

XMM-NEWTON Science Analysis System (SAS): medium and long-term strategy

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- Science Analysis System - Requirements and Implementation
- SAS 16 - start of some changes
- Remote Interface for Science Analysis (RISA)
- Medium and Long Term Strategy
- Conclusions

Requirements for XMM-Newton's scientific analysis system



>> **basis** for the **official** XMM-Newton products

Basics:

>> **interactive** analysis system to be **used by observers**

>> capable of dealing in a **similar way** with **all the data** from all the XMM-Newton instruments

Additional requirements for an observatory's data analysis system in the XXI century:

- run on different platforms >> serving users all over the world
- run on different ways >> for more and less experienced, occasional and dedicated users, X-ray and non X-ray astronomer
- user friendly >> attracting instead of repelling
- react quickly to new developments in calibration / processing >> fundamental instrument for professional science
- free of costs >> obvious but especially important for scientists in less developed countries

>> Scientific Analysis System SAS

A key player in the 5000+ achievement?

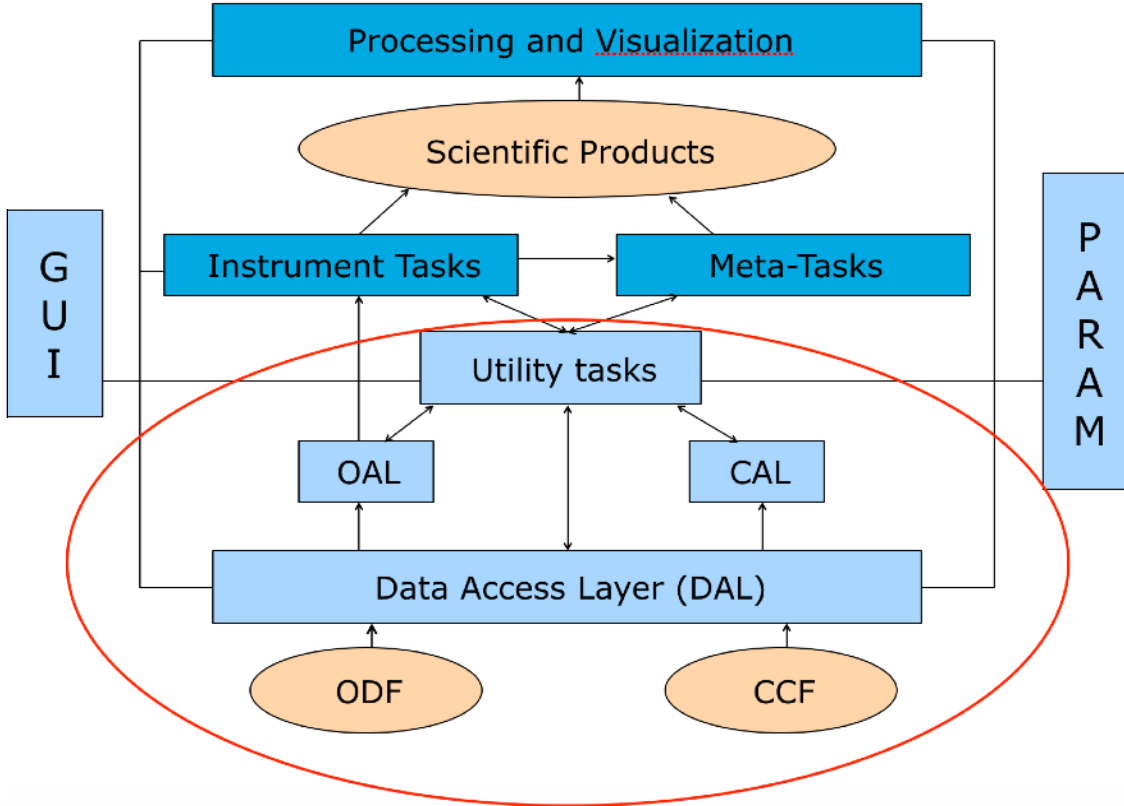
(XMM UG: ~ "high quality tool ... instrumental in high productivity of XMM")



What is SAS?

- The XMM-Newton Scientific Analysis System is a **freely distributed** suite of programs (“tasks”) for dealing with data from all XMM-Newton Instruments
- **All** tasks can run from a dedicated **GUI** or from the **command line**
- **Tasks** are written in **C++** and **F90/95**
- Perl and shell scripts constitute “**metatasks**” (users can easily construct them)
- SAS compiles on: **GNU/Linux and Mac OS X** (Solaris abandoned years ago), and it is distributed in **several flavors** and as **universal VM**
- It has been **developed** by ~ **30 programmers**, working in 6 different countries, and it is **maintained** (and further developed!) by ~ **4-5 FTEs**
- A **subset of the SAS** is used as the **official pipeline (PPS)** for reducing the data to calibrated event lists, images, spectra, source lists (and more) distributed
 - * to the PI observer ~ 2-3 weeks after the observation was performed
 - * to the world via the XMM-Newton Scientific Archive (XSA) one year later

SAS subsystems scheme



Work split:



Small team with exclusive dedication in one place



Large team geographically distributed



- Small team dealing not only with most of the SAS maintenance, but also with all of the PPS
 - only possible at the high level due to experience and excellence of team

- Distributing SAS in many binaries (32- + 64-bit versions, many Linux & Mac versions)
 - making easy its installation to the final user
 - maximising scientific return
 - ... but also increasing workload on our side

>> need to redirect efforts... first steps:

- reduce number of platforms
- simplify SAS building procedures
- start thinking in the long-term (*aka post-operational phase*)

SAS 16.0 released on 16/1/17

- SAS compiled with GNU GCC 6.2, including **gfortran 6.2** (away from NAG fortran compiler)
Compliance with newest C++ and Fortran coding standards
--- Main element of this release, it implied a very large effort by SAS team ---
(a pre-requisite for future SAS compilation at user's side...)
- **No 32bits binaries anymore** + reduction to few 64bits binaries

List of S/W changes needed for migration:

- ★ new definition of array descriptors (dope vectors)
- ★ memory mapping of array descriptors
- ★ use of specific MACRO statements for NAG
- ★ different naming convention for precompiled modules
- ★ usage of intrinsic functions - cases where conversion depends on the compiler
- ★ get_environment variable, leading blank spaces removed properly
- ★ implied_loop - different standards regarding manipulation of arrays in loops
- ★ use of reserved words - gfortran more strict
- ★ integer to string conversion - gfortran more strict
- ★ namespace errors - gfortran more strict regarding the scope of module names
- ★ memory allocation - certain parameter part of allocatable variable def not possible in gfortran
- ★ gfortran are undefined
- ★ definition of parameters in subroutines
- ★ active regarding size of variables
- ★ C++ must be initialised to null

Linux 64:

| | | |
|--------------------------|---------------|-------------|
| RHEL 6.8 | 2.6.32 | 2.12 |
| Ubuntu 16.04.1LTS | 4.4.0 | 2.23 |

Already in SAS 15

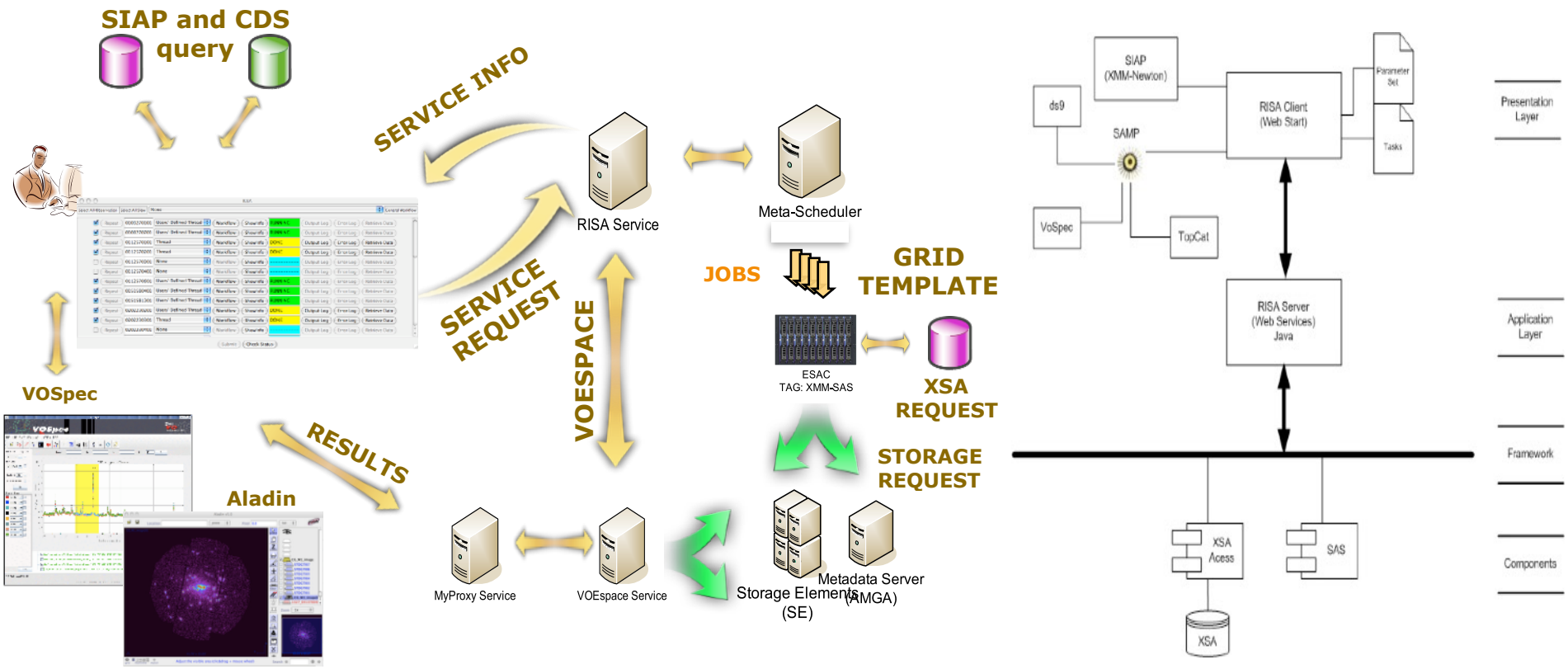
MacOS:

| | | |
|-----------------------------------|----------------------|------------------|
| MacOS 10.10.5 (Yosemite) | Darwin 14.5.0 | 1213.0.0 |
| MacOS 10.11.6 (El Capitan) | Darwin 15.6.0 | 1226.10.1 |
| MacOS 10.12.3 (Sierra) | Darwin 16.3.0 | 1238.0.0 |

New in SAS 16

+ 1 universal SAS-VMs (64bits) - Ubuntu 16.04.1

Remote Interface for Science Analysis (RISA)



Medium- and long-term strategy

On top of “normal” maintenance (and development)... working at the same time on Post-ops

- to be better prepared if something leads to termination of XMM-Newton
- to reduce the work which will be needed for legacy during the post-operational phase (limited strictly to 2 years)

Main ideas wrt SAS data processing after EoM:

- A. preserve a running SAS as long as possible
 - A1) SAS Virtual Machine ... Dockers (≥ 10 years)
 - A2) RISA (Remote Interface for Science Analysis) (5-10 years longer)
- B. give SAS code to community (*re-use (Athena...)? ... further development?*)

To make possible B means: reducing complexity = modernising

- B1) Compilers: maintaining close correspondence with new compilers
- B2) Migration to Python in 3 areas: graphical, replacing PERL, replacing calls to HEASOFT
- B3) Simplify configuration and improve documentation: making possible / easy building from source & source maintenance

Four years detailed plan (2017-2020) based on these lines

A1 - SAS is distributed since 2006 also as Virtual Machine

Estimation: such a VM could run after EoM in the most diverse OS's for ≥ 10 years

Proven: SAS-VM (2006) running today without any problem on actual OS's

A2 - RISA is a fundamental component in our long-term strategy ... it is already working though:

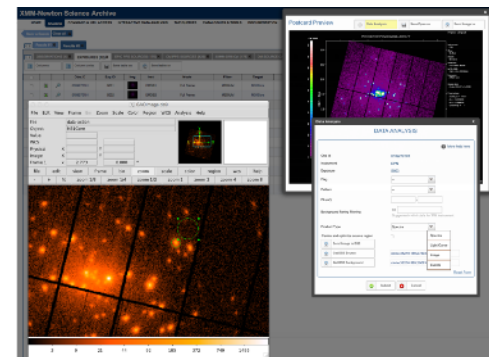
- on-the-fly reprocessing of archival data with latest SAS and calibration
- filtering and light data reduction services

>> integration in XSAv9.4

>> first steps in the way to a more complete / full RISA I/A service

RISA post-ops thought so far to be SAS-VM based ...

(> final SAS packed in one OS... extended life [5-10 years] in a central place)



See P11

XMM-Newton Solaris 8 operational machines (from 2004!) replaced these days...

>> RISA is an ideal system for experimenting replacement of SAS-VM by Dockers... (2018)
(Dockers would ease combination of SAS data reduction with other S/W)

B1) SAS 16: Transition to GNU provided gfortran compiler

at the same time, most modern C++ compiler version used: GCCv6.2

>> serious scrutiny of source code

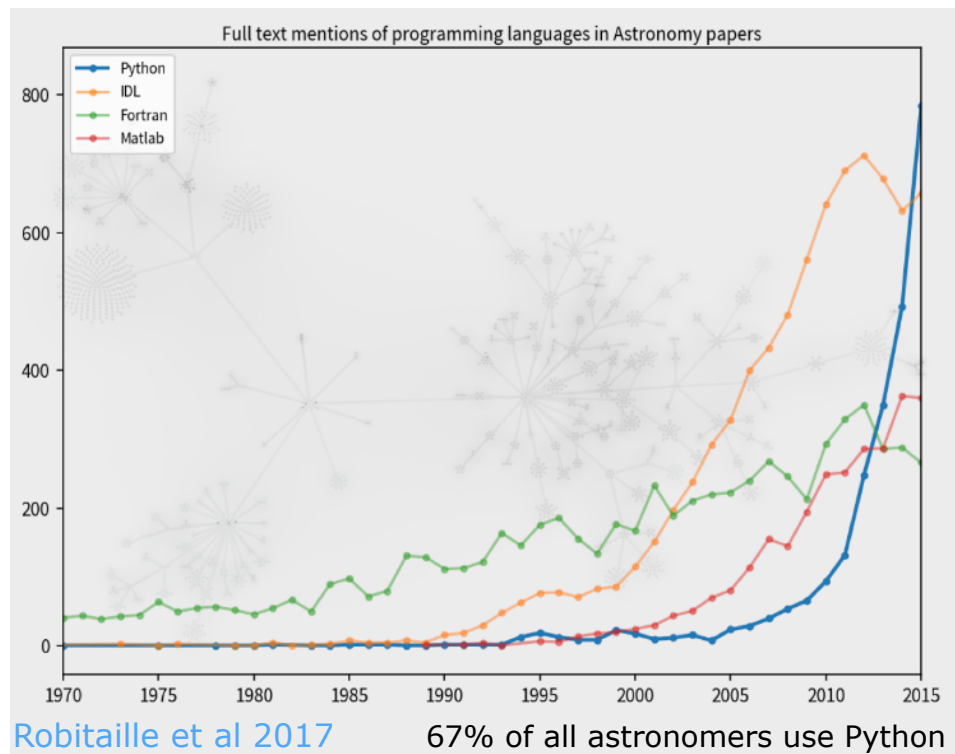
>> most up-to-date standards both in Fortran 90 and in C++

Pre-requisites for providing source code for SAS compilation at user's side

- free compilers ✓
 - code up-to-date with standards ✓ (... 2019 ... 2021 ...)
 - +
 - simplified configuration and building procedures
 - + documentation
- SAS built by SAS experts ✓
- SAS built by S/W experts (2018)
- SAS built by "normal" users (2019)

Moving areas to Python

B2 - Moving certain SAS areas to Python



Why Python?

- Simplifying SAS & PPS
 >> more maintainable
- Pre-condition for a future package to be given to the community

Stepwise introduction in SAS/PPS:

- 📁 graphics area: first products (2017)
 - 📁 graphics area: replacement of PGPLOT & Grace (2018-19)
 - 📁 scripting area: replacing PERL (yes, lot of work... 41 scripts in SAS, some pretty complex) (2019)
 - 📁 Heasoft area: replacing tasks depending on Heasoft (2020)
- t ↓

B3 - Configuration / build / documentation

Two main problems for “aliens” to deal with SAS on the source code level

- SAS is a complex piece of software >> SAS is difficult to build...
 1. replace NAG fortran compiler by gfortran ✓
 2. simplify build & configuration ... extend documentation so that SAS experts can build ✓ (2017)
 3. simplify more ... extend documentation so that S/W experts can build (2018)
 4. simplify even more ... extend documentation so that ‘aliens’ can do it (2019)
- To maintain S/W written by others is difficult (don’t tell us...!)

Internal documentation is essential - Improve so that non-experts can cope with

1. I/F type S/W (OAL, CAL, DAL) (2017-18)
2. S/W type II (beyond calibrated event lists...) (2019)
3. Rest of the S/W (2020)

This will be needed even before / independently of Post-ops

- SAS: maintenance efforts not decreasing, necessary for maximisation of scientific return
- Evolution: taking into account post-mission needs
- Optimising the timing for necessary structural changes, with the aim of
 - keeping analysis capabilities for decades after EoM
 - making possible maintenance of SAS code by community