

XMM-Newton Science Analysis Software (SAS) in Datalabs

Aitor Ibarra on behalf of XMM-Newton Team

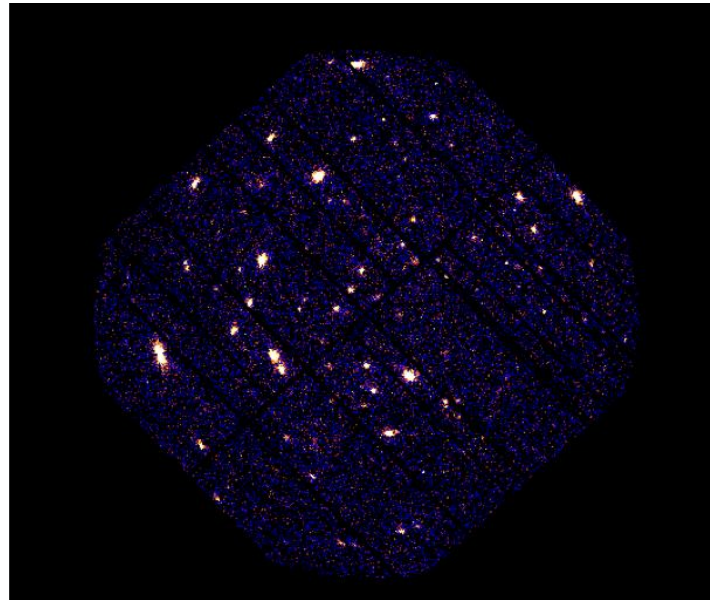
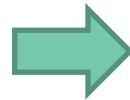
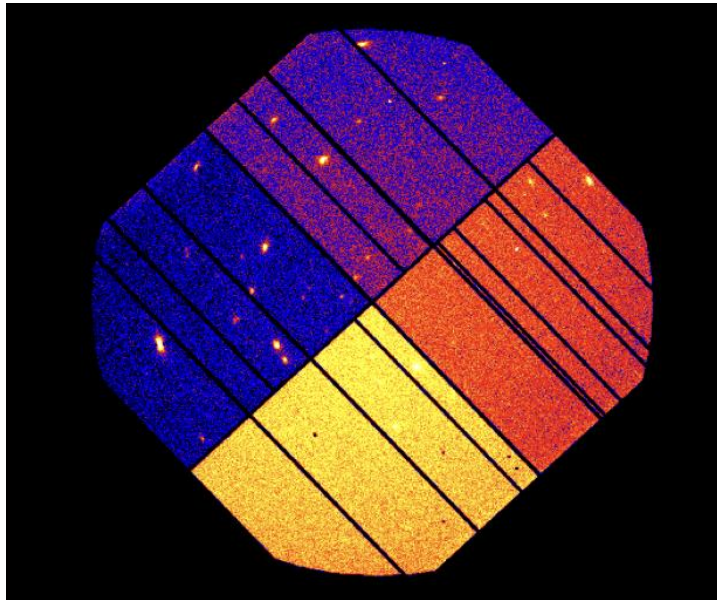
ESA Datalabs Workshop | ESAC - 25/11/2022

1. XMM-Newton Introduction
2. XMM-Newton Science Analysis System (SAS) Introduction
3. SAS evolution along the years...
4. SAS in Datalabs
 1. Data volume: SAS Calibration files (CCFs)
 2. SAS Remote Access
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XMM-Newton Science Analysis System (SAS)

Introduction

- SAS is a collection of tasks, scripts and libraries, specifically designed to reduce and analyze data collected by the XMM-Newton instruments.
- SAS is able to convert the XMM-Newton data from L0.5 (raw) to L3 (science products)
 - Applies calibrations to raw data



- Optimally screen/filter the data

SAS evolution along the years...

- SAS was designed as a stand-alone application.
 - Classical GUI interfaces
 - Command line executables

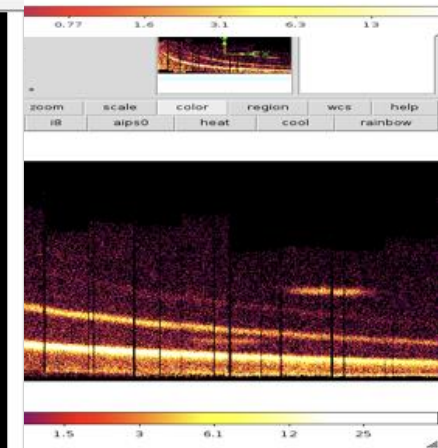
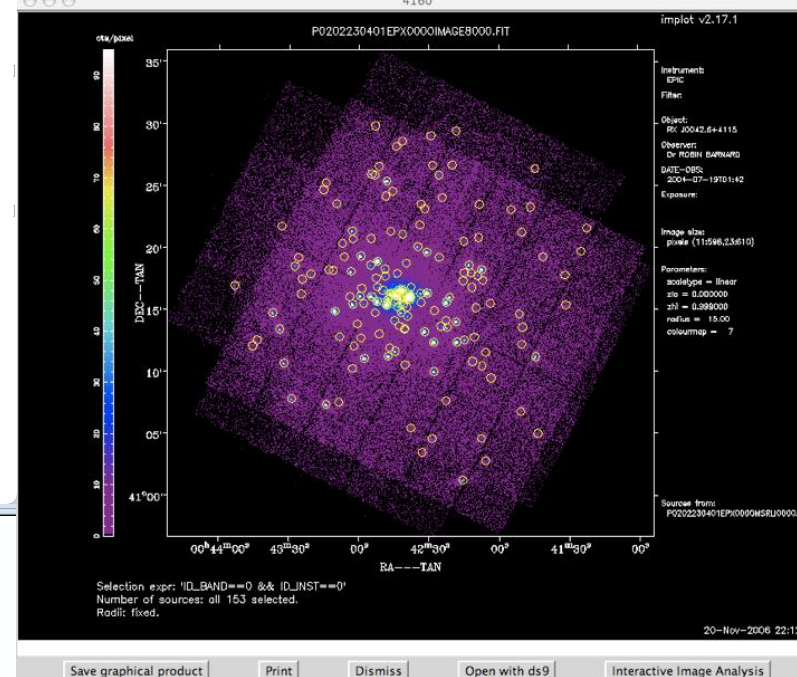
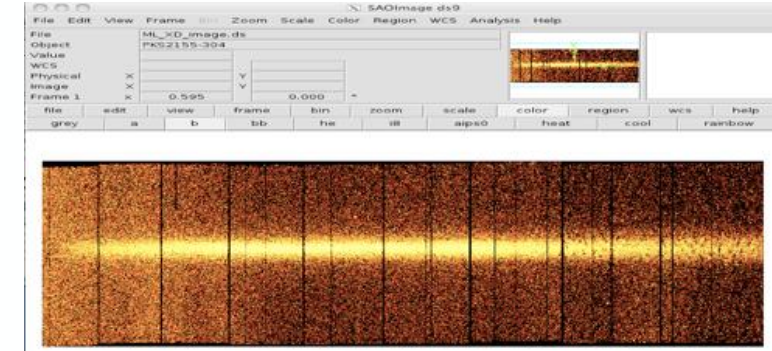
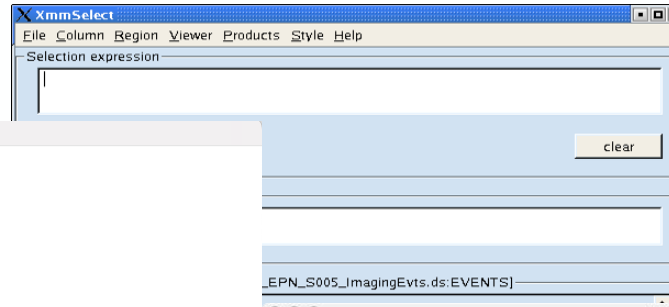
```
PN --bash--134x38
-rw-r--r-- 1 aibarra ESAAD\Domain Users 48960 Nov 18 20:40 P07808609010BX000fluxed1000.FIT
-rw-r--r-- 1 aibarra ESAAD\Domain Users 13135680 Nov 18 20:40 P0780860901R1S004RSPMAT2001.FIT
-rw-r--r-- 1 aibarra ESAAD\Domain Users 11626560 Nov 18 20:41 P0780860901R2S005RSPMAT2001.FIT
-rw-r--r-- 1 aibarra ESAAD\Domain Users 48960 Nov 18 20:41 P07808609010BX000fluxed2000.FIT
-rw-r--r-- 1 aibarra ESAAD\Domain Users 14400 Nov 18 20:41 P0780860901R1S004BGTSR_1001.FIT
-rw-r--r-- 1 aibarra ESAAD\Domain Users 14400 Nov 18 20:41 P0780860901R1S004SRTSR_1001.FIT
-rw-r--r-- 1 aibarra ESAAD\Domain Users 14400 Nov 18 20:42 P0780860901R2S005BGTSR_1001.FIT
-rw-r--r-- 1 aibarra ESAAD\Domain Users 14400 Nov 18 20:42 P0780860901R2S005SRTSR_1001.FIT
-rw-r--r-- 1 aibarra ESAAD\Domain Users 14400 Nov 18 20:42 P0780860901R1S004BGTSR_2001.FIT
-rw-r--r-- 1 aibarra ESAAD\Domain Users 14400 Nov 18 20:42 P0780860901R1S004SRTSR_2001.FIT
-rw-r--r-- 1 aibarra ESAAD\Domain Users 14400 Nov 18 20:42 P0780860901R2S005BGTSR_2001.FIT
-rw-r--r-- 1 aibarra ESAAD\Domain Users 14400 Nov 18 20:42 P0780860901R2S005SRTSR_2001.FIT
-rw-r--r-- 1 aibarra ESAAD\Domain Users 151373 Nov 18 20:42 rgsproc.log
aibarra [PN] $ ls -lrt
total 562376
-rw-r--r-- 1 aibarra ESAAD\Domain Users 9077760 Nov 18 20:37 3115_0780860901_AttHk.ds
-rw-r--r-- 1 aibarra ESAAD\Domain Users 5760 Nov 18 20:37 3115_0780860901_EPN_S003_04_Badpixels.ds
-rw-r--r-- 1 aibarra ESAAD\Domain Users 277283520 Nov 18 20:39 3115_0780860901_EPN_S003_ImagingEvts.ds
-rw-r--r-- 1 aibarra ESAAD\Domain Users 43615 Nov 18 20:39 epproc.log
-rw-r--r-- 1 aibarra ESAAD\Domain Users 1465920 Nov 24 12:27 image.ds
-rw-r--r-- 1 aibarra ESAAD\Domain Users 48960 Nov 24 12:28 rates.ds
aibarra [PN] $ sasversion
sasversion:- Executing (routine): sasversion -w 1 -V 4
sasversion:- sasversion (sasversion-1.3) [xmmsas_20211130_0941-20.0.0] started: 2022-11-25T10:01:27.000
sasversion:- XMM-Newton SAS release and build information:

SAS release: xmmsas_20211130_0941-20.0.0
Compiled on: Tue Nov 30 21:02:07 CET 2021
Compiled by: sasbuild@xmm23.local
Platform : macOS-11.6

SAS-related environment variables that are set:

SAS_DIR = /Users/aibarra/Documents/Applications/homebrew_x86_64/sas/xmmsas_20211130_0941/
SAS_PATH = /Users/aibarra/Documents/Applications/homebrew_x86_64/sas/xmmsas_20211130_0941/

sasversion:- sasversion (sasversion-1.3) [xmmsas_20211130_0941-20.0.0] ended: 2022-11-25T10:01:27.000
aibarra [PN] $
```



THEN.....

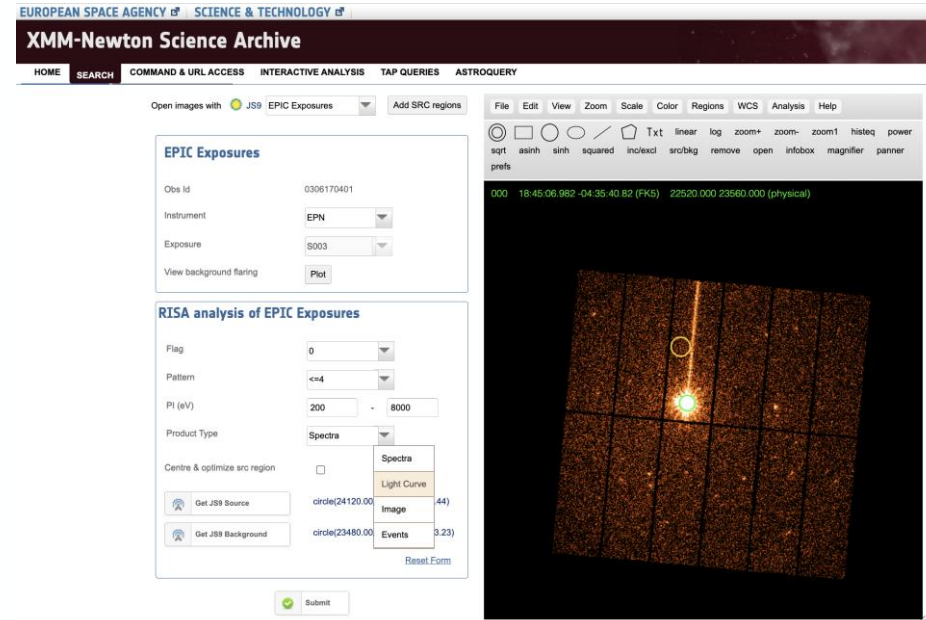
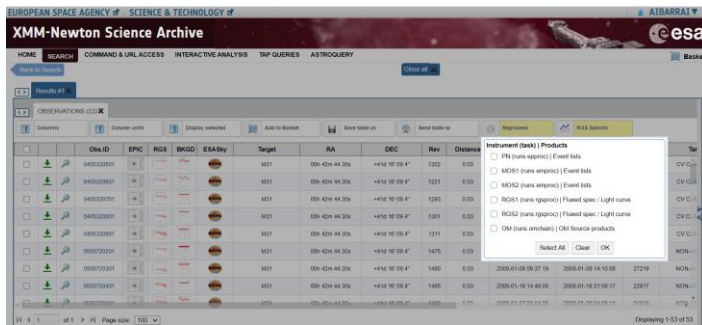
SAS evolution along the years...

- Remote Interface for Science Analysis (RISA) was developed
 - RISA is a web service able to process XMM-Newton on the grid at ESAC
 - XMM-Newton Science Archive is the RISA front-end to submit requests

REPROCESSING

SPECTRA & LIGHTCURVES & IMAGES

SPECTRA (RMF+ARF)



ObsID	Src Num	RA	DEC	Pos.Err	Det ML	Img	FC	LC	Spec	ESA Sky	Total Flux	Tot Flux Err	Tot Count Rate
0112570601	61	00h 42m 08.90s	+46° 20' 49.7"	0.5	721						2.91E-13	3.02E-14	0.0033
0112570601	62	00h 42m 40.64s	+46° 13' 28.6"	0.6	175						6.25E-14	1.91E-14	0.0338
0112570601	63	00h 43m 05.62s	+46° 12' 50.4"	0.5	483						2.24E-13	2.24E-14	0.9581
0112570601	64	00h 42m 09.47s	+46° 17' 46.7"	0.6	248						7.67E-14	1.87E-14	0.0412
0112570601	65	00h 42m 23.05s	+46° 14' 08.7"	1.0	15						2.78E-14	8.19E-15	0.0154
0112570601	66	00h 41m 51.61s	+46° 14' 39.8"	0.5	483						1.63E-13	2.25E-14	0.9631
0112570601	67	00h 42m 25.11s	+46° 13' 41.5"	0.9	48						3.88E-14	7.62E-15	0.0291
0112570601	68	00h 43m 03.01s	+46° 10' 18.2"	0.5	344						9.38E-14	1.48E-14	0.0471
0112570601	69	00h 42m 26.03s	+46° 25' 52.0"	0.6	468						2.63E-13	3.55E-14	0.8826
0112570601	70	00h 43m 21.09s	+46° 17' 52.4"	0.7	273						6.64E-14	1.21E-14	0.0464
0112570601	71	00h 42m 15.44s	+46° 20' 33.3"	0.7	261						9.28E-14	1.81E-14	0.0392
0112570601	72	00h 42m 34.24s	+46° 16' 59.9"	6.1	27						8.91E-14	5.40E-14	0.1095
0112570601	73	00h 43m 34.19s	+46° 10' 51.0"	1.0	69						3.20E-14	7.95E-15	0.0249
0112570601	74	00h 42m 11.75s	+46° 10' 50.0"	0.6	273						1.51E-13	2.43E-14	0.0411
0112570601	75	00h 41m 43.46s	+46° 21' 28.8"	0.7	251						2.22E-13	3.69E-14	0.9535

RISA statistics

- RISA statistics for 2022 (November 23th 2022):
 - Number of jobs submitted: 820
 - Users: 78

- 2019: 1351 requests → 120 users
- 2020: 985 requests → 58 users
- 2021: 1084 requests → 70 users

SAS evolution along the years...

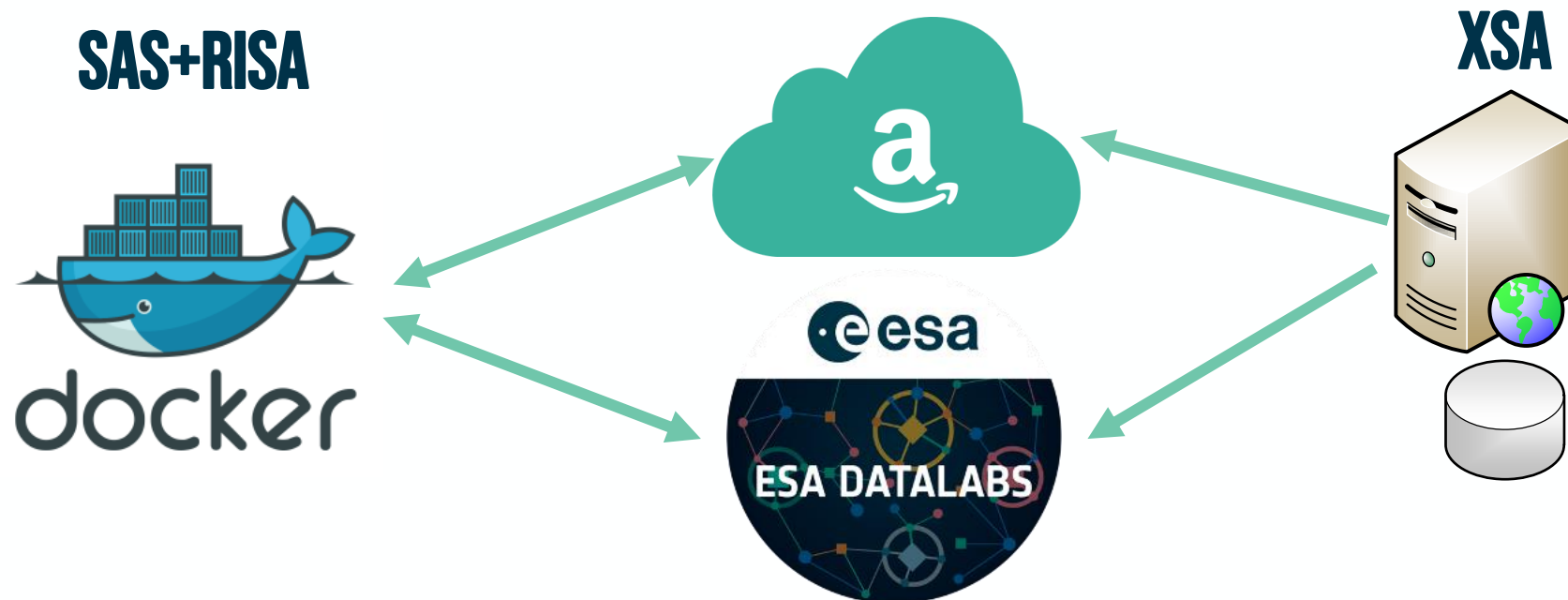
- Recently..... Python in SAS!!!!
 - New SAS python infrastructure was added in the last SAS v20.0 release (2021)
- Thanks to the SAS python infrastructure Jupyter Notebook threads were developed, enabling SAS newcomers to explore SAS capabilities easily.

The screenshot shows the XMM-Newton website interface. The top navigation bar includes 'SCIENCE MISSIONS', 'EUROPEAN SPACE AGENCY', 'SCIENCE & TECHNOLOGY', and 'SIGN IN'. The main header features the 'xmm-newton' logo and the ESA logo. The page content is titled 'XMM-Newton » Data Analysis » How to use SAS » Data Analysis Threads'. A left sidebar contains a navigation menu with items like 'Home / Latest News', 'Conferences & Meetings', 'News', 'General User Support', 'Proposers Info', 'Observers Info', 'Data Analysis', 'Archive, Pipeline & Catalogues', 'Calibration & Background', 'SOC Info', 'About XMM-Newton', 'Image Gallery', 'Publications', and 'Other Links'. The main content area is divided into sections: 'DATA ANALYSIS THREADS' (Data reduction examples for (almost) every purpose), 'SAS WATCHOUT PAGE' (Issues concerning SAS and data analysis, recommended workarounds/solutions, useful tricks and tips), 'SAS COOKBOOK' (An introduction to XMM-Newton data analysis - from NASA XMM-GOF), and 'ESAS COOKBOOK' (Cookbook for data analysis of extended sources using ESAS in SAS, (on-line and PDF) from NASA XMM-GOF. ESAS warnings and watchouts from NASA XMM-GOF). Below these sections, there is a 'SAS THREADS' section with a sub-section 'JUPYTER NOTEBOOK THREADS'. This section contains a table with the following data:

SAS Start-up and event list manipulation		
- SAS start-up thread in Python	Jupyter Notebook	html
- How to reprocess ODFs to generate calibrated and concatenated EPIC event lists	Jupyter Notebook	html
- How to filter EPIC event lists for flaring particle background	Jupyter Notebook	html

SAS evolution along the years...

- Now.... Docker technology!!!
 - During 2021, we created the first SAS docker version
 - SAS v20.0 (2021) was the first public release with a docker version.
- Why not the cloud?????
 - Pilot project was developed to migrate RISA to AWS
 - Prototype Successfully tested!!!



→ THE EUROPEAN SPACE AGENCY

ESA Datalabs [0.5.0-43-G2FD0FF1C]

Datalabs

Manage your running datalabs

[+ Launch new](#)

sas thread
jupyter jl-xmm-sas

SAS
sas jl-xmm-sas

Data Volume Catalog

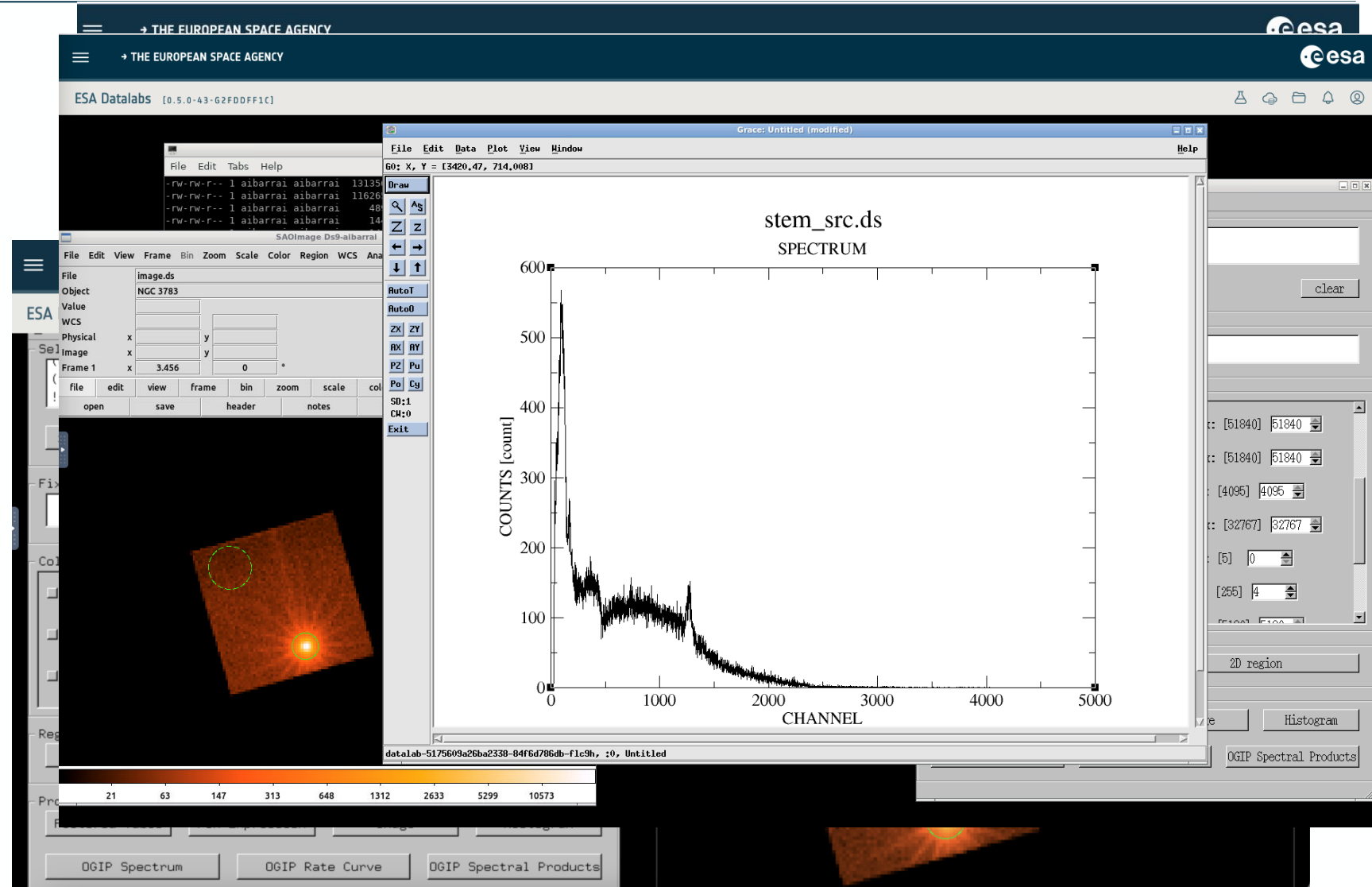
Domain Space Science (1)

XMM-Newton CCFs
Data Volume for XMM-Newton Calibration CCFs repository. Data volume made available by XMM-Newton mission.

**NOT YET IN THE OPERATIONAL DATALABS!!!
WORKING ON USE CASES**

SAS Remote Access

- Full SAS functionalities available through SAS docker in Datalabs with VNC connection.
- Access to latest version of SAS S/W.
- Access to latest version XMM-Newton Calibration files (CCFs) through *Data Volume Catalog*.
- ...



- To help users to analyse XMM-Newton data, a set of Data Analysis Threads are provided to the community.

SAS THREADS

JUPYTER NOTEBOOK THREADS

With the infrastructure of Python introduced in SAS 10, three experimental threads have been released under Jupyter Notebooks. These threads are not intended to be complete but to serve the purpose of illustrating how to use the Python interface to run SAS from a Jupyter Notebook.

SAS Start-up and event list manipulation	Jupyter Notebook	html
- SAS start-up thread in Python	Jupyter Notebook	html
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COMMON THREADS

Starting the SAS

- SAS start-up	command line
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All in one go: from raw data (ODF) to science products

- Analysis chain for point-like sources: <i>xmsextractor</i>	command line
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Guidelines for scientific analysis

- Spectral analysis with XSPEC	command line
- Timing analysis with XRONOS	command line

EPIC RELATED THREADS

All in one go: from raw data (ODF) to science products

- Analysis chain for point-like sources: <i>xmsextractor</i>	command line
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Step-by-Step

ESA Datalabs [0.5.0-43-G2FDDFF1C]

File Edit View Run Kernel Git Tabs Settings Help

Filter files by name

/ my_workspace / SAS_Threads /

Name	Last Modified
epic-bkgfiltering_singleevt.ipynb	12 days ago
epic-reprocessing.ipynb	2 days ago
SAS_image_viewer.ipynb	2 days ago
sas-startup.ipynb	2 days ago
startsas.log	2 days ago

«YOU CAN EITHER MOVE YOUR QUESTIONS OR THE DATA. [...] OFTEN IT TURNS OUT TO BE MORE EFFICIENT TO MOVE THE QUESTIONS THAN TO MOVE THE DATA.»

Jim Gray, eScience: A Transformed Scientific Method

BRING YOUR QUESTIONS TO THE DATA

There is a new paradigm, opening completely new opportunities for discovery – a data-intensive approach to science. In many domains, we have entered what could be called the golden age of surveys, with several large-scale projects, spanning decades, between finished, ongoing, and planned activities. ESA is responsible, or is a major partner, in several of these initiatives.

There is, however, a new profound change: data has become a major technological challenge. Increases by multiple orders of magnitude in dataset size means that transferring data to a scientist is often unfeasible.

ESA datalabs gives you a privileged position; bring your code directly to ESA's infrastructure – there is a great set of tools and programming languages are flexible – and execute it with direct access to ESA's archives.

The screenshot displays the ESA Datalabs environment. On the left, a file browser shows the directory structure under `/my_workspace/SAS_Threads/`, with `sas-startup.ipynb` selected. The middle pane shows the introduction and expected outcome for the `sas-startup.ipynb` notebook. The right pane shows the execution of the notebook, with the following code and output:

```
[11]: inargs=['odfid=0780860901','workdir=/media/home/my_workspace/my_ODFs/0780860901/']
```

```
[12]: w('startsas', inargs).run()
```

```
startsas - WARNING - Executing /usr/local/SAS/xmmsas_20211130_0941/lib/python/pysas/startsas/startsas.py {'odfid': '0780860901', 'workdir': '/media/home/my_workspace/my_ODFs/0780860901/', 'sasfiles': 'no', 'sas_ccf': '', 'sas_odf': '', 'level': 'ODF', 'cifbuild_opts': '', 'odfingest_opts': ''}
```

Starting SAS session

Working directory = /media/home/my_workspace/my_ODFs/0780860901/

Requesting odfid = 0780860901 to XMM-Newton Science Archive

Downloading 0780860901, level ODF. Please wait ...

Downloading URL <http://nxsa.esac.esa.int/nxsa-sl/servlet/data-action-aio?obsno=0780860901&level=ODF> to 0780860901.tar.gz ... [Done]

Creating directory 0780860901 ...

Unpacking 0780860901.tar.gz ...

Unpacking 3115_0780860901.TAR ...

Setting SAS_ODF = /media/user/my_ODFs/0780860901/0780860901

Introduction

The SAS Start-up thread provides a det Observation, and how to get the data re: other non Python SAS task, and to acc [startsas](#) and [sasver](#).

Expected Outcome

The ability to process any XMM-Newton

SAS Tasks to be Used

- [sasver](#)
- [startsas](#)
- [cifbuild](#)
- [odfingest](#)

Prerequisites

It is assumed that SAS has been installed ([SAS Watchout](#)).

Useful Links

- [pysas](#)
- [SAS web pages](#)
- [SAS download page](#)
- [SAS external software requirements](#)
- [Latest SAS on-line documentation](#)
- [SAS Threads](#)

Caveats

Last Reviewed: 30 November 20: ...
Last Updated: 15 March 2021

Procedure

Lets begin by asking four questions:

1. Where in my system have I installed the SAS software?
2. Where in my system have I stored the Calibration files?

```
sas-startup.ipynb
```

How to continue from here?

This depends on the type of products you have requested.

If you requested the Pipeline products (Level=PPS), your may begin exploring these products directly. Among them, you will find the Observation Event Files for the different instruments and a lot of information ready to be used.

If you simply requested the ODF (Level=ODF), the first step is to run the proper SAS tasks to get the Observation Event Files for each instrument. Then, you may have a look to other Threads to get familiar with specific processing tasks for each instrument.

In the next cells we show how to run from here four typical SAS tasks, three `procs` and one `chain` to process exposures taken with the EPIC PN and MOS instruments, RGS and OM.

Given that the execution of these tasks produces a lot of output, we have not run them within the notebook.

We leave this up to you!

```
[79]: os.chdir(work_dir)
```

```
[16]: w('epproc', []).run()
```

```
epproc:- Selected CCD: 7
epproc:- Selected CCD: 8
epproc:- Selected CCD: 9
epproc:- Selected CCD: 10
epproc:- Selected CCD: 11
epproc:- Selected CCD: 12
epproc:- 0 [Imaging] -> 1
epproc:- 1 [Timing] -> 0
epproc:- Considering one of the 1 exposures for mode 0 [Imaging]
epproc:- Considering exposure PNS003[index=0]
epproc:- Considering one of the 0 exposures for mode 1 [Timing]
epproc:- Selected exposure: 3 mode 0 [Imaging]
epproc:- Executing (invoked): atthkgen atthkset=../3115_0780860901_Atthk.ds timestep=1 timebegin=0 timeend=0 withtimeranges=no withpreqgti=no preqgtifile=pointings.fit -w 1 -V 4
epproc:- atthkgen (atthkgen-1.22.1) [xmmsas_20211130_0941-20.0.0] started: 2022-11-18T18:36:43.000
epproc::atthkgen:- Executing (routine): atthkgen atthkset=../3115_0780860901_Atthk.ds timestep=1 timebegin=0 timeend=0 withtimeranges=no withpreqgti=no preqgtifile=pointings.fit -w 1 -V 4
epproc::atthkgen:- atthkgen (atthkgen-1.22.1) [xmmsas_20211130_0941-20.0.0] started: 2022-11-18T18:36:43.000
epproc::atthkgen:- 20 % completed of 1st run (AHF/OM)
```

Mode: Command Ln 1, Col 1 sas-startup.ipynb

```
sas-startup.ipynb
```

```
WARNING: FixWarning: 'datefix' made the change 'Set MJD-UBS to 57733.434931 from DATE-UBS'.
Set MJD-END to 57733.647940 from DATE-END'. [astro.py.wcs.wcs]
```

```
[128]: %matplotlib inline
fig = plt.figure(figsize=(10,10))
ax = fig.add_subplot(111,projection=wcs)
ra=ax.coords[0]
dec=ax.coords[1]
ra.set_major_formatter('d.ddd')
dec.set_major_formatter('d.ddd')
ax.coords[0].set_axislabel('RA')
ax.coords[1].set_axislabel('DEC')
ax.imshow(image_data, cmap='hot', norm=LogNorm())
```

```
[128]: <matplotlib.image.AxesImage at 0x7f765f875970>
```

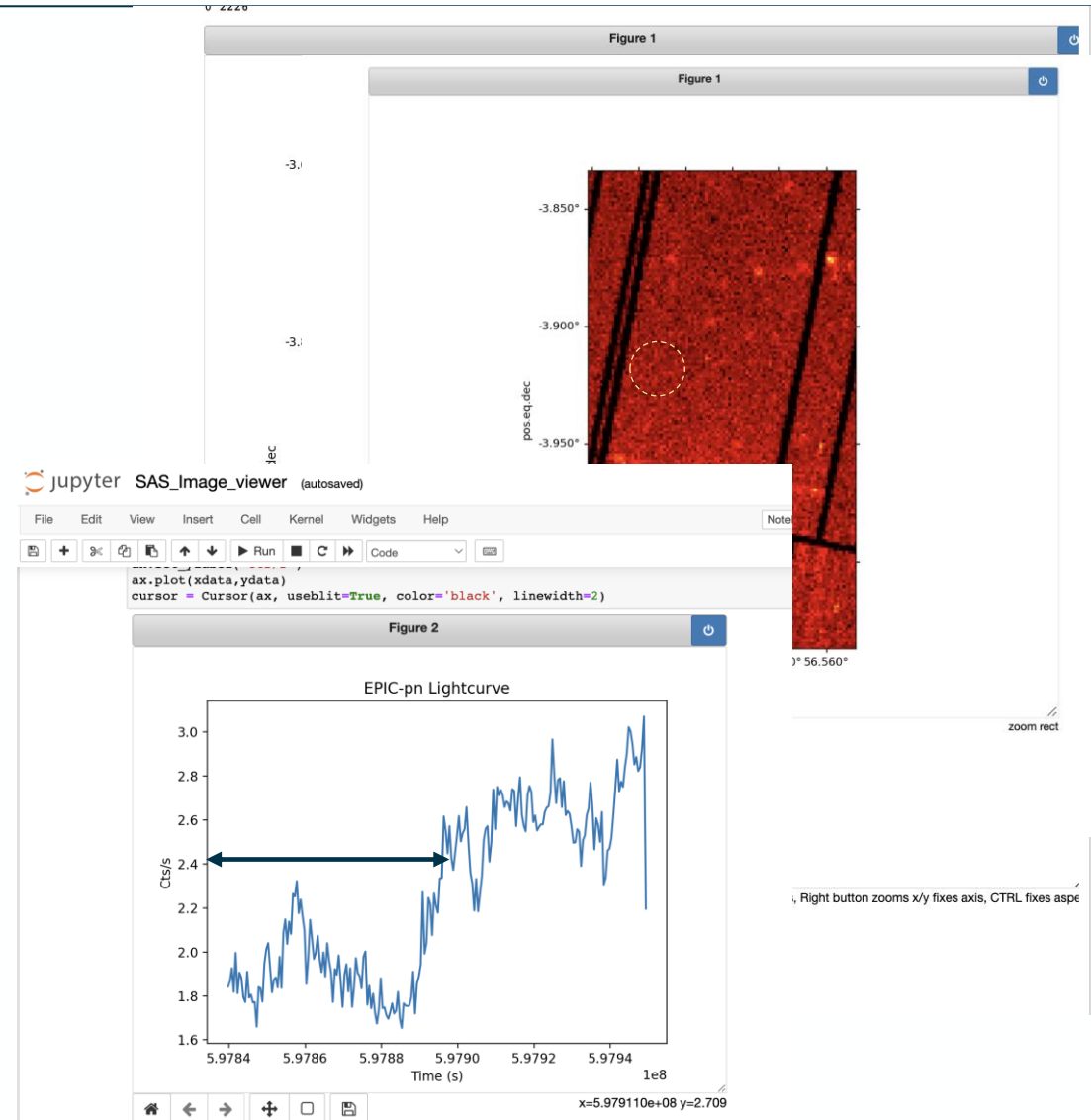
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- Thanks to the new SAS Python functionalities....
 - Develop new Jupyter Notebook for users
- Interactivity
 - Source a background regions
 - Good Time Interval selection
- SciApp?
 - Help users to create their own SAS utilities?
- More things to come...



THANKS FOR YOUR ATTENTION!!

QUESTIONS?

