Xspec

HEASOFT X-Ray Spectral Fitting Package

Astro Dev Group 14.03.2025 - Gloria Rah.

AGENDA

WINS

A quick round of celebrating successes and progress from the past week.

ISSUES

Addressing roadblocks, challenges, and lessons learned to improve our workflow.

XSPEC

A deep dive into what XSPEC is, its functionalities, and how to effectively use it.

AOB

Wrapping up with any final thoughts, questions, or spontaneous discussions.

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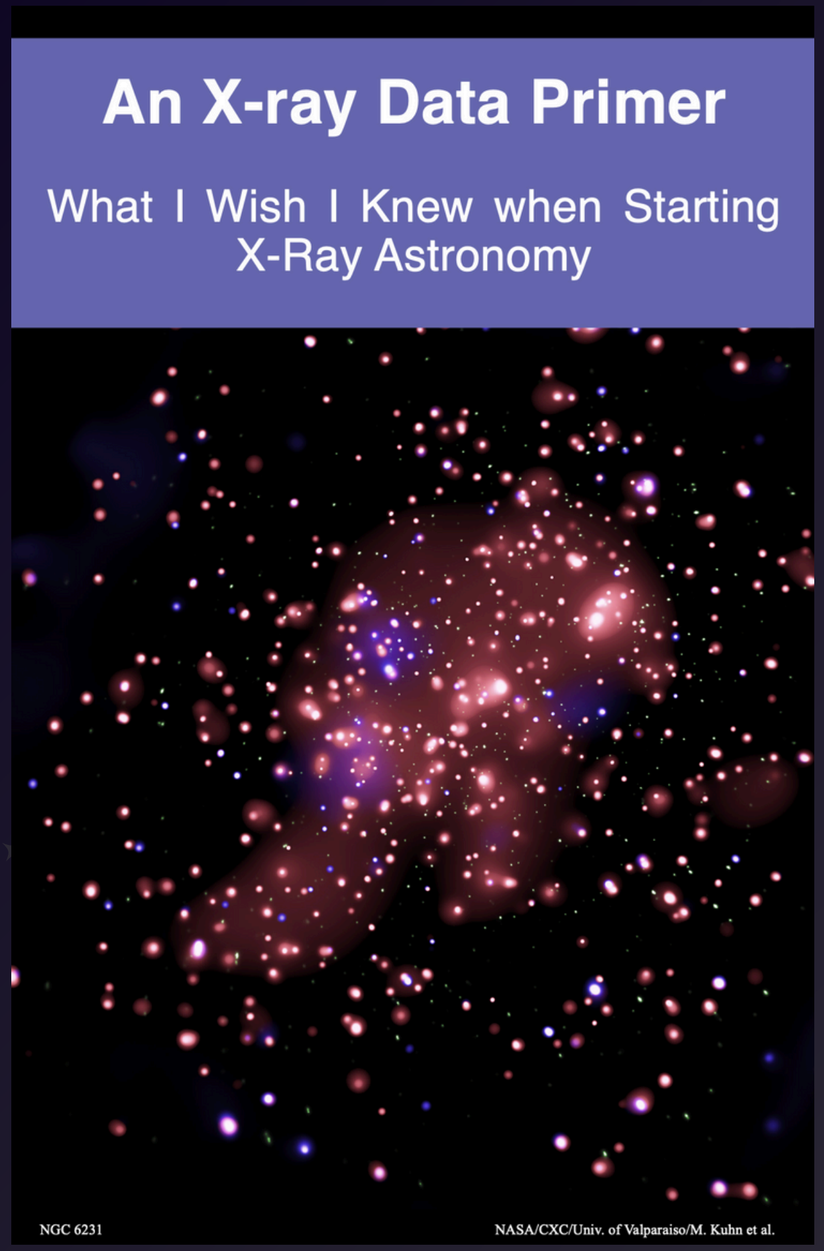

Starting X-ray Astronomy

File Type	Extension	Purpose
Source Spectrum	`.pha`	Contains X-ray spectrum (counts per energy bin)
Response Matrix	`.rmf`	Describes how the detector responds to photons of different energies
Ancillary Response	`.arf`	Accounts for telescope's sensitivity & effective area
Background Spectrum	`.pha`	Background noise spectrum to be subtracted from source data
Good Time Intervals (optional)	`.gti`	Defines observation periods unaffected by high background noise

https://cxc.harvard.edu/cdo/xray_primer.pdf

HEASOFT

HEASoft (High Energy Astrophysics Software) is a software package developed by NASA's High Energy Astrophysics Science Archive Research Center (HEASARC) for analysing data from high-energy astrophysics missions. It is widely used by astronomers to process and analyze X-ray and gamma-ray data from space telescopes like Swift, NuSTAR, Chandra, XMM-Newton, and Fermi.

Data Reduction & Analysis

Tools for processing raw data from space-based X-ray and gamma-ray observatories.

Spectral Analysis

Includes software like **XSPEC**, which is used to fit astrophysical spectra.

Xspec

Spectral analysis and model fitting

Timing Analysis

Tools for analyzing variability in X-ray and gamma-ray sources.

Xronos

Timing analysis for light curves

Image Processing

Software for creating and manipulating X-ray images.

Ximage

X-ray image processing and visualization

https://heasarc.gsfc.nasa.gov/docs/software/heasoft/

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- Originally developed in 1983 by Keith Arnaud at NASA's Goddard Space Flight Center, initially written in Fortran and later expanded with C and Python interfaces (PyXspec).

Why Use XSPEC?

- Widely Used: It is the standard tool for X-ray spectral analysis in high-energy astrophysics.
- Flexible: Allows for easy model fitting, parameter estimation, and statistical analysis.
- Extensive Model Library: Includes various built-in spectral models for emission, absorption, and more.
- Open Source & Customizable: Users can add custom models in C or Fortran.

Drawbacks

- Steep Learning Curve: The command-line interface and scripting can be complex for beginners.
- Limited GUI Features: While some graphical tools exist, much of the work requires command-line inputs.
- Installation Complexity: Installing XSPEC can be tricky, especially on certain Linux distributions or macOS.
- Heavy Dependencies: Requires multiple libraries like HEASoft, Python, and Fortran compilers.

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SETTING UP

Typhon

ssh -X
typhon.star.bris.ac.uk

HEASOFT Initialisation

```
$ export HEADAS=/opt/local/rocky8/heasoft-6.34/x86_64-pc-linux-gnu-libc2.28/
$ alias heainit=". $HEADAS/headas-init.sh"
$ heainit
```

Launch XSPEC

```
$ xspec
```

https://www.star.bris.ac.uk/local/notes/heasoft.html

COMMANDS

XSPEC is a command-driven, interactive program. You will see a prompt **XSPEC12>** whenever input is required.

DATA

Load spectral data and calibration data such as backgrounds and responses, and specify channel ranges to be fit.

> data
> backgrnd
> response
> arf
> ignore

MODEL

Define and manipulate theoretical models and their parameters, and compute additional information such as fluxes or line identifications.

> model
> untie
> newpar
> freeze
> thaw
> addcomp
> delcomp

FIT

Initiate the fitting routines, control the parameter set, perform statistical tests and compute confidence levels.

> fit
> statistic
> steppar
> error
> chain

PLOT

Generate about 50 different kinds of 2-dimensional plots.

> cpd /xw
> setplot
> plot
da / model / spectrum / residual / ratio / contour

> iplot
> hardcopy

See Chapter 5 (section 5.1) of the manual for a summary of XSPEC commands
https://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/XspecManual.pdf

DATA COMMANDS

XSPEC is a command-dri

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> data
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> response
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> ignore

To load only one spectral data

XSPEC12> data filename_src.pha	Load the spectral data (usually the source spectrum)
XSPEC12> backgrnd filename_bkg.pha	Load the background spectrum file
XSPEC12> response filename.rsp	Load the response file *.rsp or *.rmf
XSPEC12> arf filename.arf	Load the ancillary file *.arf
XSPEC12> setplot energy	Working with the energy band (default: channel)
XSPEC12> ignore bad	Ignore spectral bins flagged as bad
XSPEC12> ignore **-0.2 10.0-**	Ignore energy range below 0.2 keV and above 10 keV

The decimal annotation `.` when using ignore is needed to indicate energy, otherwise, it would be interpreted as channels if integer

$ grppha src.pha output.pha COMM="chkey backfile bkg.pha && chkey respfile file.rmf && chkey ancrfile file.arf && group min 20 && exit"

To set up multiple data groups

XSPEC12> data 1:1 file1 1:2 file2 2:3 file3

DATA GROUP # DATA SET #

See Chapter 5 (se
https://heasarc.g

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XSPEC12> data 1:1 file1 1:2 file2 2:3 file3
                    | |
DATA GROUP #    DATA SET #
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MODEL COMMANDS

XSPEC provides a wide range of spectral models to fit observed data and extract physical parameters from astronomical sources.
The main types of XSPEC models are:

Additive Models – Represent components that emit radiation (power-law, blackbody, thermal, ...)
Multiplicative Models – Modify spectra by absorbing or altering photon energies (interstellar absorption, comptonisation effect, ...)
Convolution Models – Apply mathematical transformations to spectra (doppler broadening, relativistic effect, reflection effect, ...)
Mixing Models – Used for multi-source or multi-zone systems

MODEL

Define and manipulate theoretical models and their parameters, and compute additional information such as fluxes or line identifications.

XSPEC Models

To use only one model

```
XSPEC12> model                          View models available on XSPEC
XSPEC12> model  model_name              Define the model to be used
XSPEC12> newpar  1  20.0                Changing the value of an individual parameter
                    |    |
          PARAMETER INDEX      NEW PARAMETER VALUE
                    |
XSPEC12> freeze  1                      Fixing parameter #1 at its current value
XSPEC12> thaw  1                        Allow parameter #1 to vary freely
```

To set up multiple model

```
XSPEC12> model  tbabs*jet+kerrconv(optxagnf)
```

FITTING COMMANDS

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> statistic
> steppar
> error
> chain

XSPEC Manual

Before starting the fitting process you can use the following commands to review and save your input commands

`XSPEC12> show all`

Showing all the data, models used, parameters and all fitting details. **show data** or **show param** could also be used for specific view for data or parameters only.

`XSPEC12> save all file.xcm`

Save all the previous input commands into a .xcm file

`XSPEC12> @file.xcm`

Execute the .xcm file

Some key fitting commands in XSPEC

`XSPEC12> fit`

Start the fitting in the default algorithm Levenberg-Marquardt

`XSPEC12> statistic cstat`

Chi-squared is the default fitting statistic assuming a Gaussian distribution. Cstat is used for Poisson distribution.

`XSPEC12> chain`

Using the Markov Chain Monte Carlo (see section 5.5.2 of the manual)

`XSPEC12> error 1 2`

Estimating the 90% confidence ranges for parameters #1 and #2

Calculating the confidence contour levels for parameters #1 vs #2. The default plot shows use 3 confidence levels (1σ, 2σ, 3σ)

`XSPEC12> steppar 1 0.2 1.4 50 2 50.0 750.0 50`

Parameter #1 — Minimum value — Maximum value — Number of steps — Parameter #2

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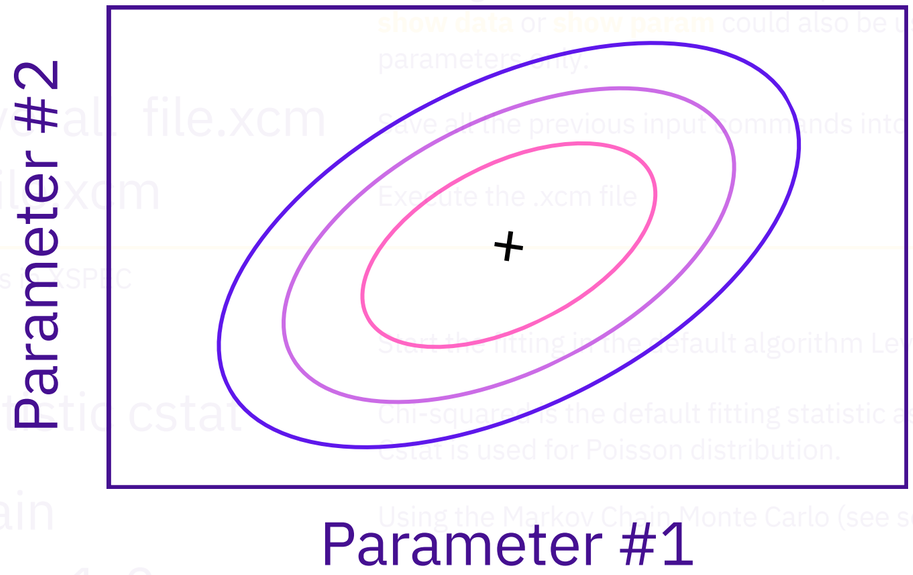

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> cpd /xw
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QDP/PLT summary

Before running any plot commands, ensure that XSPEC knows where to send the output.

XSPEC12> cpd /xw — Set plotting device to X11 window, ensuring plots appear in a pop-up window

Some key plotting commands in XSPEC

XSPEC12> plot ldata	Displays the observed spectrum with error bars, using logarithmic scales
XSPEC12> plot eeufspec	Shows the unfolded energy spectrum (energy × flux), useful for seeing the intrinsic spectral shape
XSPEC12> plot model	Plots the best-fit model without the observed data, displaying the theoretical prediction
XSPEC12> plot ratio	Plots the data-to-model ratio, helping visualize where the fit deviates from the data
XSPEC12> plot contour	Visualizes confidence regions for two free parameters in a model

XSPEC12> iplot	Modifying the default plots
PLT> label title My Plot	Editing the plot title
PLT> hardcopy myplot.eps/cps	Save the plot as a color PostScript file
PLT> wenv myplot	Generate numerical data (.qdp) and plot setting (.pco) files
PLT> @myplot.pco	Upload the saved plot settings

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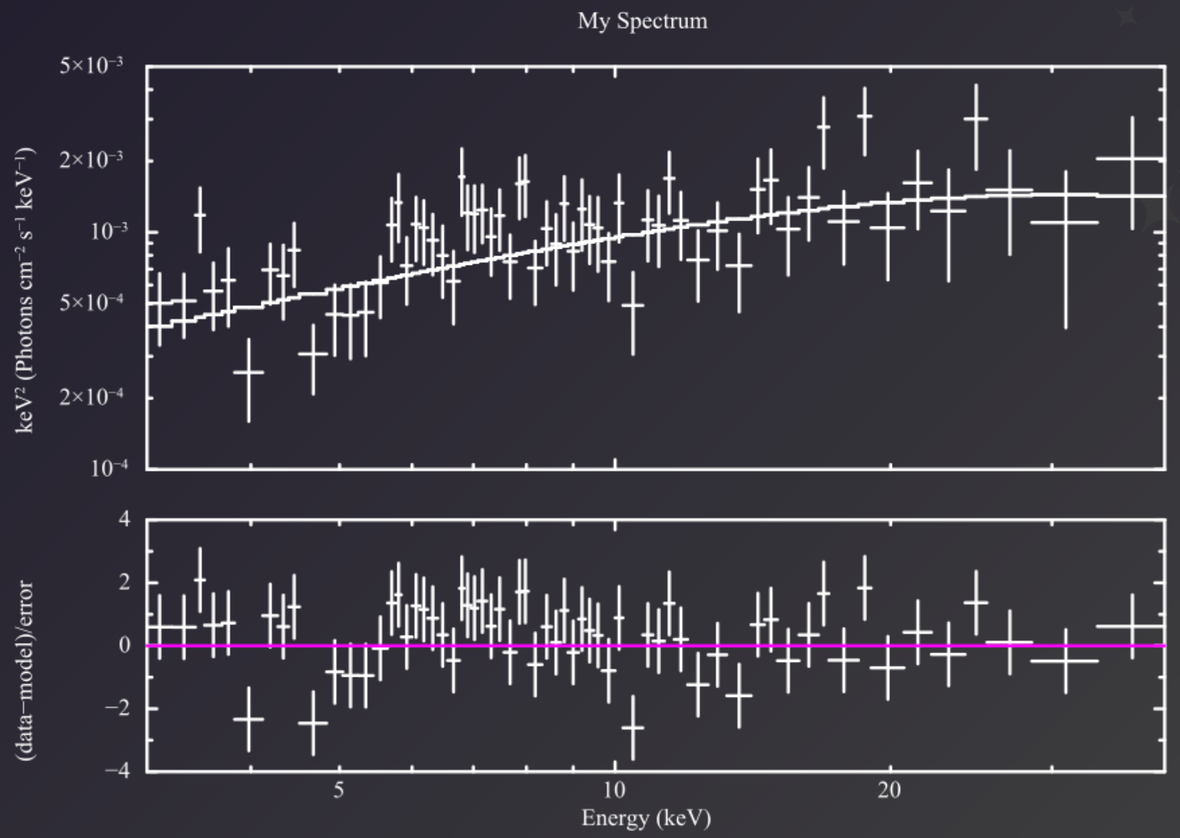
DEMOS #1

QDP/PLT Details

```
# Regrouping and binning
$ grppha source.pha data_group.pha COMM="chkey backfile background.pha &&
 chkey respfile redistribution.rmf && chkey ancrfile ancillary.arf && group min 10 && exit"
```

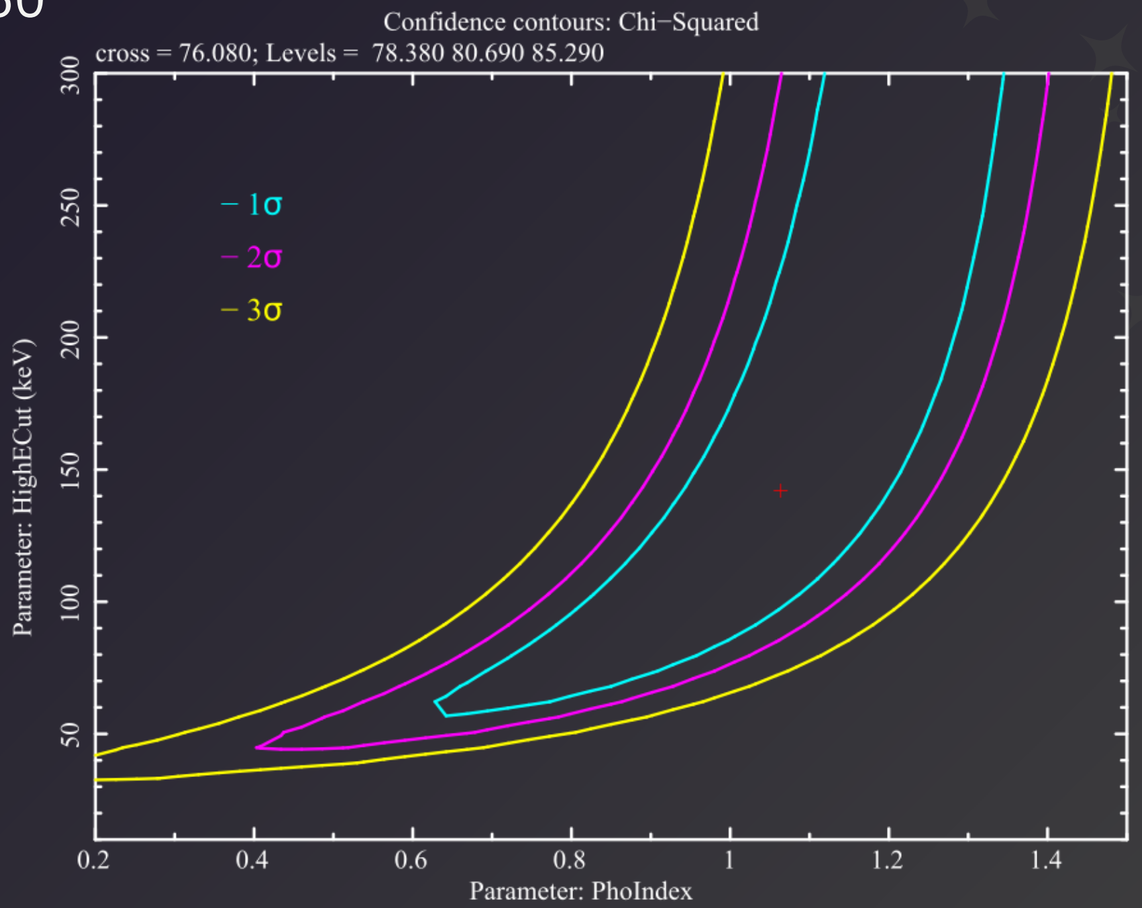
```
# Simple fitting
XSPEC12> cpd /xw
XSPEC12> data data_group.pha
XSPEC12> setplot energy
XSPEC12> ignore bad
XSPEC12> ignore **-3.0 40.0-**
XSPEC12> model zcutoffpl
XSPEC12> newpar 3 3.29
XSPEC12> show all
XSPEC12> fit
XSPEC12> plot eeufs delchi
XSPEC12> iplot
PLT> label title My Spectrum
PLT> font roman
PLT> lw 5
```

```
PLT> lw 5 on 1..3
PLT> win 1
PLT> rescale Y 1e-4 5e-3
PLT> vp 0.15 0.5 0.9 0.9
PLT> win 2
PLT> rescale Y -4 4
PLT> vp 0.15 0.2 0.9 0.45
```



DEMOS #2

```
# Contour Plot
XSPEC12> steppar 1 0.2 1.5 50 2 10.0 300.0 50
XSPEC12> plot contour
XSPEC12> iplot
PLT> image off
PLT> time off
PLT> font Roman
PLT> lw 5
PLT> contour lw 5, 5, 5, 5
PLT> la 2 pos 0.4 250 col 2 cs 1.2 "- 1\gs"
PLT> la 3 pos 0.4 230 col 3 cs 1.2 "- 2\gs"
PLT> la 4 pos 0.4 210 col 4 cs 1.2 "- 3\gs"
PLT> hardcopy my-plot.eps/cps
PLT> wenv my-plot
PLT> @my-plot.pco
```

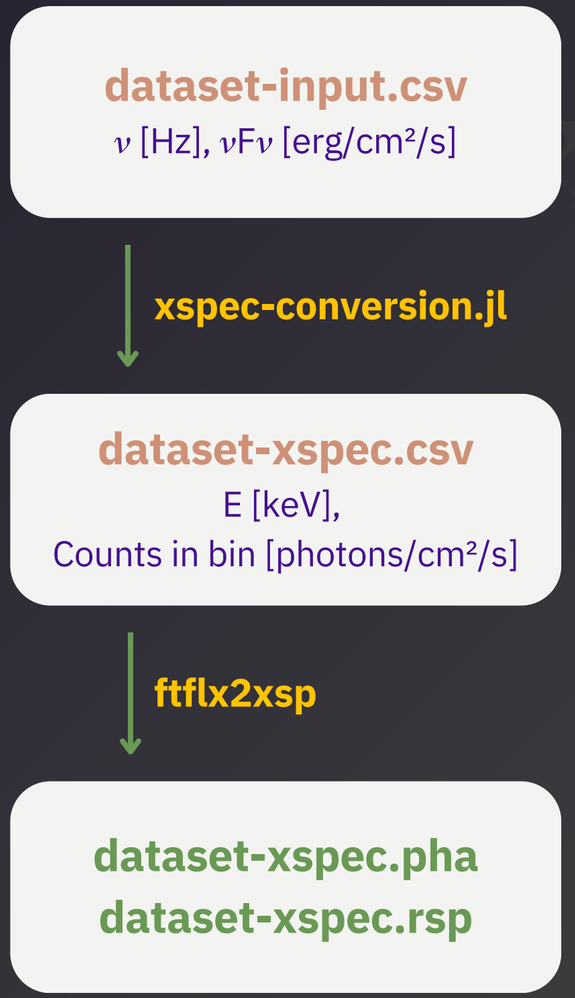


Multiwavelength data fitting with XSPEC

```
# This Julia script creates a binned dataset that is more compatible with XSPEC
using CSV
using DataFrames

file = CSV.File(@__DIR__() * "/../data/dataset-input.csv"; comment="#")
E = 4.14E-18 * file.nu[1:25]
E_low = 4.14E-18 * file.nu[1:25] .* 0.95
E_high = 4.14E-18 * file.nu[1:25] .* 1.05
ΔE = E_high .- E_low
νF_ν = file.nuFnu[1:25]
F_ν = νF_ν ./ file.nu[1:25]
f_E = 1.51E26 .* F_ν ./ E
int_f_E = ΔE .* f_E
int_f_E_err = 0.1 * int_f_E
df = DataFrame(E_low=E_low, E_high=E_high, flux=int_f_E, flux_err=int_f_E_err)
CSV.write(@__DIR__() * "/../data/dataset-xspec.csv", df; delim=' ', writeheader=false)

println("Now you need to run the following in the data directory with HEASOFT initialised")
println("  ftflx2xsp dataset-xspec.csv dataset-xspec.pha dataset-xspec.rsp")
println("The output will use default units of keV and photons/cm^2/s")
```



ALTERNATIVES TOOLS

Tool	Developed by	Website	Key Features	Best for
Sherpa	Chandra X-ray Center (CXC)	https://cxc.cfa.harvard.edu/sherpa/	Python-based, supports scripting and automation, Bayesian methods, integrates with CIAO	Users familiar with Python who prefer a flexible, programmable interface
ISIS	MIT	https://space.mit.edu/asc/isis/	Command-line driven, scriptable in S-Lang and Python, optimized for high-resolution spectroscopy, supports XSPEC models	Researchers working with high-resolution X-ray data (e.g., Chandra, XMM-Newton)
SPEX	SRON Netherlands Institute for Space Research	https://www.sron.nl/astrophysics-spex/	Specialized in plasma modeling, more accurate atomic models than XSPEC, advanced ionization balance calculations	Researchers analyzing thermal plasmas in clusters of galaxies, AGNs, and supernova remnants
PyXspec	NASA (as part of XSPEC)	https://heasarc.gsfc.nasa.gov/xanadu/xspec/python/html/	Python interface for XSPEC, offers the same functionality as XSPEC but in Python, more user-friendly than XSPEC's CLI	Users who prefer Python scripting but still want access to XSPEC's extensive model library
xspec_emcee & 3ML	Multi-mission astrophysics community	https://threeml.readthedocs.io/	Integrates XSPEC models with Bayesian inference (MCMC methods), supports multi-wavelength analysis, modern and flexible with Python	Users interested in Bayesian methods and multi-mission data analysis

SpectralFitting.jl vs XSPEC

Feature	SpectralFitting.jl	XSPEC
Language	Julia	C, Fortran (with Python interface)
Performance	Faster (optimized for numerical computing)	Slower, but efficient for complex models
Ease of Use	Modern syntax, easier to write and maintain	Command-line interface, steeper learning curve
Built-in Models	Limited (still developing)	Extensive library of spectral models
Extensibility	Custom models can be easily added in Julia	Custom models in C/Fortran
Statistical Methods	Julia's powerful fitting libraries (e.g., Optim.jl, Turing.jl for Bayesian fitting)	Built-in fitting methods (C-stat, χ^2, MCMC, etc.)
Interoperability	Can work with Julia ecosystem (DataFrames.jl, Plots.jl, etc.)	Integrates with HEASoft, PyXspec for Python users
GUI Support	None (command-line & scripting)	Limited, mostly command-line
Community & Support	Smaller, developing	Large, widely used in astrophysics
Installation	Easier (Julia package manager)	More complex (requires HEASoft & dependencies)

https://github.com/fjebaker/SpectralFitting.jl

AGENDA

WINS

A quick round of celebrating successes and progress from the past week.

ISSUES

Addressing roadblocks, challenges, and lessons learned to improve our workflow.

XSPEC

A deep dive into what XSPEC is, its functionalities, and how to effectively use it.

AOB

Wrapping up with any final thoughts, questions, or spontaneous discussions.

AGENDA

WINS

A quick round of celebrating successes and progress from the past week.

AOB

Wrapping up with any final thoughts, questions, or spontaneous discussions.