XRISM X-Ray Imaging and Spectroscopy Mission

XRISM Data Processing Pipeline and Software

Michael Loewenstein for the XRISM Science Data Center (SDC)

Matt Holland (PDL), Tahir Yaqoob and Eric Miller, Bob Hill, Trisha Doyle, Patty Hall, Efrain Perez-Solis, and Efrem Braun (alumnus)

This talk

Will cover

- XRISM processing pipeline
- XRISM processing ftools (including reprocessing scripts) and CalDB
- Some details on the MXS and energy assignment
- XRISM post-processing and data analysis ftools (briefly)
- XRISM / Hitomi differences
- XRISM software status and plans (briefly)

Will *not* cover

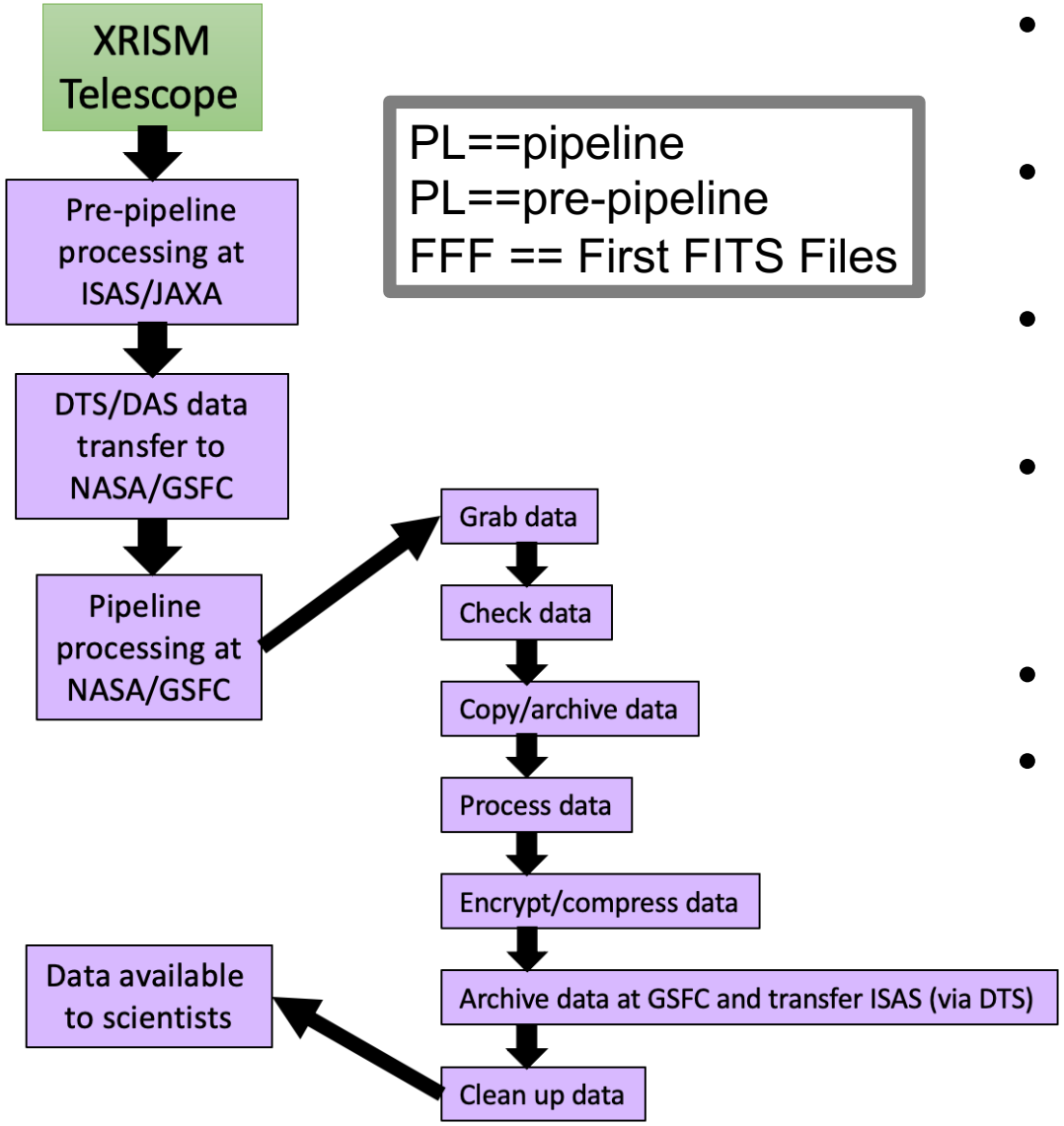
- Data (archive) organization, naming conventions, retrieval
- Coordinate system definitions
- Time assignment
- Bright source details (E. Hodges-Kluck)
- Extended source details (F. Mernier)

Will *focus* on Resolve

The SDC

- Handles all processing of record from observation scheduling to delivery of pipeline output to data archives.
- Provides proven, standards-based community software tools needed for data processing (calibration, screening), data product extraction, and data product analysis.
- Manages XRISM ground system software and data systems involved in maintaining the XRISM Calibration Database (CalDB) derived from deliveries from the Xtend, Resolve (and XMA) instrument teams.
- Supports the XRISM Guest Observer Facility (GOF) in user-support activities.

How the Data Flow



PL==pipeline
PL==pre-pipeline
FFF == First FITS Files

- Telemetry from XRISM arrives at ISAS
- PPL converts the telemetry data into FFF
- Data are transferred to the PL virtual machines
- Data are verified and prepared for pipeline processing
- Data are processed
- Data (encrypted) are transferred to the archives

The PL operates in a (mostly) automated manner

Data Processing - General

XRISM X-Ray Imaging and Spectroscopy Mission

- Checks input files for validity
- Determines nominal pointing - aberattitude, attconvert, aspect
- Calculates Optical Axis (sky) – coordpnt
- Calculates quartz clock temperature trend (backup timing) – xatrendtemp (ahrendtemp)
- Collects necessary HK, orbit, and attitude information into “make-filter” (mkf) and “extended HK” (ehk) files (for screening, coordinate assignment) – xamkehk (ahmkehk)
- Calibrates, cleans for each instrument; extracts preview products

- Most tasks make use of the XRISM CalDB (Calibration Database) where all necessary calibration information is stored and indexed.
- The SDC is constructing the pre-flight CalDB that will be updated based on commissioning and in-flight calibration activities.

XRISM CalDB

(Calibration Database)

What's in the CalDB

XRISM X-Ray Imaging and Spectroscopy Mission

GEN (misson-independent) **5 files**
Atomic data (2), rigidity (1), leap seconds (1), solar geophysical data (1)

XRISM (54 files)

GEN (all instruments) **10 files**
Timing files (3), XMA optical constants (1), XMA vignetting (1), atomic line data (1), filter file configuration (1), event selection expressions (1), SAA bounds (1), col. defs.(1)

RESOLVE **26 files**
Teldef (1), QE (1), blocking filter (1), contamination (1), bad pixels (1), instrument map (1), pixel map (1), rmf params (1), FW files (5), gate valve (1), gain (1), antico (1), time coefficients (1), mxsparam (1), secondary pulses (1), pulse templates(1), XMA (5), clipping(1)

XTEND **18 files**
Teldef (1), QE (1), contamination (1), instrument map (1), bad pixels (1), mask (1), rmf params (1), video temp (1), charge trail (1), CTI (1), split thresh (1), pixel pattern (1), gain (1), XMA (5)

What's in the (Current) CalDB

XRISM X-Ray Imaging and Spectroscopy Mission

- Hitomi-based data (e.g., XMA) to be updated for first XRISM public release
- Optical axes at center of Resolve 6x6 array and nominal aimpoint for Xtend
- Preliminary deliveries of XRISM-based data (from ground testing) to be updated for XRISM public release
  - MXS parameters CalDB file
  - Temperature vs. Frequency relation for timing
  - Other timing parameters
  - Resolve gain
  - Resolve RMF
  - Xtend bad pixels
  - Resolve & Xtend "teldef" files (detector layout)
- Final pre-flight versions of XRISM-based data (from ground testing)

Pre-Launch CalDB

XRISM X-Ray Imaging and Spectroscopy Mission

- Optical axes refined based on ground-based misalignment measurements, but will be further refined using inflight calibration data.
- XMA calibration will have large (~10-20%) systematics above ~8 keV, to be improved post-launch.
- Au optical constants for XMA mirror reflectivity same as Hitomi.
- No Resolve bad pixels.
- Contamination for both Resolve and Xtend set to zero.
- Xtend RMF line-spread function narrower than measured on ground, so users will need to include additional line broadening in models.

Xtend PL Processing

(in brief)

Data Proc. – Xtend Calibration

XRISM X-Ray Imaging and Spectroscopy Mission

- Calculate Xtend CCD mode GTI (for expo map) – xtdmodegti (sximodegti)
- Assign higher level coordinates - coordevt
- Merge inner 3x3 and outer 5x5 pulse heights – xtdphas (sxiphas)
- Set initial data quality STATUS flags (for screening) – xtdflagpix (sxiflagpix)
- Assign grade and initial energy (PI) – xtdpi (sxipi)
- Update grade and PI w/ grade-dependent CTI correction – xtdpi (sxipi)
- ID and output flickering pixels among clean events – searchflickpix/coordevt
- Update STATUS flags w/ flickering pixel information – xtdflagpix (sxiflagpix)

Data Proc. – Xtend Clean

XRISM X-Ray Imaging and Spectroscopy Mission

- Filter times
  - HK (nominal instrument status)
  - Telemetry (not saturated)
  - Pointing accuracy, stability
  - Safe angle above Earth, sunlit Earth limb
  - Away from SAA in time and orbit
- Screen events for
  - Grade
  - Data quality (STATUS; not in a “bad” detector area, pixel, row, etc)

(ahtigen + ahscreen)

Resolve Software Concepts

Detector channels
(fixed)

30	32	34	26	24	23
29	31	33	25	22	21
27	28	35	18	20	19
1	2	0	17	10	9
3	4	7	15	13	11
5	6	8	16	14	

12

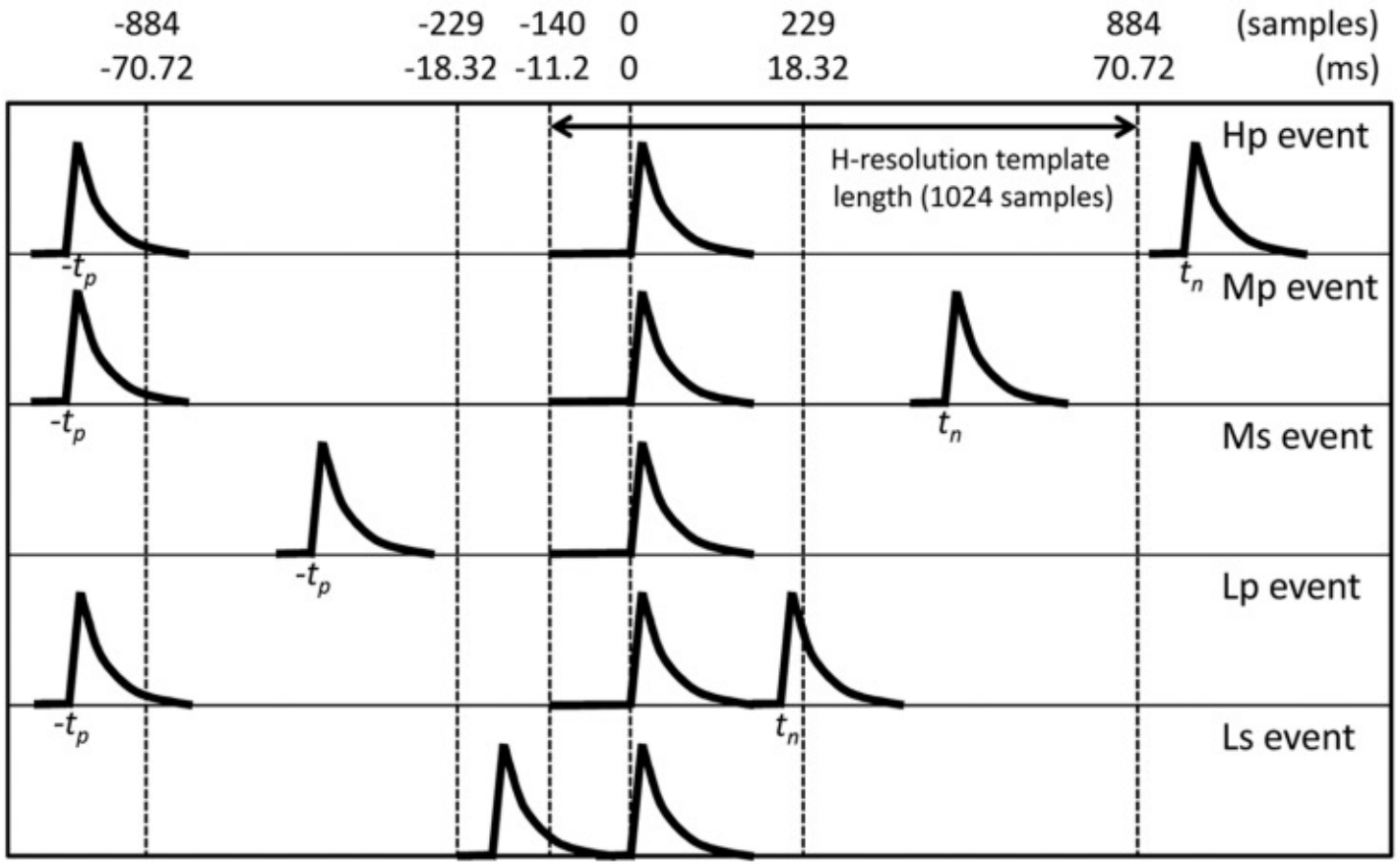
Resolve Event File Columns

XRISM X-Ray Imaging and Spectroscopy Mission

Column	Description	Range
ITYPE	Resolution Grade; ITYPE=0: HP, ITYPE=1: MP, ITYPE=2: MS, ITYPE 3: LP, ITYPE 4: LS, ITYPE 5: BL, ITYPE 6: EL, ITYPE 7: Rj	0-7
PIXEL	Pixel number (pixel 12 is the calibration pixel)	0-35
RISE_TIME	Measured time from baseline to peak for Resolve pulse	0-255
PI	Linearized Energy Channel	0-60000
STATUS	16 bit Event Flag (14 in use)	
	STATUS[1]: in (0) or out (1) of all-pixel GTI file	0-1
	STATUS[2]: in (0) or out (1) of individual-pixel GTI	0-1
	STATUS[3]: coincident with antico events (1)	0-1
	STATUS[4]: coincident with other event within a temporal proximity	0-1
	STATUS[5]: coincident with pixel 12 event	0-1
	STATUS[6]: coincident with pixel 12, and recoil energy test satisfied	0-1
	STATUS[7]: coincident with event in wiring proximity (electrical crosstalk) – short timescale	0-1
	STATUS[8]: largest PHA in electrical crosstalk group – short timescale	0-1
	STATUS[9]: coincident with MXS, direct mode*	0-1
	STATUS[10]: coincident with MXS afterglow, direct mode*	0-1
	STATUS[11]: coincidence with MXS, indirect mode*	0-1
	STATUS[12]: coincident with MXS afterglow, indirect mode*	0-1
	STATUS[13]: coincident with event in wiring proximity (electrical crosstalk) – long timescale	0-1
	STATUS[14]: largest PHA in electrical crosstalk group – long timescale	0-1

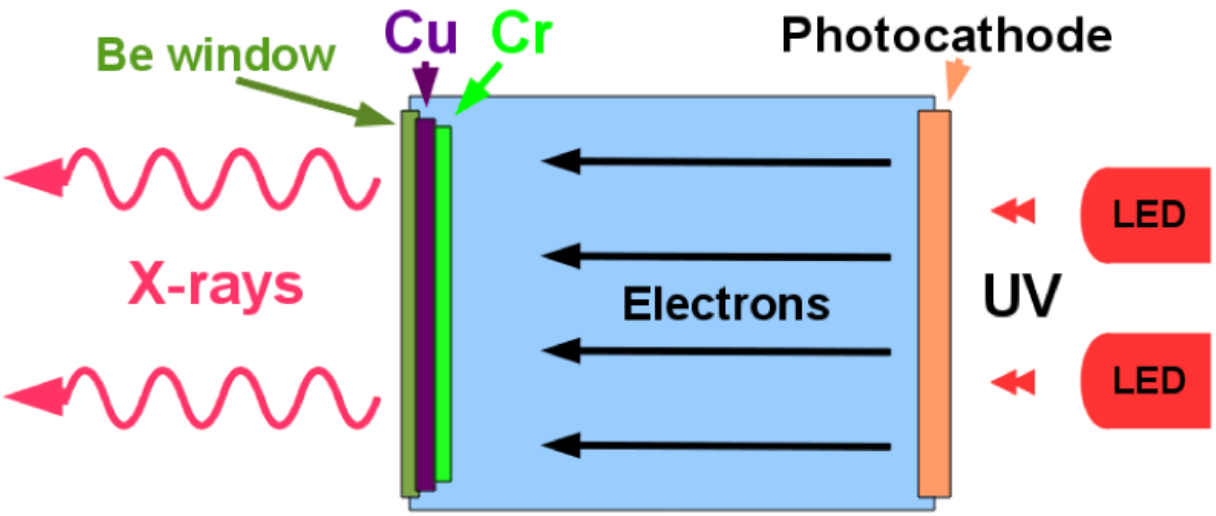
Resolve Grade (ITYPE)

	$t_p \le \delta t_2$	$\delta t_2 < t_p \le \delta t_1$	$\delta t_1 < t_p$
$t_n \le \delta t_2$	L_S	L_S	L_P
$\delta t_2 < t_n \le \delta t_1$	L_S	M_S	$\mathbf{M_P}$
$\delta t_1 < t_n$	L_S	M_S	$\mathbf{H_P}$



The Resolve MXS

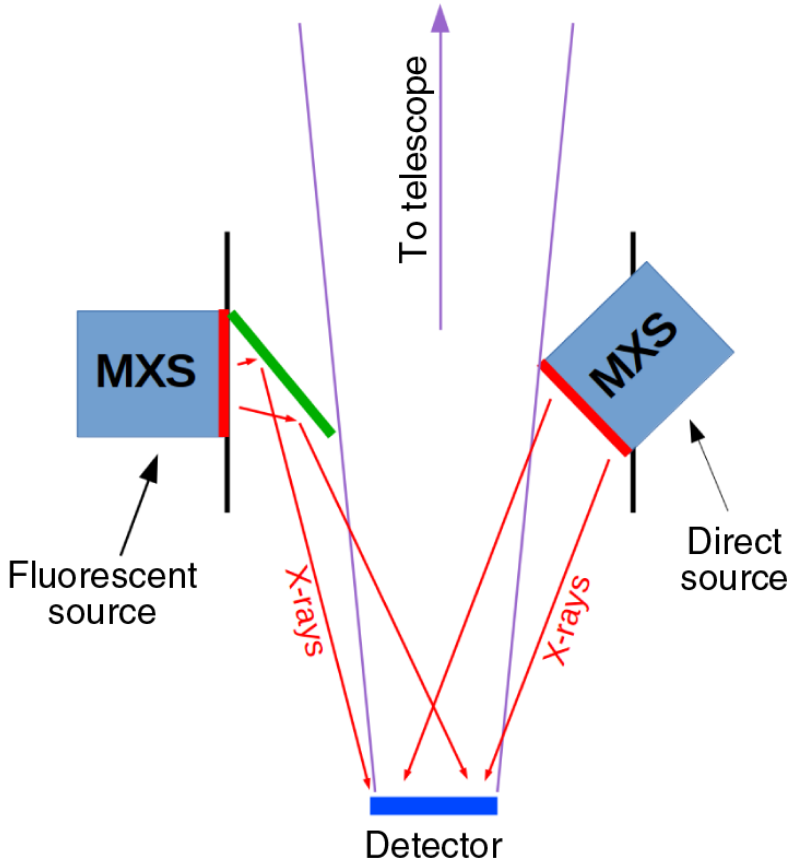
- The modulated X-ray source (MXS) is the primary source for Resolve energy scale calibration, illuminating each pixel with X-rays generated using LEDs operating with a short pulse period and low duty cycle. The pulsed emission dominated by narrow features of known energy.
- This enables continuous pixel-by-pixel energy gain drift monitoring while avoiding contamination of the astrophysical source.

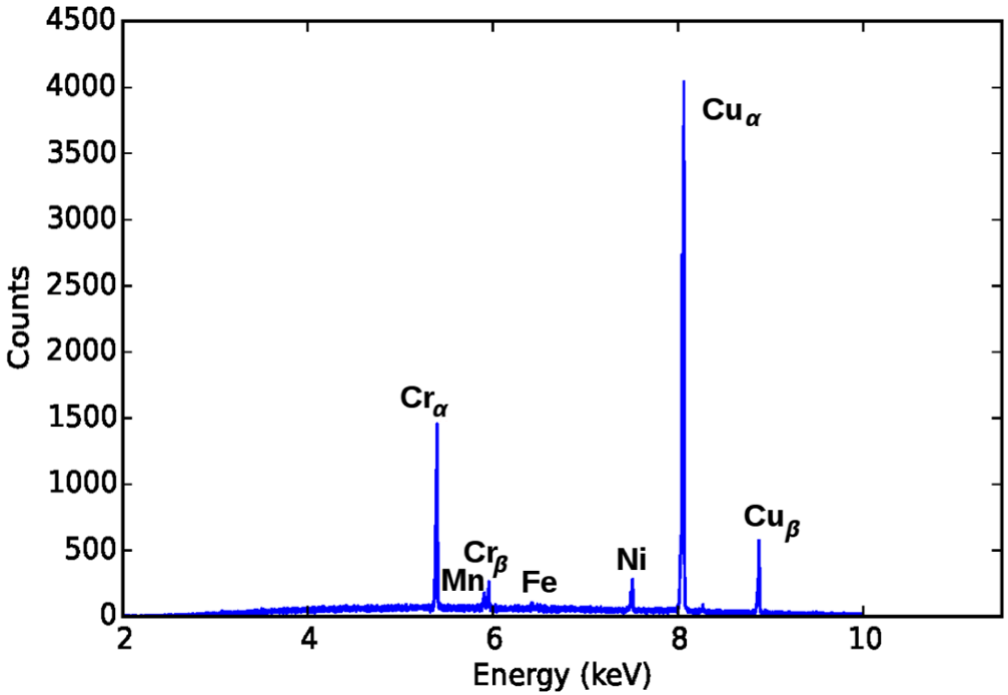


https://doi.org/10.1117/1.JATIS.4.1.011204

The Resolve MXS

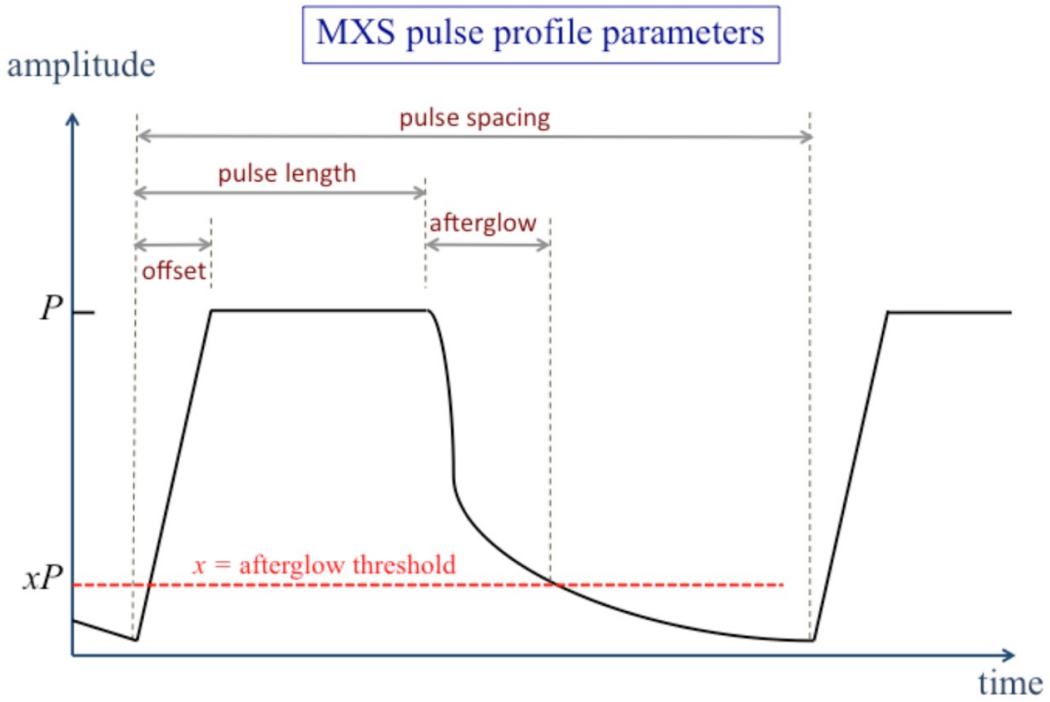
- There are **direct** (LED1/3 on the nominal/redundant side) and indirect (LED2/4 on the nominal/redundant side). The K-shell lines emission lines **directl**y generated by the Cr/Cu anode are primarily used for energy assignment.





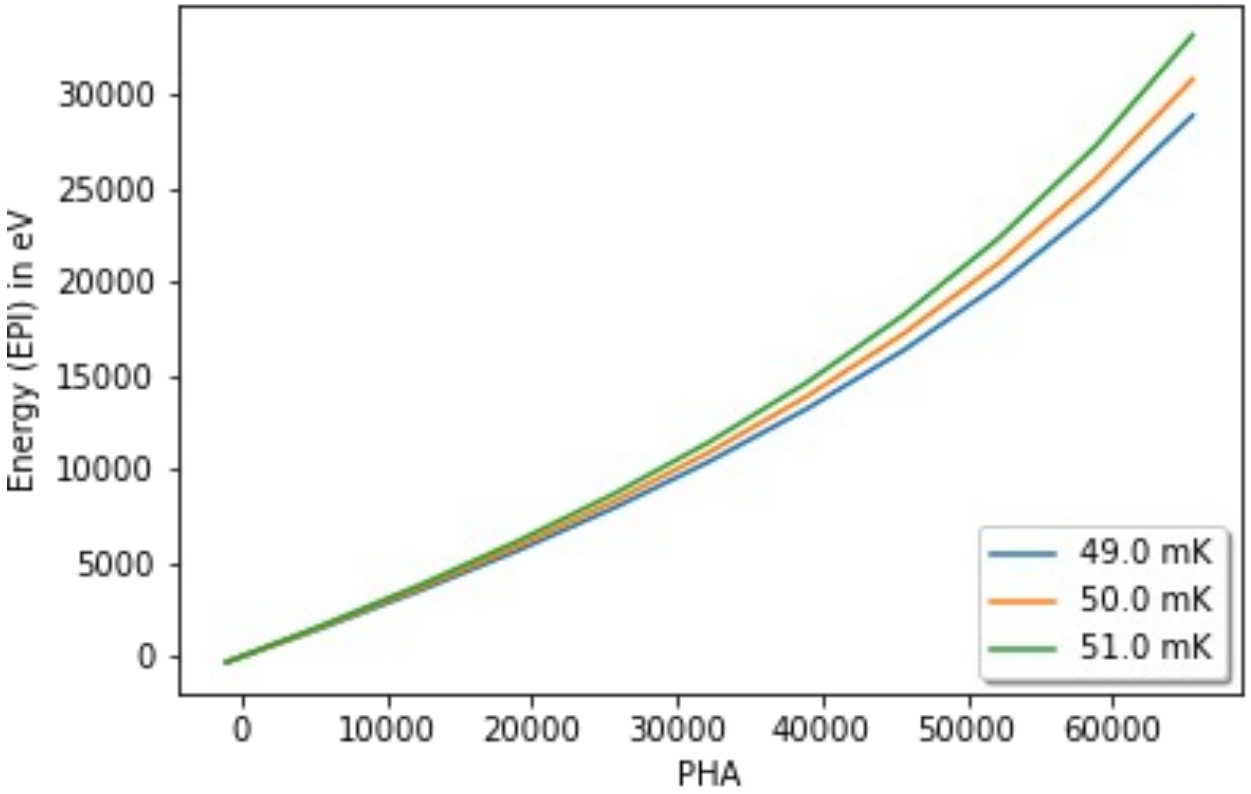
MXS Pipeline Ftools

- The XRISM ftools tasks rslmxstime and rslmxsgti calculate “MXS Pulse ON” and “MXS Pulse OFF” time intervals for each LED. The former is used for gain tracking, the latter - extended to include an afterglow tail - to omit times with MXS X-rays from cleaned event files.
- rslmxstime calculates the basic MXS Pulse-ON GTI per LED, and rslmxsgti combines and inverts these in several ways.
- Pulse parameters from HK
  1. Pulse length → afterglow
  2. Pulse spacing
  3. Peak intensity (LED Current) → offset
- Parameter optimization and operations tradeoffs (bright, but not too bright; frequent, but not too frequent).



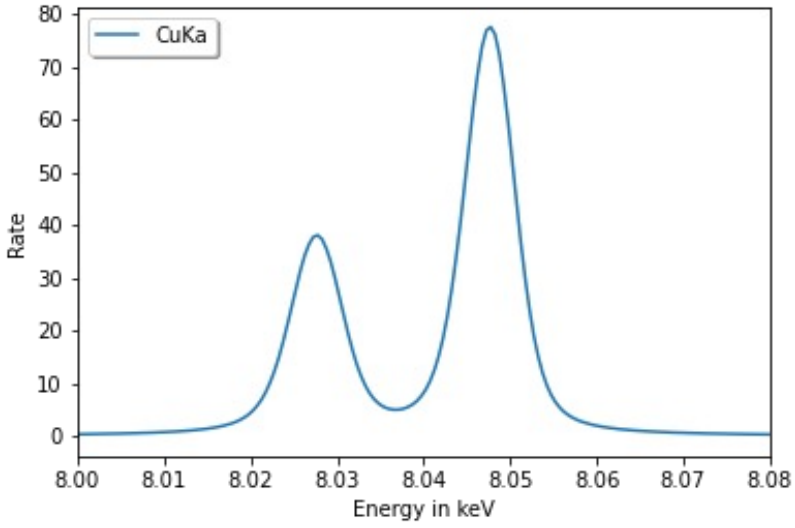
Gain and energy assignment

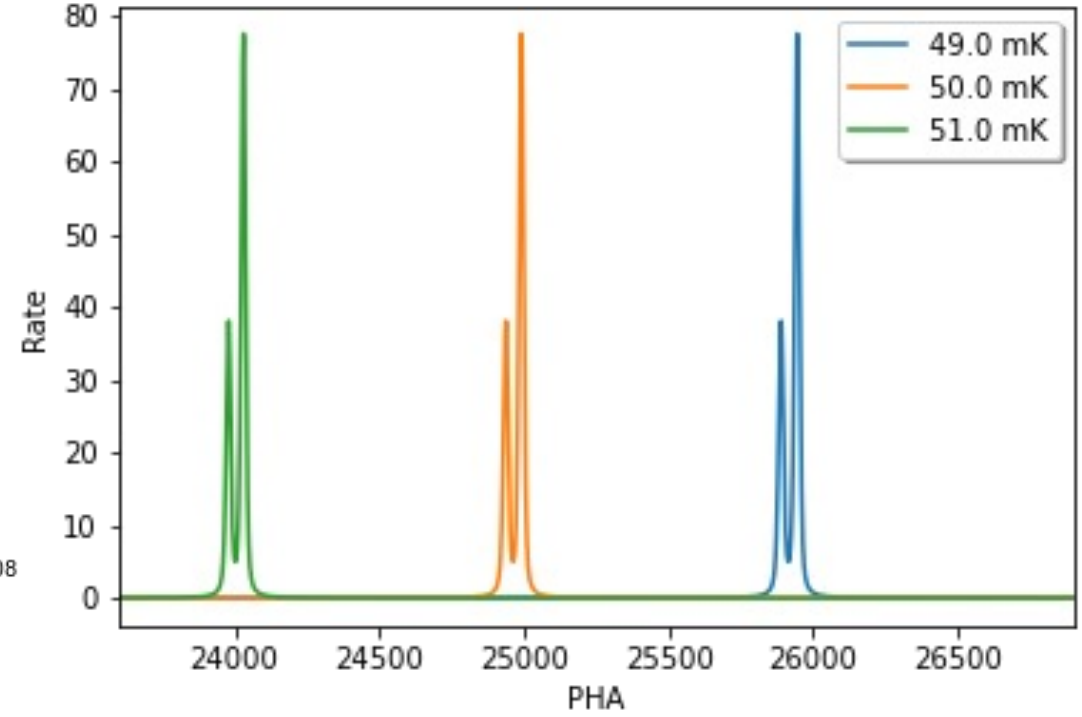
- Gain curve: Energy as a function of PHA (pulse height amplitude) and operating temperature
- Separately calculated for High, Mid, and Low resolution events for each pixel



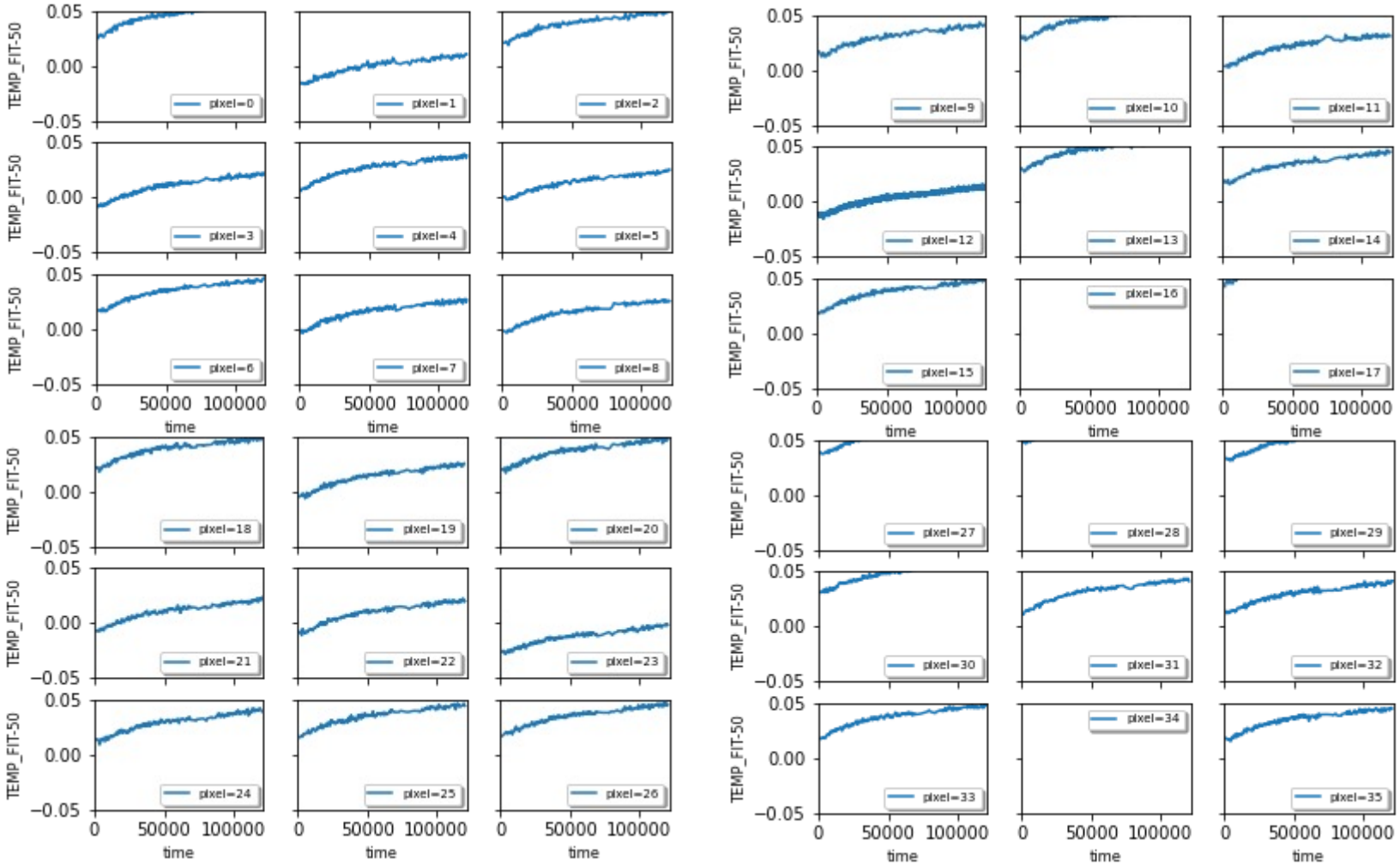
Energy assignment

- Extract spectra from an onboard calibration source in time intervals over the observation exposure.
- Use knowledge of the intrinsic line energy and shape, and the measured PHA to derive the effective temperature.





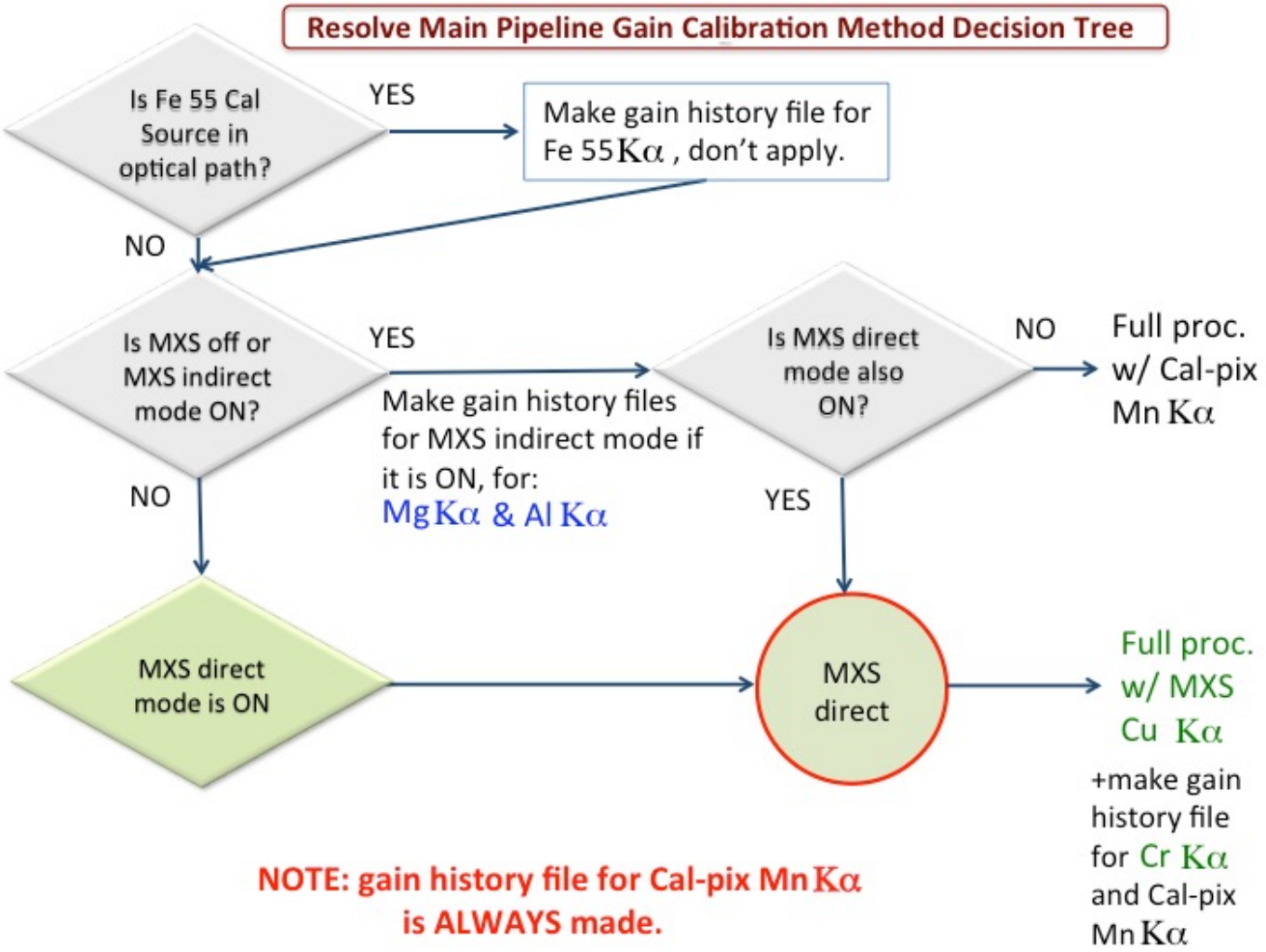
Gain Histories (per pixel)



Methods and lines

Cal method	Cal lines	Pipeline Gain History	Pipeline energy assignment
Cal-pix	MnKa, MnKb	Always (MnKa)	If no MXS direct
Fe55	MnKa, MnKb	If FW set to Fe55 (MnKa)	For calibration
MXS (direct)	Cuka, Cukb, Crka, Crkb	If MXS direct on (CuKa, CrKa)	Primary method
MXS (indirect)	AlKa, AlKb, MgKa, MgKb	If MXS indirect on (AlKa, MgKa)	For calibration

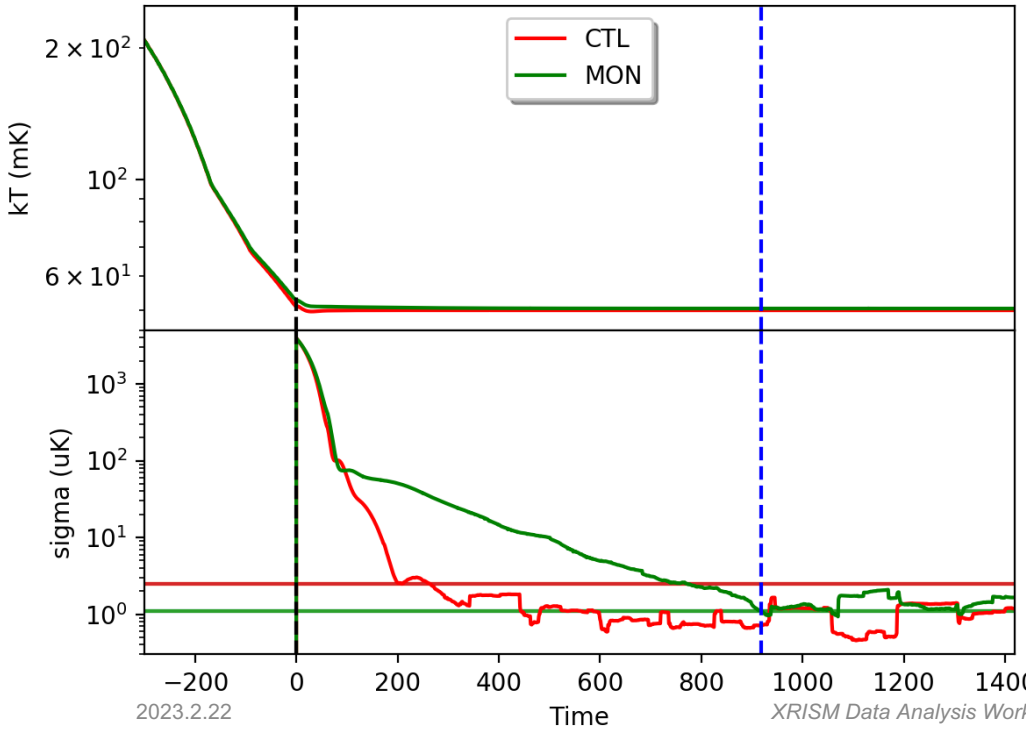
Methods and lines



- Use MXS if direct mode is enabled, otherwise use cal-pixel.
- Make all possible gain history files

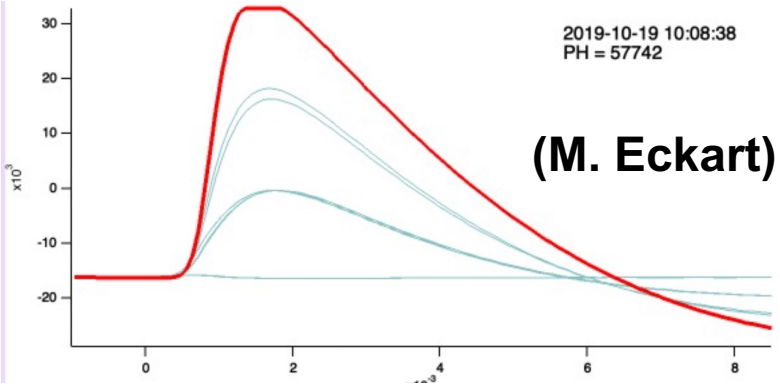
Data Proc. – Resolve Cal.

- Calculate ADR temperature fluctuations (for ADR GTI) – rslctsfluct (new)
- Calculate ADR GTI (screening) – rsladrgti (new)
- Calculate MXS GTI (screening, energy assignment) – rslmxsgti (mxsgti)
- Invert LOST GTI file (expo map) – gtiinvert
- Assign antico energy (PI) – rslanticolc (sxsanticolc)
- Assign higher level coordinates – coordevt



Data Proc. – Resolve Cal.

- Assign pulse clipping flag (screening) – rslplsclip (new)



- Set energy-independent data quality STATUS flags (screening) – rslflagpix (sxsflagpix)
- Associate groups of secondary with primary events (energy assignment) – rslsecid (sxssecid)
- Compute the energy scale drift correction (energy assignment) – rslgain (sxsgain)
- Assign initial energy (PI) – rslpha2pi (sxspha2pi)
- Set energy-dependent data quality STATUS flags – rslflagpix (sxsflagpix)
- Re-assign groups of secondary events with primary – rslsecid (sxssecid)
- Correct secondary event raw pulse heights - rslseccor (sxsseccor)
- Assign final energy (PI) – rslpha2pi (sxspha2pi)

Data Proc. – Resolve Clean

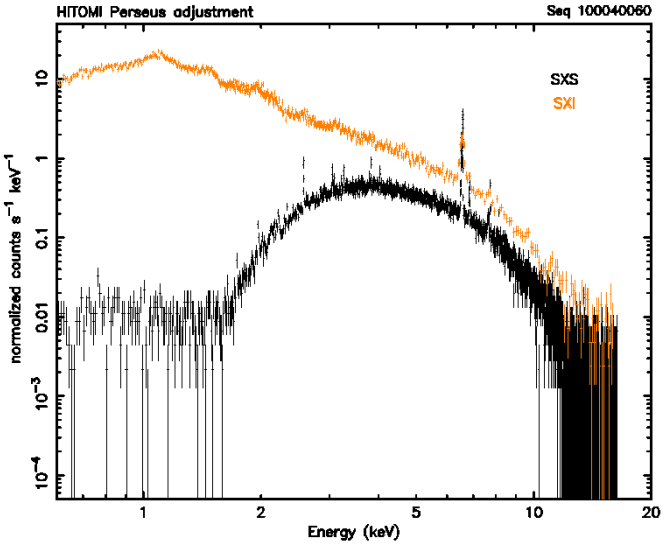
XRISM X-Ray Imaging and Spectroscopy Mission

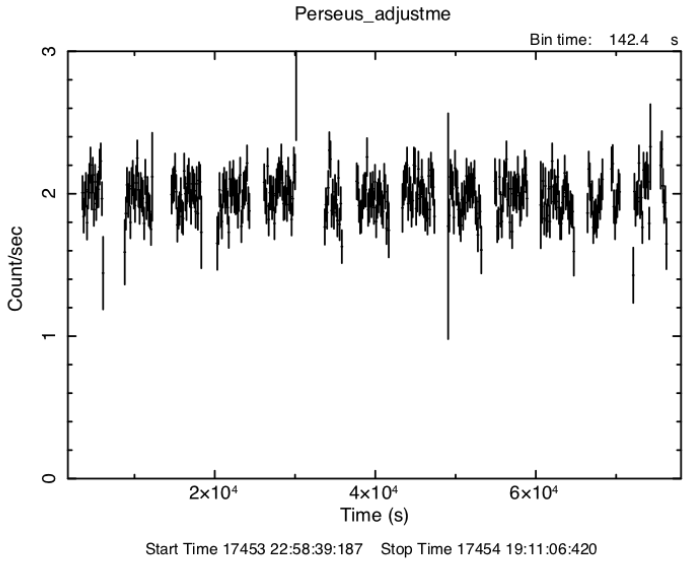
- Filter times for
  - HK (nominal instrument status)
  - Telemetry (not saturated)
  - Pointing accuracy, stability
  - Safe angle above Earth, sunlit Earth limb
  - Away from SAA in orbit
  - ADR (not recycling, settling down)
  - MXS (not pulsing, not in afterglow)
- Screen events for
  - Grade (ITYPE<5)
  - Data quality (based on STATUS)
  - Pulse shape (SLOPE_DIFFER, QUICK_DOUBLE)

(ahtigen + ahscreen)

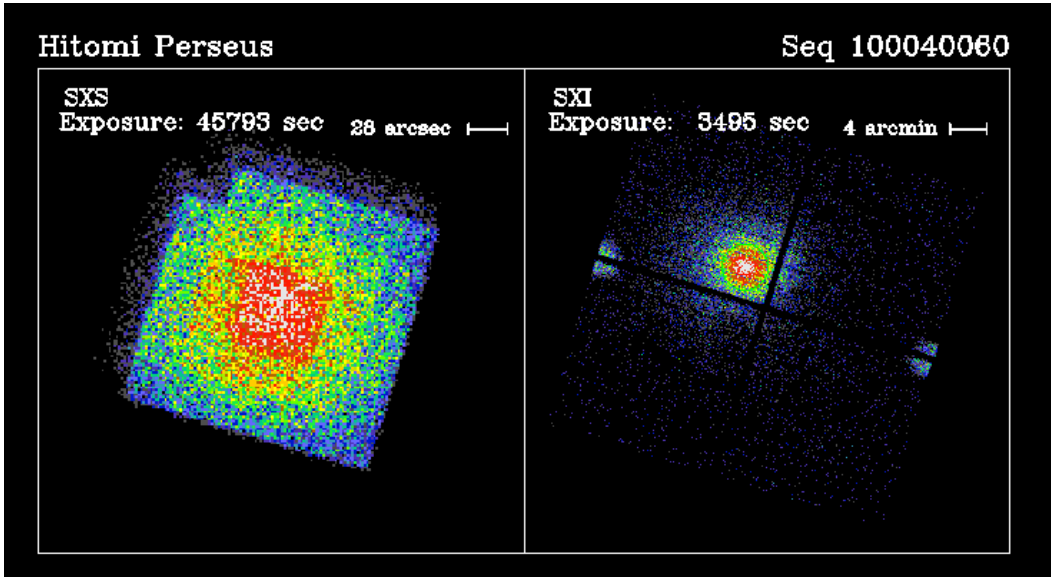
Preview products

- The pipeline constructs a set of standard light curves, images, spectra and response files.





- These ”preview products” are intended for a ***quick*** assessment of the data.

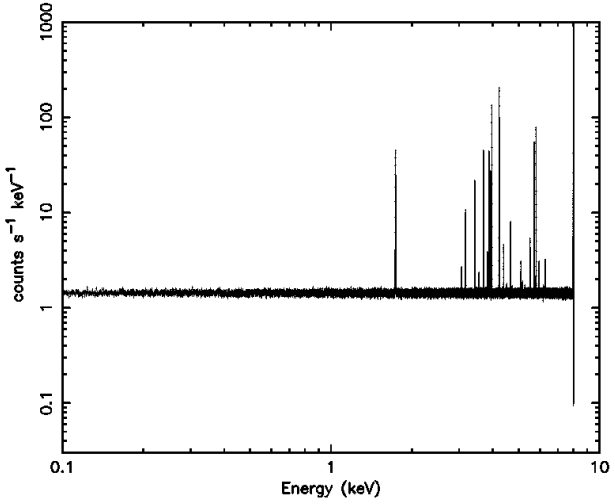


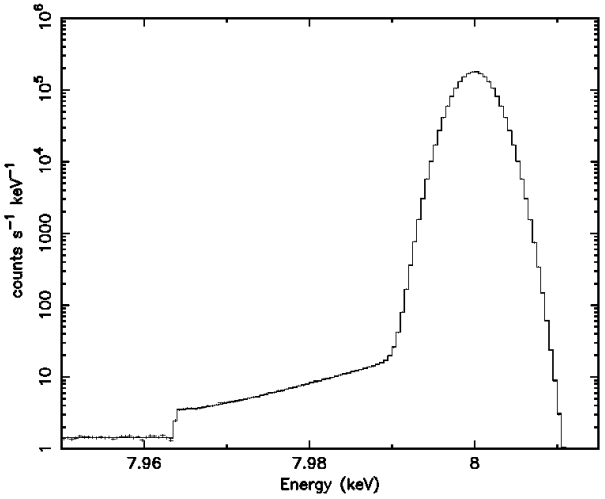
User Data Reprocessing

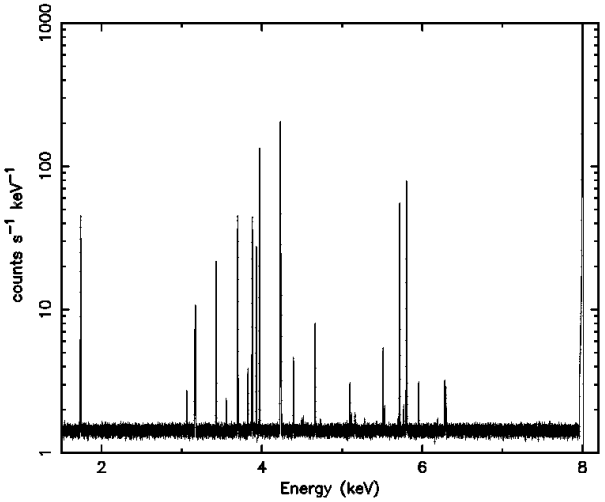
- XRISM Users should reprocess data when there has been an update to pipeline software and/or CalDB since the data was archived; or, if a user wants to apply a non-standard calibration or screening criteria.
- Resolve and/or Xtend data may be reprocessed using the xapipeline script that is part of the standard software library (set the instrument parameter to ALL, Xtend, or Resolve).
- Resolve/Xtend data may also be reprocessed using the rslpipeline/xtdpipeline scripts.
- Users may start/finish the reprocessing at the calibration, screening, or preview product generation stage. The ‘pre-calibration’ steps of mkf/ehk and ADR GTI and MXS GTI file generation may be skipped (in which case the pre-existing files may be used).
- Users essentially have access to all of the parameters for all of the tools that comprise the pipeline – so the full sequence of individual tools rarely if ever need to be run (except by the SDC and instrument teams for verification).
- The pipeline tools include a randomization seed – output from multiple, identical runs may not be precisely identical.

Post-pipeline tools - RMF

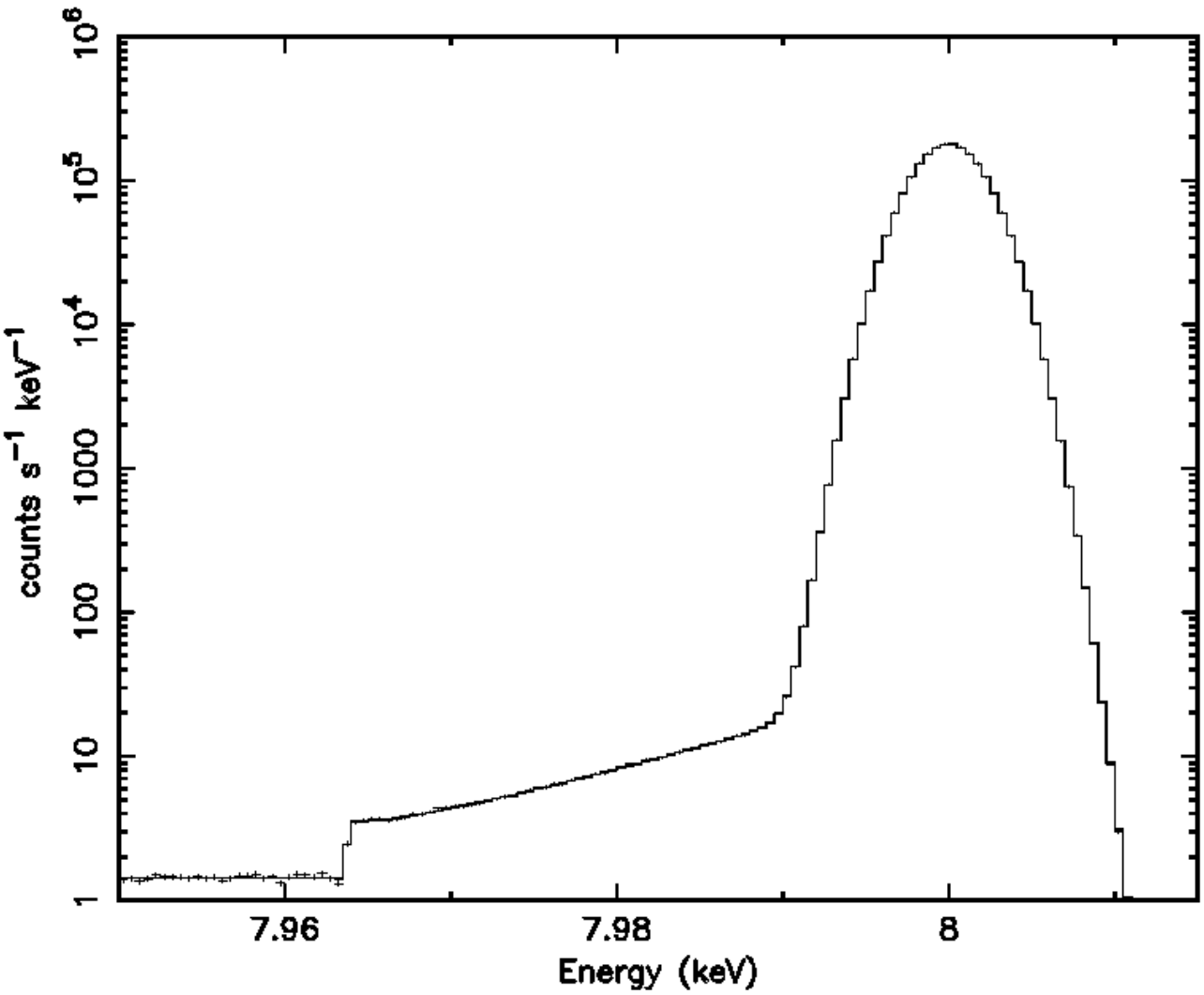
Size	Gaussian core	Exponential tail	Si K alpha emission line*	Escape peaks	Electron loss continuum
Small (s)	✓	✗	✗	✗	✗
Medium (m)	✓	✓	✗	✗	✗
Large (l)	✓	✓	✓	✓	✗
X-large (x)	✓	✓	✓	✓	✓



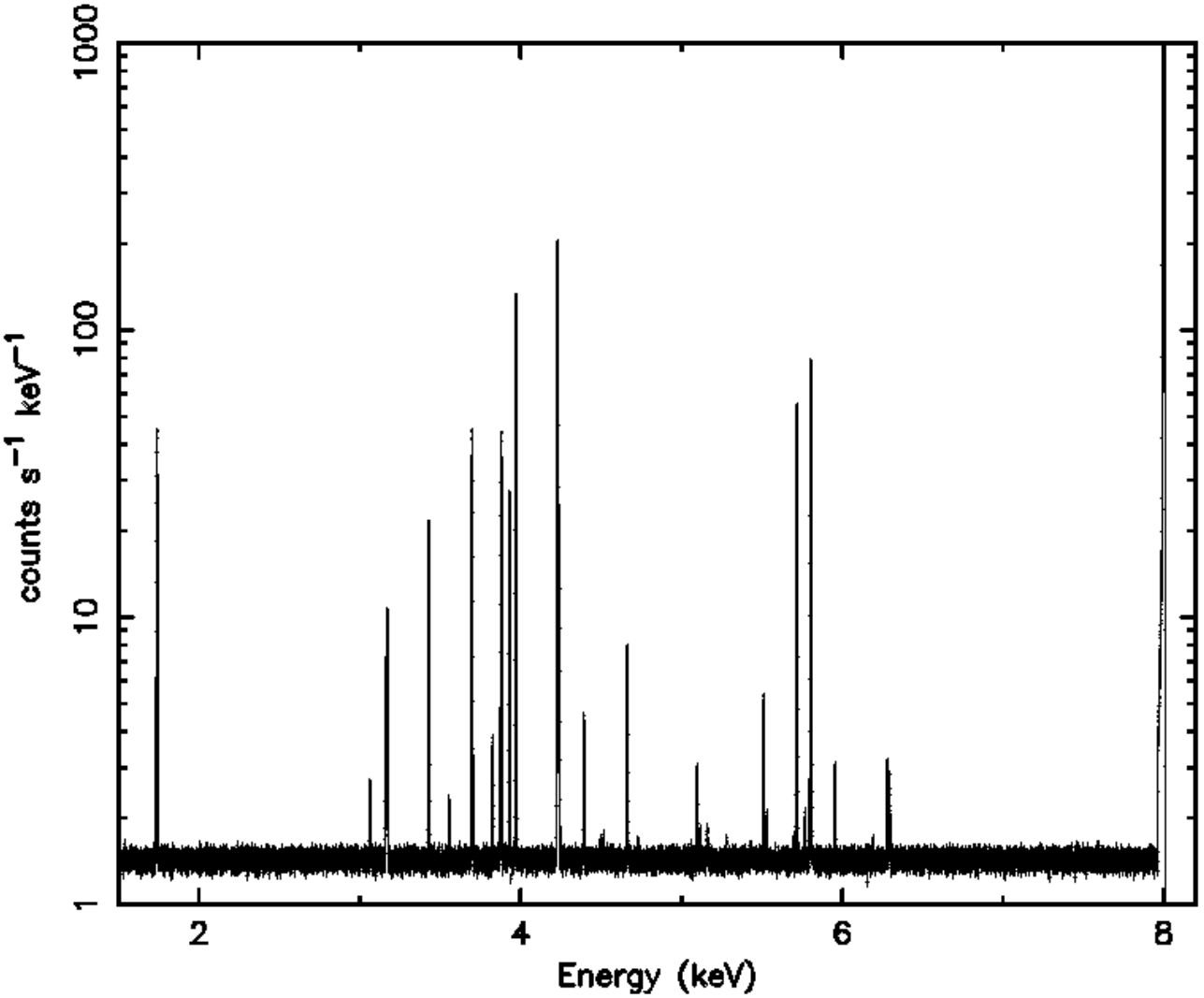




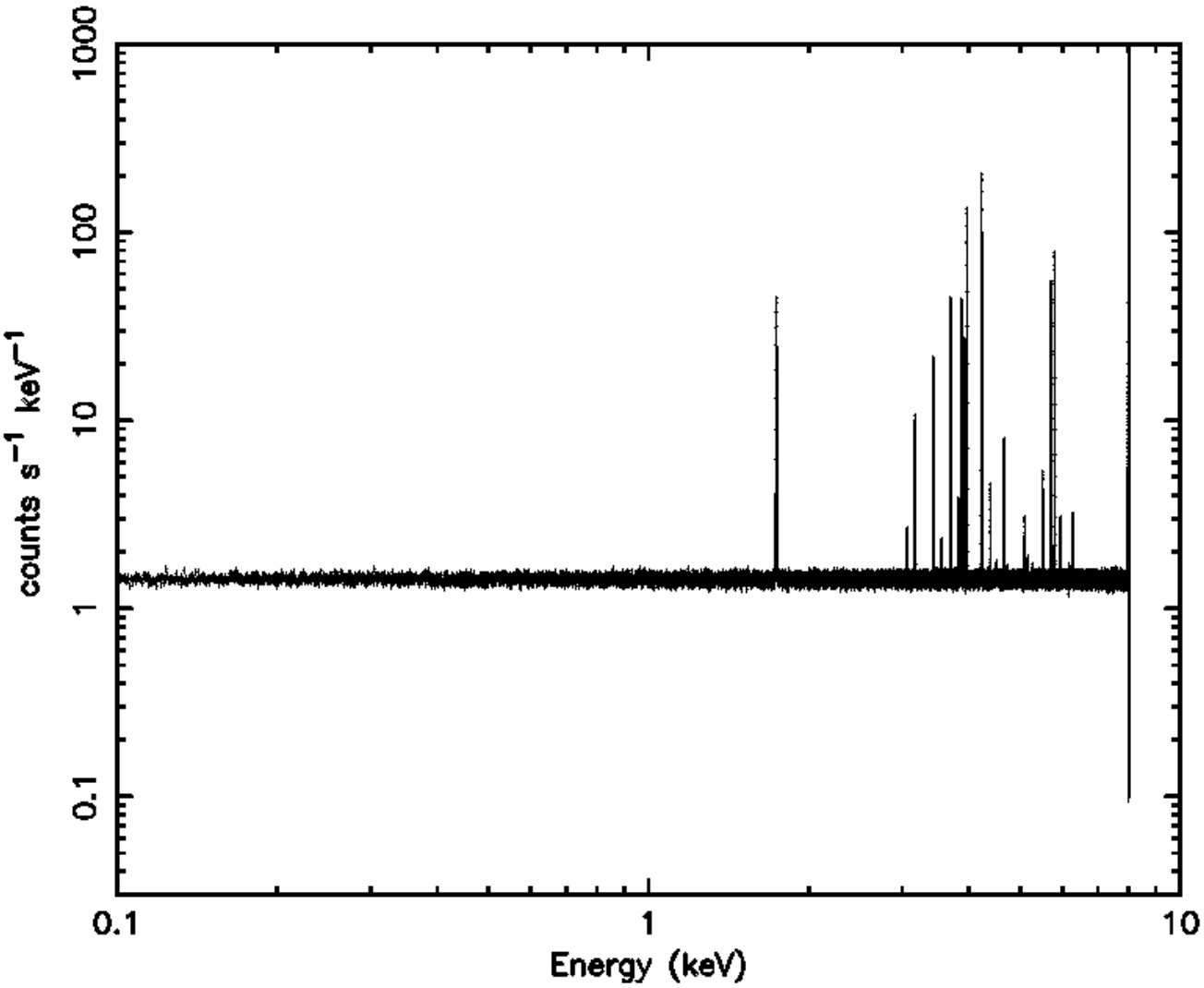
Post-pipeline tools - RMF



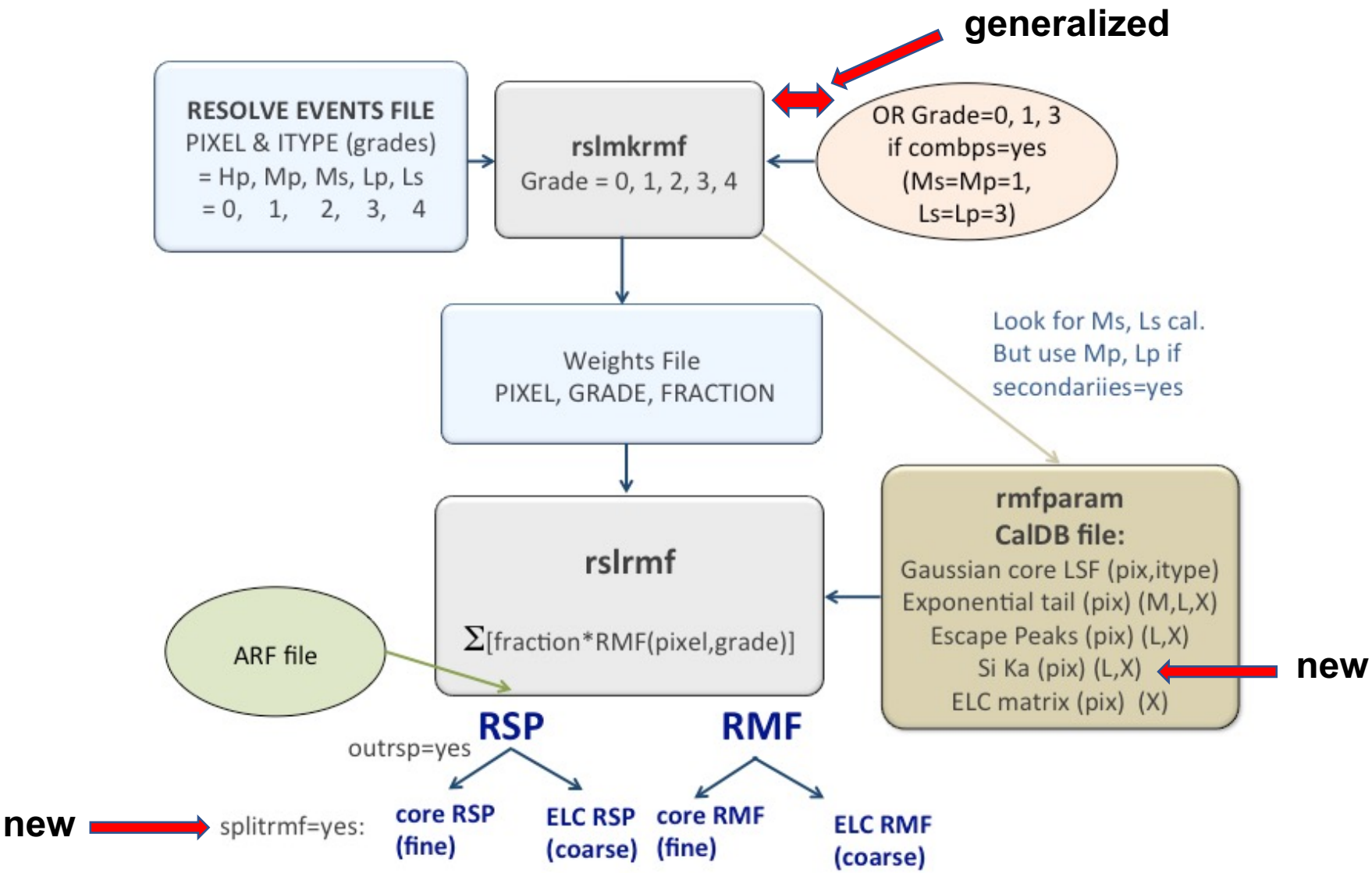
Post-pipeline tools - RMF



Post-pipeline tools - RMF



Post-pipeline tools - RMF

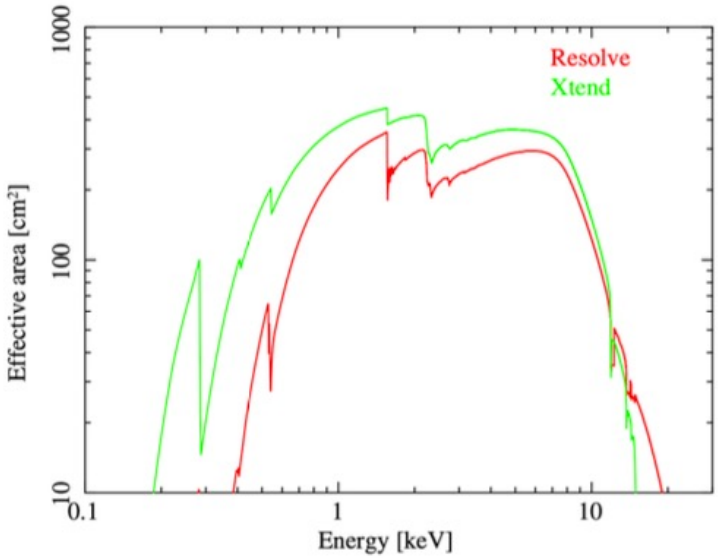


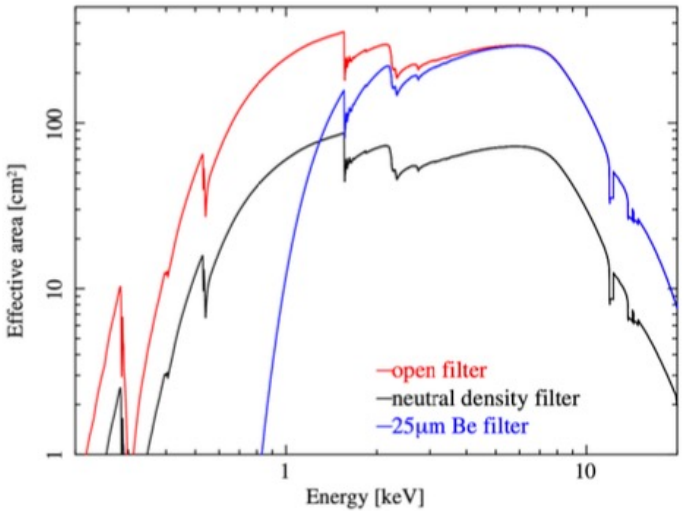
Post-pipeline tools - ARF

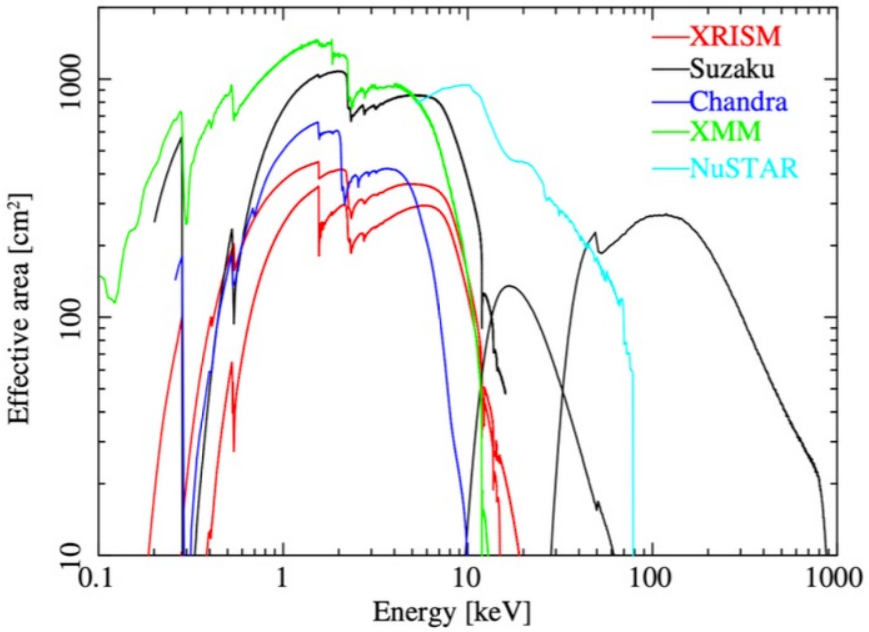
XRISM X-Ray Imaging and Spectroscopy Mission

- An ARF describes the *effective* area of an X-ray telescope as a function of energy – essentially the *geometric* area multiplied by the efficiency at which photons may be detected.
- The xaarfgen task creates an ancillary response function (ARF) file for the XRISM Resolve and Xtend instruments using raytracing simulation.
- Inputs include
  - Exposure map – Where the telescope is looking and for how long (pointing histogram, effective exposure per pixel)
  - Location of the source in the sky
  - Spatial distribution and extent of the source (point-like or extended)
  - Extraction region (match to spectrum)
  - Physical model of the telescope and any obstructions in the optical path (geometry, material composition and their optical properties)
  - Detector efficiency
  - Filter transmission curves
- The xaarfgen task invokes the raytracing task xrtraytrace, using the above inputs, to run a monte-carlo simulation of the photon paths through the X-ray telescope.

Post-pipeline tools - ARF







XRISM Quick Reference

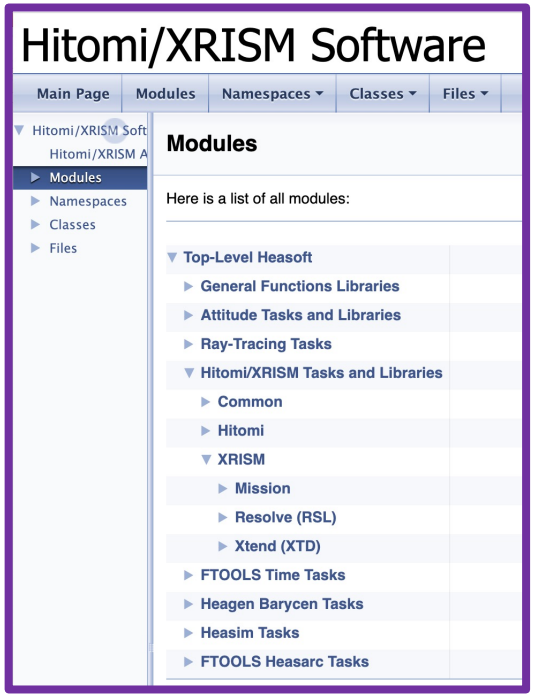
Post-pipeline tools - NXB

- The non-X-ray background (NXB) is an irreducible background that is not due to X-ray photons (mostly high-energy charged particles) collected by the optics and focused on the detector.
- Xtend and Resolve will accumulate a database – that will be accessible online and downloadable - of NXB events during Earth occultations when XRISM is pointed toward the dark limb of the Earth.
- Xtend and Resolve NXB generators (xtdnxbgen, rslnxbgen) extract events from the NXB database, matching the spacecraft and instrument conditions and settings.
- The Resolve NXB is expected to be low in cleaned event lists (~0.0003 cts/sec/pixel for Hitomi SXS), but will have an additional MXS component TBD.

- Some notable updates (in addition to the new tasks mentioned) are as follows:
  - Software / CalDB (not including CalDB content, bug fixes)
    - MET origin from 2014-01-01 to 2019-01-01
    - Resolve MXS pulse delay, pulse offset, afterglow treatment
    - Unified Resolve energy scale
    - New Resolve pixel dependencies (QE, non-core LSF)
    - New Resolve grade dependencies (trigger-to-arrival time correction)
    - Xtend RMF accounts for response to incoming photon energy of peak output channel
    - Additional flexibility in Xtend event flagging
    - Updated algorithm (e.g., CTI correction) treatment in Xtend energy assignment
    - Resolve RMF accounts for Si Ka emission fluorescent line
    - Resolve RMF energy dependence of ELC, split RMF with separate ELC extensions
    - Additional complexity (accuracy, tuning capabilties) in modeling the optics (external objects such as the TS, inner foils, FW, GV)

Hitomi → XRISM

- All Hitomi tasks are maintained as part of a dual architecture where common code may be shared.
- Most XRISM tasks have diverged from their Hitomi cognates (improvements, bug fixes), but changes are mostly “under the hood”.
- Some Hitmomi tasks are deprecated (obsolete or redundant)
  - sxsperseus, sxsregext, sxsextend
- Comprehensive Functional and Lightweight Field Test for automated regression-checks of validated unit-tests.
  - (LFT) delivered to end users as part of ftool release
- Documentation
  - Improved help files
  - Doxygen - bridges the code and help files
    - Easy access and documentation of XRISM software
    - Full access to task code and associated codes/libraries
    - Easy to navigate code components
    - Structure follows the directory structure of HEASoft.
- Final internal pre-flight release: Spring 2023 (XRISM V1.0 release candidate)
- First HEASoft release: After commissioning (XRISM; commissioning updates plus bug fixes)

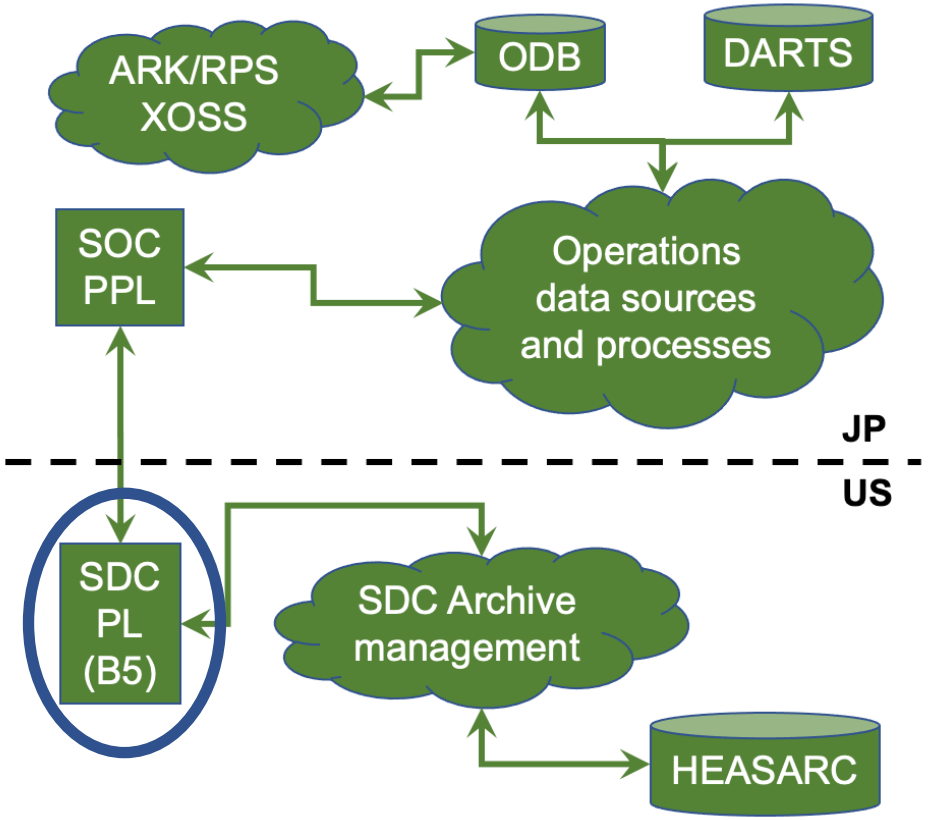


EXTRA SLIDES

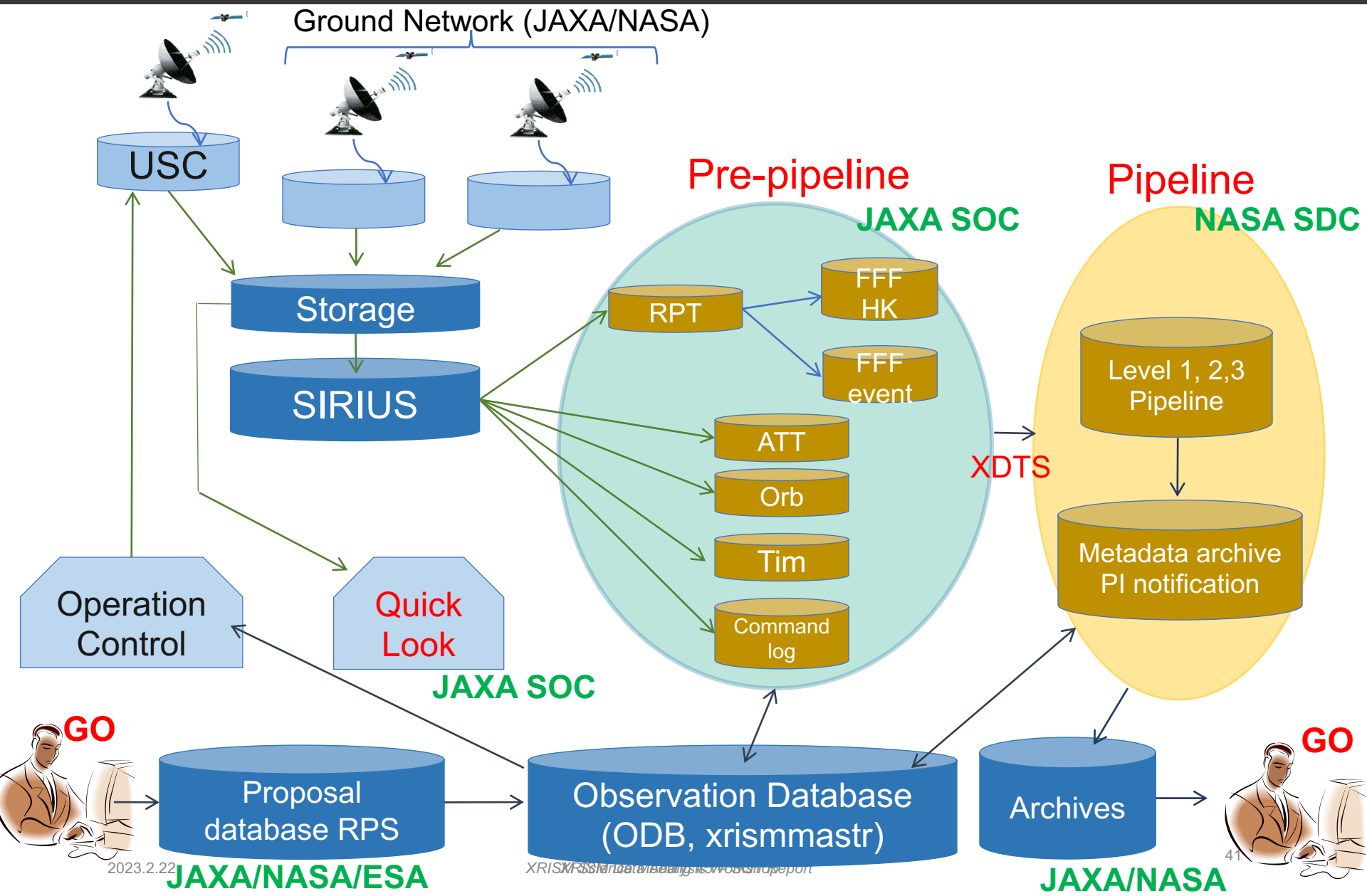
The SOT = SDC + SOC

The XRISM pipeline (PL) is a collection of daemons running on a set of virtual machines hosted at the NASA/GSFC. Each daemon is responsible for a different aspect of data transfer, processing, and validation (next slide).

The PL converts first FITS files (FFFs) – basic event and housekeeping telemetry in FITS format with time-tagging - constructed by the pre-pipeline (PPL) located at JAXA/ISAS, into calibrated and screened FITS files suitable for scientific investigation, and into trend products used to monitor instrument health and performance.



Data Processing/Distribution in Detail



MXS extras

		MXSTYPE		
		NOM (nominal)	RED (redundant)	OFF
MXSLED13 (direct)	Bright, medium, or dim	LED1 is ON	LED3 is ON	N/A
	OFF	LED1 is OFF	LED3 is OFF	All LEDs are OFF
MXSLED24 (in-direct)	Bright, medium, or dim	LED2 is ON	LED4 is ON	N/A
	OFF	LED2 is OFF	LED4 is OFF	All LEDs are OFF

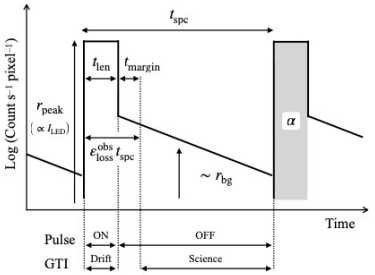


Fig. 3. Pulse parameters.

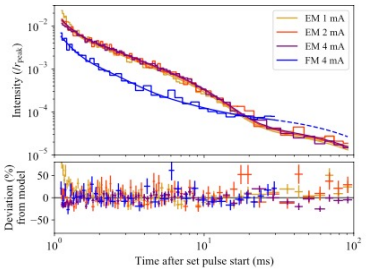


Fig. 4. Afterglow profile.

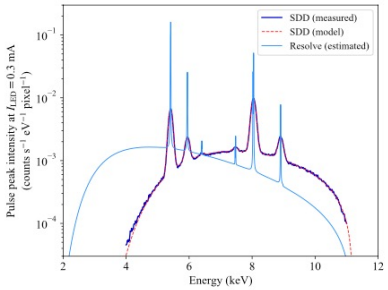
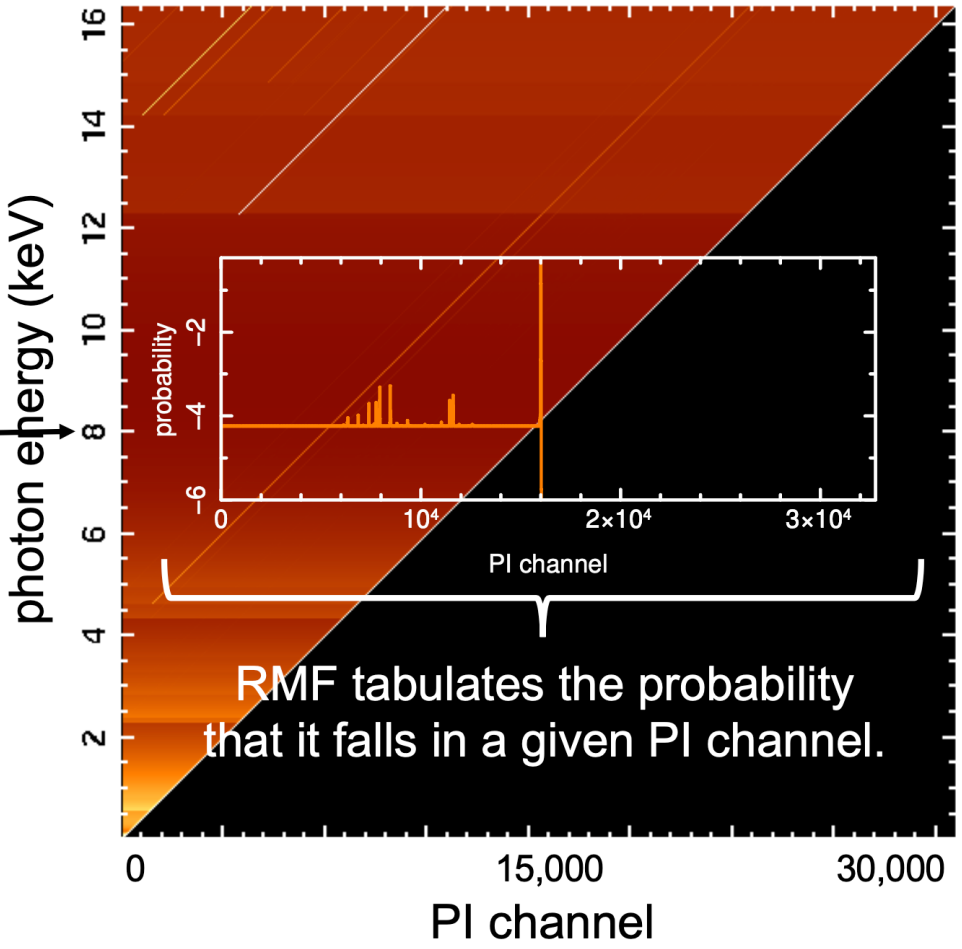


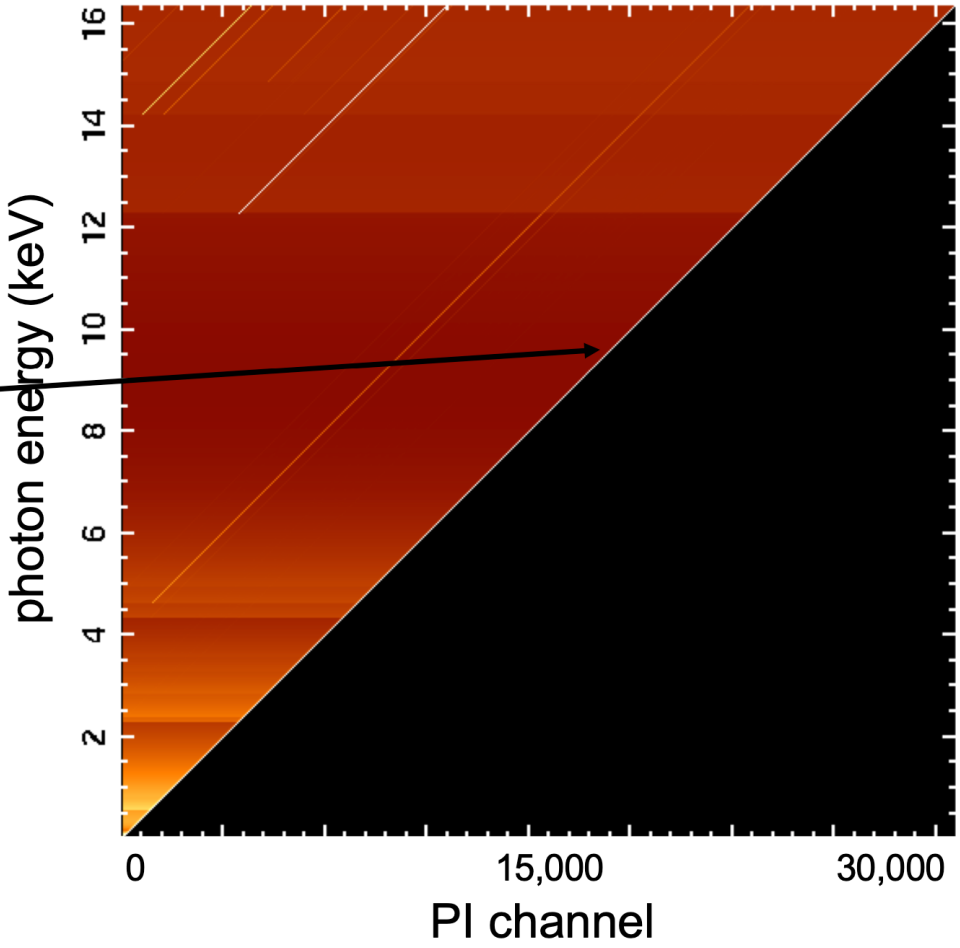
Fig. 5. MXS spectrum.

Photon arrives at 8 keV.



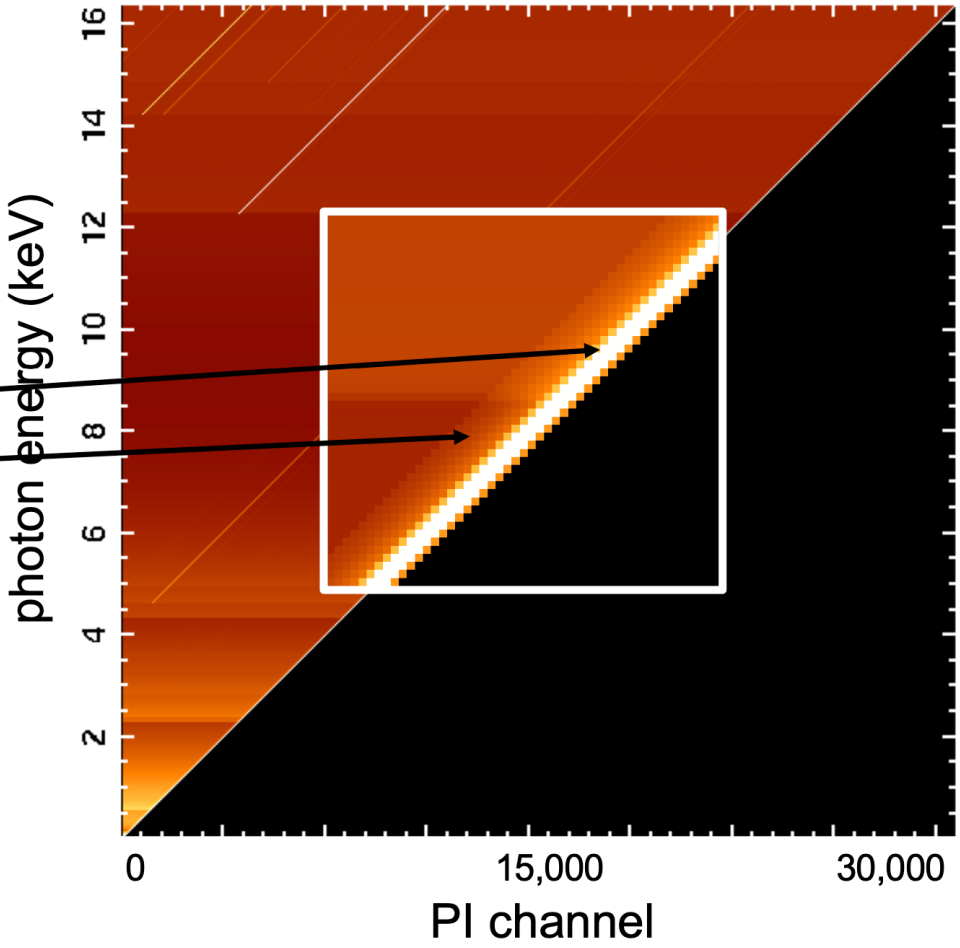
RMF extra

- Photons are redistributed to other, mostly lower detected energy (PI).
- RMF components for SXS/Resolve:
  - Gaussian main peak
  - Exponential shoulder/tail
  - Escape peaks
  - Electron loss continuum (ELC)



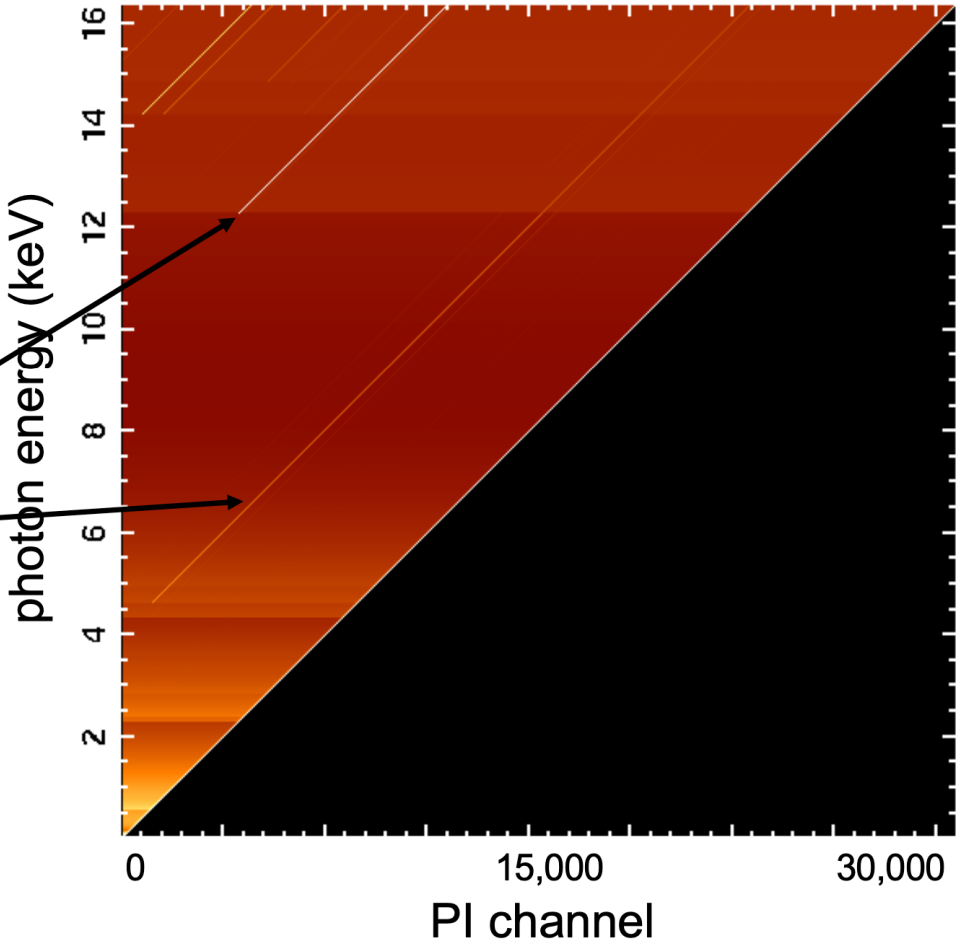
RMF extra

- Photons are redistributed to other, mostly lower detected energy (PI).
- RMF components for SXS/Resolve:
  - Gaussian main peak
  - Exponential shoulder/tail
  - Escape peaks
  - Electron loss continuum (ELC)



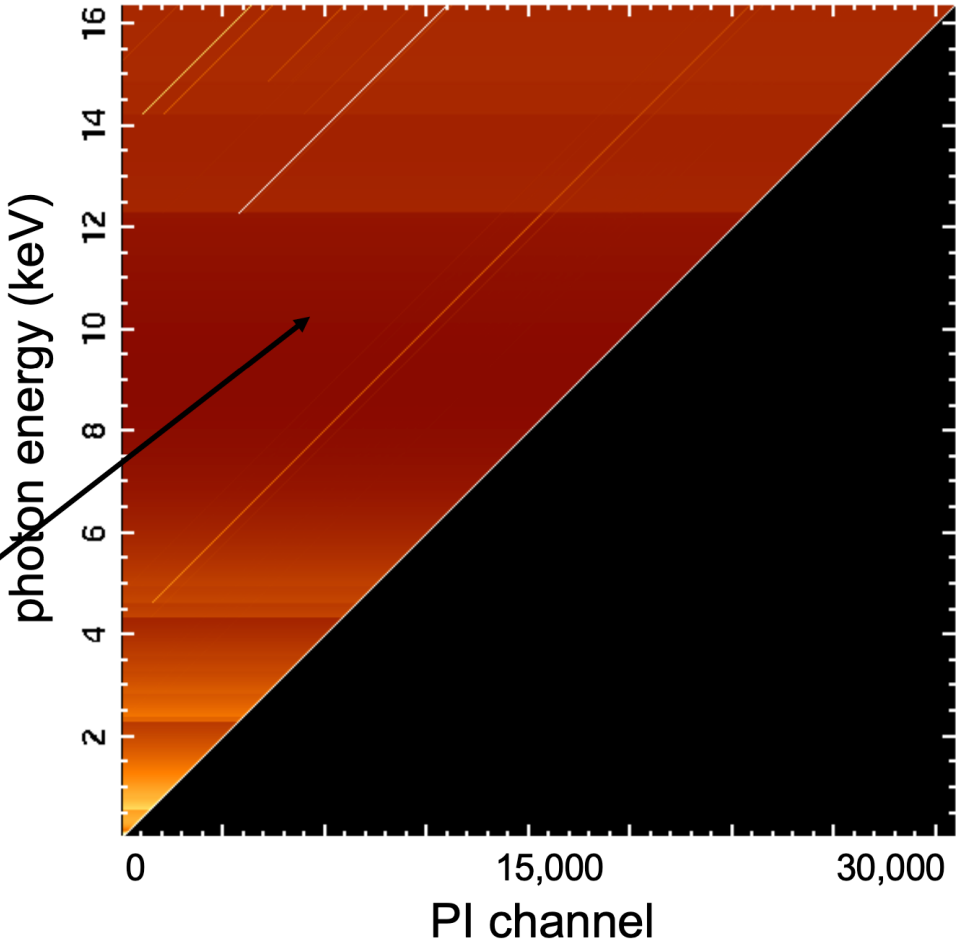
RMF extra

- Photons are redistributed to other, mostly lower detected energy (PI).
- RMF components for SXS/Resolve:
  - Gaussian main peak
  - Exponential shoulder/tail
  - Escape peaks
  - Electron loss continuum (ELC)

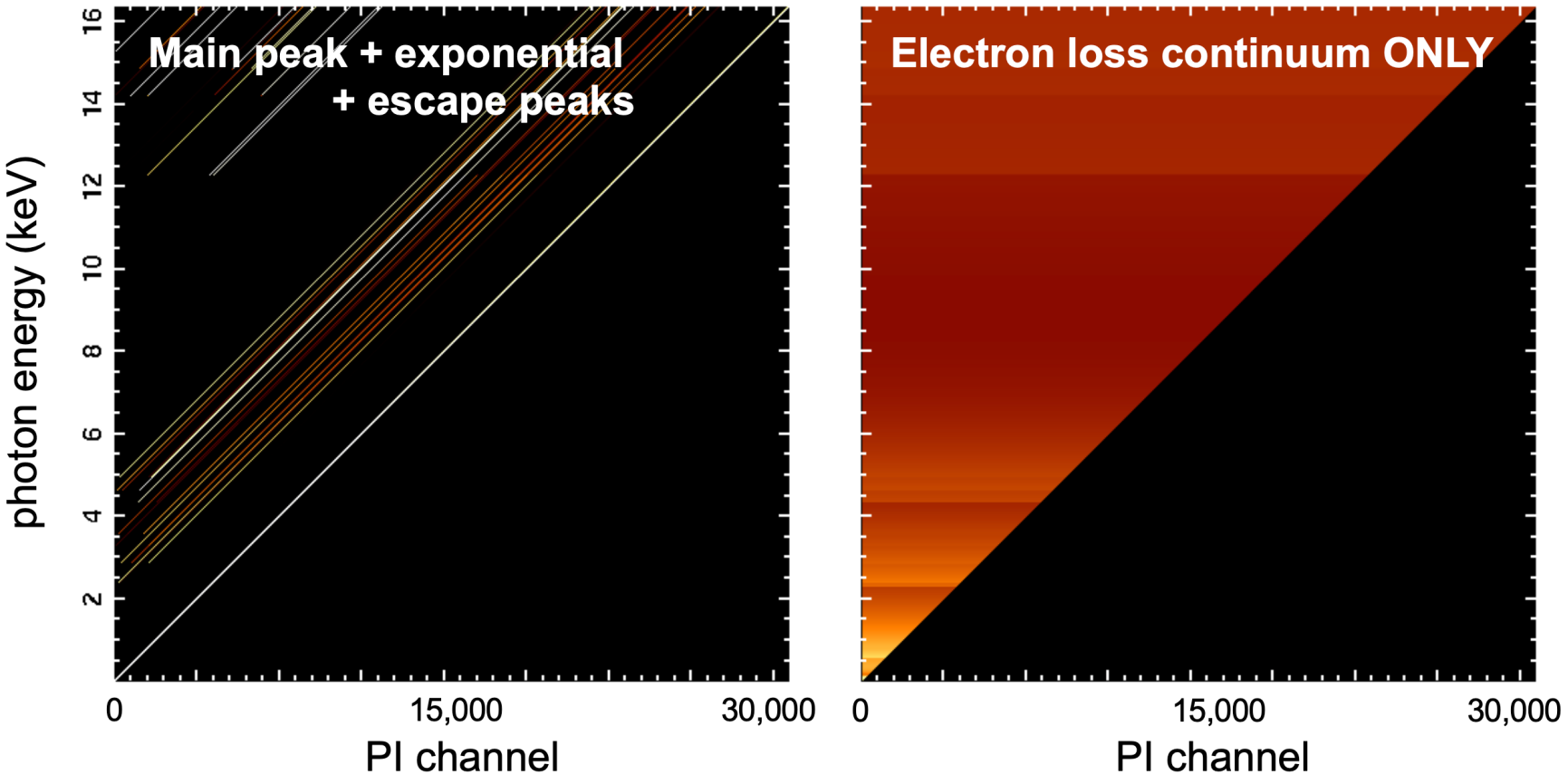


RMF extra

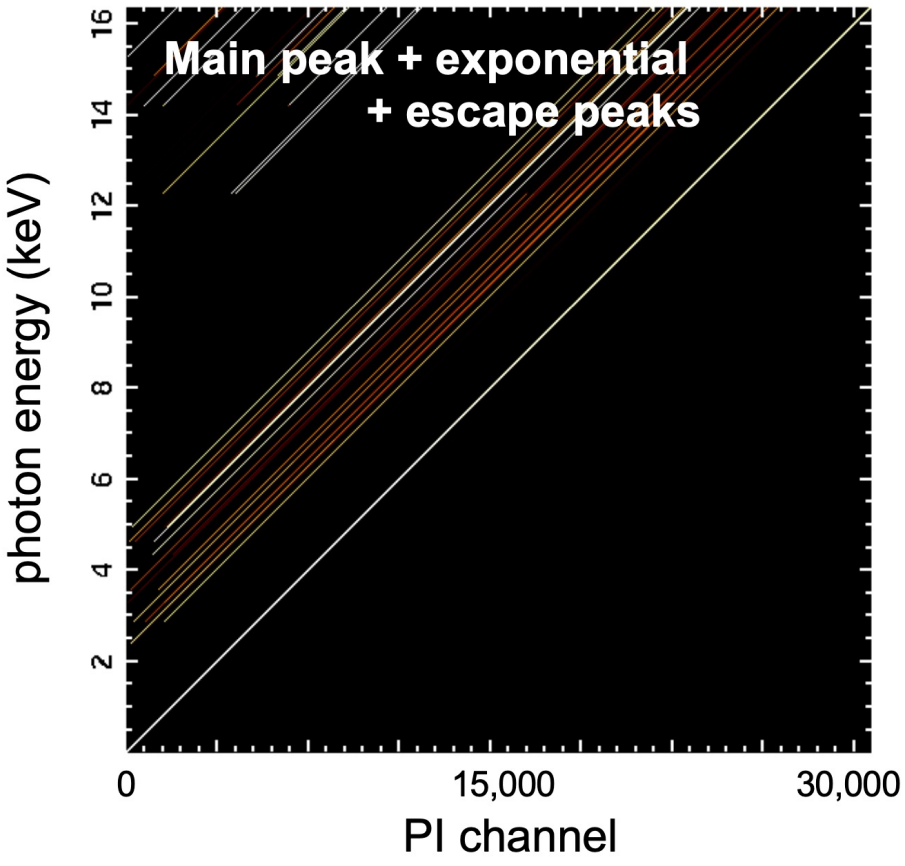
- Photons are redistributed to other, mostly lower detected energy (PI).
- RMF components for SXS/Resolve:
  - Gaussian main peak
  - Exponential shoulder/tail
  - Escape peaks
  - Electron loss continuum (ELC)



RMF extra


Main peak + exponential
+ escape peaks
photon energy (keV)
2
4
6
8
10
12
14
16
0
15,000
30,000
PI channel
Electron loss continuum ONLY
0
15,000
30,000
PI channel

RMF extra

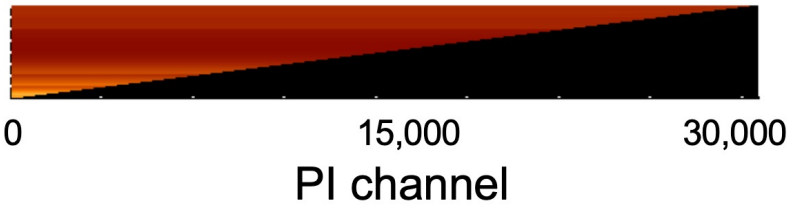


Electron loss continuum ONLY

Bin this up in model energy since it varies slowly with E.

Doesn't depend on source spectrum.

Shown 8x binned, 130 MB.



Raytrace/ARF Coming Attractions

XRISM X-Ray Imaging and Spectroscopy Mission

Work is in progress on enhancements and additions to the raytracing and ARF generation suite of software.

1. Enhancements have been made to the core raytracing program xrtraytrace to accommodate geometrical changes to the inner foil structure, and to implement more accurate thermal shield modeling.
2. A new tool, xmasim, is being developed that is a driver for xrtraytrace, adding many capabilities.
3. Enhancements planned for the ARF generator tool that introduce options for distributed computation of the effective area, with statistical errors, and on-the-fly raytracing of the Resolve filters and gate valve.
4. PSF library planned for Resolve, enabling spectroscopy that accounts for cross-contamination of spatial regions due to the PSF spatial redistribution.
5. Will include the effects of dust scattering on the PSF and effective area.
6. Prototype work has started in order to run xrtraytrace on AWS Batch

Graphical Overview of the Suite