

XMM-Newton

XMM-Newton Science Analysis System 19.0 scientific validation

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1 Introduction

The SAS scientific validation (SV) is performed on a standard set of XMM-Newton observations, which cover all commissioned observational modes, and a number of observations, specially chosen for testing new aspects of the data reduction corresponding to the version to be validated. Table 1 lists all the datasets used for the validation of SAS version 19.0. Some of these observations are particularly suitable to test calibration-related items, as specified in the rightmost column of Tab. 1. These datasets are partly intended as a standard reference, which has been and will be used to verify the performances of all SAS versions. However, additional datasets may occasionally be used to test version-specific SAS items. This is the case, for instance, for the datasets discussed in Sect. 2 of this report. Datasets discussed in a given report and not listed in Tab. 1 do not belong to the reference datasets, and are therefore not intended to be discussed in later SAS versions validation reports.

1.1 Methodology

The SV for SAS v19.0 consisted of the following steps:

1. all the datasets listed in Tab. 1 were processed through the SAS 19 based testing Pipeline System (PPS) running at the SOC, and
2. the same datasets were also processed through the SAS reduction meta-tasks:
`e[mp]proc, om[ifg]chain, rgsproc`
3. all the SAS threads were ran as documented, for checking the integrity of the software and the validity of the threads
4. products generated by the above steps were used as a basis for the *interactive SV analysis*. Standard scientific products (images, light curves, spectra, source lists) were generated and analysed as described in Tab. 2. This allowed us to:
 - test the SAS interactive tasks.
 - verify the calibration accuracy obtained with SAS v19.0, and compare it with the expected accuracy on the basis of the calibration status at the time the SV is performed.
5. SAS v19.0 includes a substantial improvement in the support for Python scripting and programming. Python packages included in SAS 19 are:
 - (a) `pysas`: Core SAS Python package. Includes modules `sastask.py`, `parser.py`, `param.py`, `error.py`, `runtask.py` and `wrapper.py`. The wrapper can be used to run any SAS native task from Python.
 - (b) `xmmextractorGUI`: GUI counterpart for the `xmmextractor` SAS task.
 - (c) `pkgmaker`: A fully rewritten in Python version of the same Perl package which allow to create any new SAS package either in Python or in the other SAS programming languages, C++, Fortran or Perl. For new packages in Python, it provides the required package structure and components.
 - (d) `sasver`: The twin in Python of the SAS tool `sasversion`.

- (e) `startsas`: A Python package that initiates analysis of an ODF by producing the CIF and SAS summary file from a given input ODF id. Aimed to be used in interactive Python sessions such as from Jupyter Notebooks.
- 6. in addition the whole cross-calibration database has been reduced by standard analysis scripts based on SAS but including also model fitting through Xspec.

Table 1: SV datasets

Instrument	Mode	Object	Revolution Obs. ID	ID	Calibration item
EPIC MOS	Full Frame	Lockman Hole	544 0147511601	1	Astrometry + source detection
	"	G21.5.09	060 0122700101	2	Effective area
	"	M31	2847 0761970101	2	Extended source
	Small Window (W2)	Mkn 421	165 0099280201	3	
	Large Window (W3)	PKS0558-504	153 0129360201	4	Effective area
	Timing Uncompressed	Her X-1	207 0134120101	5	Timing
EPIC-pn	Full Frame	Lockman Hole	544 0147511601	1	Astrometry
	Full Frame/Small Window	PKS0558-504	153 0129360201	4	Effective area
	Full Frame	M31	2847 0761970101	2	Extended source
	Large Window	AB Dor	185 0133120201	6	
	Small Window	PKS0558-504	084 0125110101	7	Effective area
	Fast Timing	Her X-1	207 0134120101	5	Timing
		Crab	698 0160960201	8	
	Fast Burst	Crab	411 0153750301	9	Timing
		Crab	411 0153750501	10	Timing
	Extended Full Frame	G21.5-0.9	060 0122700101	2	Effective area
	Slew Data		1388 9138800002	18	Slew data processing
	Slew Data		1450 9145000003	19	Slew data processing
RGS	SPEC+Q	PKS0558-504	084 0125110101	7	
		Mkn 421	165 0099280201	3	Effective area
	"	AB Dor	185 0133120201	6	Wavelength scale
	"	AB Dor	338 0134521301	11	Wavelength scale
	"	AB Dor	462 0134521601	12	Wavelength scale
	"	AB Dor	572 0134522201	13	Wavelength scale
	"	EXO0748-67	044 0119710201	20	Time jumps
	"	MCG-6-30-15	108 0111570201	21	Time jumps
OM	Image Mode	BPM 16274	261 0125320701	14	Photometry
	Fast Mode	X1822-371	228 0111230101	15	
	FF Low Resolution	BPM 16274	261 0125320701	14	Astrometry
	Optical grism	Hz2	503 0125910901	16	Wavelength scale & flux calibration
	UV Grism	HD13499 (offset)	657 0125911301	17	Wavelength scale & flux calibration
	Image+Fast mode	1ES 1553+11.3	2882 0727780301	23	Jupiter patch flagging

Table 1: SV datasets

Instrument	Mode	Object	Revolution Obs. ID	ID	Calibration item
	Image+Fast mode	1ES 1553+11.3	3242 0727780501	24	Jupiter patch flagging

1.2 Validation schedule

This SAS version will be released in two Linux OS 64 versions (Red Hat Enterprise and Ubuntu LTS) as well as one macOS version (Catalina), to cover a broad band of kernels. One Virtual machine will be made available for 32 bit OSs.

The schedule for the validation foresees a total of around 8 weeks for performing the different tasks (for the period from going into release track mode to final release). This was the projected schedule:

- SAS into release track mode
- SAS builds on different platforms
- SAS 19 binaries (Linux & macOS)
- Processing of all the standard datasets, on Linux
- Installation of SAS 19 binary in XCal grid
- Communication to validators about success and data location
- Preparation of a SAS 19 based PPS test version
- Processing of standard datasets by testing pipeline
- Processing of standard datasets also on macOS + cross-checks
- Processing of XCal archive
- First I/A analysis of standard data
- Evaluation of XCal
- Screening of PPS processed standard datasets
- Analysis of Python integration
- Integrity checks running all the existing SAS threads
- Dedicated analysis (see section 2)
 1. Use an image to define an extraction region in evselect
 2. Allow RA, DEC selection
 3. Combine spectra from different cameras
 4. Produce QPB products
 5. RGS background smooth technique

6. EPIC-pn BURST mode CTI

7. esas

8. Source-searching tasks

- Summary reports
- Final SV individual reports
- Release notes + SAS 19 web pages contents ready + XMM Newsletter text
- SAS 19 distribution tar files ready
- SAS 19 release
- SAS VM produced
- Final SV Report compilation

1.3 Calibration data used

SASv19 was validated using the full public calibration constituents available on 30 June 2020, plus the following components which at this date were not yet public:

- EPN_CTL0053.CCF, EPN_CTL0054.CCF which were made public before the SAS 19 release but the RDPHA correction for BURST mode EPIC-pn data will only take effect with SAS 19.
- EMOS1_FWC_0003, EMOS2_FWC_0003, EPN_FWC_0003.CCF
- XMM_FLARE_0001.CCF
- XMM_SCALEFACTORS_0001.CCF
- XMM_SPDETMAP_0001.CCF
- XMM_SWCX_0001.CCF
- EMOS1_QPB_0001.CCF, EMOS2_QPB_0001.CCF, EPN_QPB_0001.CCF. Note that these calibration files are not strictly speaking CCFs and are actually stored in the testprods directory of the SAS.

2 New and updated in SAS 19.0

Version 19.0 is a main yearly release of the SAS. The release contains the following changes which have been specifically tested.

2.1 New in SAS 19.0: use an image to define an extraction region in evselect

Using the construct "expression=IMAGE('imagefile')" an image, spectrum or time series can be produced from the positive parts of a mask, in evselect. Product files should be further processable in downstream software such as arfgen, rmfgen and epiclccorr.

2.2 New in SAS 19.0: Allow RA, DEC selection

The expressions, "(RA,DEC) in circle(rrr,ddd,radius_deg)" and "(RA,DEC) in box(rrr,ddd,half_wid_x_deg,half_wid_y_deg)" are now supported within evselect.

2.3 Updated in SAS 19.0: combine spectra from different cameras

epicspeccombine and multiespecget were introduced in SAS 18 as experimental tasks. These have now been upgraded to standard SAS tasks.

2.4 New in SAS 19.0: produce QPB products

A new task, qpbselect, which produces spectra or images from quiescent particle background (QPB) data has been introduced. This task uses all of the filter wheel closed data contained in the *_FWC*.CCF files, scaling them by a factor related to the number of discarded lines found in the observation of interest after filtering for GTIs.

2.5 Updated in SAS 19.0: RGS background smooth technique

A new background smoothing technique has been introduced. This is experimental and will initially be issued as 'SOC-only'.

2.6 Updated in SAS 19.0: EPIC-pn BURST mode CTI

A new rate-dependent correction calibration has been derived for Burst mode observations. These use the new CCFs, EPN_CTL0053/0054.CCF.

2.7 esas

The esas package is undergoing a major upgrade to integrate it more fully into the rest of the SAS package. In this release only the tasks espfilt and emanom should have changed. Other routines should run as before.

2.8 Python support within SAS

The infrastructure of Python in SAS has been reorganized and extended to allow the integration and development of real Python packages and modules, allowing the user to create a set of Python applications within SAS. Simultaneously, new Python modules have been developed to allow users to run any SAS native task from pure Python sessions running standalone or under Jupyter Notebooks.

2.9 Updated in SAS 19.0: source detection

Small changes were introduced into the source detection tasks to:

- Correct the pile-up estimate for extended sources
- Changes to esplinemap in smoothing mode which may affect source parameters

3 Validation results: standard tests

3.1 Processing of standard datasets

All the datasets listed in Tab. 1 have been processed without errors using the SAS 19 release candidate `xmmsas_20200825_1931` using Ubuntu 18.04LTS. The same datasets were also processed without failure on the mac with os 10.15.6 (Catalina). Processing times were of the order of 11-12 hrs on Linux (RHEL and Ubuntu) and 11-12 hrs on MacOS.

3.1.1 EPIC data - standard set

The standard EPIC datasets were processed without any obvious errors being produced. Results were compared with the processing from SAS 18 and were found to be consistent.

3.1.2 RGS data - standard dataset

The standard set of validation data processed with the SASv19.0 build of August 17 2020 (`xmmsas_20200817_0927`) have been examined. Output products of `rgsproc` have been compared with the result of processing with previous versions of SAS. There are no significant differences.

3.1.3 OM data processing

We have verified the results of SAS 19 on the standard OM validation data sets. Comparisons of the photometry, astrometry, grism spectroscopy and fast mode products processed with SAS 19, against those from SAS 18, all show very good consistency. Checks against reference data (e.g. GAIA DR2 for astrometry, and spectrophotometric standards for photometry and spectroscopy) confirm the validity and stability of SAS 19 for the OM.

As in previous SAS deliveries, this Science validation has been devoted to checking and confirming that the main functionalities already present in previous versions are maintained, in other words, we confirm the overall stability of the system. The reader is thus referred to previous Science Validation Reports for more detailed comments or descriptions.

3.1.4 Repeatability of OM filter photometry

Several spectrophotometric standard stars are observed regularly with OM in order to establish and monitor the photometric and flux calibrations. We have reprocessed all the data from one of them, BPM16274, using SAS 19.

Table 2: Comparison elements

Calibration Item	Test products	Test items
Astrometry + source detection	Source lists	Nr. of sources, positions, fluxes
Effective Area	Spectra + Light curves	Model results, harness ratios
Timing	Light curves + Fourier transforms	Periodicities
Wavelength scale	Spectra + Light curves	Line positions and strengths
Photometry	Source lists	Fluxes

The results are presented in Table 3. For comparison we give also the results obtained with SAS 18 - note the SAS18 results are based on calibration data at the time of the SAS18 release. The data used span the mission baseline, up to revolution 3552 (to ensure the same data are used) but exclude observations after revolution 3224 where the source was observed within the so-called 'Jupiter' patch, where the sensitivity degradation is not corrected for.

The quoted errors are the standard deviations of the data about the mean values, given as a percentage of the mean.

We see that after all corrections are applied, the standard deviation of the count rate of the star obtained in each filter is less than 2.5%. The data also confirm that SAS 19 delivers very similar count rate results to SAS 18 ($< 1\%$ differences).

Table 3: A comparison of the average count rates (per filter) of all observations of the standard star, BPM16274, up to revolution 3552 (but excluding those where the source is affected by the Jupiter patch degradation), processed with SAS 19.0 and SAS 18

SAS	UVW2	UVM2	UVW1	U	B	V
19	14.63	29.99	72.37	112.13	106.93	32.81
error (%)	1.6	1.0	1.0	0.8	0.9	2.2
18	14.67	30.17	72.72	112.40	107.10	33.09
error (%)	1.6	1.0	1.0	0.8	0.9	2.4

3.1.5 Test pipeline checks

All the validation dataset ODFs were successfully processed in a SASv19 based Pipeline.

3.1.6 XCal data

The new SAS version SASv19.0 was compared with its previous version SASv18.0 by performing spectral extractions of 348 individual exposures of 52 targets of various source types throughout all the epochs of the mission that are included in the XMM-Newton SOC cross-calibration archive

- 211 exposures of on-axis point targets of various source types, mainly with continuum dominated spectra, from isolated neutron stars to AGN.
- 101 exposures of 2 different thermal supernova remnants
- 12 exposures of 4 different galaxy clusters
- 24 off-axis point sources (AGN).

All results of the spectral extractions using the two different versions of the SAS show comparable differences between the camera returned fluxes (Fig. 1).

Fits of the very soft isolated Neutron star, RXJ1856.6-3754, were performed over the whole history of observations (Fig. 2). Results are compatible between SAS v18.0 and the new SAS v19.0. Similarly the line strengths returned by a multi-component fit to the SNR 1E0102.2-7219 were compared between SAS 19 and SAS 18 (Fig. 3) giving consistent results.

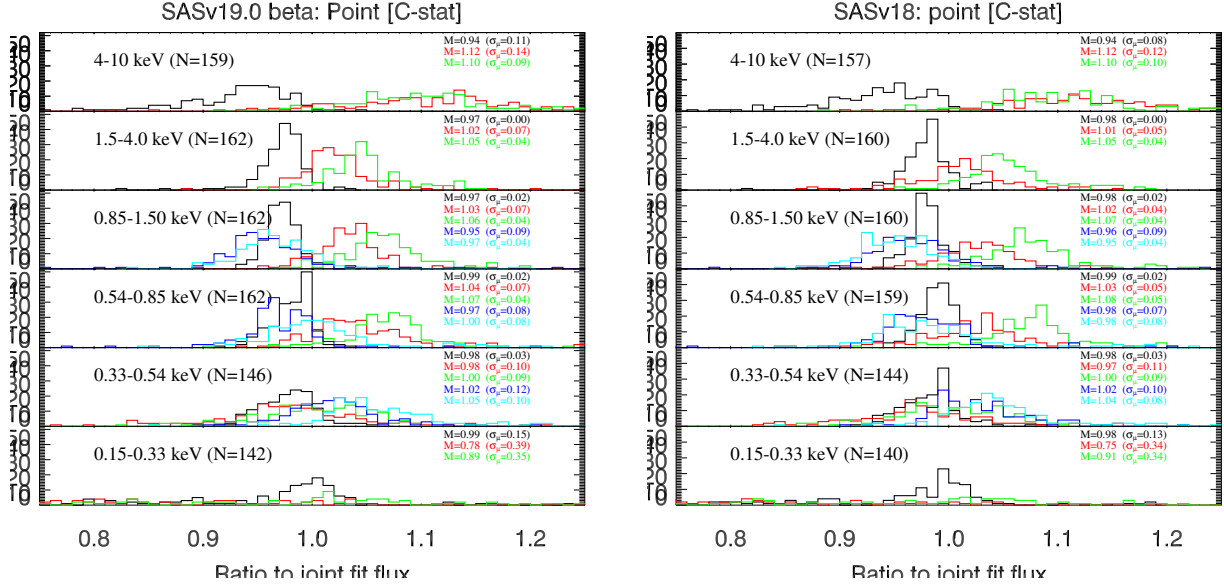


Figure 1: *Left panel:* comparison of fluxes returned on a set of point sources by the three EPIC cameras and the RGS, using SAS v19.0. *Right panel:* comparison of fluxes using SAS v18.0.

3.2 Processing with SAS built on a different flavour than the one used - Compatibility

The two Linux versions (Centos 7.3 and Ubuntu 18.04LTS) have been successfully used on a variety of different systems, including RedHat 7 and 8 and Ubuntu 20.04LTS, to check for compatibility issues. SAS built on macOS Catalina was executed on Macs running the Mojave operating systems without problems.

3.3 Dedicated analysis

3.3.1 G21.5-0.9

The non-thermal SNR G21.5-0.9 has been used as one of the standard targets for the validation of the EPIC effective area calibration. Additionally, this source has proven useful in multi-mission cross-calibration studies (Tsujiimoto et al. 2011). Its spectrum can be well modelled by a simple power-law combined with a photoelectric absorption.

In observation 0122700101, G21.5-0.9 was observed with MOS in Full Frame mode and PN in Extended Full Frame Mode (all using Medium Filter) for 30 ks. MOS and PN source spectra were extracted from a circular region (~ 2.5 arcmin radius) around the SNR, and spatially filtered through their common exposure mask. MOS background spectra were obtained from annular regions around the source, whereas PN background was obtained from neighbouring source free regions. EPIC data were reduced with SAS 19.0 and spectra were extracted with standard event pattern selection.

The results of the comparison of PN and MOS are summarised in Fig. 4, and are essentially in agreement with the previous SAS science validation study. This is as expected, as no significant changes in energy scale calibration have been introduced in the meantime.

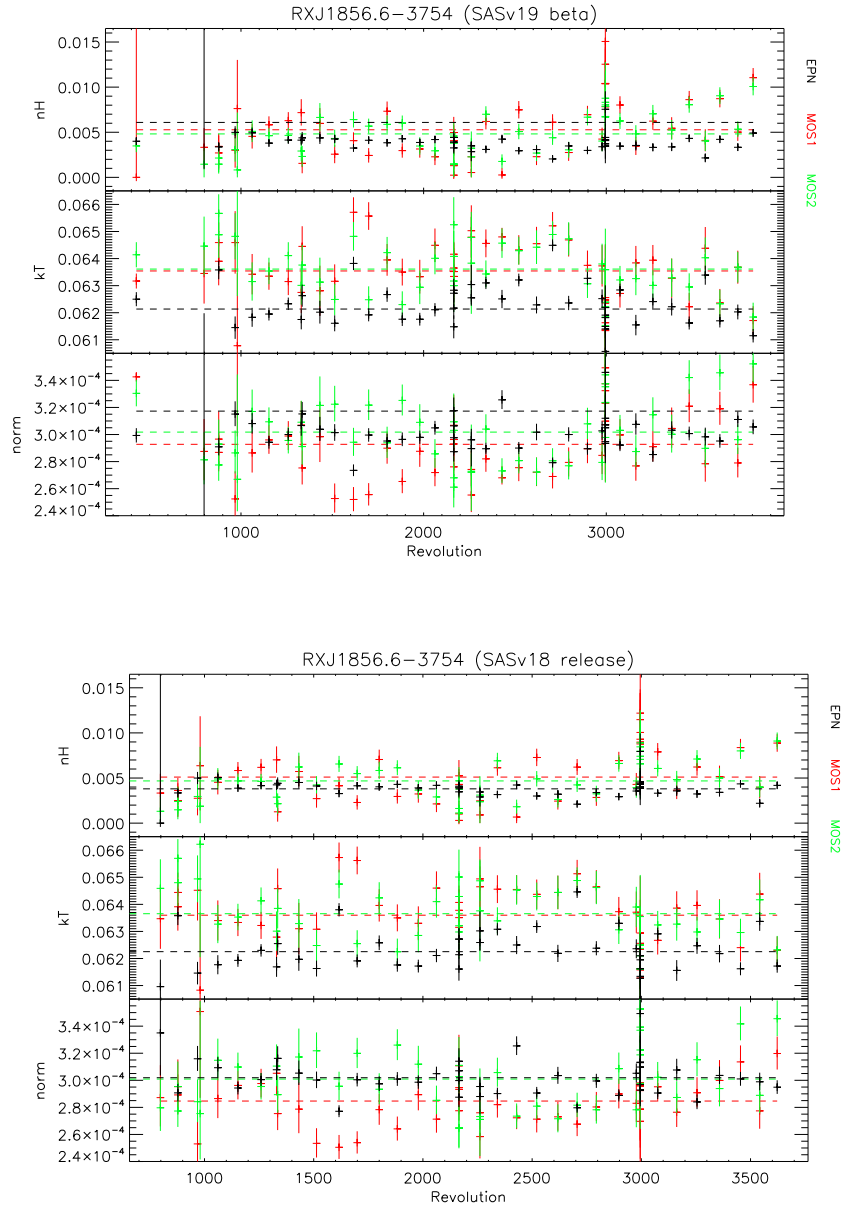


Figure 2: Spectral parameters of an absorbed black-body model fitted to historical spectra of RXJ 1856.6-3754. Upper: SAS v19.0, lower: SAS v18.0.

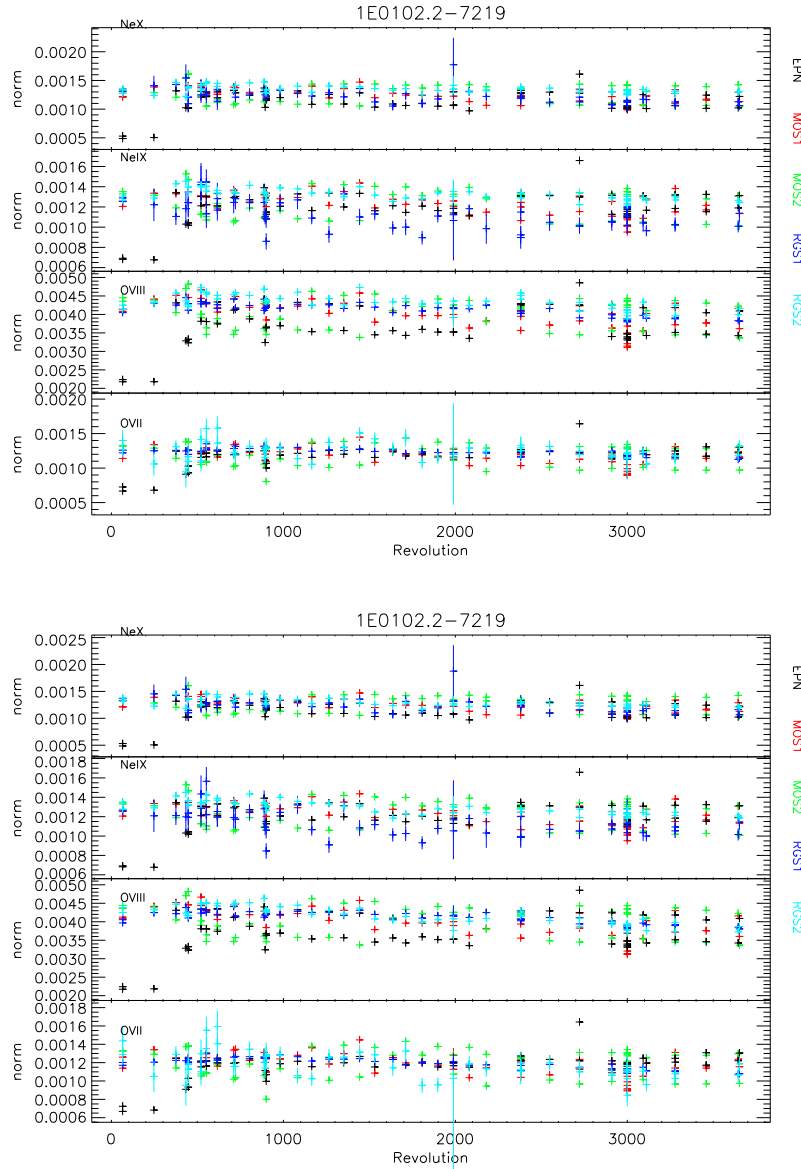


Figure 3: Measured line strengths, as a function of epoch, for spectral fits to the SNR 1E0102.2-7219 with SAS v19.0 (upper) and SAS v18 (lower).

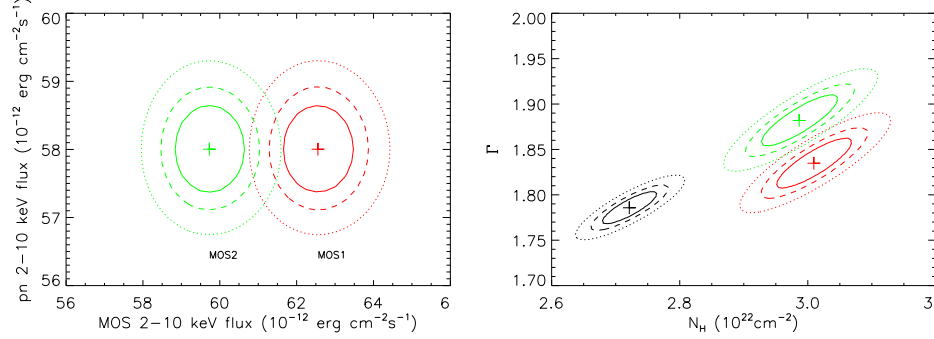


Figure 4: Comparison of PN versus MOS spectral fits of G21.5-0.9. Spectra based on data reduced with SAS 19.0, using standard pattern selection. *Left panel:* the 2-10 keV flux confidence contours for PN versus MOS1 (red) and MOS2 (green). *Right panel:* column density versus photon index confidence contours for PN (black), MOS1 (red), MOS2 (green). Levels shown are at 68%, 90% and 99% confidence.

3.3.2 PKS 0558-504

PKS 0558-504 is a well studied radio loud Narrow Line Seyfert 1 galaxy (e.g. Siebert et al. 1999), and has been observed by *XMM-Newton* as calibration target. Its 2-10 keV spectrum is characterised by a spectral slope $\Gamma \sim 2.2$, and the 0.2-2 keV emission is dominated by a large and featureless soft excess.

EPIC spectra of ObsIds 0125110101 and 0129360201 are compared as part of this science validation. In the exposures compared here, PN was operated in Small Window Mode, and both MOS instruments in Large Window Mode. Data were reduced with SAS 19.0 (using the respective latest calibration files), and resulting spectra were fit in the 0.3–10 keV band with a model consisting of a power-law and bremsstrahlung component with an ISM absorption model (Papadakis et al. 2010). As the MOS data are subject to pile-up the spectra were extracted from annular regions with core exclusion radii of $10''$.

The best fit results are summarised in Tables 4 and 5. The main differences between instruments are due to the imperfect relative effective area calibration, resulting in fluxes which are formally not consistent across all three instruments.

Table 4: Comparison of MOS and PN spectral fits to PKS 0558-504 (ObsId 0125110101) with a power-law plus bremsstrahlung model.

Instrument	kT keV	Γ	Flux $10^{-11} \text{ erg cm}^{-2} \text{ s}^{-1}$	
			(0.3–2.0 keV)	(2.0–10.0 keV)
PN	$0.27^{+0.03}_{-0.03}$	$2.22^{+0.06}_{-0.06}$	$2.48^{+0.03}_{-0.03}$	$1.07^{+0.07}_{-0.06}$
MOS1	$0.21^{+0.06}_{-0.04}$	$2.24^{+0.13}_{-0.15}$	$2.12^{+0.02}_{-0.02}$	$0.94^{+0.05}_{-0.06}$
MOS2	$0.32^{+0.05}_{-0.08}$	$2.13^{+0.17}_{-0.14}$	$2.30^{+0.02}_{-0.02}$	$0.92^{+0.05}_{-0.05}$

Table 5: Comparison of MOS and PN spectral fits to PKS 0558-504 (ObsId 0129360201) with a power-law plus bremsstrahlung model.

Instrument	kT keV	Γ	Flux $10^{-11} \text{ erg cm}^{-2} \text{ s}^{-1}$	
			(0.3–2.0 keV)	(2.0–10.0 keV)
PN	$0.35^{+0.03}_{-0.03}$	$2.12^{+0.04}_{-0.04}$	$2.44^{+0.01}_{-0.01}$	$1.18^{+0.02}_{-0.02}$
MOS1	$0.40^{+0.09}_{-0.08}$	$1.92^{+0.16}_{-0.19}$	$2.54^{+0.02}_{-0.02}$	$1.35^{+0.06}_{-0.06}$
MOS2	$0.26^{+0.06}_{-0.05}$	$2.22^{+0.11}_{-0.10}$	$2.47^{+0.02}_{-0.02}$	$1.17^{+0.05}_{-0.05}$

3.3.3 Standard tests of esas

The full thread for **esas** images extraction has been run on the observation 0097820101 of the Abel 1795 galaxy cluster for EPIC-pn and MOS data. In detail the following tasks have been run:

- epchain withoutoftime=true
- epchain
- emchain
- emanom eventfile=mos1S001.fits keepcorner=FALSE
- emanom eventfile=mos2S002.fits keepcorner=FALSE
- espfilt eventfile=mos1S001.fits method=histogram elow=2500 ehigh=8500 withsmoothing=yes smooth=51 rangescale=6.0 allowsigma=3.0 keepinterfiles=false
- espfilt for MOS2 and EPIC-pn
- cheese prefixm='1S003 2S004' prefixp=S005 scale=0.5 rate=1 dist=40.0 clobber=0 elow=300 ehigh=10000 mlmin=15 clobber=1
- pn-spectra prefix=S005 caldb=/xdata/ccf/pub/extras/esas_caldb mask=1 elow=400 ehigh=2000 quad1=1 quad2=1 quad3=1 quad4=1
- mos-spectra prefix=1S003 caldb=/xdata/ccf/pub/extras/esas_caldb region=regm1.txt mask=1 elow=400 ehigh=2000 ccd1=1 ccd2=1 ccd3=1 ccd4=1 ccd5=0 ccd6=1 ccd7=1
- pn_back prefix=S005 caldb=/xdata/ccf/pub/extras/esas_caldb diag=0 elow=400 ehigh=2000 quad1=1 quad2=1 quad3=1 quad4=1
- mos_back prefix=1S003 caldb=/ccf/pub/extras/esas_caldb diag=0 elow=400 ehigh=2000 ccd1=0 ccd2=1 ccd3=1 ccd4=1 ccd5=0 ccd6=1 ccd7=0
- proton prefix=S005 caldb=/ccf/pub/extras/esas_caldb specname=pnS005-obj.pi ccd1=1 ccd2=1 ccd3=1 ccd4=1 elow=400 ehigh=2000 spectrumcontrol=1 pindex=0.972080 pnorm=0.131099

- proton prefix=1S003 caldb=/ccf/pub/extras/esas_caldb specname=mos1S003-obj.pi ccd1=0 ccd2=1 ccd3=1 ccd4=1 ccd5=0 ccd6=0 ccd7=0 elow=400 ehigh=2000 spectrumcontrol=1 pindex=0.972080 pnorm=0.131099
- rot_det_sky mode=1 prefix=S005 elow=400 ehigh=2000 detx=-1079.810798 dety=1482.314823 skyx=450.91 skyy=450.91 maskfile=1 clobber=1
- rot_det_sky mode=2 prefix=S005 elow=400 ehigh=2000 detx=-1079.810798 dety=1482.314823 skyx=450.91 skyy=450.91 maskfile=1 clobber=1
- rot_det_sky mode=1 prefix=1S003 elow=400 ehigh=2000 detx=-1414.414144 dety=-1389.413894 skyx=450.91 skyy=450.91 maskfile=1
- rot_det_sky mode=2 prefix=1S003 elow=400 ehigh=2000 detx=-1414.414144 dety=-1389.413894 skyx=450.91 skyy=450.91 maskfile=1
- comb caldb=/ccf/pub/extras/esas_caldb withpartcontrol=1 withsoftcontrol=1 withswcxcontrol=0 elowlist=400 ehighlist=2000 mask=1 prefixlist="1S003 2S004 S005"
- adapt smoothingcounts=50 detector=0 thresholdmasking=0.02 binning=2 elow=400 ehigh=2000 withmaskcontrol=no withpartcontrol=yes withsoftcontrol=yes withswcxcontrol=no

The updated task `espfilt` (`espfilt-3.4.4`) was tested and found to be working, as was the new task, `emanom`.

From the above list of tasks, from *cheese* onwards, the tasks were found to work as with SAS v18 with one caveat. The old *cheese* takes the file names as output by `pn-filter` and `mos-filter`. As these two tasks are no longer used, *cheese* can not find the file names it needs. There is no way of telling *cheese* via command-line parameters the names of the files. So the files output by the new `espfilt` task have to be renamed before running *cheese*. The files need to be renamed in the following way:

```
cp pnS005-fovevc.fits pnS005-clean.fits
cp pnS005-fovevcot.fits pnS005-clean-oot.fits
cp mos1S003-fovevc.fits mos1S003-clean.fits
cp ms21S004-fovevc.fits mos2S004-clean.fits
```

In summary:

1. There is a new task: `emanom` to get anomalous chip information. This task works fine.
2. `pn-filter` and `mos-filter` have been removed and replaced by `espfilt`. Although as of today, `pn-filter` and `mos-filter` are still present in the distribution.
3. The above list of tasks was run successfully in a 64 bit machine to produce a mosaic image of the three instruments with point sources removed (also smooth version of image produced). For simplicity, only the energy range `elow=400 ehigh=2000` was used.

4 Validation results: New and updated features in SAS 19

4.1 New in SAS 19.0: use of an image as an extraction region

Functionality was tested on a Linux desktop, using the pre-processed event lists from the observation 0122700101 of the SNR G21.5-09. Testing procedure:

- Generate MOS1/pn image from the mos1/pn event list, using energy band [1,2] keV, allow for images with different binSize, i.e. pixel size. Experiment with binSize=20 (1"/pixel) and binSize=80 (default, 4"/pixel).
- Use the generated MOS1/pn image to create a mask with a circular region centred on (RA_OBJ,DEC_OBJ) from the MOS1/pn image header and with radius 1 arcmin.
- Create two filtering expressions for evselect: one with

```
(RA,DEC) in CIRCLE (RA_OBJ,DEC_OBJ,radius)
```

and another one with

```
IMAGE(<X_mask_image>)
```

- Spectral extraction:
 - Extract with evselect two output spectra with the two filtering expressions (all the other parameters are identical).
 - Compare the two output spectra.
 - Try with a mask image with no overlap with the observation (i.e. changing CRVAL2 to be more than 1 degree away) and check evselect.
 - Try with a mask image with much smaller size; the current MOS1 image with binSize=80 is of shape 648x648 pixels, will try with 100x100 pixels.
- Light-curve extraction:
 - Extract with evselect two output light curves with the two filtering expressions (all the other parameters are identical) in different energy bands. No barycenter correction.
 - Correct the light-curves with epiclccorr
 - Compare the two output light curves

It was noted that the input image must contain integer values, otherwise an error message is issued. This is adequately documented. The following warning message is always generated:

```
warning (DssCompForm), Two 2-d filters with the name POS have been found  
to different components. Cannot write data subspace.
```

This warning has been removed with dsslib 5.12.1 (SPR-7561).

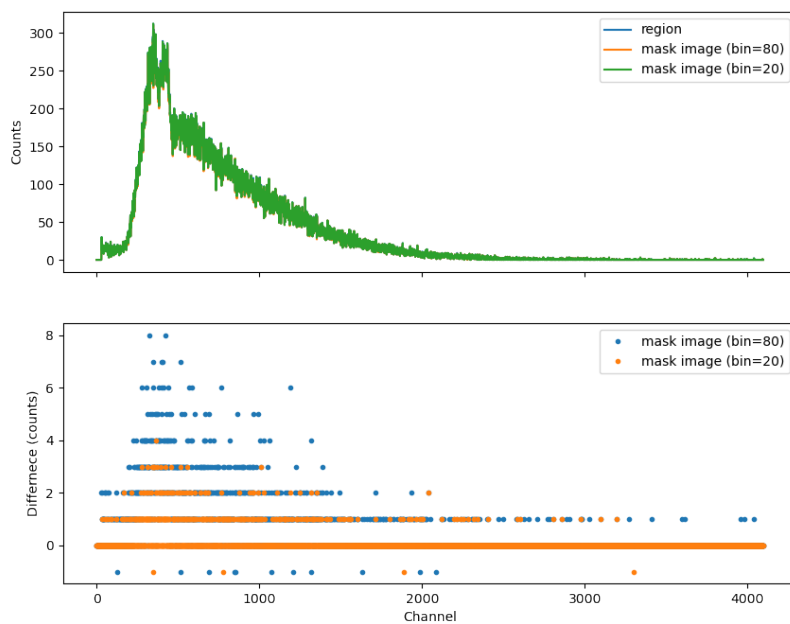


Figure 5: Upper: Counts spectrum of G21.5-09 extracted with images of pixel size 20 and 80 detector pixels. Lower: The difference in counts between the two extractions.

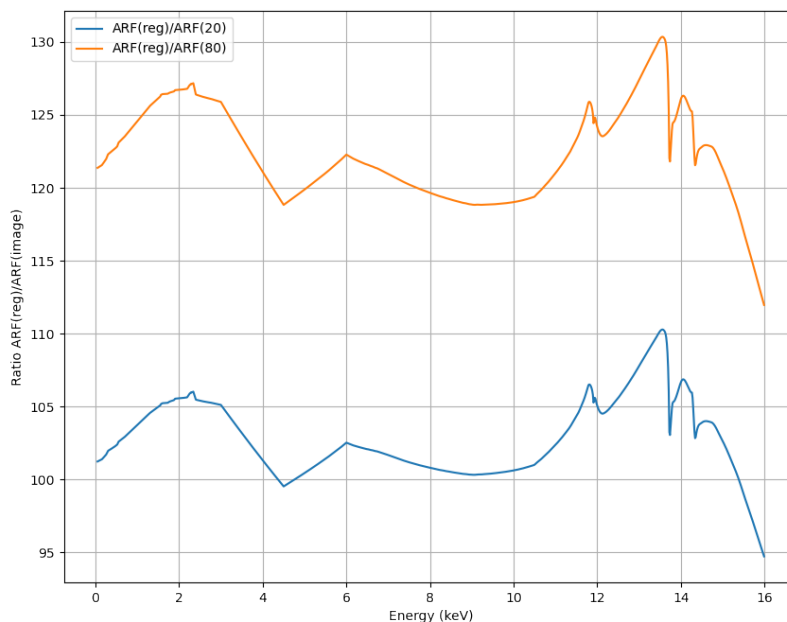


Figure 6: The ratio of the effective area returned by arfgen from a spectrum extracted with an image, compared with a spectrum extracted using a circular region. arfgen has been run assuming a point source and applying the encircled energy correction.

4.1.1 Using MOS1-based mask image

Comparing the spectra filtered with MOS1 mask with 1"/pixel and 4"/pixel against filtering with a region shows minimal differences due to the binning (Fig. 5).

Using a mask image with a very different sky position does not result in an error message but evselect produces a warning that no events were selected. This is correct behaviour.

Using zoomed in image with 300x300 pixels, cropping the MOS1 mask image to 5x5 arcmin. The results are identical with the non-cropped, original size MOS1 image.

4.1.2 ARF files

Checking the produced ARF files, arfgen was executed with the same parameters, the differences are the RMF files and the input spectral sets.

Point source: there is a huge difference in the ARF files, comparing the two 'SPECRESP' extension (Fig. 6).

Extended source: Checking the produced ARF files with arfgen and using extendedsource=yes option. The ratio of the effective areas agrees to within $\sim 1\%$. (Fig. 7).

4.1.3 Using PN-based mask image

Comparing the spectra filtered with pn mask with 4"/pixel against filtering with a region shows the expected behaviour with a max of 6 counts difference out of 150 (Fig. 8). The effective areas

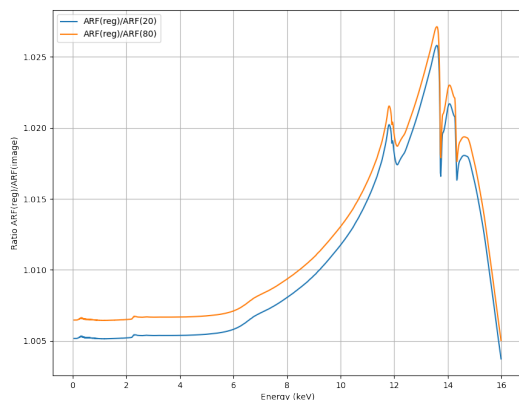


Figure 7: The ratio of the effective area returned by arfgen from a spectrum extracted with an image, compared with a spectrum extracted using a circular region. arfgen has been run assuming an extended source.

produced by arfgen agree to $< 1\%$.

4.1.4 Results on Light Curves

Running evselect with two filtering expressions to create a rates file was successful using a MOS-1 based image with $4''/\text{pixel}$. However, epiclccorr failed with

```
epiclccorr::evselect:- selected 36693 rows from the input table.
** epiclccorr::evselect: error (NoRegion), No region information available
for this filter type.** epiclccorr: error (invalidInvocation),
Execution failed of evselect(evselect-3.71) [xmmsas_20200817_0927-19.0.0]
```

This was fixed with dsslib 5.12.2.

4.2 New in SAS 19.0: Allow RA, DEC selection

The dataset 544_0147511601 was used to check the changes in evselect. For the test, we extracted with SAS19 both images and spectra for the object labeled as src 11 by edetect_chain. Both "circle" and "box" shapes were used, and the extraction was repeated writing the coordinates of the extraction regions both as (X,Y) and (RA,DEC):

(X,Y)

```
circle(22648.315,26017.652,500)
box(22699.759,25998.37,1350.3144,733.01416,0)
circle(25175.322,24995.278,1000) - bkg, for the spectral analysis
```

(RA,DEC)

```
circle(163.2457831,57.5083696,0.0069444)
box(163.2444524,57.5081027,0.0187544,0.0101808,0)
circle(163.1804390,57.4941968,0.0138889) - bkg, for the spectral analysis
```

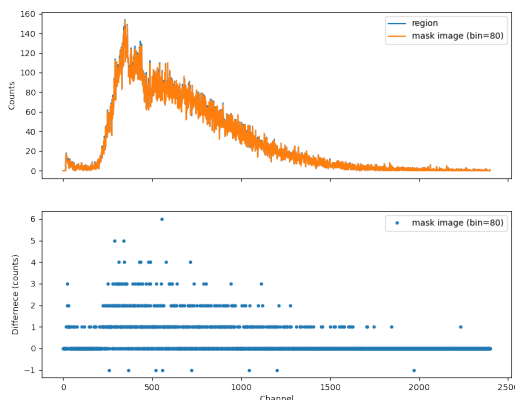


Figure 8: Counts spectrum using an image mask and a circular region.

Spectra and images were extracted without errors, and the results for extraction using (X,Y) or (RA,DEC) are consistent (Fig. 9, 10).

For comparison, spectra and images were extracted also with SAS18; as expected, the attempt with the (RA,DEC) expression ends with an error message:

```
** evselect: error (UnknownColumn), No column named 'RA' in table '/tmp/file17h0Lb:EVENTS'
No column named 'DEC' in table '/tmp/file17h0Lb:EVENTS'
Column 'RA' does not exist in table '/tmp/file17h0Lb:EVENTS'
```

4.3 Updated in SAS 19.0: combine spectra from different cameras

This was tested using the observations referred to in the data processing thread: H1426+428, OBSID=0310190101 and the Circinus Galaxy, OBSID=0111240101. PPS products produced with the SAS 18 pipeline were used with the following procedure:

- Download the PPS products
- Use the image in band 8 to select the source and background regions and save it in Equatorial coordinates.
- Filter the event lists for GTI and FLAGS.
- Use the cleaned event lists from step 3 to extract source and background spectra with expression using (RA,DEC) and run backscale.
- Generate RMF and ARF. Note that special spectral channel selection and spectral bin size is necessary. As well as a special switch in rmfgen for pn.
- Run epicspeccombine with the generated spectra.

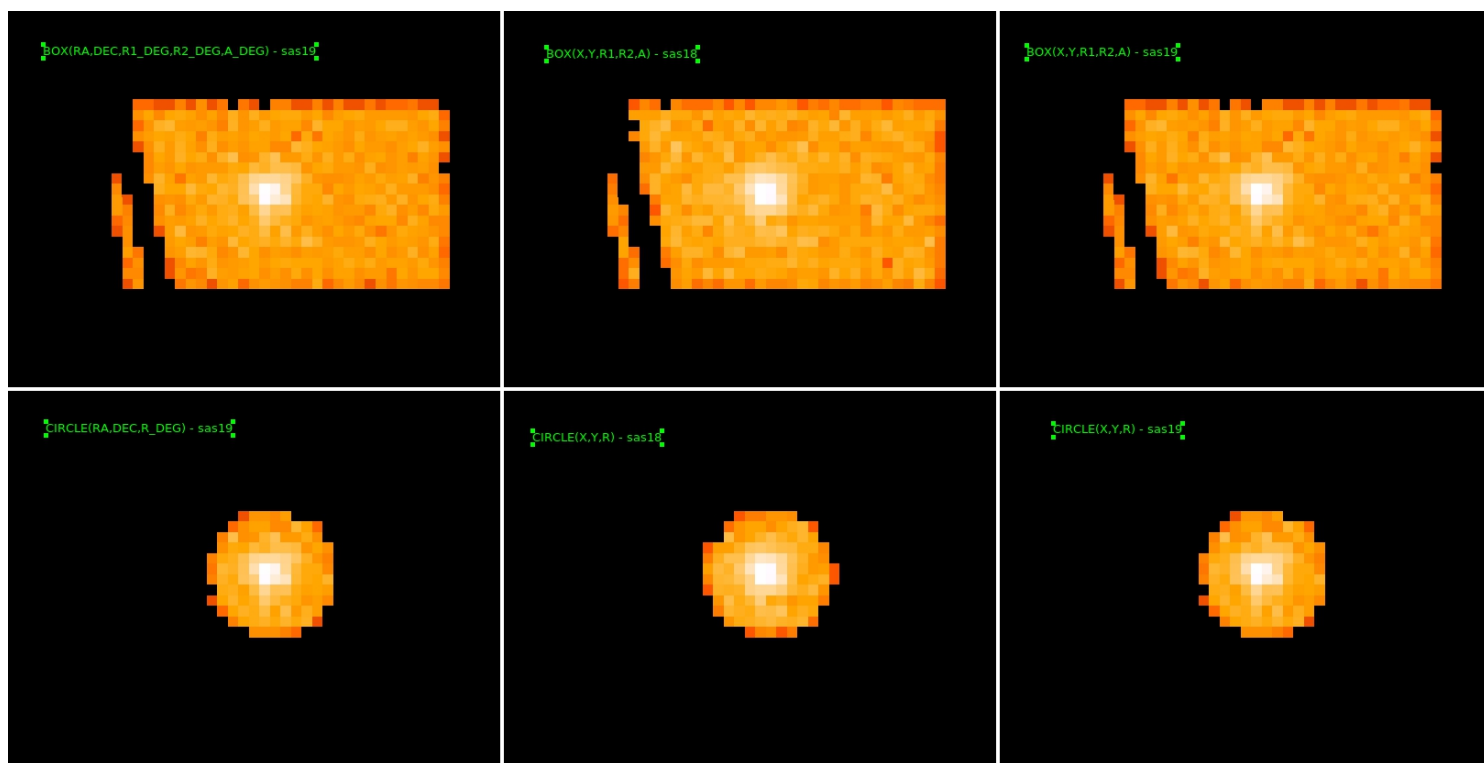


Figure 9: Comparison between the images extracted with SAS18 (central column) and SAS19 assuming the (RA,DEC) expression (left column) and the (X,Y) expression (right column); up: box extraction shape; bottom: circle extraction shape.

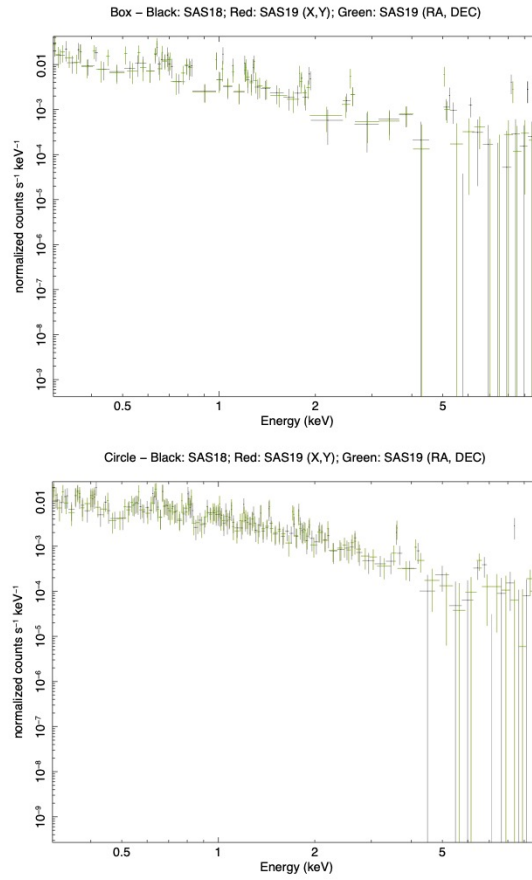


Figure 10: Comparison between the spectra extracted with SAS18 (black) and SAS19 using the (RA,DEC) expression (green) and the (X,Y) expression (red, completely overlapping); up: box extraction shape; bottom: circle extraction shape.

The tests were successful. The tested task `epicspeccombine` behaved as expected (Fig. 11). In the case that the RMFs were not generated as explained in the thread (i.e. not using the options - `withenergybins=yes` `energymin=0.1` `energymax=12.0` `nenergybins=2400`) then the task fails with a Segmentation fault (core dumped) and the error message is not helpful to understand why it failed. In this case some intermediate files are kept: `TEST_rsp_0.ds`, `TEST_rsp_1.ds`, `TEST_rsp_2.ds`.

This problem was fixed in `epicspeccombine` v0.2.1 (see SPR-7566).

A numerical comparison was made using an observation of the AGN NGC 6814 (Fig. 12). Spectral fits using a fixed model were applied to the individual EPIC cameras and separately to the combined spectrum. The residuals are generally small except for an excess of MOS flux at 0.6–0.7 keV likely due to cross-calibration differences between the cameras.

4.4 New in SAS 19.0: produce QPB products

Tests were ran on EPIC-pn data from observation 0804860201. A source spectrum and image were created. These were given as input products to the task using the command:

```
qpbselect table=3407_0804860201_EPN_S003_ImagingEvts.ds
productname=imagepn.ds outevfile=QPBevfile.fits
outprod=QPBproduct.fits attfile=P08048602010BX000ATTTSR0000.FIT
```

A QPB image and spectrum were correctly generated (Fig. 13).

A run of the software on an EPIC-pn observation with an `ExtendedFullFrame` observing mode resulted in the correct error message:

```
** qpbselect::evqpb: error (WrongInstSubmode), Instrument Mode not supported
```

similarly, running the task on EPIC-MOS data produced:

```
** qpbselect: error (WrongInstrument), Wrong instrument: EMOS1 - qpbselect only works with EP
```

4.5 Updated in SAS 19.0: EPIC-pn BURST mode CTI

To test the rate dependent calibration results with `EPN_CTI_0053/0054.CCF`, using SAS19 against those of SAS18, two test observations were chosen with different averaged count rates: Aql X-1, ObsID=0303220301, 2005-04-11 (264 ± 0.7 cts/s, in the spectral extraction region, see below) and MAXI J1535-571, ObsID=079571200, 2017-09-14 (5518 ± 3 cts/s, in the spectral extraction region, see below).

Data reduction and extraction of the spectra and standard products followed the standard procedures outlined in the SAS Threads (<https://www.cosmos.esa.int/web/xmm-newton/sas-threads>). We first used SAS18 and then repeated the procedures using SAS19. For the calibration correction using SAS18, we used a customized SAS18 routine to be able to use the `EPN_CTI_0053/0054.CCF` files. The procedure was:

- run `epproc burst=yes`
- Extract the EPIC-PN spectra in a rectangular region from raw 1 to 180, centered on the brightest column with a half-width of 10 columns (i.e., 21 columns in total).
- Subtract a background spectrum chosen in a region with columns 1 to 5 inclusive.

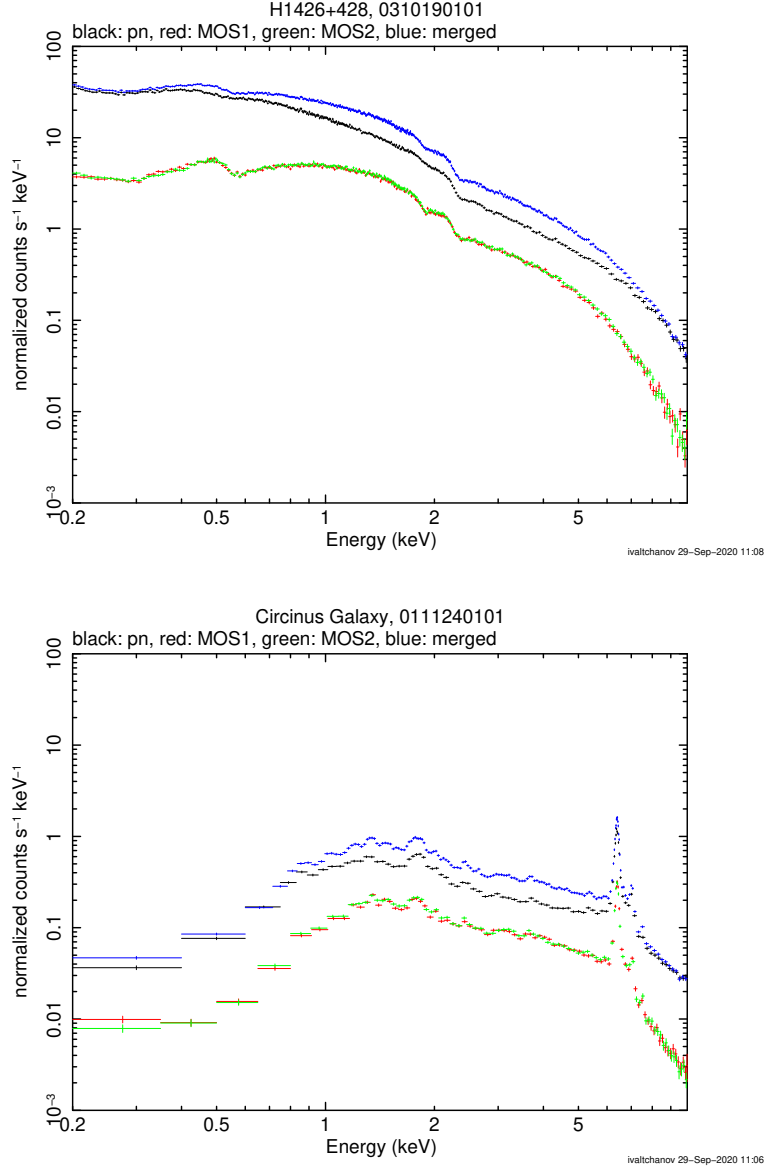


Figure 11: Upper: comparison between the images extracted with SAS18 (central column) and SAS19 assuming the (RA,DEC) expression (left column) and the (X,Y) expression (right column); up: box extraction shape; bottom: circle extraction shape. Lower: comparison between the spectra extracted with SAS18 (black) and SAS19 using the (RA,DEC) expression (green) and the (X,Y) expression (red, completely overlapping); up: box extraction shape; bottom: circle extraction shape.

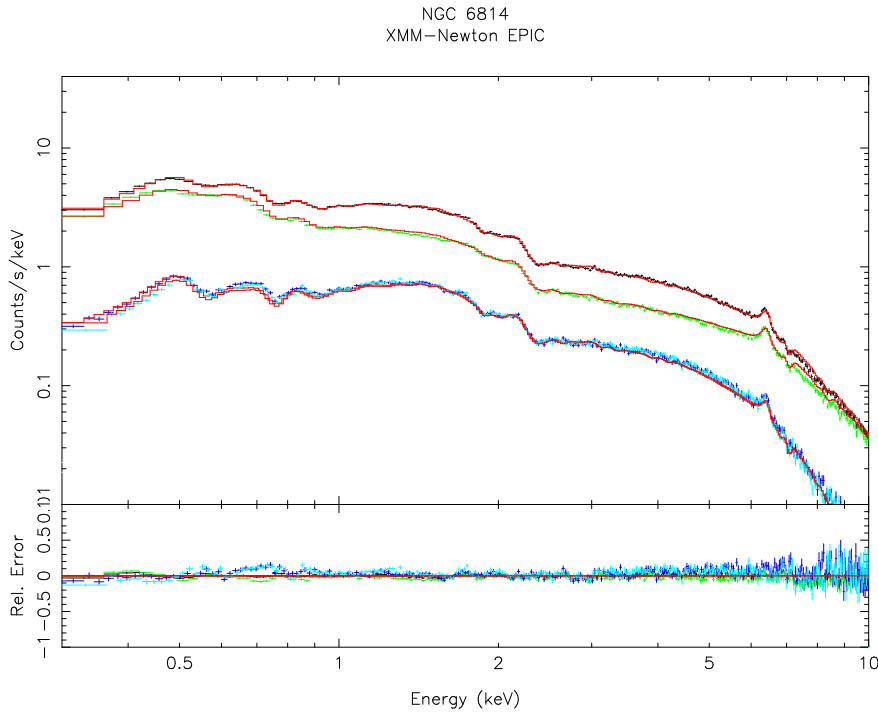


Figure 12: A fit to the individual EPIC MOS (light blue, dark blue), EPIC pn (green) and combined EPIC (black) spectra. Fit parameters were taken from the best fit to the combined spectrum. Small normalisation differences have been allowed between the fits which do not exceed 5%.

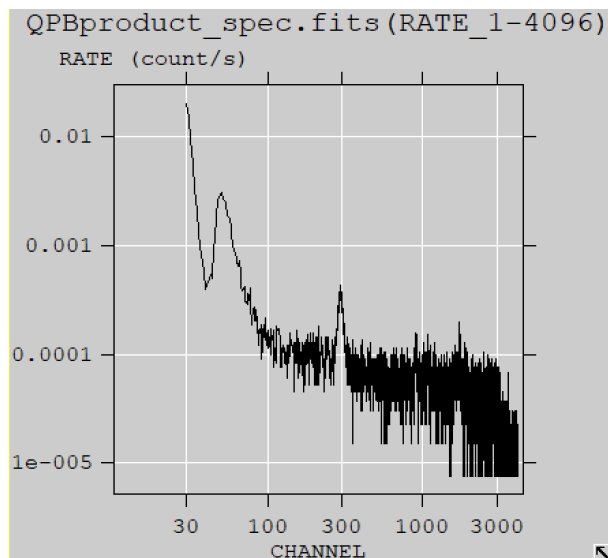
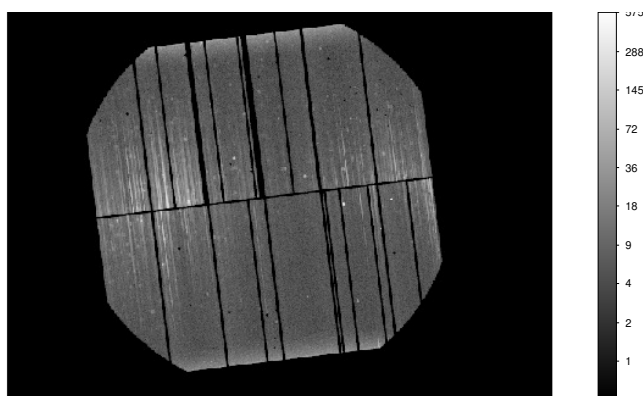


Figure 13: Upper: An image created from FWC events scaled by the discarded line value for observation 0804860201. Lower: A spectrum created from FWC events for observation 0804860201.

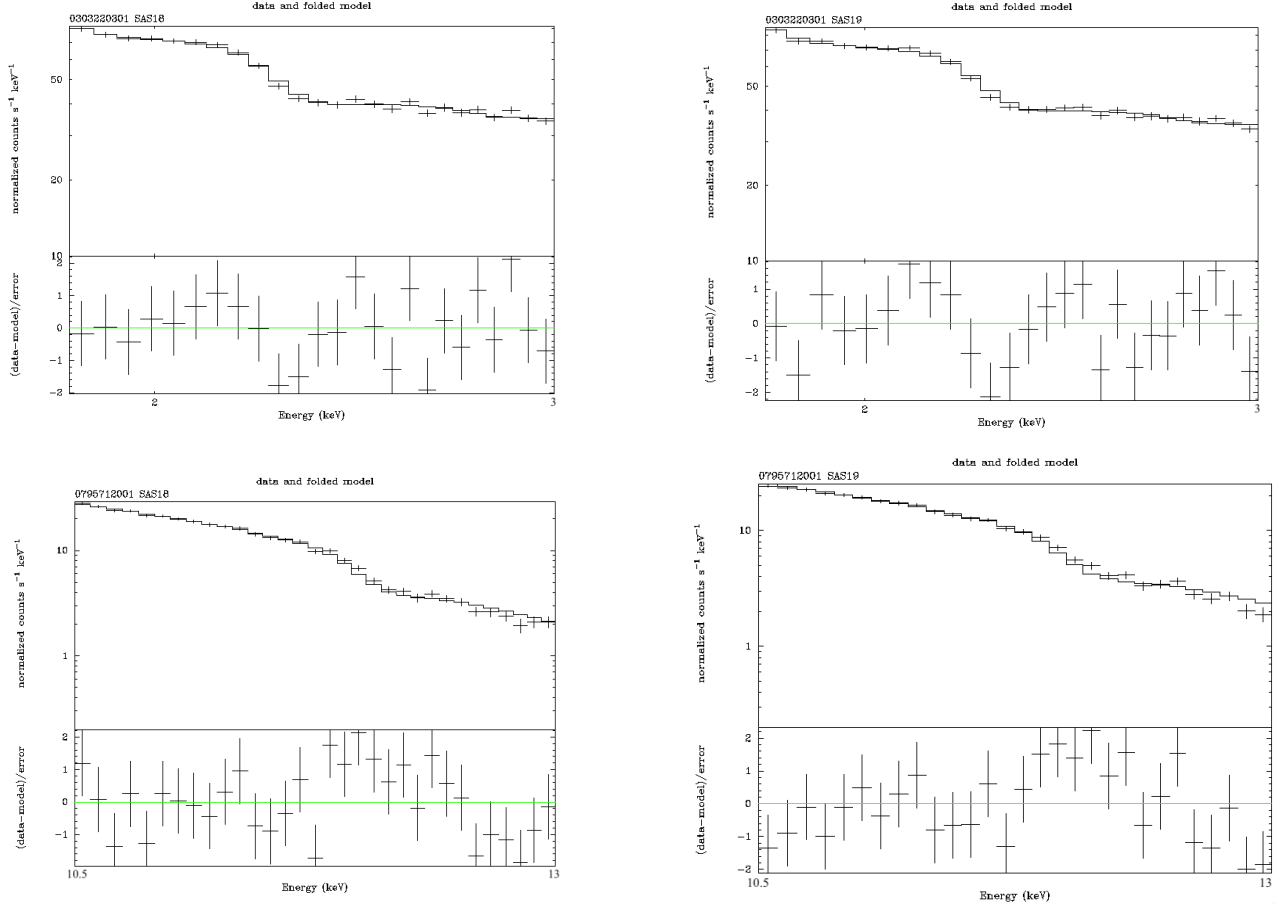


Figure 14: Fits of the testing sample spectra at the Au instrumental edges: Au L-edge at 2.2 keV (obsID 033220301; upper) and Au M-edge at 11.9 keV (obsID 079571200; lower). The comparison between data extraction and calibration corrections using SAS18 (left) and SAS19 (right) shows consistent spectra and fits, within statistical uncertainties.

- test the results of the calibration correction by spectral analysis of the instrument edges around 2 keV and 12 keV.

Fits to these edges were made with simple power laws using SAS18 and SAS19 (Fig. 14). The results are consistent within statistical uncertainties.

4.6 Updated in SAS 19.0: source detection

The dataset 544.0147511601 was processed with both SAS18 and SAS19; in both cases, the source detection has been performed following the corresponding thread:

<https://www.cosmos.esa.int/web/xmm-newton/sas-thread-src-find>

In the following, we consider as detected only sources with a likelihood of detection DET_ML not lower than 25.

We found 145 sources with SAS18 and 147 sources with SAS19 (Fig. 15).

The positions are consistent, with differences of between 1 and 5 arcsec.

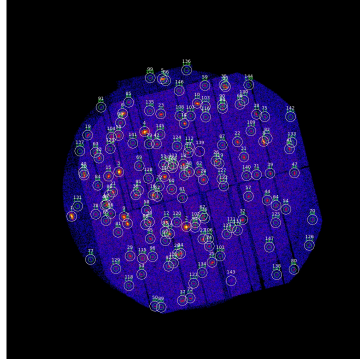


Figure 15: Image from SAS19 with sources detected in SAS19 superimposed as white bigger circles and sources detected in SAS18 as smaller green circles.

All sources found in SAS18 are also found in SAS19; two sources are found in SAS19 and not in SAS18: in both cases, the likelihood of detection is near the threshold:

DET_ML_19 = 29.101633, DET_ML_18 = 22.608942, threshold 25 DET_ML_19 = 25.176706, DET_ML_18 = 23.296957, threshold 25

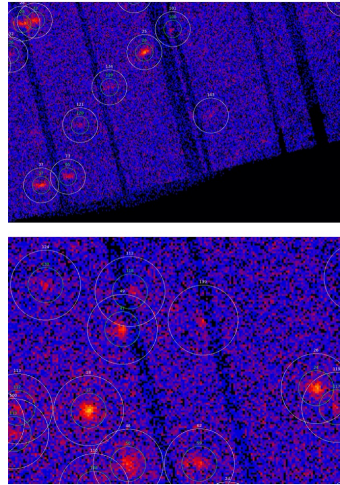


Figure 16: zoom showing the only two differences in detection (src139 and src143 from SAS19, white bigger circles).

The distributions in counts are consistent (Fig. /reffig:dethist).

Finally, one faint source (RATE \sim 0.004 and \sim 0.008 c/s in SAS18 and SAS19, respectively) is considered as extended in SAS19 (EXT=2.6) and not in SAS18 (EXT=0) (Fig. 18).

4.7 New in SASv19.0: New default parameters in rgsrmfgen and rgsproc

Starting in SASv19.0, a time and wavelength dependent correction will be applied by default to the RGS effective area. The application of this correction leads to an accuracy of the order of $<$

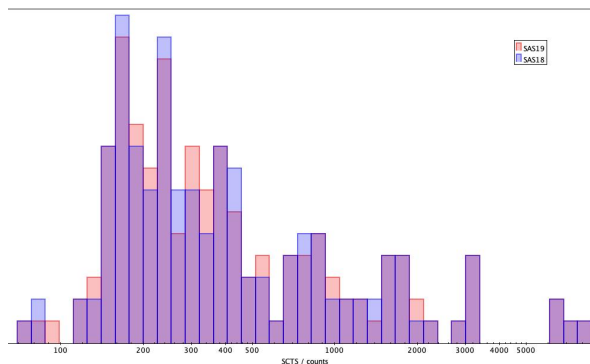


Figure 17: Distribution of source counts in SAS18 and SAS19.

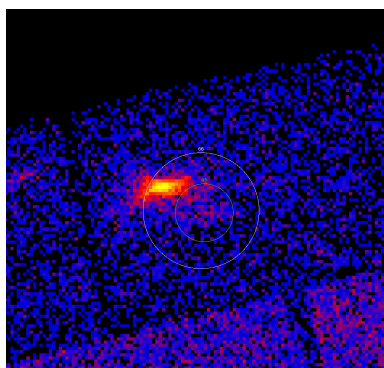


Figure 18: Extended sources detected by SAS18 and SAS19 (larger white circles).

2% over most of the RGS wavelength band (see <https://xmmweb.esac.esa.int/docs/documents/CAL-SRN-0340-1-0.pdf>).

This is done by setting the default value of the `rgsrmfgen` and `rgsproc` parameter `witheffectiveareacorreption` to `yes`.

Since new RGS-to-EPIC-pn Rectification factors were derived using this correction (see <https://xmmweb.esac.esa.int/docs/documents/CAL-SRN-0372-1-0.pdf>), care must be taken when using the `rgsrmgen/rgsproc` parameter `withrectification`:

- `withrectification = no`
`witheffectiveareacorreption = yes`
are the default values.
- `withrectification=yes`
`witheffectiveareacorreption=yes`
is correct, though is not the default.

`withrectification=no`
`witheffectiveareacorreption=no`.
is correct, but would prevent the application of the correction.
- `withrectification=yes`
`witheffectiveareacorreption=no`.

is not correct, as it will result in inconsistent results.

In this case the user is warned and `witheffectiveareacorrection` is automatically set to `yes`:

```
rgsproc: warning (RectificationDefaults), withrectification parameter  
was set to YES. In this case, witheffectiveareacorrection will be changed  
to YES automatically
```

4.8 Updated in SASv19.0: User is warned when there are no Qdumps available

While the default method to compute the CCDs energy offsets is to use the values derived from averaged diagnostic images taken over three consecutive orbits, it is possible to use the diagnostic images that are transmitted to ground interleaved with the science data during the observation ("Q-dumps"). This is done through the `rgsproc` parameter `calcoffsets`, that has to be set to the non-default value `yes`.

In case "Q-dumps" are not available for the observation, SAS will issue a warning:

```
rgsproc: warning (NoQDumps), Problem while running rgsoffsetcalc. No QDumps found
```

5 Validation results: Python support

Python support was tested.

5.1 SAS Python-based tasks

`xmmextractorGui`: A number of issues were found with this task.

- Login not accepting credentials correctly.
- Failure filtering PN GTIs with PG script
- `RGSPROC` is run even when it is deselected in the panel
- Change of output directory not taking effect.

The first two of these issues were resolved with an upload of `xmmextractorGui` v0.3. The other two are not deemed to be showstoppers.

`pkgmaker`: Was tested in a development environment and worked successfully for all types of packages, Python, Perl, C++ and Fortran. The structure of a newly created Python package worked successfully, the package could be built normally.

`wrapper`: The wrapper component of `pysas` was tested inside a Jupyter Notebook. The module `wrapper` was imported as

```
In [ ]: from pysas.wrapper import Wrapper as w
```

The execution of a non-Python task was executed by:

```
In [ ]: w(.epproc., []).run()
```

`startsas`: tested for ODF and PPS retrieval and initial processing in a python notebook in jupyterlab.

6 Conclusion

The validation exercise resulted in updated versions of the following tasks:

- *epicspeccombine* (v0.2.1)
- *evqpb* (v0.6.4)
- *dsslib* (v5.12.2)
- *xmmextractorGUI* (v0.3)

The SAS scientific validation process concluded that SAS 19 was validated and should be released.

During the exercise it was realised that the task *omsources* was not working correctly in multiple ways, problems which could not be resolved on a short timescale. This task will be changed to have a SOC-only distribution with the intention of having it ready for SAS 20.

A new task, *rgsbkgsmoothing*, has been introduced as SOC-only. It will be tested and made available to the public with SAS 20.

References

- Papadakis, I.E. et al. 2010, A&A 510, A65
Siebert, J. et al. 1999, A&A 348, 678
Tsujimoto, M. et al. 2011, A&A 525, A25