two extensions of the same FITS file (Fig. 3). An *Xspec* release >= **v12.11.0** is required to correctly load the X-IFU RMF with the extended LSF. The size of the FITS file depends on the chosen binning factor of the LR component, which must be linear with respect to the nominal binning in order to be loaded by *Xspec*. If the nominal binning of 29931 is used, only the 3×, 11× and 33× binning factors are available. In order to test a larger selection of binning factors, the last channel is removed from the RMF - and the associated ARF FITS file - to get a total number of 29930 channels and the 2×, 5×, 10×, 41×, 73×, 82×, 146× binning factors. The size of the new RMF FITS file is listed in Table 1.

full RMF	**1x (29931)**	**2x (29930)**	**5x (29930)**	**10x (29930)**	**11x (29931)**	**33x (29931)**	**41x (29930)**	**73x (29930)**	**82x (29930)**	**146x (29930)**
3.6 GB	2.7 GB	1.9 GB	780 MB	420 MB	390 MB	170 MB	150 MB	115 MB	110 MB	90 MB

Table 1: RMF with extended LSF size for different binning factors.

4. PERFORMANCE AND ACCURACY TESTING

The model used for testing the performance and accuracy, i.e. run time and best fit parameters, is obtained from an HITOMI/SXS observation with gate valve closed (no flux below 2 keV). The model is an absorbed power-law plus a gaussian (*tbabs* × *powerlaw* + *gaussian*). A single simulation is generated with the RMF using the full extended LSF model with no resolution optimization. The optimized RMF is then loaded and the spectrum is fitted with all parameters free to obtain the best fit results and the 90% confidence errors (Fig. 4).

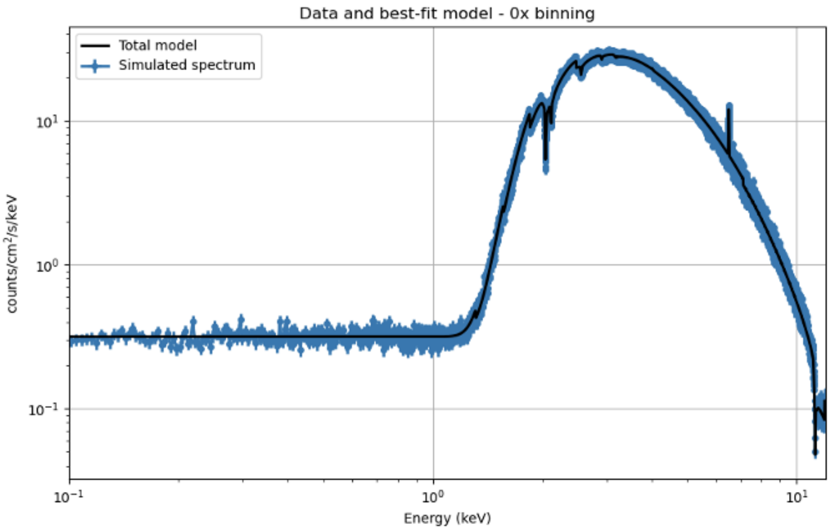

Fig. 4: Simulated spectrum (100 ks exposure, in blue) and best fit model (in black).

The time for creating and loading the RMF and fitting the spectrum is shown in Fig. 5 (left panel). The time required to create the RMF is well above 100 s for all the binning factors, the reason being that the computation of the low energy threshold for the exponential tail is time consuming and the use of a constant cut could be introduced in the next releases of the code to optimize the performance of the RMF production. The time to load the RMF falls below 10 s for a binning factor larger than 10×. The time required to fit the spectrum is below 3 s for a binning factor of 10× and close to 1 s for a binning factor larger than 40×. The gain in performance saturates for a binning factor above 40×, corresponding to a size of about 150 MB. The best-fit values and 90% confidence errors are not affected by the binning factor (Fig. 5, right panel). Similar results are obtained for the XRISM RMF optimization study [10], although with lower errors associated with the fit as expected.

It should be noted that the present test only aims at a preliminary trade-off analysis of accuracy and performance but further studies applied to dedicated science cases are needed to evaluate the impact of the extended LSF in the X-ray data analysis.

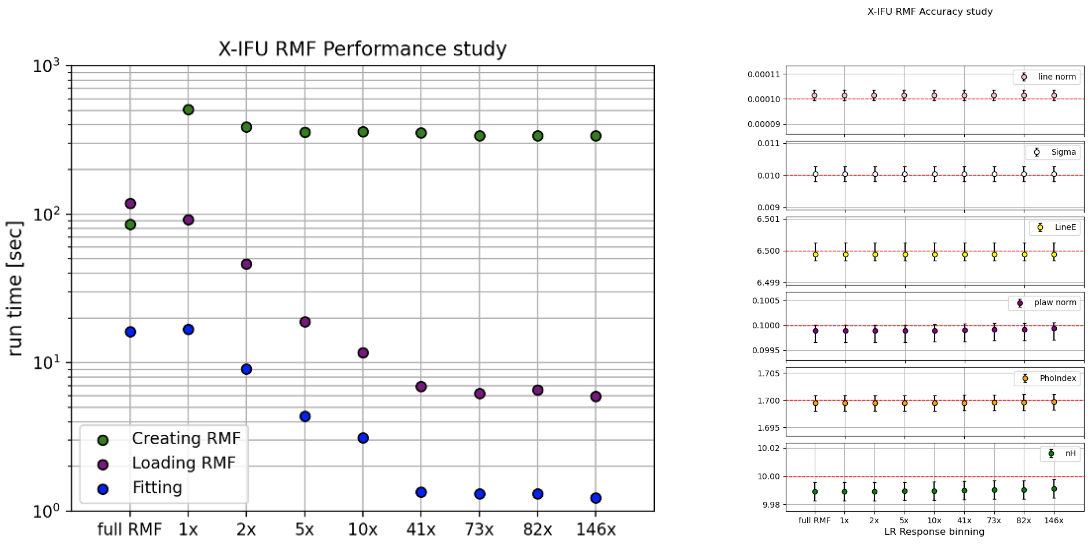

Fig. 5: Performance (left panel) and fitting accuracy (right panel) as a function of the binning factor for the LR component of the LSF.

5. USAGE OF THE RMF WITH EXTENDED LSF

The presence of the HR and LR LSF components in the RMF is transparent to the user, and its usage is the same as the nominal RMF but an *Xspec* release >= **v12.11.0** is required.

The nominal RMF is *XIFU_CC_BASELINECONF_2018_10_10.rmf* and can be downloaded from: http://x-ifu-resources.irap.omp.eu/PUBLIC/RESPONSES/CC_CONFIGURATION/

The RMF with extended LSF is obtained with a binning factor of 33×. The HR component has the nominal channel binning (29931) and can be used with the standard X-IFU ARF files.

6. CONCLUSIONS

The present document describes the first release of the X-IFU RMF with extended LSF to be used for scientific data analysis. The extended LSF model does not include the presence of escape peaks and X-ray fluorescence lines, these features are currently under investigation and will be added in future releases of the X-IFU RMF.