X-ray Software Packages

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- with useful advice over the years from-

John Davis, John Houck, Dave Huenemoerder, Jörn Wilms

Outline

- Overview of Software Packages & Their Purposes
- Flexible Image Transport System (FITS)
  - Data Visualization: fv, prism, DS9
  - Reading & Writing FITS files
- Spacecraft Specific Software
  - CALDB
- Data Analysis Packages
- Your Responsibilities
  - How to Install Software, Send Bug Reports, and Write Software

Purpose of Software Packages

- Read, Write, Visualize Astrophysical Data - Primarily from Binary Files
  - Standard Format - Flexible Image Transport System
  - Other Formats: HDF5, ASCII, ... (but not universal)
- Data Reduction - Temporal/Spatial/Energy/Grade Filters, and Spacecraft Specific Procedures
  - Create Images, Spectra, Lightcurves, Backgrounds, Responses, ...
- Data Analysis - Apply Models to Reduced Products

Spacecraft Specific or Not?

- Analysis usually begins “agnostic” - reading/writing, visualizing
- Proceeds through a spacecraft specific stage, especially for the creation of response files (and often backgrounds)
  - Spacecraft determines which software package
- Analysis often then becomes agnostic again - spectra, lightcurves, and images from many different missions can be handled in similar manners.

3 Systems, +1 Independent

- High Energy Astrophysics Software:
  HEASOFT (Current Version 6.11)
  - CFITSIO, FV, FTOOLS, XSELECT, XSPEC, XRONOS
- Chandra Interactive Analysis of Observations:
  CIAO (Current Version 4.3)
  - Data Model (DM), Crates, Prism, ChIPs, Sherpa
- Scientific Analysis System:
  SAS (Current Version 11.0.0)
- DS9 (Current Version 6.2)

Scripts Tie Pieces Together

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    "XANADU"
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“HERA”

“XANADU”

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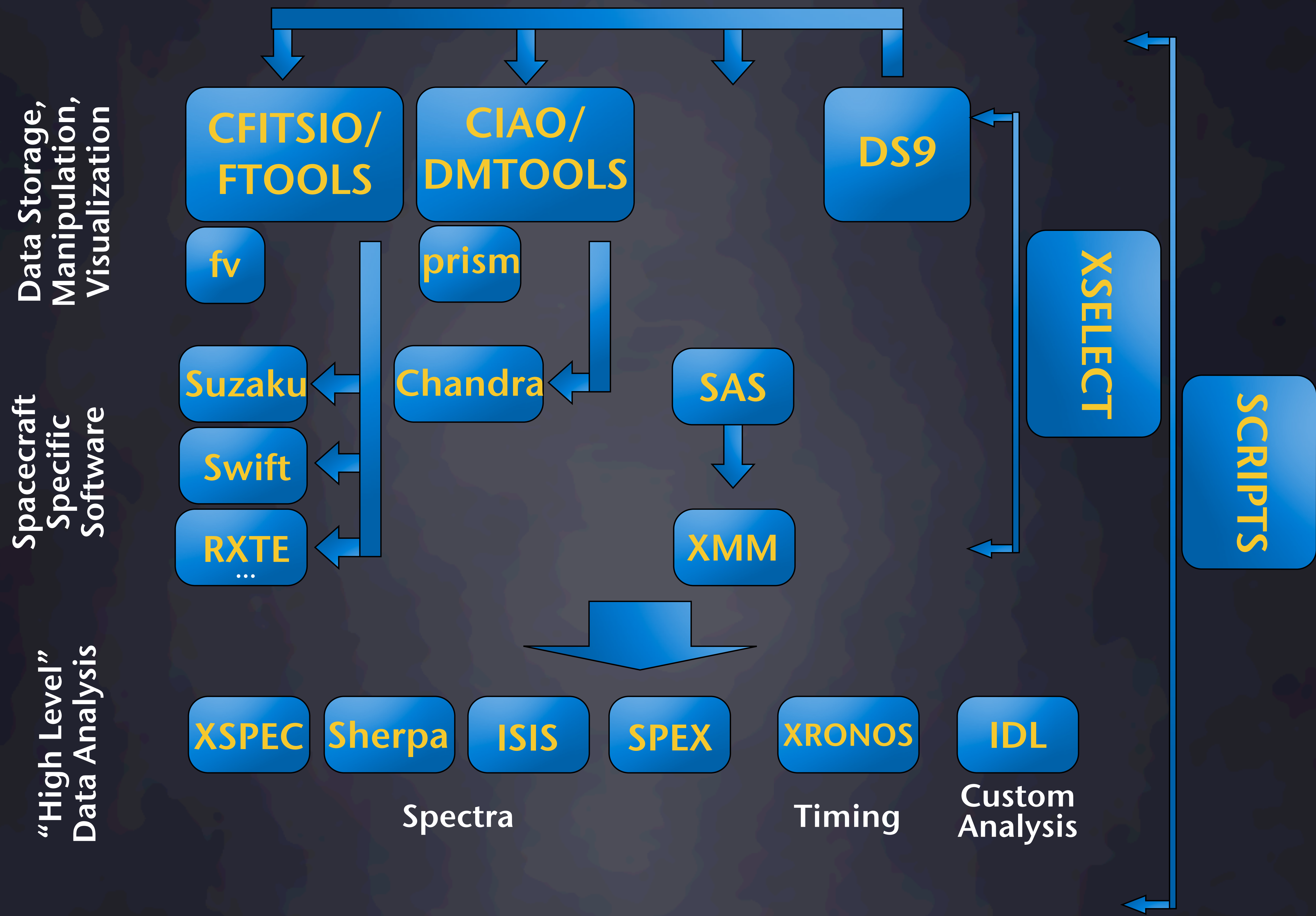
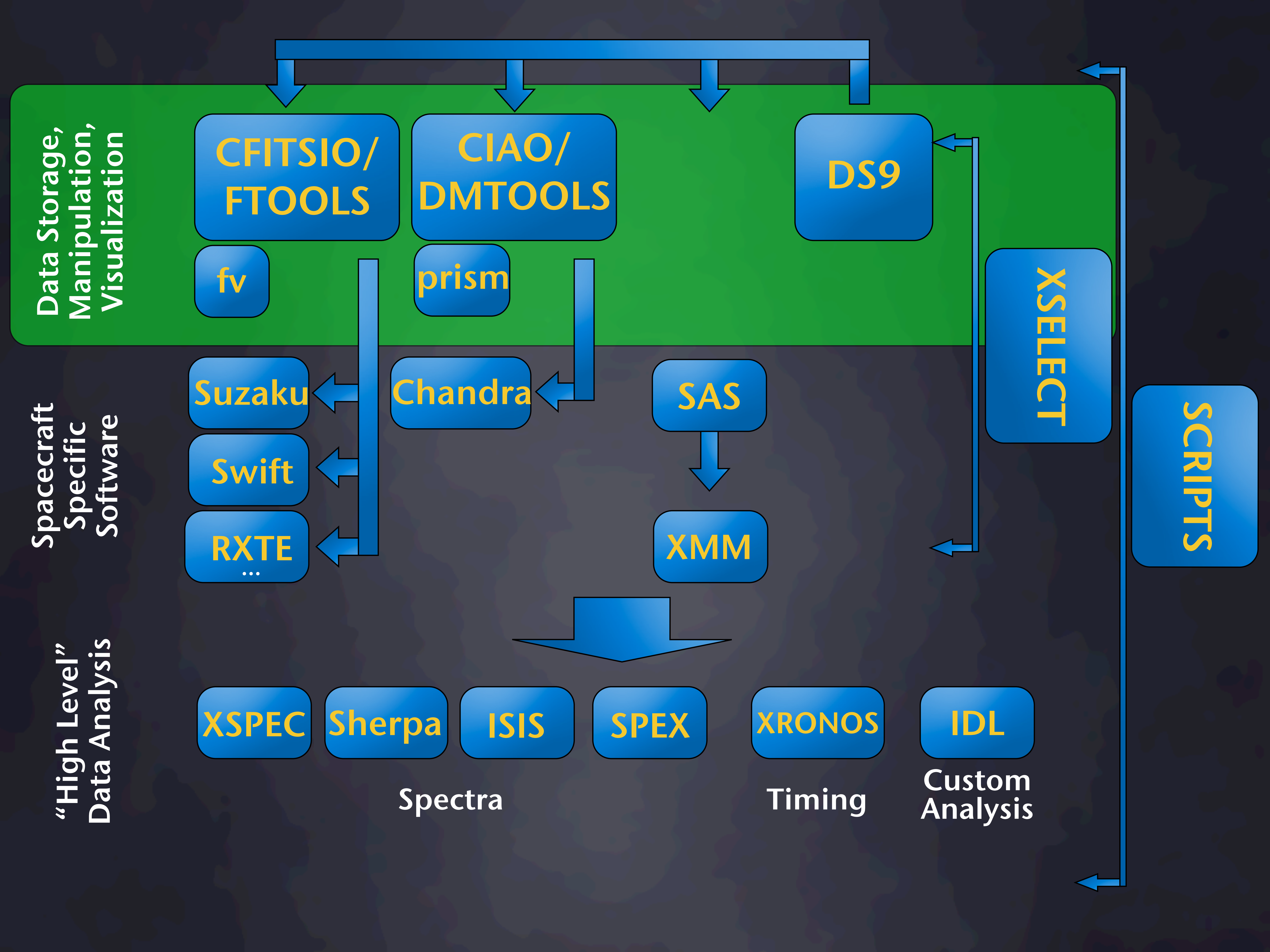
Scripts Tie Pieces Together

Plus Additional High Level Analysis Systems

- Interactive Spectral Interpretation System (ISIS- Current Version 1.6.1-43)
- Spectral X-ray and UV modeling, analysis, and fitting (SPEX- Current Version 2.02.04)
- Interactive Data Language (IDL) + Packages
  - Spitzer Analysis System
  - PINTofALE (Package for Interactive Analysis of Line Emission)



Data Storage, Manipulation, Visualization
Spacecraft Specific Software
"High Level" Data Analysis
CFITSIO/ FTOOLS
CIAO/ DMTOOLS
DS9
fv
prism
XSELECT
SCRIPTS
Suzaku
Chandra
SAS
Swift
RXTE
...
XMM
XSPEC
Sherpa
ISIS
SPEX
XRONOS
IDL
Spectra
Timing
Custom Analysis


Data Storage, Manipulation, Visualization
CFITSIO/ FTOOLS
CIAO/ DMTOOLS
DS9
fv
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Spacecraft Specific Software
Suzaku
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SCRIPTS
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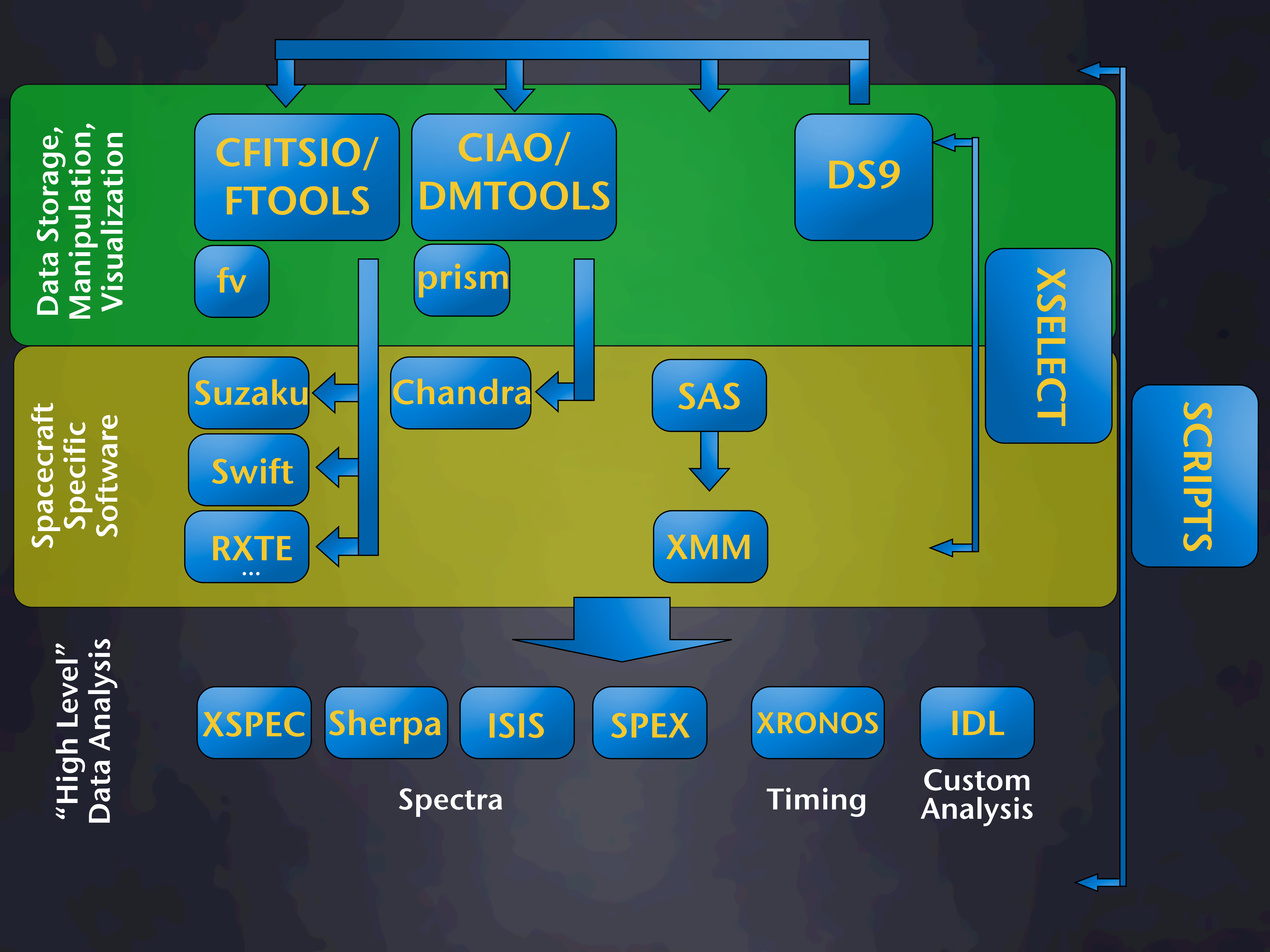
Timing
Custom Analysis



Data Storage, Manipulation, Visualization
CFITSIO/ FTOOLS
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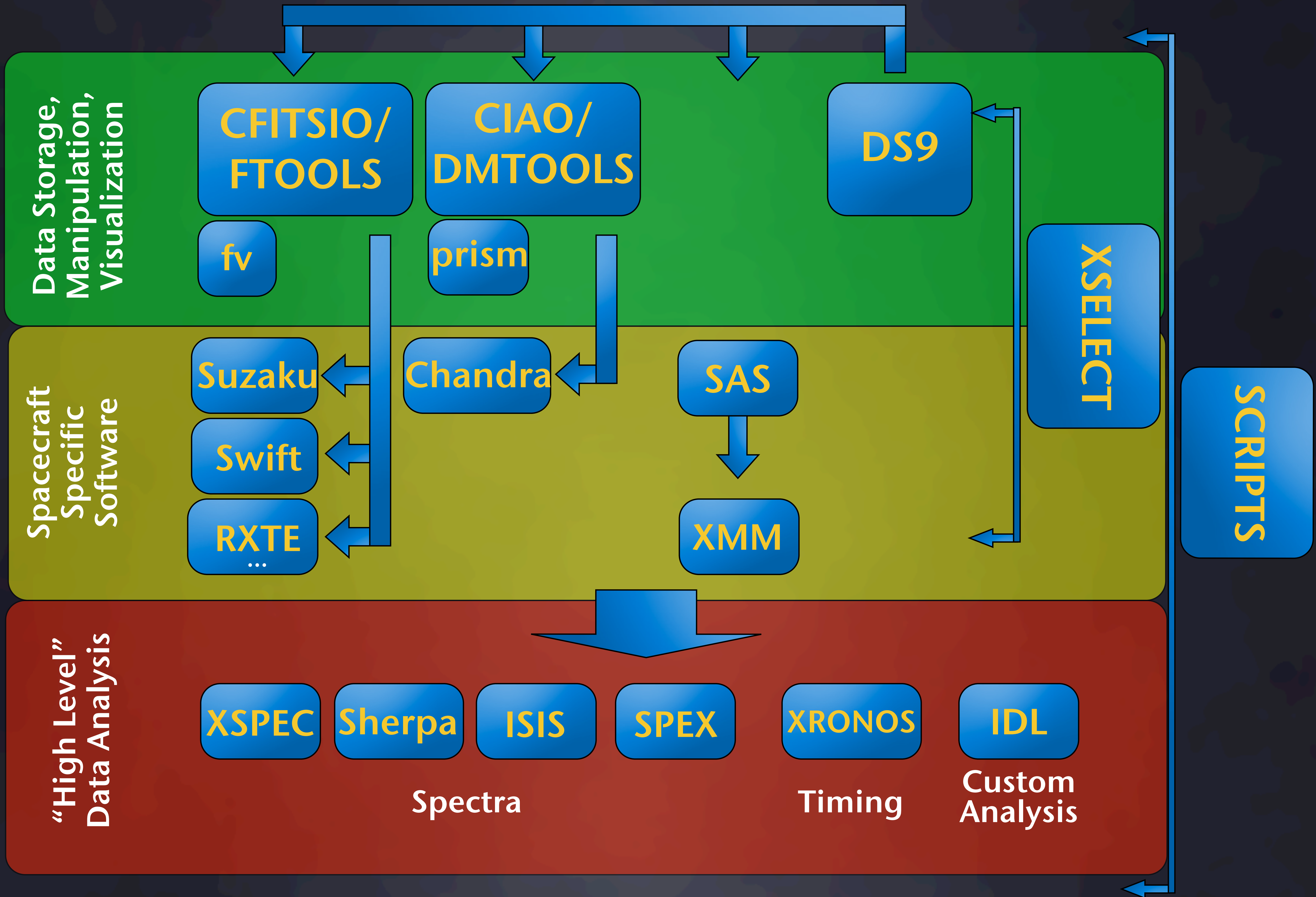

Data Storage, Manipulation, Visualization
CFITSIO/ FTOOLS
CIAO/ DMTOOLS
DS9
fv
prism
XSELECT
Spacecraft Specific Software
Suzaku
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Chandra
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"High Level" Data Analysis
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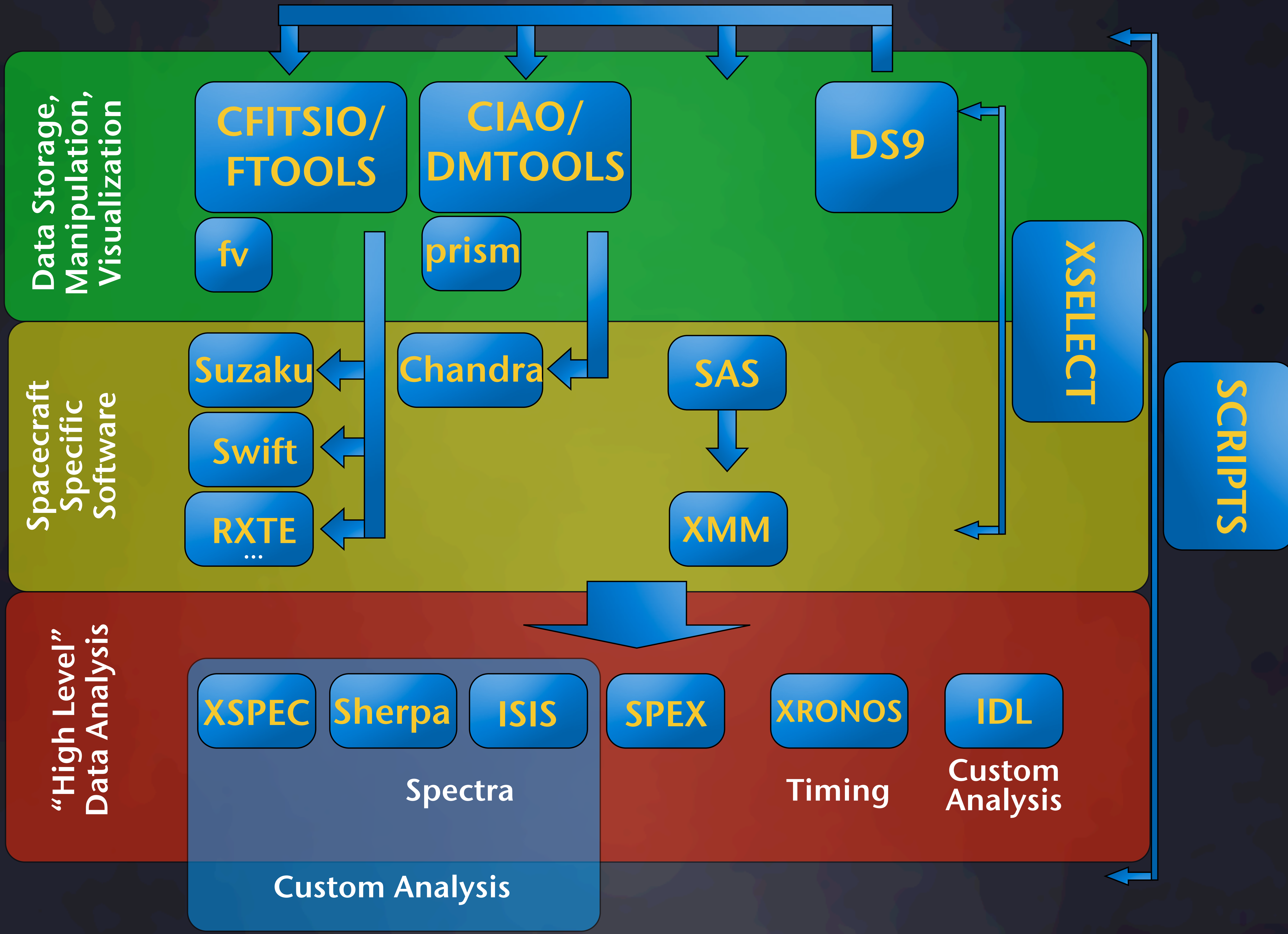

Data Storage, Manipulation, Visualization
CFITSIO/ FTOOLS
CIAO/ DMTOOLS
DS9
fv
prism
XSELECT
Spacecraft Specific Software
Suzaku
Swift
RXTE
...
Chandra
SAS
XMM
SCRIPTS
"High Level" Data Analysis
XSPEC
Sherpa
ISIS
SPEX
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Timing
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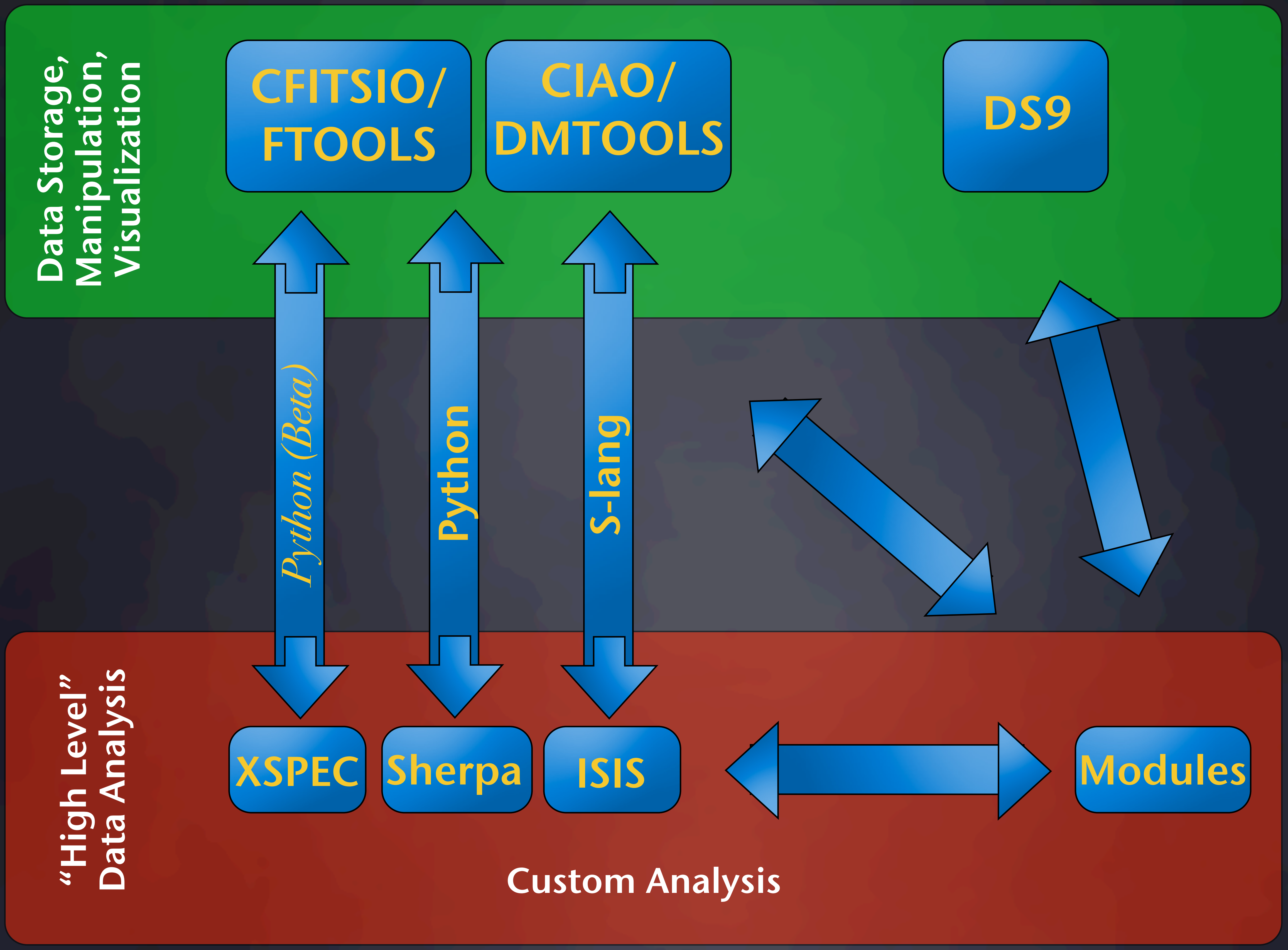
Custom Analysis


Data Storage, Manipulation, Visualization
CFITSIO/ FTOOLS
CIAO/ DMTOOLS
DS9
Python (Beta)
Python
S-lang
"High Level" Data Analysis
XSPEC
Sherpa
ISIS
Modules
Custom Analysis

FITS Format

(http://heasarc.nasa.gov/docs/heasarc/fits.html)

- Binary File Format that is “Self Documenting”
- Named Extensions, containing Headers and Data
- Extensions can be referred to by Name or Number
- Headers Describe Contents, Format, Processing History
- Keywords contain descriptive data
- Data are rows & columns containing values, arrays, images …

FITS Format

(http://heasarc.nasa.gov/docs/heasarc/fits.html)

- Standard types of astrophysical files, e.g., spectra or Ancillary Response Files (ARF) have specific format requirements
- OGIP (Office of Guest Investigator Programs) http://heasarc.nasa.gov/docs/heasarc/ofwg/ofwg_intro.html
- Analysis Packages can be More or Less Tolerant of lack of "OGIP Compliance"
- Most missions strive to be consistent, others openly scoff (I'm looking at you INTEGRAL …)

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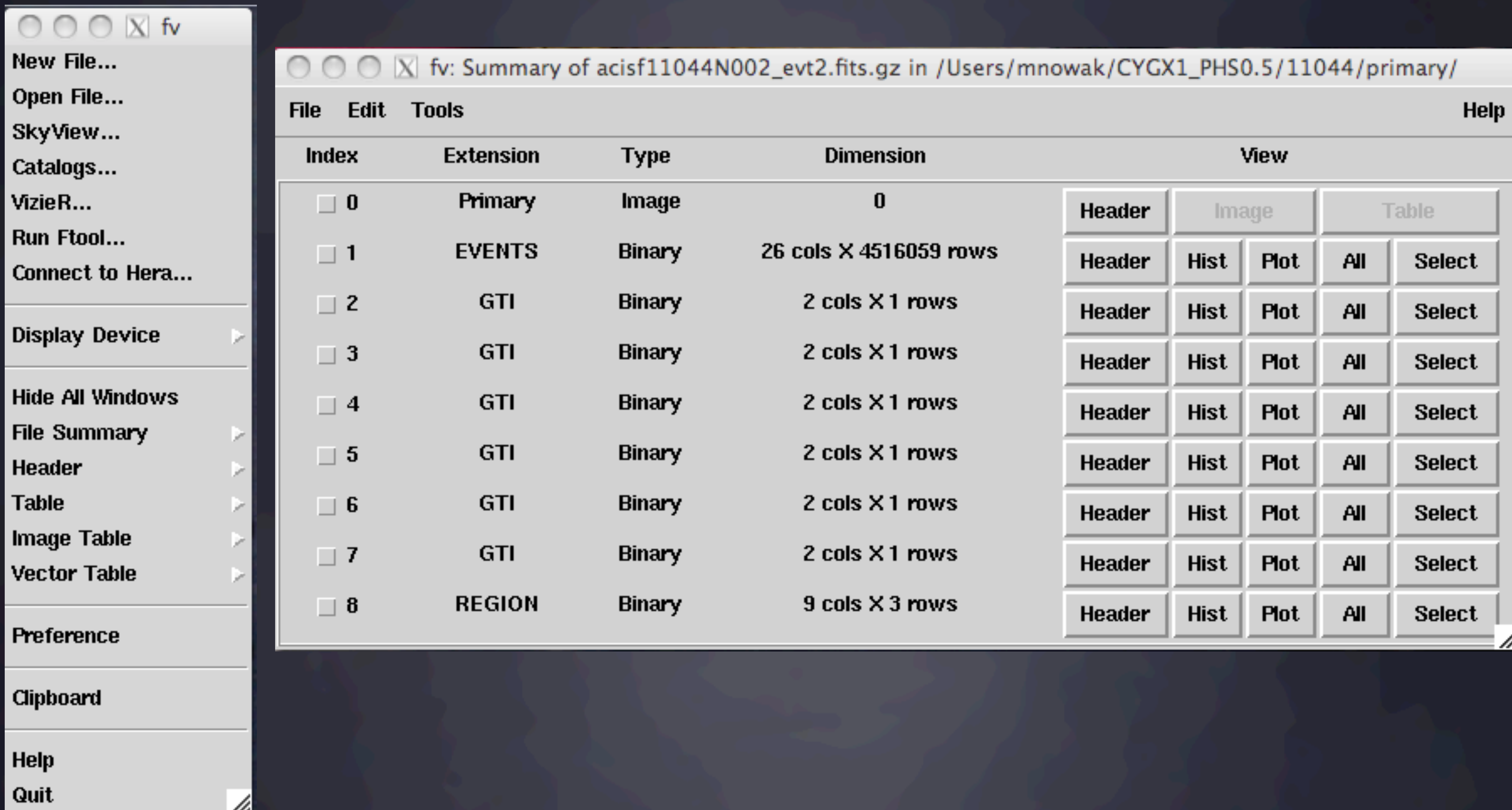

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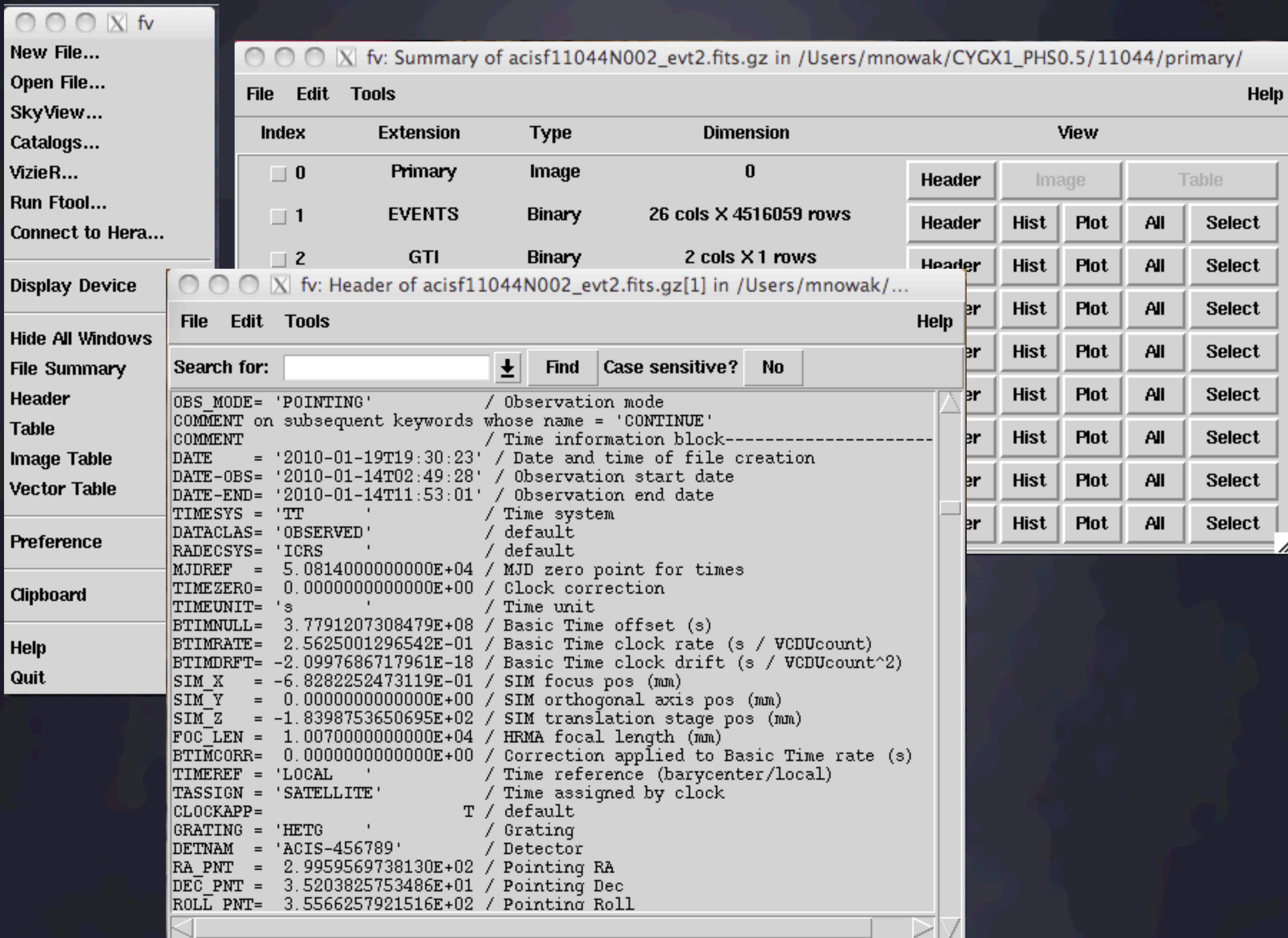

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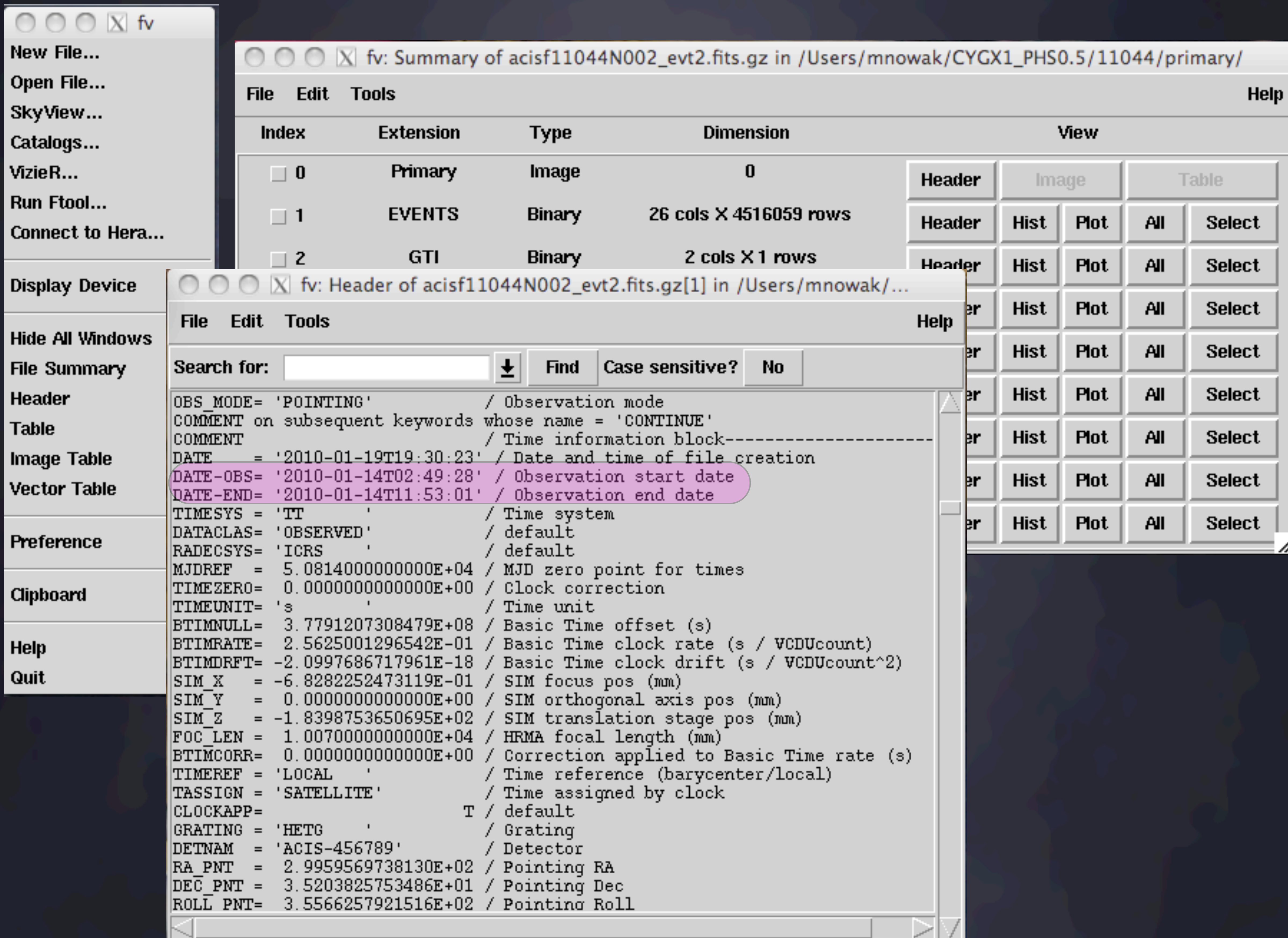

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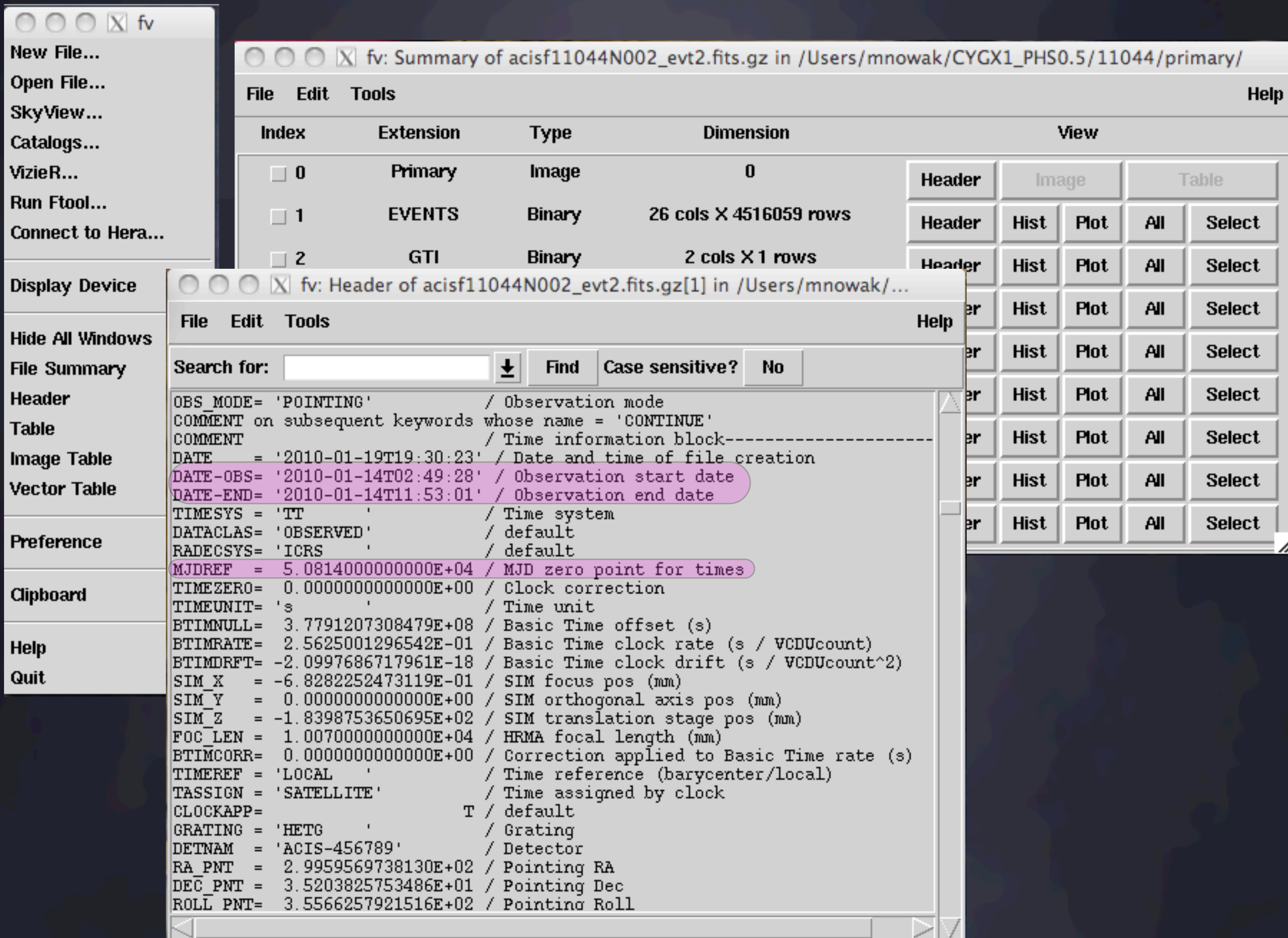

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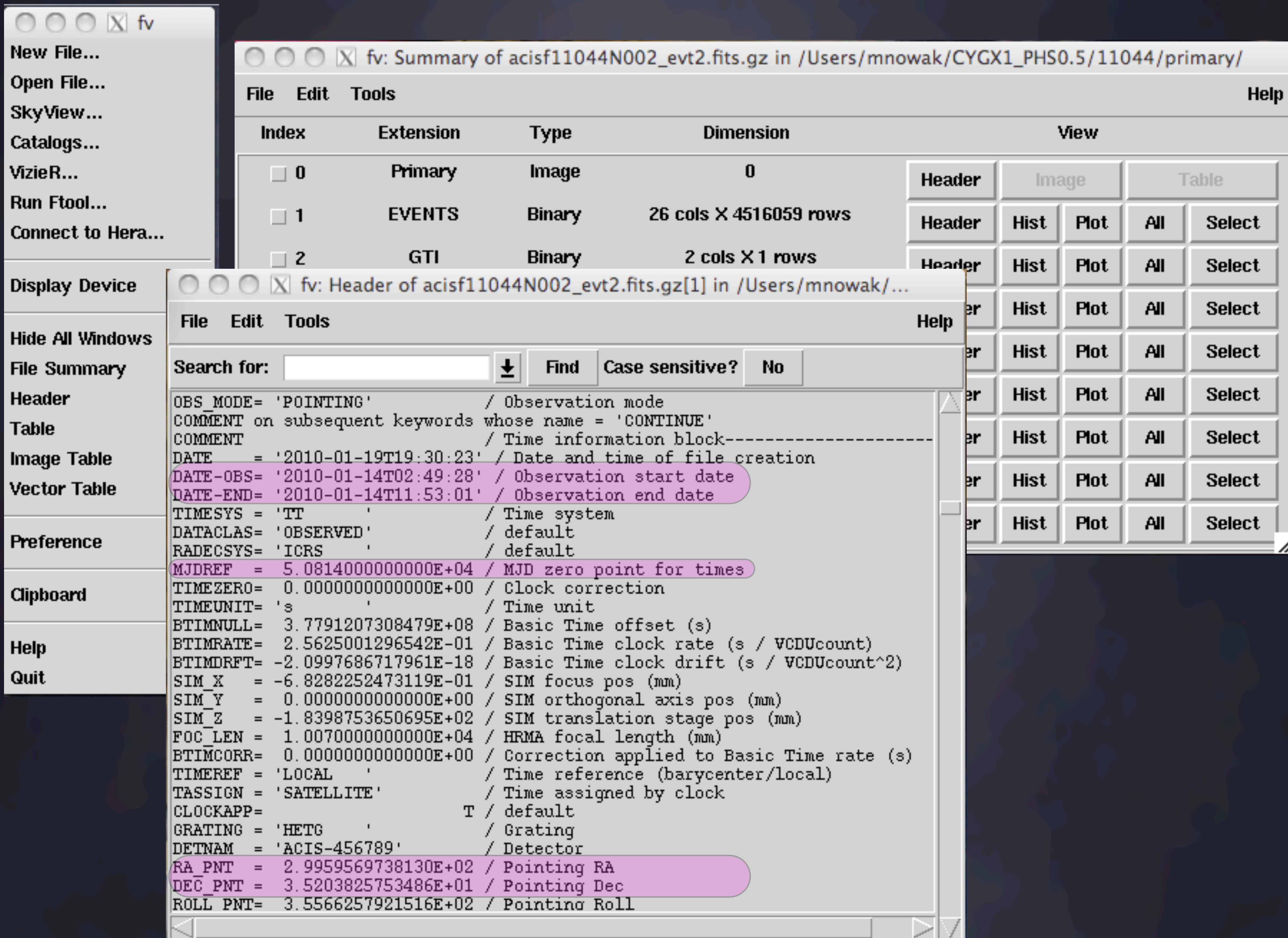

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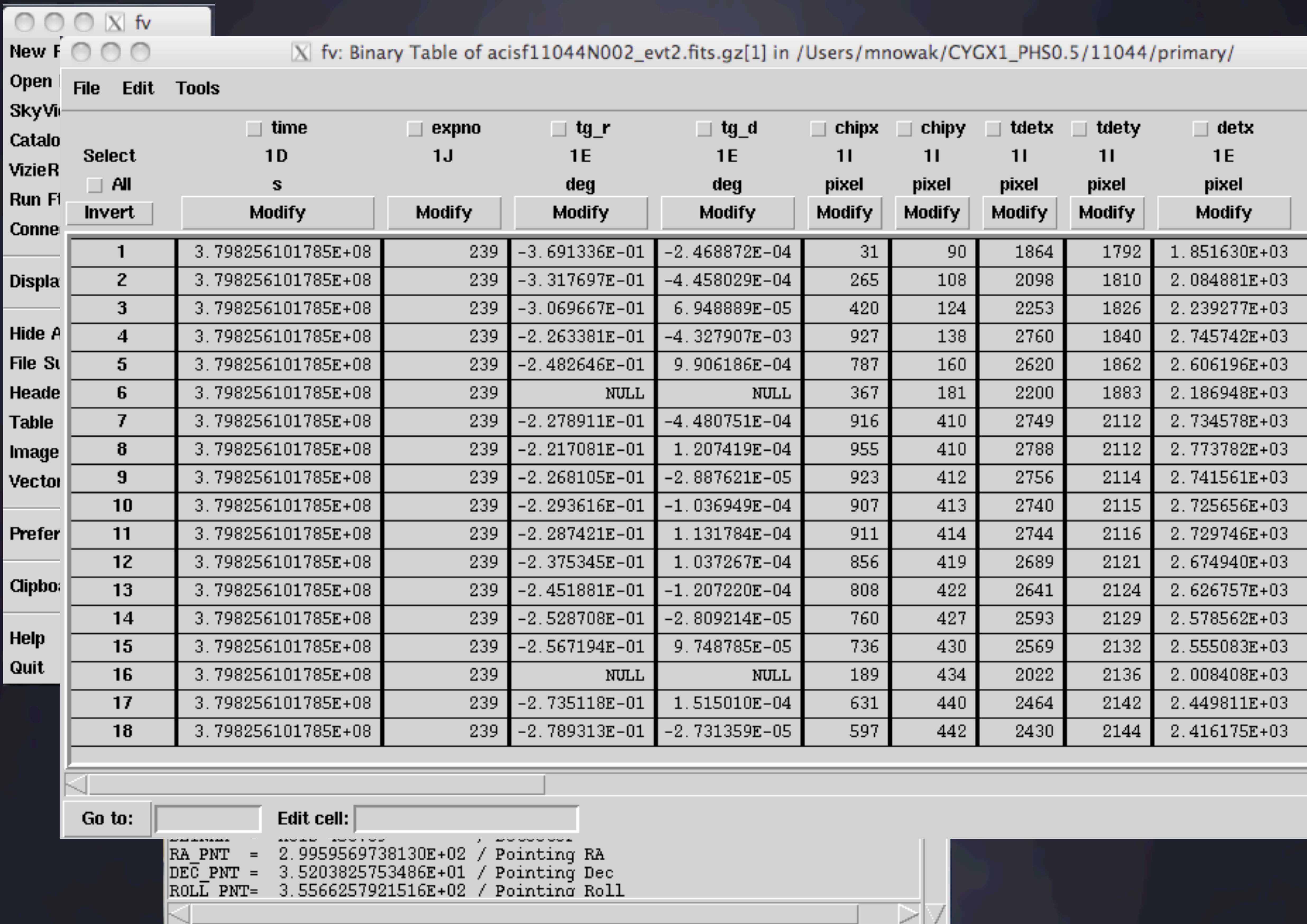

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All	s		deg	deg	pixel	pixel	pixel	pixel	pixel
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2	3.798256101785E+08	239	-3.317697E-01	-4.458029E-04	265	108	2098	1810	2.084881E+03
3	3.798256101785E+08	239	-3.069667E-01	6.948889E-05	420	124	2253	1826	2.239277E+03
4	3.798256101785E+08	239	-2.263381E-01	-4.327907E-03	927	138	2760	1840	2.745742E+03
5	3.798256101785E+08	239	-2.482646E-01	9.906186E-04	787	160	2620	1862	2.606196E+03
6	3.798256101785E+08	239	NULL	NULL	367	181	2200	1883	2.186948E+03
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13	3.798256101785E+08	239	-2.451881E-01	-1.207220E-04	808	422	2641	2124	2.626757E+03
14	3.798256101785E+08	239	-2.528708E-01	-2.809214E-05	760	427	2593	2129	2.578562E+03
15	3.798256101785E+08	239	-2.567194E-01	9.748785E-05	736	430	2569	2132	2.555083E+03
16	3.798256101785E+08	239	NULL	NULL	189	434	2022	2136	2.008408E+03
17	3.798256101785E+08	239	-2.735118E-01	1.515010E-04	631	440	2464	2142	2.449811E+03
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DEC_PNT =  3.5203825753486E+01 / Pointing Dec
ROLL_PNT=  3.5566257921516E+02 / Pointing Roll
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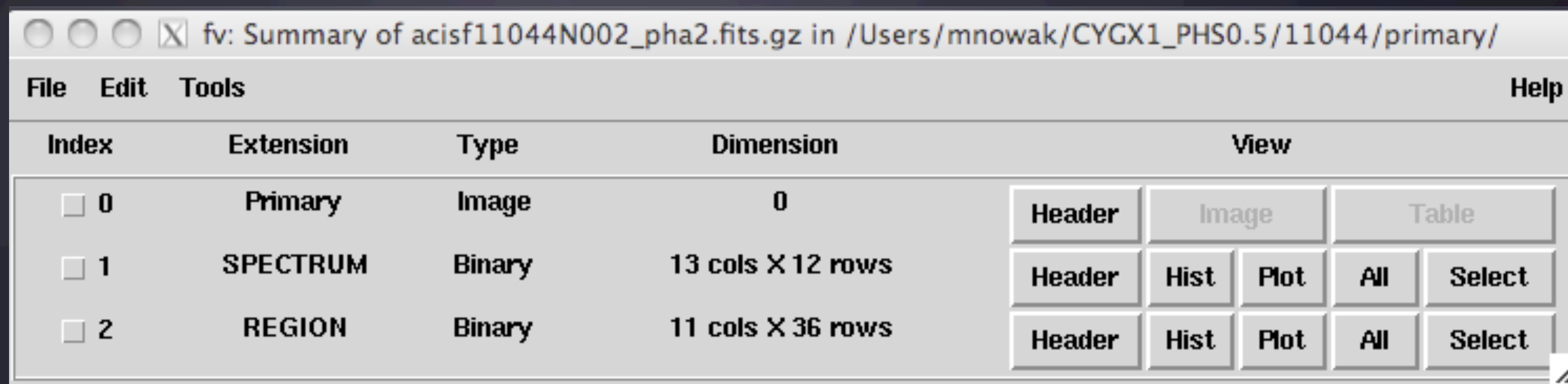

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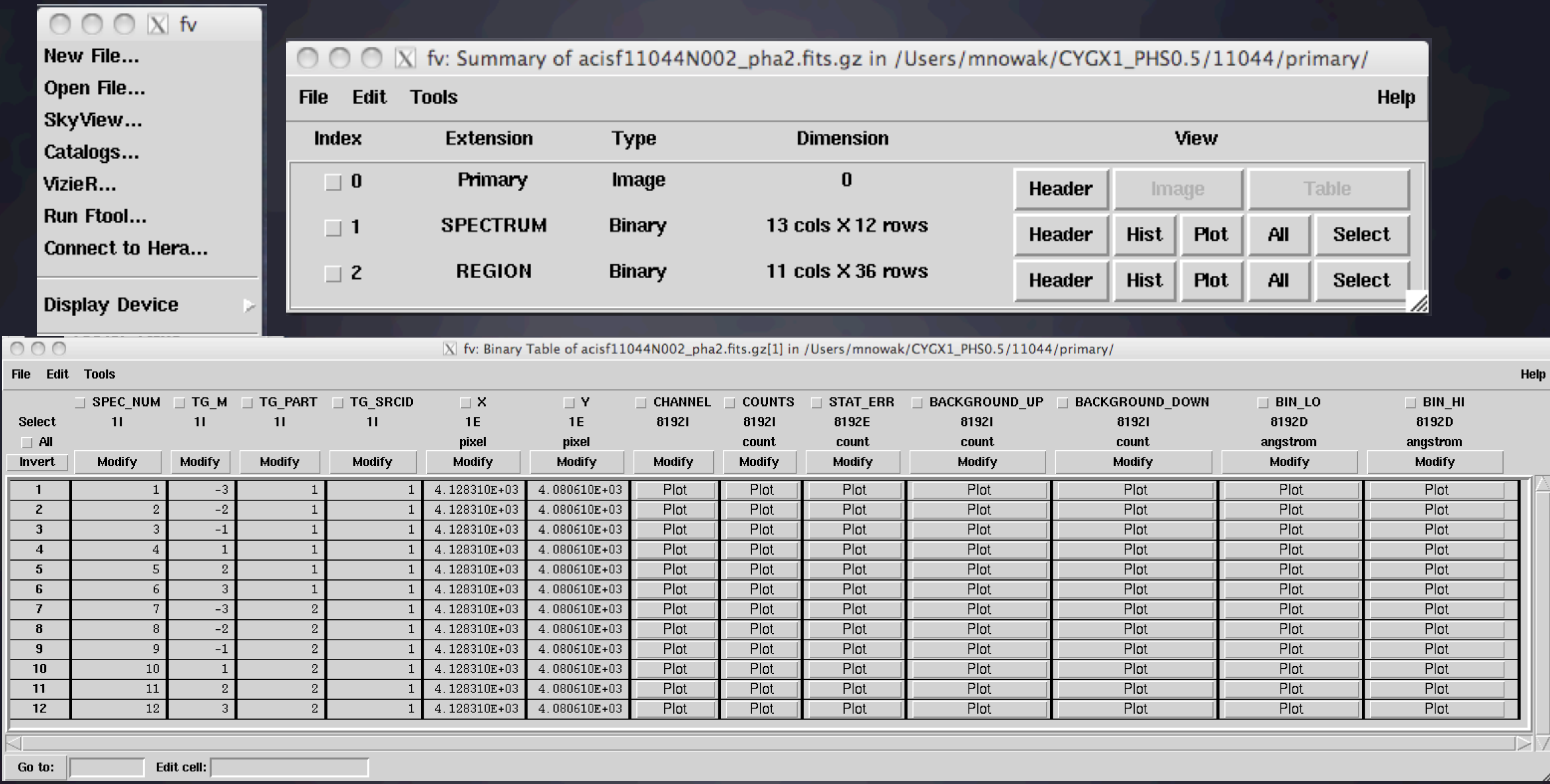

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All					pixel	pixel		count	count	count	count	angstrom	angstrom
Invert	Modify	Modify	Modify	Modify	Modify	Modify	Modify	Modify	Modify	Modify	Modify	Modify	Modify
1	1	-3	1	1	4.128310E+03	4.080610E+03	Plot	Plot	Plot	Plot	Plot	Plot	Plot
2	2	-2	1	1	4.128310E+03	4.080610E+03	Plot	Plot	Plot	Plot	Plot	Plot	Plot
3	3	-1	1	1	4.128310E+03	4.080610E+03	Plot	Plot	Plot	Plot	Plot	Plot	Plot
4	4	1	1	1	4.128310E+03	4.080610E+03	Plot	Plot	Plot	Plot	Plot	Plot	Plot
5	5	2	1	1	4.128310E+03	4.080610E+03	Plot	Plot	Plot	Plot	Plot	Plot	Plot
6	6	3	1	1	4.128310E+03	4.080610E+03	Plot	Plot	Plot	Plot	Plot	Plot	Plot
7	7	-3	2	1	4.128310E+03	4.080610E+03	Plot	Plot	Plot	Plot	Plot	Plot	Plot
8	8	-2	2	1	4.128310E+03	4.080610E+03	Plot	Plot	Plot	Plot	Plot	Plot	Plot
9	9	-1	2	1	4.128310E+03	4.080610E+03	Plot	Plot	Plot	Plot	Plot	Plot	Plot
10	10	1	2	1	4.128310E+03	4.080610E+03	Plot	Plot	Plot	Plot	Plot	Plot	Plot
11	11	2	2	1	4.128310E+03	4.080610E+03	Plot	Plot	Plot	Plot	Plot	Plot	Plot
12	12	3	2	1	4.128310E+03	4.080610E+03	Plot	Plot	Plot	Plot	Plot	Plot	Plot

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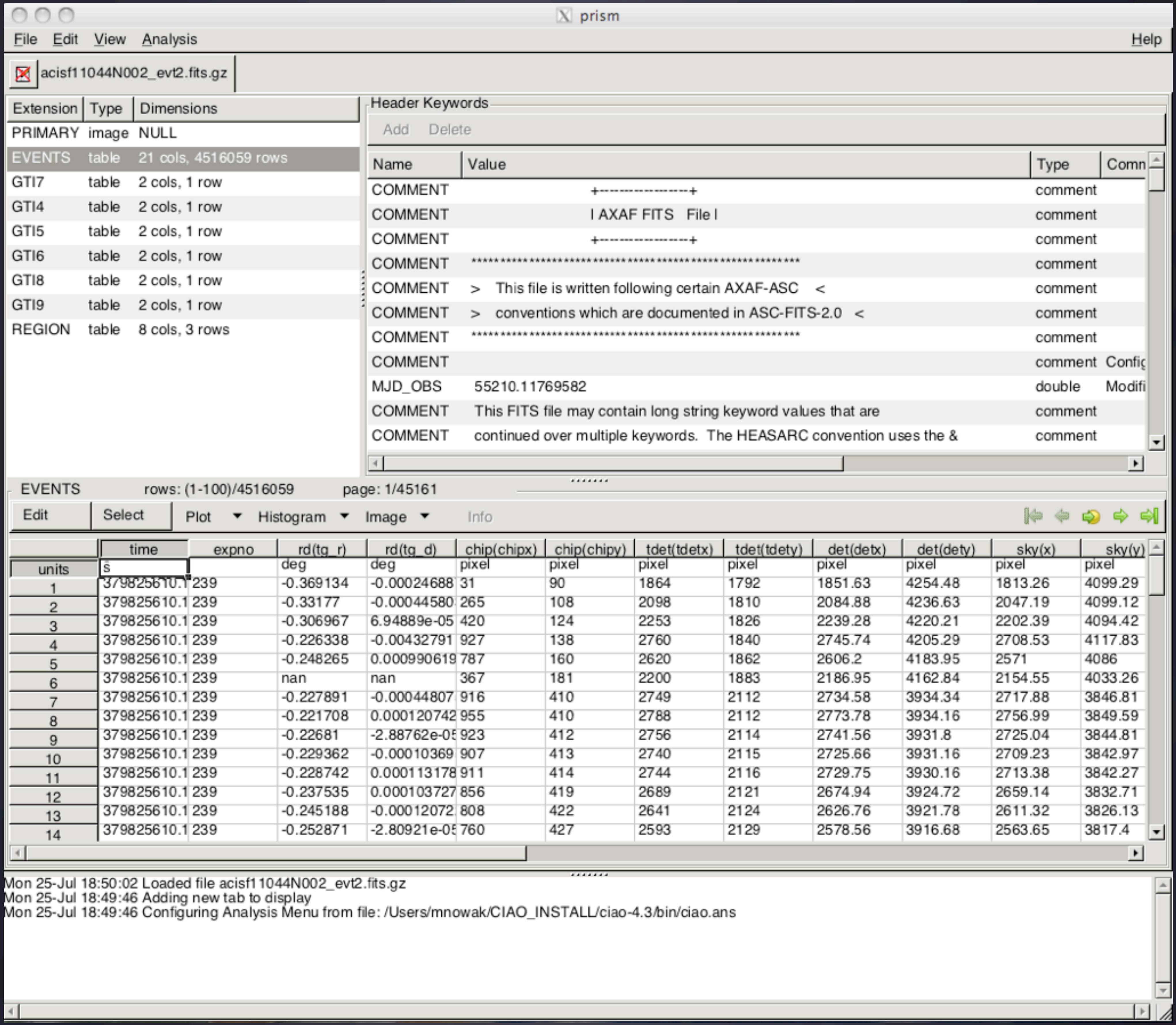

prism

File Edit View Analysis Help

acisf11044N002_evt2.fits.gz

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EVENTS	table	21 cols, 4516059 rows
GTI7	table	2 cols, 1 row
GTI4	table	2 cols, 1 row
GTI5	table	2 cols, 1 row
GTI6	table	2 cols, 1 row
GTI8	table	2 cols, 1 row
GTI9	table	2 cols, 1 row
REGION	table	8 cols, 3 rows

Header Keywords

Add Delete

Name	Value	Type	Comn
COMMENT	+------------------+	comment	
COMMENT	I AXAF FITS File I	comment	
COMMENT	+------------------+	comment	
COMMENT	**	comment	
COMMENT	> This file is written following certain AXAF-ASC <	comment	
COMMENT	> conventions which are documented in ASC-FITS-2.0 <	comment	
COMMENT	**	comment	
COMMENT		comment	Config
MJD_OBS	55210.11769582	double	Modifi
COMMENT	This FITS file may contain long string keyword values that are	comment	
COMMENT	continued over multiple keywords. The HEASARC convention uses the &	comment	

EVENTS rows: (1-100)/4516059 page: 1/45161

Edit Select Plot Histogram Image Info

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units	s		deg	deg	pixel	pixel	pixel	pixel	pixel	pixel	pixel	pixel
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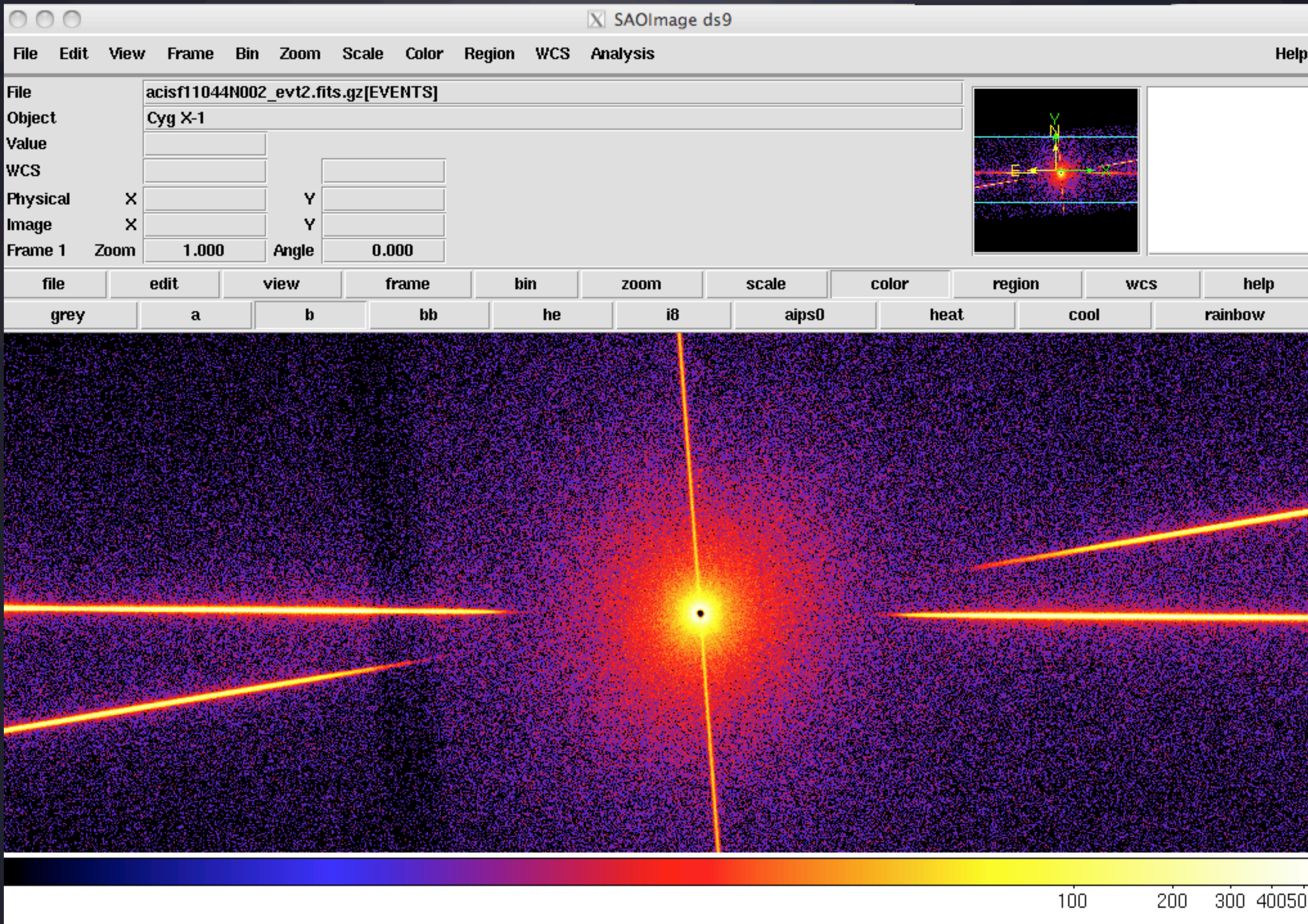
9	379825610.1	239	-0.22681	-2.88762e-05	923	412	2756	2114	2741.56	3931.8	2725.04	3844.81
10	379825610.1	239	-0.229362	-0.00010369	907	413	2740	2115	2725.66	3931.16	2709.23	3842.97
11	379825610.1	239	-0.228742	0.000113178	911	414	2744	2116	2729.75	3930.16	2713.38	3842.27
12	379825610.1	239	-0.237535	0.000103727	856	419	2689	2121	2674.94	3924.72	2659.14	3832.71
13	379825610.1	239	-0.245188	-0.00012072	808	422	2641	2124	2626.76	3921.78	2611.32	3826.13
14	379825610.1	239	-0.252871	-2.80921e-05	760	427	2593	2129	2578.56	3916.68	2563.65	3817.4

Mon 25-Jul 18:50:02 Loaded file acisf11044N002_evt2.fits.gz
Mon 25-Jul 18:49:46 Adding new tab to display
Mon 25-Jul 18:49:46 Configuring Analysis Menu from file: /Users/mnowak/CIAO_INSTALL/ciao-4.3/bin/ciao.ans

unix%> ds9 acisf11044N002_evt2.fits.gz &



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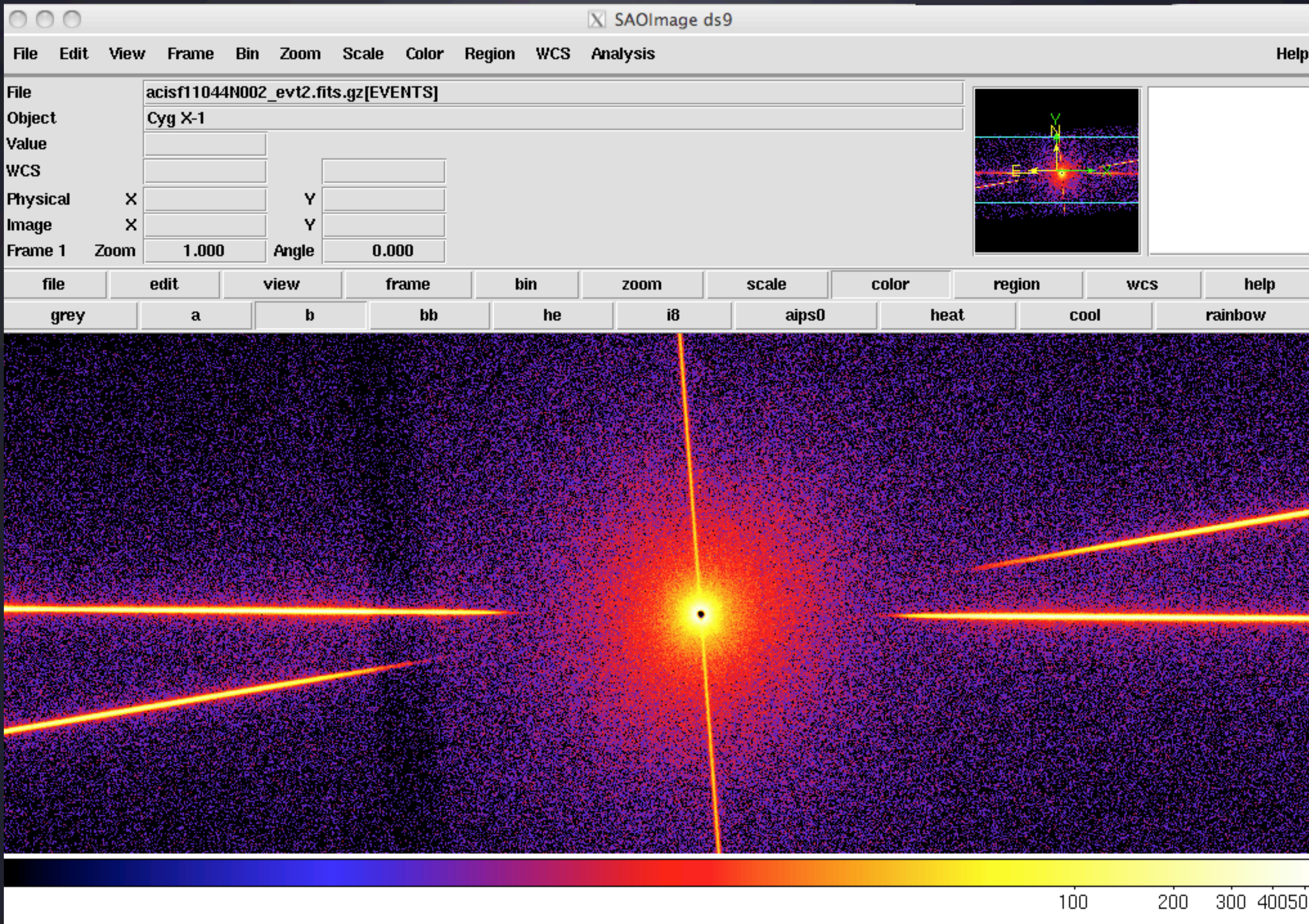

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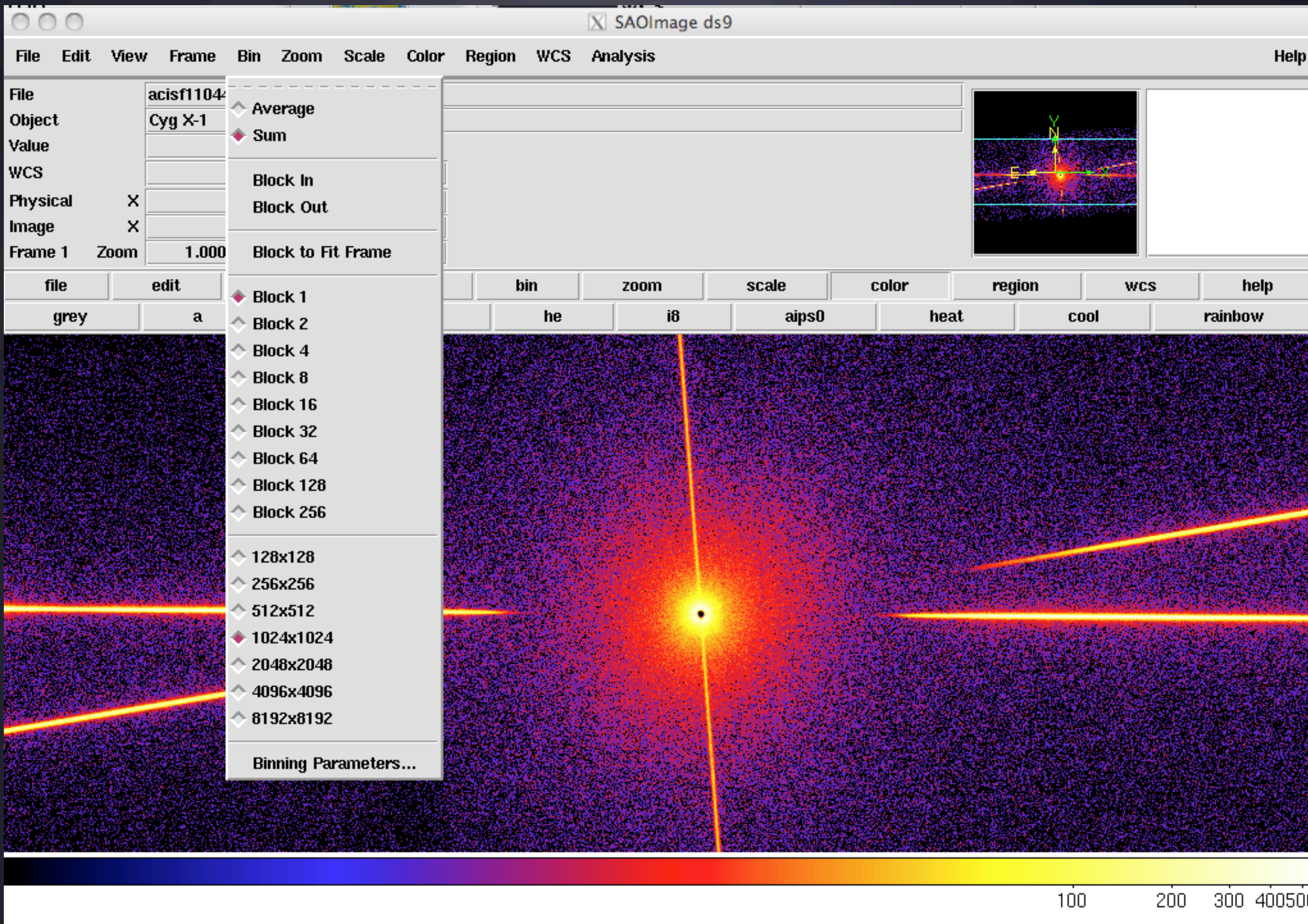

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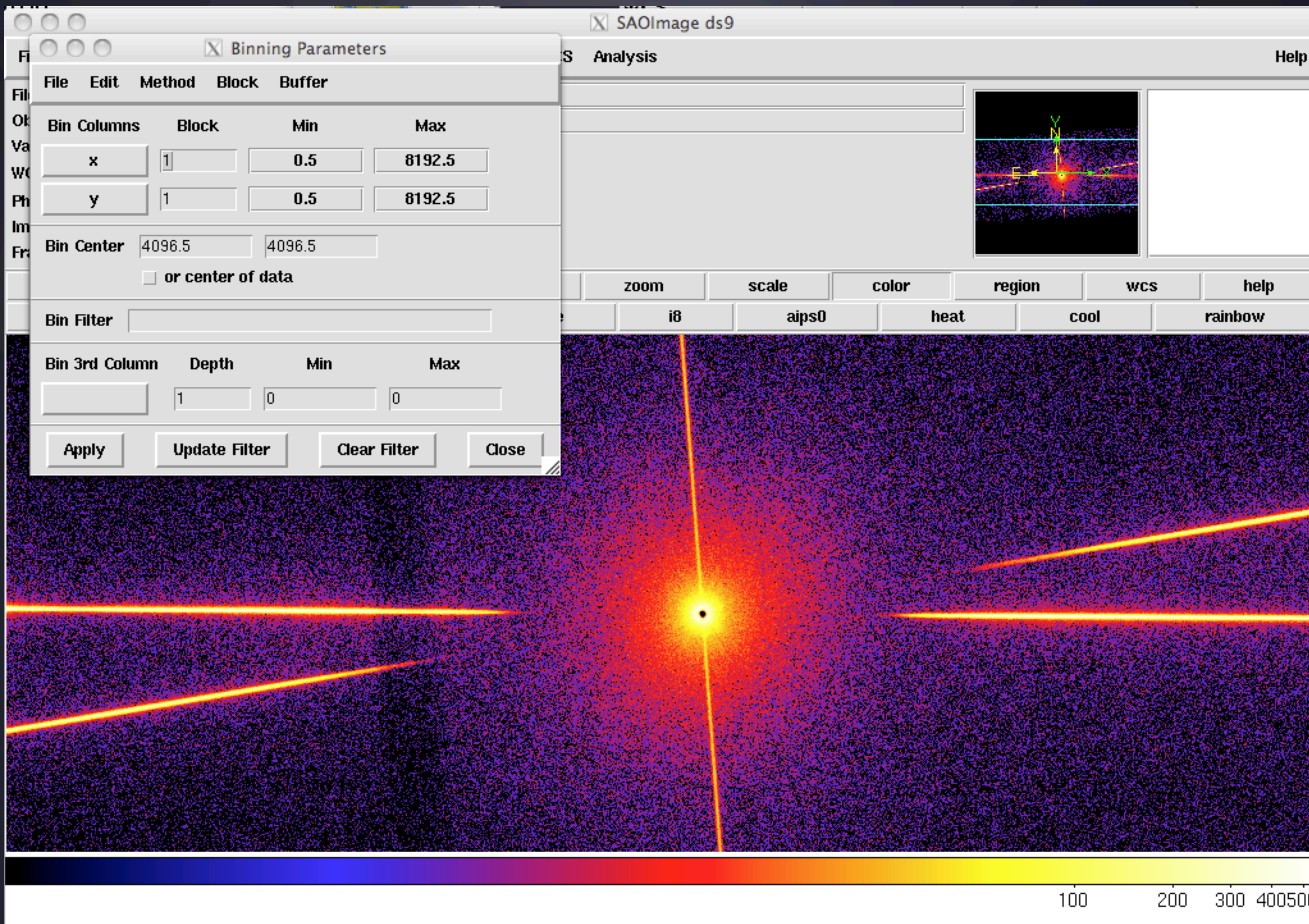

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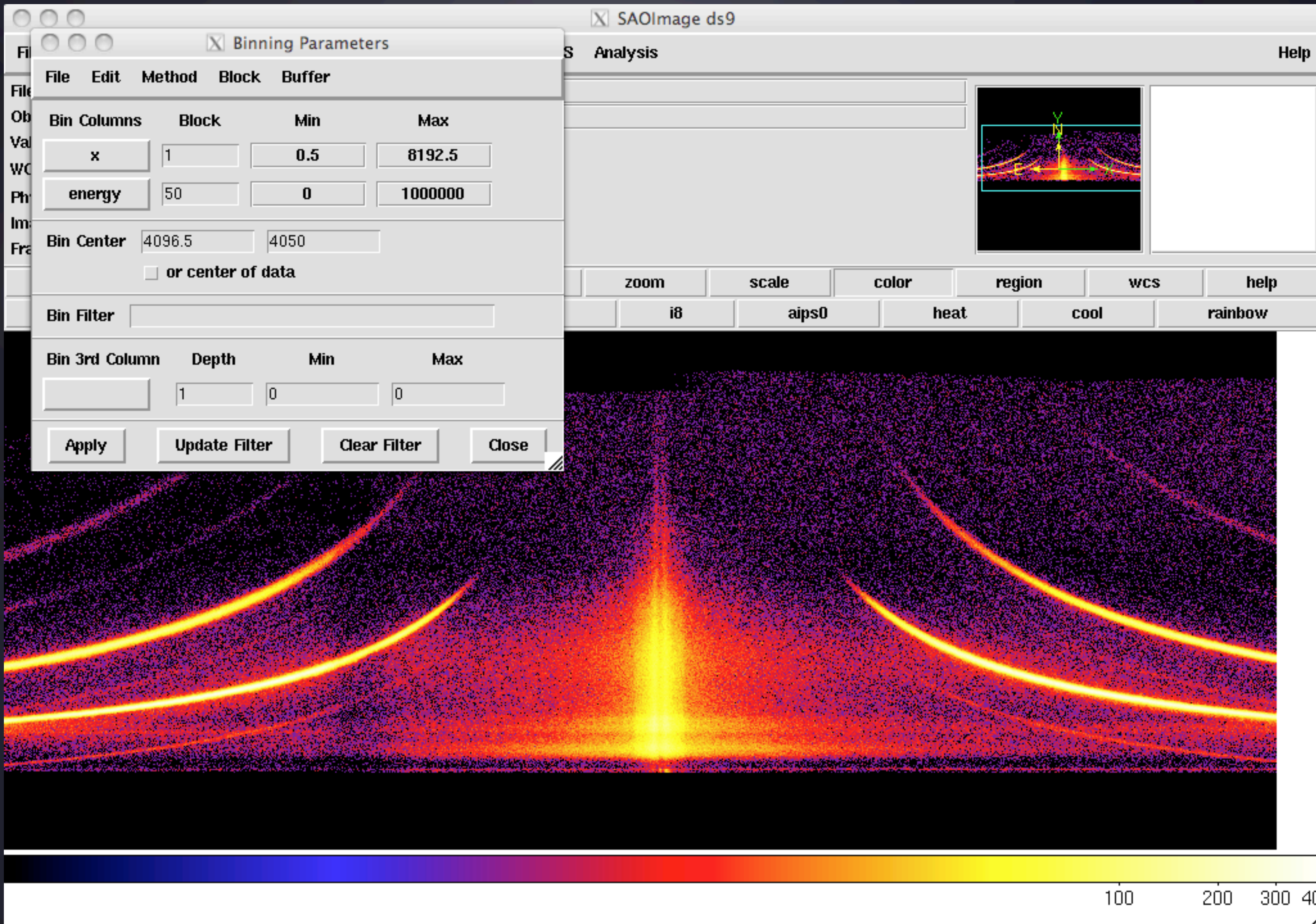

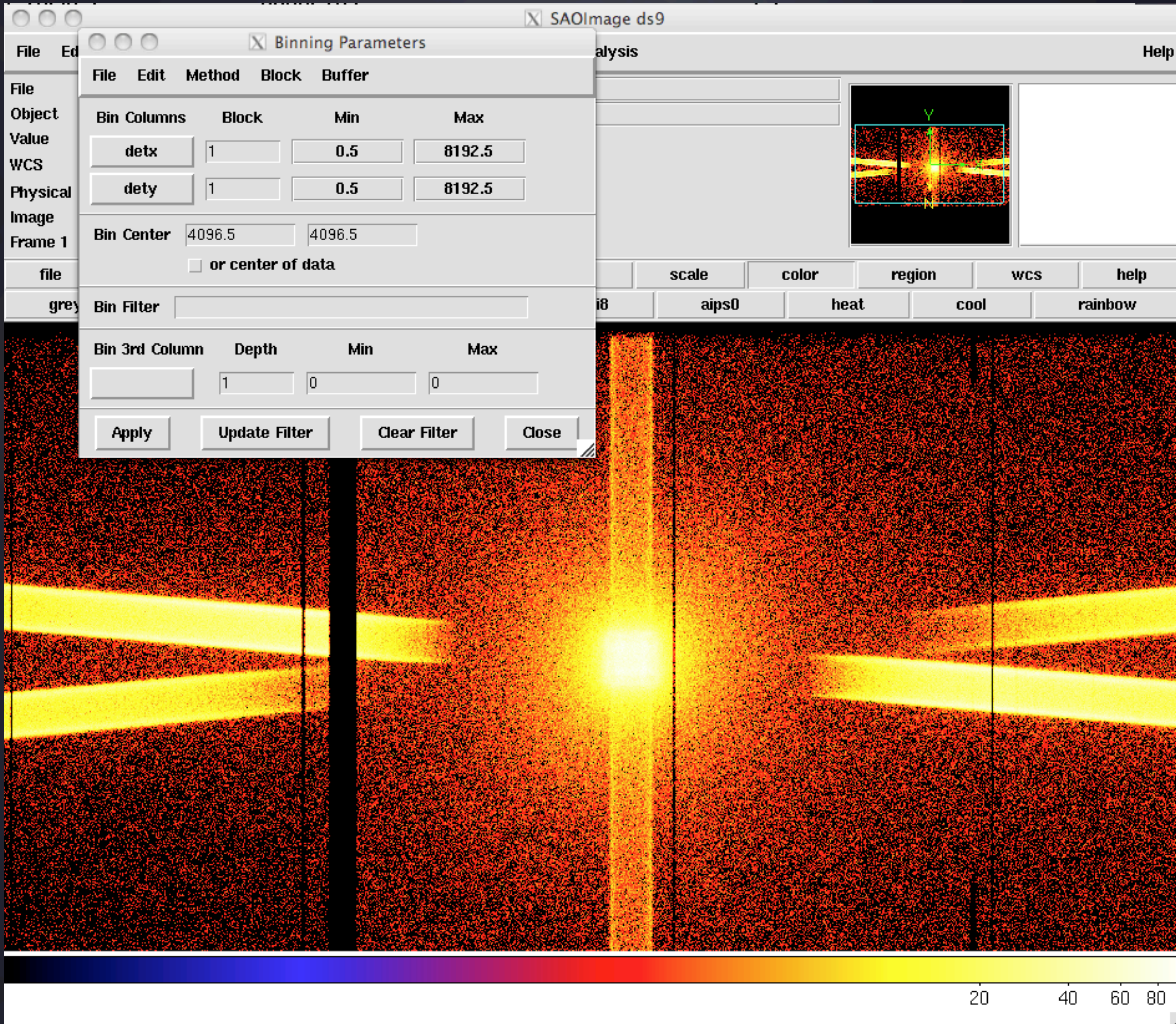
SAOImage ds9
Binning Parameters
File
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Method
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Buffer
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Bin Center
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Bin Filter
Bin 3rd Column
Depth
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Apply
Update Filter
Clear Filter
Close
File
Object
Value
WCS
Physical
Image
Frame 1
Help
file
scale
color
region
wcs
help
aips0
heat
cool
rainbow
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80

READING & WRITING: HEASOFT–FITSIO & FTOOLS

(http://heasarc.gsfc.nasa.gov/lheasoft/)

- CFITSIO library: Suitable for compiled programs (Fortran, C, C++)
    - Interfaces exist for scripting languages (S-lang, Python, Ruby, TCL, Perl, MATLAB, IDL)
    - Overlapping functionality in script packages (IDL, Python via PyFITS)
- FTOOLS functions: Command line interfaces
    - Suitable for use in Shell/Perl Scripts

HEASOFT – FTOOLS

(http://heasarc.gsfc.nasa.gov/docs/software/ftools)

- Tools have a variety of parameters (plist), that can be set before running (pset), or on the command line
  - Command line interface is less “hidden”; therefore, less prone to error, cleaner for scripts
  - Be careful to update default parameters every new HEASOFT release! (punlearn)
- Wide variety of tools - fdump (list contents), fcopy (copy contents), fextract (extract an extension), fstatistic (statistics of columns), ftcopy (copy with filters), fltime (filter file by time), …

READING & WRITING: CIAO–CRATES & DM

(http://cxc.harvard.edu/ciao/ahelp/crates.html, http://cxc.harvard.edu/ciao/ahelp/dm.html)

- CRATES – A high level Python interface for Input/ Output of data files
  - Used in ChIPs and Sherpa
  - Can be used with other Python packages
- Data Model functions: Command line interfaces
  - Suitable for use in Shell/Perl Scripts

CIAO – Data Model

(http://cxc.harvard.edu/ciao/ahelp/dm.html)

- Tools have a variety of parameters (plist), that can be set before running (pset), or on the command line
  - Command line interface is less “hidden”; therefore, less prone to error, cleaner for scripts
  - Be careful to update default parameters every new CIAO release! (punlearn)
- Wide variety of tools - dmlist (list contents), dmcopy (copy contents), dmextract (extract data), dmstat (statistics of columns), ...

Parameter Files

- Usually found in your home directory:
  - HEASOFT – /home/me/pfiles/*
  - CIAO – /home/me/cxcds_param4/*
- *Not All Parameters are Prompted for by Tools!*
  - Unprompted parameters take on defaults; *often* are parameters that needn't/shouldn't be changed
- Check parameter files directly; read FITS history
- When in doubt, set all parameters explicitly
- For scripts, set PFILES environment to a dedicated directory (avoids jobs clobbering each other)

Spacecraft Specific Reduction

- Three Primary Choices for X-ray Astronomy:
  - CIAO – Chandra Observations
    - Includes (& Usually Requires) DS9
  - SAS – XMM-Newton Observations
    - Requires HEASOFT, DS9, & GRACE
  - HEASOFT – (Almost) Everything Else
    - RXTE, Suzaku, Swift, (some of) INTEGRAL (->OSA)
    - ASCA, CGRO, EXOSAT, ROSAT, Einstein, HEAO-1

Data Analysis Steps I.

- "Raw" Telemetry is converted to a FITS data file
  - "Level 0" -> "Level 1"
  - Processing Pipeline step, usually not accessible/ reproducible by an ordinary user
- "Level 1" files can still have many detector effects included in the file
  - False Events: flaring pixels, time tags, etc.
  - "Bad Grades": Cosmic Ray hits
  - Uncorrected positions, times, gain (energy), ...

Data Analysis Steps II.

- Further Cleaning/Filtering Provided by Pipelines
    - “Level 1” -> “Level 2”
    - “Standard” Choices are Applied
    - (Most) False Events Removed & Corrections Made
- You may have other choices and/or calibration may have improved, requiring reprocessing
- You likely will want to subdivide the data, e.g., remove times of high background, or select specific Space/Time/Energy cuts

Data Analysis Steps IIa.

- You Do Want to Change Spacecraft Specific Filters & Corrections, e.g., CTI Correction, Bad Pixels, etc.
- Spacecraft Specific Software needs to be used
  - acis_process_events -> Chandra data
  - xispi -> Suzaku data, ... etc.
- Software will properly update FITS headers to account for changes in integration Time or Area

Data Analysis Steps IIb.

- Applying “Generic” Time/Space/Energy Filters
- In Principle, Multiple Software Packages Work
  - CIAO: Data Model with filters
  - HEASOFT: Xselect (extractor run under the hood)
  - SAS: evselect or xmmselect (XMM only!)
- Software Updates Exposures, Areas, etc., in Headers
  - Warning: Sometimes information needed later is only properly passed along by “principal” system, e.g., Suzaku “works best” under HEASOFT

Data Analysis Steps III.

- Extraction of “High Level” Data Products
  - Spectra
  - Lightcurves
  - Images – DS9 Often Used to Define Regions
- In Principle, Multiple Software Packages Work
  - CIAO: Data Model with filters
  - HEASOFT: Xselect (extractor run under the hood)
  - SAS: evselect or xmmselect (XMM only!)

XSELECT

- Attempts to Combine IIa, IIb, and III All in One Package
- Not Really a GUI, Not Really a Command Line System, Not Quite a Programmable Environment
- Runs extractor “under the hood”, but hides (obfuscates?) the details
- Can be worked into Shell Scripts, but given that XSELECT expects user interaction it is easier to incorporate into Perl/Python scripts

Data Analysis Steps IV.

- Create Associated Files to Aid Analysis
- Responses (RMF & ARF), Exposure Maps, Background Files (& their Responses [maybe])
- Spacecraft Specific Software Required!
- Follow the ABC Guides!
- Try to understand *why* a step is being done; don't try to automate until you understand the pitfalls!

Helpful Starting Points

- Chandra Analysis: http://asc.harvard.edu/ciao/guides
- XMM Analysis: http://xmm.esa.int/sas
- Suzaku Analysis: http://heasarc.nasa.gov/docs/suzaku/analysis/abc
- RXTE Analysis: http://heasarc.nasa.gov/docs/xte/recipes/cook_book.html
- Swift Analysis: http://heasarc.nasa.gov/docs/swift/analysis/start
- INTEGRAL Analysis: http://www.isdc.unige.ch/integral/download/osa_doc

CALDB

- Calibration Database Required for Analyses
- Check Spacecraft Sites periodically for Updates & Caveats. Learn the files to apply in each situation
- Use Consistent Software & Calibration Database
- New Software with Old Calibration Files, or visa versa, sometimes can produce wrong results
- This is where having the correct Parameter Files can be crucial! (New Software+New CALDB+Old Parameters = Wrong Results!)

Analysis

- You've got your Spectra, Images, and Lightcurves, *now what?*
- Analyze with your favorite software package!
- Products are back to "Standard Forms" so packages work well on products from a wide range of spacecraft
- Timing – XRONOS is specifically designed for timing
  - I have never used it
  - I used IDL (<= 2001), & now ISIS (>2001)
  - Lots of custom code out there ...

Analysis

- Imaging Analysis –
  - Sherpa will convolve Chandra PSF with simple 2D models & fit a 2D histogram
  - Some fraction of image analysis reduces 2D -> 1D, and then any spectral package applies
  - My limited experience is simple 2D models applied to 2D histograms using ISIS
  - You'll see examples from people far more experienced than me in this arena...

Analysis

- Spectral Analysis –
  - Lots of choices, with the four major choices being XSPEC, Sherpa, ISIS, SPEX
  - XSPEC is the oldest & most established, so many models will be written with XSPEC in mind
  - Sherpa is ≈ the youngest; lectures on advanced use on Saturday
  - SPEX is in some ways a “specialty” package for high-resolution X-ray spectroscopy
  - I use ISIS for most of my mathematical analysis (spectra, timing, & other things)

Comparison of Packages:

	XSPEC Models	XSPEC Local Models	Scripted Models	User Scripts	Data Product Access	Other Fit Kernels	User Fit Kernels	User Optim. Methods	User Fit Stats
XSPEC	All	Yes	Limited	TCL, Python	Limited	Gain	No	No	No
Sherpa	Most	With Effort	Python	Python	Yes	No	Yes	Yes	Yes
ISIS	All	Yes	S-lang	S-lang	Yes	Gain, Pileup	Yes	Yes	Yes
SPEX	Few	No	No	No	No	No	No	No	No

	Non-X-ray Data	Atomic Data Access	Model Caching	Multi-core Errors	Multi-core Fits	Multi-System Errors	Multi-System Models
XSPEC	With Fake RMF, ARF	No	Limited	No*	No*	No	No
Sherpa	Yes	No	Yes	Yes	No	No	No
ISIS	Yes	Yes	Yes	Yes	Yes	Yes	Yes
SPEX	No	Yes	?	No*	No*	No	No

*Some internal code is, or can be, parallelized upon compilation

Your Responsibilities:

- You will use & install a lot of software over your astrophysical career.
- You will probably write a lot of scripts, and maybe even spectral fit models, or even a software package.
- Undoubtedly, sometime, somewhere you will run into some problems.
- There are things you can do to help yourself, and things you can do to help us help you.

Installing Software:

- *Don't* have anyone else to install software for you. *Know what's going where on your machine!*
- Use a consistent set of compilers and libraries. E.g., all 32-bit built with gcc/gfortran/g++ 4.4.1. *Know what compilers and libraries you are using!*
  - unix%> gcc --version
  - Builds: setenv CC ; setenv CXX ; setenv FC
  - Linux: package management systems, e.g., apt-get can be helpful in creating a consistent system
  - Apple: it's the Wild West, between Xcode, Fink, MacPorts, & Downloaded Packages
    - I use Fink/MacPorts sparingly, and hand-install compilers (sourceforge.net) and many libraries

Installing Software:

- Install software in sane, “standard” locations, for example, /usr/local or /opt
- Don’t default paths to access software automatically – use start up scripts when you need the program
  - Our programs try to play nice with one another, but some mistakes happen …
  - It’s easy to end up with multiple copies of CFITSIO, PGPLOT, … Using one program at a time decreases the chance of inconsistent libraries

Writing Bug Reports:

- If we've made a mistake, let us know! But give us the info we need to figure it out:
  - Clear, informative subject line on e-mail
  - Tell us what version of the software, caldb, compilers, and operating system you are using
  - Send us copies of any log files and and the complete text of any error messages
  - Send us figures, with clear labels and detailed descriptions, that illustrate the issues. *Figure names* should make it obvious what you mean!
  - If possible, write us a script that reproduces the problem. Point us to a place where we can download the script and data that you used

Writing Software:

- If You are going to use existing code (e.g., Numerical Recipes), either:
  - Compile it in via an existing library, or,
  - Change the subroutine name in *your* code! (Fortran, especially, will happily use the first instance of a name it finds)
- Avoid generic names, e.g., directories called “data”. “agn_torus_data” would be a better name.
- Be descriptive in variable, subroutine, data, directory, and code names. And ...
  - Comments, Comments, Comments ...

Writing Software:

- Put comments and contact info and dates in your code. Use version numbers! E.g., ISIS 1.6.1-35
- -35: minor changes (mostly bug fixes), .1: new functionality, but backward compatibility preserved, .6: significant changes, backward compatibility not guaranteed, 1: major changes!
- If you change *anything*, change the version number! I mean *anything, change the number!*
- Version control is your friend, for software, scripts, papers... I highly recommend git

Writing Software:

- The basics of git are straightforward:

```
unix%> git init
unix%> git add .isisrc_plots
unix%> git commit -a
```

- git lets you track changes:

```
unix%> git show
unix%> git log
```

- git lets you go back to earlier versions:

```
unix%> git checkout <commit-hash>
unix%> git revert <commit-hash>
```

- Your life will be much happier! For more, see tutorials at: http://git-scm.com/documentation