An X-Ray Spectral Fitting Package

User's Guide for version 12.5.1

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Updates to the manual

July 2009 (v12.5.1 release)

- Gain command has new source:spectrum syntax. Gain parameters can now use newpar, freeze, thaw, untie, and error commands by prefixing the command name with the letter 'r'.
- New Xspec.init numerical differentiation option mentioned in Overview and Spectral Fitting sections, and the fit and method commands.
- Improved the description of the critical delta and tolerance parameters in the fit, method, and error commands.
- Steppar now prompting for case of new minimum found, and can now operate on gain parameters.
- Setplot wave x-axis units option, set from Xspec.init file.
- Appendix F updated with new version string function.
- Added the delta option to the xset page.
- Added an example of a tclout error string.
- New udmget option for initpackage.
- New tclout sigma and tclout steppar delstat options.
- The goodness command now states that the default is nosim.
- Added par9 to kerrdisk and removed par4 from disk model.
- Moved previous release notes into new appendix I.

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- Additional section added to appendix F.
- New tclout gain option.
- Updates to nsmax and simpl model descriptions.

Nov 2008 (v12.5.0 release)

- New model files for cflux, diskir, kerrconv, kerrdisk, nsmax, nthcomp, partcov, recorn, simpl, swind1, spexpcut, and zxipcf. Removed model files for rgsxsrc and bvapec (merged into bapec).
- Added mdefine command to "Model Commands" section.
- Added new section "Tcl Scripts" to "XSPEC Commands".
- Cleaned up and reorganized Appendix C "Adding models to XSPEC"
- Moved description of changes between v11 and v12 out of the introduction and into new Appendix H.

- Table added to xset command description for cross-referencing models with the variables they set in xset's <string name> database.
- Tclout command: goodness option added.
- Response command: added "{n}" syntax description.
- Model command description: fewer constraints in "Syntax Rules" and new use of unnamed models with active/inactive option.
- Chain command: run option has high-chatter output.
- In Appendix F, XSFunctions now has dependence on XSModel.
- In Appendix G, new function in RandomizerBase class.
- Slight modifications to descriptions in model files apec, c6mekl, compbb, equil, gnei, meka, mekal, nei, npshock, pshock, raymond, sedov, and zhighect, and command descriptions for addline, flux, modid, and plot.

1. XSPEC

XSPEC is a command-driven, interactive, X-ray spectral-fitting program, designed to be completely detector-independent so that it can be used for any spectrometer. XSPEC has been used to analyze data from HEAO-1 A2, *Einstein Observatory,* EXOSAT, Ginga, ROSAT, BBXRT, ASCA, CGRO, IUE, RXTE, Chandra, XMM-Newton, Integral/SPI, Swift and Suzaku. There now over 1000 papers listed on ADS which cite the Arnaud 1996 XSPEC reference.

This manual describes XSPEC v12.5, which is available on Linux (gcc 3.2.2 and later), MacOSX/Darwin (gcc 3.3 and later) , Solaris (2.6-9; WS6.0 and later). New users are advised to read **Chapter 2**, which introduces spectral fitting and the XSPEC approach, **Chapter 3**, which gives an overview of the program commands, and **Chapter 4**, which contains walkthroughs of XSPEC sessions. They should then experiment with XSPEC and, if necessary, look up individual commands in **Chapter 5**, or descriptions of the spectral models in use, in **Chapter 6**.

The User Interface for XSPEC, which employs a **tcl** scripting shell and the XSPEC parser are described in **Appendix A**. Users possessing X-ray spectra with small numbers of counts per bin are referred to **Appendix B**, which describes the C-statistic option. Users interested in adding their own models can read how to do so in **Appendix C**. **Appendix D** describes the **PLT** plotting package which XSPEC currently uses for graphical output. Some of the tools (FTOOLS, fortran programs, scripts) that can operate on XSPEC files are listed in **Appendix E**. The XSPEC model library can be linked into other programs following the instructions in **Appendix F**. **Appendix G** describes how to use your own proposal distribution for Markov Chain Monte Carlo. Finally, **Appendix H** includes some notes on the changes between XSPEC v11 and v12.

1.1 New in v12.5.1

- Gain parameters can now be used in the error, freeze, newpar, thaw, and untie commands by prefixing the command name with the letter ‘r’ (for “response parameter”, the more general category to which gain parameters belong). Steppar can now also handle gain parameters. Gain parameters can be displayed either with “show parameter” or the new “show rparameter” option.
- The gain command syntax has changed when using multiple sources. To better conform with the rest of XSPEC, it now requires <source number>:<spectrum number> rather than the reverse.
- Gain parameter limit values can be stored in response files, using the keywords GSLOP_MIN, GSLOP_MAX, GOFFS_MIN, and GOFFS_MAX.
- All input and output data filenames can now include CFITSIO/FTOOLS extended-syntax for specifying particular HDUs. As a result, XSPEC can now handle files which contain both ARFs and RMFs in multiple extensions.
- Partial derivative calculations during fitting can now be performed numerically rather than with an approximated analytical expression. This option is chosen in the Xspec.init initialization file.

- If a new minimum is found during a steppar run, steppar now prompts the user for acceptance of the new values. Also the delta statistic column of a stepar run is now obtainable with the tclout steppar delstat option.
- The output warning message has been improved in the case where Levenberg-Marquardt fitting runs into a zero diagonal element in the second derivative matrix. Similarly, the more frequent pegged-parameter messages (due to running into hard limits) is now output at higher chatter levels only.
- All calls to the xanlib dynamic memory allocation function udmget have been removed from the Fortran models in XSPEC's models library. The relevant code has been converted to C++. If a user's local models library still requires the udmget code, they'll need to run initpackage with the new -udmget option.
- Additional enhancements previously released as patches to 12.5.0:
  - Steplot wave x-axis units can be toggled from Hz to angstroms through WAVE_PLOT_UNITS entry in Xspec.init file.
  - New tclout gain and sigma options.
  - New xs_getVersion function available for those linking their own programs to the XSPEC models library.
  - The show parameters option can now take a range of parameters for displaying subsets.
- All bug fixes to v12.5.0 released as patches a - an are included in v12.5.1. In addition the following problems have been corrected.
  - After running the ARF command, any gain previously applied to the associated RMF will be removed. Previously it was erroneously applying the gain to the new ARF.
  - Additional header file inclusions needed in code files to compile with g++-4.4.0
  - Extra line-feed characters removed from Ascii text files in the modelData directory. These were causing problems on Solaris 10 w/f90.
  - The nthcomp model's internal arrays were hardcoded to a maximum size of 5000 energy bins. The size is now dynamically allocated. (This also affects the diskir model.)
  - A Levenberg-Marquardt fit now immediately stops if the fit statistic becomes NaN due to an erroneous model calculation.
  - C++-style comments have been removed from xsFortran.h for the benefit of users compiling their own C programs with the models library.
  - Plotting fix for case where "setplot area" is selected and no models are currently loaded.
  - Model parsing fix for case of nested parentheses with no '+' operator, ie. A(B(C*D)).

1.2 How to find out more information

XSPEC is distributed and maintained under the aegis of the GSFC High Energy Astrophysics Science Archival Research Center (HEASARC). It can be downloaded as part of HEAsoft

http://heasarc.gsfc.nasa.gov/docs/software/lheasoft/download.html

XSPEC is available either as binaries or source. We recommend downloading the source and compiling locally to avoid potential system library conflicts and allow installation of any patches we release. If you have any problems compiling or running XSPEC please e-mail us at

xanprob@athena.gsfc.nasa.gov

The XSPEC Web page comprises links to the anonymous ftp site, a Web version of the manual, and several useful documents, including a list of known bugs. The Web address is

http://xspec.gsfc.nasa.gov/

with the list of issues and available patches at

http://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/bugs.html

and additional models which can be added at

http://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/newmodels.html

Further useful information can be found on the XSPEC Wiki at

https://astrophysics.gsfc.nasa.gov/XSPECwiki/XSPECPage

and the xspector blog at

http://xspector.blogspot.com/

1.3 History

The first version of XSPEC was written in 1983 at the Institute of Astronomy, Cambridge, under VAX/VMS by Rick Shafer. It was written to perform spectral analysis of data from the ESA EXOSAT X-ray observatory, which was launched that year. XSPEC is a descendant of a series of spectral-fitting programs written at NASA/Goddard Space Flight Center for the OSO-8, HEAO-1 and EO missions. The initial design was the fruit of many discussions between Rick Shafer and Andy Szymkowiak. Rick Shafer subsequently joined the EXOSAT group, where he enhanced the VAX/VMS version in collaboration with Frank Haberl. Meanwhile, Keith Arnaud ported XSPEC to a Sun/UNIX operating system. The two implementations of XSPEC diverged for several years until a determined and coordinated effort was made to recover a single version. The results of that effort was XSPECv6, described in the first edition of this manual. Subsequent editions have covered later versions of the program. In recent years XSPEC has become the *de facto* standard for X-ray spectroscopic analysis for the ROSAT mission and the *de jure* standard for the BBXRT, ASCA, and RXTE missions. It is now in extensive use for all current X-ray and gamma-ray missions. An extensive re-engineering effort was started in the fall of 1998 to improve long-term maintainability,

allow significant new features to be added, and support the analysis of spectra from coded-mask instruments.

1.4 Acknowledgements

This project would not have been possible without ignoring the advice of far more people than can be mentioned here. We would like to thank all our colleagues for their suggestions, bug reports, and (especially) source code. The GSFC X-ray astronomy group are particularly thanked for their patience exhibited while functioning as the beta test site for new releases. The initial development of XSPEC was funded by a Royal Society grant to Prof. Andy Fabian and subsequent development was partially funded by the European Space Agency's EXOSAT project and is now funded by the HEASARC at NASA/GSFC.

1.5 References

Arnaud, K.A., 1996, Astronomical Data Analysis Software and Systems V, eds. G. Jacoby and J. Barnes,p17, ASP Conf. Series volume 101.

Dorman, B., and Arnaud, K. A. 2001, Astronomical Data Analysis Software and Systems X eds. F.R. Harnden, Jr., F.A. Primini, and H. E. Payne, vol. 238, p. 415

Dorman, B., Arnaud, K. A., and Gordon, C. A. XSPEC12: Object-Oriented X-Ray Data Analysis, AAS HEAD meeting No. 35, #22.10

2. Spectral Fitting and XSPEC

2.1 Introduction

This chapter comprises a brief description of the basics of spectral fitting, their application in XSPEC, and some helpful hints on how to approach particular problems. We then provide more details on the way XSPEC provides flexibility in its approach to the minimization problem. We also describe the data formats accepted.

2.2 The Basics of Spectral Fitting

Although we use a spectrometer to measure the spectrum of a source, what the spectrometer obtains is not the actual spectrum, but rather photon counts (C) within specific instrument channels, (I). This observed spectrum is related to the actual spectrum of the source (f(E)) by:

$$C(I) = \int_0^\infty f(E) R(I,E) dE$$

Where R(I,E) is the instrumental response and is proportional to the probability that an incoming photon of energy E will be detected in channel I. Ideally, then, we would like to determine the actual spectrum of a source, f(E), by inverting this equation, thus deriving f(E) for a given set of C(I). Regrettably, this is not possible in general, as such inversions tend to be non-unique and unstable to small changes in C(I). (For examples of attempts to circumvent these problems see Blissett & Cruise 1979; Kahn & Blissett 1980; Loredo & Epstein 1989).

The usual alternative is to choose a model spectrum, f(E), that can be described in terms of a few parameters (i.e., f(E,p1,p2,...)), and match, or "fit" it to the data obtained by the spectrometer. For each f(E), a predicted count spectrum (C_p(I)) is calculated and compared to the observed data (C(I)). Then a "fit statistic'" is computed from the comparison and used to judge whether the model spectrum "fits" the data obtained by the spectrometer.

The model parameters then are varied to find the parameter values that give the most desirable fit statistic. These values are referred to as the *best-fit parameters*. The model spectrum, f_b(E), made up of the best-fit parameters is considered to be the *best-fit model*.

The most common fit statistic in use for determining the "best-fit" model is χ^2, defined as follows:

$$\chi^2 = \sum (C(I) - C_p(I))^2 / (\sigma(I))^2$$

where σ(I) is the (generally unknown) error for channel I (e.g., if C(I) are counts then σ(I) is usually estimated by $\sqrt{C(I)}$; see e.g. Wheaton et.al. 1995 for other possibilities).

Once a "best-fit" model is obtained, one must ask two questions:

1. How confident can one be that the observed C(I) can have been produced by the best-fit model f_b(E)? The answer to this question is known as the "goodness-of-fit"

of the model. The χ^2 statistic provides a well-known-goodness-of-fit criterion for a given number of degrees of freedom (ν, which is calculated as the number of channels minus the number of model parameters) and for a given confidence level. If χ^2 exceeds a critical value (tabulated in many statistics texts) one can conclude that f_b(E) is *not* an adequate model for C(I). As a general rule, one wants the "reduced χ^2" (χ^2/ν) to be approximately equal to one $(\chi^2 \sim \nu)$. A reduced χ^2 that is much greater than one indicates a poor fit, while a reduced χ^2 that is much less than one indicates that the errors on the data have been over-estimated. Even if the best-fit model (f_b(E)) *does* pass the "goodness-of-fit" test, one still cannot say that f_b(E) is the *only* acceptable model. For example, if the data used in the fit are not particularly good, one may be able to find many different models for which adequate fits can be found. In such a case, the choice of the correct model to fit is a matter of scientific judgment.

2. For a given best-fit parameter (p1), what is the range of values within which one can be confident the true value of the parameter lies? The answer to this question is the "confidence interval" for the parameter.

   The confidence interval for a given parameter is computed by varying the parameter value until the χ^2 increases by a particular amount above the minimum, or "best-fit" value. The amount that the χ^2 is allowed to increase (also referred to as the critical $\Delta\chi^2$) depends on the confidence level one requires, and on the number of parameters whose confidence space is being calculated. The critical $\Delta\chi^2$ for common cases are given in the following table (from Avni, 1976):

Confidence	Parameters		
	1	2	3
0.68	1.00	2.30	3.50
0.90	2.71	4.61	6.25
0.99	6.63	9.21	11.30

2.3 The XSPEC implementation

To summarize the preceding section, the main components of spectral fitting are as follows:

- A set of one or more observed spectra $\boldsymbol{D}(I)$ with background measurements B(I) where available
- The corresponding instrumental responses $\boldsymbol{R}(I,E)$
- A set of model spectra $\boldsymbol{M}(E)$

- These components are used in the following manner:
- Choose a parameterized model which is thought to represent the actual spectrum of the source.
- Choose values for the model parameters.
- Based on the parameter values given, predict the count spectrum that would be detected by the spectrometer in a given channel for such a model.
- Compare the predicted spectrum to the spectrum actually obtained by the instrument.
- Manipulate the values of the parameters of the model until the best fit between the theoretical model and the observed data is found.

Then calculate the "goodness" of the fit to determine how well the model explains the observed data, and calculate the confidence intervals for the model's parameters.

This section describes how XSPEC performs these tasks.

C(I): The Observed Spectrum

To obtain each observed spectrum, $C(I)$, XSPEC uses two files: the data (spectrum) file, containing *D*(I), and the background file, containing *B*(I). The data file tells XSPEC how many total photon counts were detected by the instrument in a given channel. XSPEC then uses the background file to derive the set of background-subtracted spectra *C*(I) in units of counts per second. The background-subtracted count rate is given by, for each spectrum:

$$C(I) = \frac{D(I)}{a_{D(I)} t_D} - \frac{b_{D(I)}}{b_{B(I)}} \frac{B(I)}{a_{B(I)} t_B}$$

where $D(I)$ and $B(I)$ are the counts in the data and background files; t_D and t_B are the exposure times in the data and background files; $b_{D(I)}$ and $b_{B(I)}$, $a_{D(I)}$ and $a_{B(I)}$ are the background and area scaling values from the spectrum and background respectively, which together refer the background flux to the same area as the observation as necessary. When this is done, XSPEC has an observed spectrum to which the model spectrum can be fit.

R(I,E): The Instrumental Response

Before XSPEC can take a set of parameter values and predict the spectrum that would be detected by a given instrument, XSPEC must know the specific characteristics of the instrument. This information is known as the detector response. Recall that for each spectrum the response $R(I,E)$ is proportional to the probability that an incoming photon of energy E will be detected in channel I. As such, the response is a continuous function of E. This continuous function is converted to a discrete function by the creator of a response matrix who defines the energy ranges E_J such that:

$$R_D(I,J) = \frac{\int_{E_{J-1}}^{E_J} R(I,E)dE}{E_J - E_{J-1}}$$

XSPEC reads both the energy ranges, E_J, and the response matrix $R_D(I,J)$ from a response file in a compressed format that only stores non-zero elements. XSPEC also includes an option to use an auxiliary response file, which contains an array $A_D(J)$ that is multiplied into $R_D(I,J)$ as follows:

$$R_D(I,J) \rightarrow R_D(I,J) \circ A_D(J)$$

This array is designed to represent the efficiency of the detector with the response file representing a normalized Redistribution Matrix Function, or RMF. Conventionally, the response is in units of cm^2.

M(E): The Model Spectrum

The model spectrum, $M(E)$, is calculated within XSPEC using the energy ranges defined by the response file :

$$M_D(J) = \int_{E_{J-1}}^{E_J} M(E)dE$$

and is in units of photons $cm^{-2}s^{-1}$. XSPEC allows the construction of composite models consisting of additive components representing X-ray sources (e.g., power-laws, blackbodys, and so forth), multiplicative components, which modify additive components by an energy-dependent factor (e.g., photoelectric absorption, edges, ...). Convolution and mixing models can then perform sophisticated operations on the result. Models are defined in algebraic notation.

For example, the following expression:

phabs (power + phabs (bbody))

defines an absorbed blackbody, phabs(bbody), added to a power-law, power. The result then is modified by another absorption component, phabs. For a list of available models, see **Chapter 6**.

Fits and Confidence Intervals

Once data have been read in and a model defined, XSPEC uses a fitting algorithm to find the best-fit values of the model parameter. The default is a modified Levenberg-Marquardt algorithm (based on CURFIT from Bevington, 1969). The algorithm used is local rather than global, so be aware that it is possible for the fitting process to get stuck in a local minimum and not find the global best-fit. The process also goes much faster (and is more likely to find the true minimum) if the initial model parameters are set to sensible values.

The Levenberg-Marquardt algorithm relies on XSPEC calculating the 2^{nd} derivatives of the fit statistic with respect to the model parameters. By default these are calculated analytically, with the assumption that the 2^{nd} derivatives of the model itself

may be ignored. This can be changed by setting the USE_NUMERICAL_DIFFERENTIATION flag to "true" in the Xspec.init initialization file, in which case XSPEC will perform numerical calculations of the derivatives (which are slower).

At the end of a fit, XSPEC will write out the best-fit parameter values, along with estimated confidence intervals. These confidence intervals are one sigma and are calculated from the second derivatives of the fit statistic with respect to the model parameters at the best-fit. These confidence intervals are not reliable and should be used for indicative purposes only.

XSPEC has a separate command (**error** or **uncertain**) to derive confidence intervals for one interesting parameter, which it does by fixing the parameter of interest at a particular value and fitting for all the other parameters. New values of the parameter of interest are chosen until the appropriate delta-statistic value is obtained. XSPEC uses a bracketing algorithm followed by an iterative cubic interpolation to find the parameter value at each end of the confidence interval.

To compute confidence regions for several parameters at a time, XSPEC can run a grid on these parameters. XSPEC also will display a contour plot of the confidence regions of any two parameters.

2.4 A more abstract and generalized approach

The sections above provide a simple characterization of the problem. XSPEC actually operates at a more abstract level and considers the following:

Given a set of spectra $\boldsymbol{C}(\mathrm{I})$*, each supplied as a function of detector channels, a set of theoretical models* $\{\boldsymbol{M}(\mathrm{E})_j\}$ *each expressed in terms of a vector of energies together with a set of functions* $\{\boldsymbol{R}(\mathrm{I,E})_j\}$ *that map channels to energies, minimize an objective function S of* $\boldsymbol{C}$*,* $\{\boldsymbol{R}(\mathrm{I,E})_i\}$*,* $\{\boldsymbol{M}(\mathrm{E})_j\}$ *using a fitting algorithm, i.e.*

$$\boldsymbol{S} = \boldsymbol{S}\left(\boldsymbol{C}, \sum_k \boldsymbol{M}_j^k \circ \boldsymbol{R}_j^k\right)$$

In the default case, this reduces to the specific expression for χ^2 fitting of a single source

$$\boldsymbol{S} = \chi^2 = \sum_i (\boldsymbol{C}_i - \boldsymbol{R}_i \circ \boldsymbol{M}_i)^2$$

where i runs over all of the channels in all of the spectra being fitted, and using the Levenberg-Marquadt algorithm to perform the fitting.

This differs from the previous formulation in that the operations that control the fitting process make fewer assumptions about how the data are formatted, what function is being minimized, and which algorithm is being employed. At the calculation level, XSPEC requires spectra, backgrounds, responses and models, but places fewer constraints as to how they are represented on disk and how they are combined to compute

the objective function (statistic). This has immediate implications for the extension of XSPEC analysis to future missions.

New data formats can be implemented independently of the existing code, so that they may be loaded during program execution. The 'data format' includes the specification not only of the files on disk but how they combine with models.

Multiple sources may be extracted from a spectrum. For example, it generalizes the fitting problem to minimizing, in the case of the χ^2 statistic,

$$\chi^2 = \sum_i \left(C_i - \sum_j \boldsymbol{R}_{ij} \circ \boldsymbol{M}_j \right)^2$$

and *j* runs over one or more models. This allows the analysis of coded aperture data where multiple sources may be spatially resolved.

Responses, which abstractly represent a mapping from the theoretical energy space of the model to the detector channel space, may be represented in new ways. For example, the INTEGRAL/SPI responses are implemented as a linear superposition of 3 (fixed) components.

Instead of explicitly combining responses and models through convolution XSPEC places no prior constraint on how this combination is implemented. For example, analysis of data collected by future large detectors might take advantage of the form of the instrumental response by decomposing the response into components of different frequency.

Other differences of approach are in the selection of the statistic of the techniques used for deriving the solution. Statistics and fitting methods may be added to XSPEC at execution time rather than at installation time, so that the analysis package as a whole may more easily keep apace of new techniques.

2.5 XSPEC Data Analysis

XSPEC is designed to support multiple input data formats. Support for the earlier SF and Einstein FITS formats are removed. Support for ASCII data is planned, which will allow XSPEC to analyze spectra from other wavelength regions (optical, radio) transparently to the user.

2.5.1 OGIP Data

The OGIP data format both for single spectrum files (Type I) and multiple spectrum files (Type II) is fully supported. These files can be created and manipulated with programs described in **Appendix E** and the provided links. The programs are described more fully in **George et al. 1992**. (the directories below refer to the **HEAsoft** distribution).

- Spectral Data: **callib/src/gen**/rdpha2.f, wtpha3.f
- Responses: **callib/src/gen** rdebd4.f, rdrmf5.f, wtebd4.f, wtrmf5.f. The "rmf" programs read and write the RMF extension, while the "ebd" programs write an extension called EBOUNDS that contains nominal energies for the detector channels.

- Auxiliary Responses: **callib/src/gen** rdarf1.f, and wtarf1.f

2.5.2 INTEGRAL/SPI Data

XSPEC also includes an add-in module to read and simulate INTEGRAL/SPI data, which can be loaded by the user on demand. The INTEGRAL/SPI datasets are similar to OGIP Type II, but contain an additional FITS extension that stores information on the multiple files used to construct the responses.

The **INTEGRAL** Spectrometer (**SPI**) is a coded-mask telescope, with a 19-element Germanium detector array. The Spectral resolution is ~500, and the angular resolution is ~3°. Unlike focusing instruments however, the detected photons are not directionally tagged, and a statistical analysis procedure, using for example cross-correlation techniques, must be employed to reconstruct an image. The description of the XSPEC analysis approach[1] which follows assumes that an image reconstruction has already been performed; see the SPIROS utility within the INTEGRAL offline software analysis package (**OSA**), OR, the positions on the sky of all sources to be analyzed are already known (which is often the case). Those unfamiliar with INTEGRAL data analysis should refer to the **OSA documentation**. Thus, the INTEGRAL/SPI analysis chain must be run up to the event binning level [if the field of view (FoV) source content is known, e.g. from published catalogs, or from IBIS image analysis], or the image reconstruction level. SPIHIST should be run selecting the "PHA" output option, and selecting detectors 0-18. This will produce an OGIP standard **type-II PHA spectral file**, which contains multiple, detector count spectra. In addition, the SPIARF procedure should be run once for each source to be analyzed, plus one additional time to produce a special response for analysis of the instrumental background. If this is done correctly, and in the proper sequence, SPIARF will create a table in the PHA-II spectral file, which will associate each spectrum with the appropriate set of response matrices. The response matrices are then automatically loaded into XSPEC upon execution of the **data** command in a manner very transparent to the user. You will also need to run SPIRMF (unless you have opted to use the default energy bins of the template SPI RMFs). Finally, you will need to run the FTOOL SPIBKG_INIT. Each of these utilities - SPIHIST, SPIARF, SPIRMF and SPIBKG_INIT - are documented elsewhere, either in the INTEGRAL or (for SPIBKG_INIT the HEAsoft) software documentation.

There are several complications regarding the spectral de-convolution of coded-aperture data. One already mentioned is the source confusion issue; there may be multiple sources in the FoV, which are lead to different degrees of shadowing on different detectors. Thus, a separate instrumental response must be applied to a spectral model for each possible source, for each detector. This is further compounded by the fact that INTEGRAL's typical mode of observation is “dithering.” A single observation may

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[1] This is one of several possible analysis paths. The most commonly used method involves the SPIROS utility in spectral extraction mode, which leads to a effective-area corrected, background subtracted "pseudo-count" spectra. A (single) customized XSPEC RMF is then applied to approximate the photon-to-count redistribution for model fitting.

consist of ~10's of individual exposures at raster points separated by ~2°. This further enumerates the number of individual response matrices required for the analysis. If there are multiple sources in the FoV, then additional spectral models can be applied to an additional set of response matrices, enumerated as before over detector and dither pointing. This capability - to model more than one source at a time in a given Chi-Square (or alternative) minimization procedure - did not exist in previous versions of XSPEC. For an observation with the INTEGRAL/SPI instrument, where the apparent detector efficiency is sensitive to the position of the source on the sky relative to the axis of the instrument, the χ^2 statistic is:

$$\chi^2 = \sum_p \sum_d \sum_I \left\{ \frac{\left[D_{d,p}(I) - \sum_j \sum_E R^j_{d,p}(I,E) \circ M_j\left(E;\mathbf{x}_s\right) - B_{d,p}(I;\mathbf{x}_b) \right]}{\sigma(I)_{d,p}} \right\}^2$$

where:

p, d	run over instrument pointings and detectors;
I	runs over individual detector channels
j	enumerates the sources detected in the field at different position (θ,ϕ)
E	indexes the energies in the source model
$\mathbf{x_s}$	parameters of the source model, which is combined with the response
$\mathbf{x_b}$	parameters of the background model, expressed as a function of detector channel

Examination of this equation reveals one more complication; the term B represents the background, which, unlike for chopping, scanning or imaging experiments, must be solved for simultaneously with the desired source content. The proportion of background-to-source counts for a bright source such as the Crab is ~1%. Furthermore, the background varies as a function of detector, and time (dither-points), making simple subtraction implausible. Thus, a model of the background is applied to a special response matrix, and included in the de-convolution algorithm.

2.6 References

Arnaud, K.A., George, I.M., Tennant, A.F., 1992. Legacy, 2, 65.

Avni, Y., 1976. ApJ, 210, 642.

Bevington, P.R., 2002, 3rd Edition. Data Reduction and Error Analysis for the Physical Sciences, McGraw-Hill.

Blissett, R.J., Cruise, A.M., 1979. MNRAS, 186, 45.

George, I.M., Arnaud, K.A., Pence, W., Ruamsuwan, L., 1992. Legacy, 2, 51.

Kahn, S.M., Blissett, R.J., 1980. ApJ, 238, 417.

Loredo, T.J., Epstein, R.I., 1989. ApJ, 336, 896.

Press, W.H., Teukolsky, S.A., Vetterling, W.T., Flannery, B.P., 1992. Numerical Recipes (2nd edition), p687ff, CUP.

Wheaton, W.A. et.al., 1995. ApJ, 438, 322.

3. XSPEC Overview and Helpful Hints

3.1 Syntax

XSPEC is a command-driven, interactive program. You will see a prompt

```
XSPEC12>
```

whenever input is required. Command recall and inline editing are available using the arrow keys. XSPEC uses Tcl as its user interface, providing looping, conditionals, file I/O and so on. For further details of the Tcl syntax, consult the "Description of Syntax" section, the **User Interface** appendix, and links therein.

3.2 How to return to the XSPEC> prompt

The string /* acts as an emergency escape back to the XSPEC prompt. This string in answer to any question should bounce XSPEC out of whatever it is doing and back to the command prompt.

3.3 Getting Help

Quick help: If you are uncertain about command syntax, typing a command followed by a "?" will print a one-line summary. The **help** command :

```
XSPEC12> help
```

without arguments will bring up the full XSPEC manual in a PDF document reader (e.g. Adobe™ Acrobat Reader), or will open a browser to the XSPEC manual home page either locally or on the HEASARC site. See "Customizing XSPEC" later in this section to see how to select between these options, and how to assign a PDF reader and web browser to XSPEC. Typing

```
XSPEC12> help <command>
```

will display the manual section corresponding to <command>. Help for individual model components can be displayed by

```
XSPEC12> help model <modelName>
```

if all else fails you can e-mail your questions to the XSPEC team at

xanprob@athena.gsfc.nasa.gov

3.4 Commands

XSPEC commands can be divided into 6 categories: Control, Data, Model, Fitting, Plotting and Setting, as follows:

Control commands include items such as controlling logging, obtaining help, executing scripts, and other miscellaneous items to do with the program control rather than manipulating data or theoretical models.

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

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

Fit commands initiate the fitting routines, control the parameter set, perform statistical tests and compute confidence levels.

Plot commands generate about 50 different kinds of 2-dimensional plots

Setting commands change a variety of XSPEC internals which control details of models, statistics, and fitting methods.

These command types are summarized below. For full details see Chapter 5.

3.5 Issuing Commands

In an interactive session, the command interpreter accepts the shortest unambiguous abbreviation for any command. Since the interpreter is built on the Tcl language, some possible XSPEC command abbreviations might coincide with both XSPEC and Tcl commands. In this case, the interpreter will print the multiple possibilities and stop. Command abbreviations may be specified in a start-up script ($HOME/.xspec/xspec.rc) – see **Appendix A** for details.

Inside a script, command abbreviations are not recognized. This behavior can be overridden but we do not recommended it: however, specific abbreviations can be defined in the custom startup script.

Operating-system commands can be given from within XSPEC simply by typing the command, as at the shell prompt: however, if wild cards are needed (e.g. **ls *.pha**) the operating system command must be preceded by **syscall**. Note that an XSPEC abbreviation which corresponds to a system command will run the latter.

3.6 Control Commands

Control commands include those for:

writing program information: **log**, (save session to an ASCII file) **script** (record a set of commands), **save** (save commands needed to restore the current program state), **autosave** (automatically run the save command at specified intervals);

controlling program output: **chatter** (control the amount of program output), **query** (give an automatic response to prompts), **tclout** and **tcloutr** (create Tcl variables for manipulation in scripts)

displaying status information **show**, **time**, and **version**

ending the session: **exit** (or quit)

displaying online help **help** and ‘?”. Help can be given either in summary, in specific manual pages, a manual section, or the entire manual.

3.6.1 Query, chatter and shutting XSPEC up (somewhat)

The **fit** command will run a certain number of iterations and then query the user whether he or she wants to continue. While useful under most circumstances, the constant questioning can be a pain if one leaves XSPEC running and expects to find it finished when one gets back, or if one habitually runs scripts. One way around this problem is to reset the number of iterations before the question is asked by giving a single argument. For example,

```
XSPEC12> fit 100
```

will run 100 iterations before asking a question.

A more drastic solution is to use the **query** command.

```
XSPEC12> query yes
```

This will suppress all questions and assume that their answer is yes, while

```
XSPEC12> query no
```

will suppress all questions but assume that their answer is no.

The amount of output that XSPEC writes is set by the **chatter** command, which takes two arguments applying to the terminal and to the log file.

3.6.2 Scripts and the Save command

XSPEC commands can be written into a file and then executed by entering

```
XSPEC12> @filename
```

Alternatively, from the shell prompt

```
% xspec - filename &
```

for batch execution (remember to end the script in file `filename.xcm` with **exit** if you want the program to terminate after completion!). Note that the default suffix for xspec scripts is `.xcm`

The **save** command writes the current XSPEC status to a command file, which later can be run to reset XSPEC to the same configuration. XSPEC has a mechanism to save the current status automatically. This is controlled through the **autosave** command.

This command is very useful when reading a large number of data sets and/or fitting complicated models. If autosaving is operating (the default) then the equivalent of

```
XSPEC12> save all xautosav.xcm
```

is run after each command, so if a disaster occurs it is possible to recover.

3.6.3 Miscellaneous

Information on the current XSPEC status can be printed out using the **show** command. The **time** command writes out system-timing information, and the version command writes out the version number and the build time and date. Finally, XSPEC can be terminated with the **exit** or **quit** commands.

3.7 Data Commands

XSPEC is designed to allow complicated, multi-instrument analysis, so most commands can take arguments specifying more than one data set. Arguments in XSPEC are separated by either blanks or commas. A single argument can define a range. The ranges are delimited by a dash (–). A colon (:) is used to separate ranges (e.g., the phrase 1–2:11–24 refers to channels 11–24 in files 1 and 2).

3.7.1 Reading data and modifying calibration and auxiliary files

XSPEC reads in spectra from spectral files using the **data** command. Several datasets may be specified in one command. Several datasets may be stored in a single file and accessed separately. A particular dataset in use may be replaced by another or dropped entirely. The input data file contains pointers to background, redistribution and auxiliary response files, but these pointers may be overridden by the **backgrnd**, **response**, and **arf** commands. All these commands have the same syntax as **data**. An auxiliary background file, called the correction file (an absolute subtraction with zero variance), also can be included using the **corfile** command. Its use is described in the section on fitting. The current response can be replaced by a diagonal version using **diagrsp**. A dummy response for testing purposes can be defined using **dummyrsp**.

3.7.2 Controlling channels being fitted

PHA channels may be left out of fitting using the **ignore** command and included again using the **notice** command. These commands have a syntax allowing the same channels to be specified for more than one input file. The ignored and noticed ranges can be specified either as channels or as energies. If the command **setplot wave** has been entered, real ranges are interpreted as wavelengths.

3.7.3 Simulations

The **fakeit** command is used to generate simulated data. The current response matrix and model (a model must be defined prior to using the **fakeit** command) are used to create fake data. The user is prompted for various options. To make fake data when only a response matrix is available, give the command

```
XSPEC12> fakeit none.
```

XSPEC will prompt the user for the response and ancillary filenames from which to build the simulated data. It is important to note that a model must be defined prior to issuing this command.

3.7.4 Data groups

The most common use of XSPEC is to fit one or more data sets with responses to a particular model. However, it is often useful to be able to fit simultaneously several data sets with a model whose parameters can be different for each data set. A simple example would be a number of data sets that we expect to have the same model spectrum shape but different normalizations. XSPEC caters to this need through the use of data

groups. When files are read in they can be labeled as belonging to a particular data group. When a model is defined a set of model parameters is allocated for each data group. These parameters can all vary freely or they can be linked together across data groups as required.

To set up data groups, the **data** command should be given as in the following example :

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

which sets up two data groups. The first data group comprises data sets from file1 and file2, and the second data group takes the data set from file3. Now when a model is defined, XSPEC will give two sets of model parameters, one for the first datagroup and one for the second.

3.8 Model Commands

XSPEC allows users to fit data with models constructed from individual components. These components may be either additive, multiplicative, mixing, or convolution. Multiplicative components simply multiply the model by an energy-dependent factor. Convolutions apply a transformation to the model component they operated on whereby the output can be affected by a range of input energies, such as in smoothing operations. Mixing components are two dimensional and designed to transform fluxes between different spatial regions (such as in projection). Multiplicative, and convolution components can act on individual components, on groups of components, or on the entire model, whereas mixing transformations apply to the whole model.

The **model** command defines the model to be used and prompts for the starting values of its parameters. The user also can set the allowed ranges of the parameter. Parameters can be linked to an algebraic function of the other parameters, and unlinked using the **untie** command. The value of an individual parameter can be changed with the command **newpar** (and the current setting queried with **newpar 0**). Parameters can be fixed at their current value with the **freeze** command and allowed to vary freely with the **thaw** command. Individual components can be added or subtracted from the model using **addcomp**, **delcomp**, and **editmod**. The plasma emission and photoelectric absorption models require an assumption about relative elemental abundances.

The **flux** command calculates the flux from the current model in the given energy range. This energy range must be within that defined by the current response matrix. If a larger energy range is required, then the **energies** command can be given to compute the model over the desired range. The **lumin** command calculates the luminosity for the source redshift given. The **eqwidth** command determines the equivalent width of a model component, usually a line. The user of either of these last two commands should read the help descriptions carefully. The Tcl script **addline** can be used to automatically add lines to a model. These can be identified using **identify** and **modid**.

New model components which can be described by a simple algebraic formula can be set up using **mdefine** and used in the same way as the standard models except they will run slower being interpreted rather than compiled.

3.8.1 Models with multiple responses and background models

Multiple models and responses can be assigned to a single spectrum. This generalizes and replaces the '/b' technique of specifying background models in v11. In the FITS file format, a single response file can be associated with a spectrum either through a header keyword or a table column entry. XSPEC always assigns this response to a spectrum's source number 1. The **model** command by default also creates new models for source number 1. The **response** command in tandem with **model** can be used to create additional sources. For example to add a background model to loaded spectrum 1, first load a 2nd response:

```
XSPEC12> response 2:1 resp2.rsp
```

then define a background model to apply to source 2:

```
XSPEC12> model 2:my_background_model_name wa(po)
```

This model will now apply to spectrum 1 **and any other** spectrum that has a response loaded for source 2. To apply a different background model to spectrum 2, load a response for source 3 rather than 2:

```
XSPEC12> response 3:2 another_response.rsp
XSPEC12> model 3:another_background_model ga
```

An **arf** can also be assigned to a particular source number and spectrum:

```
XSPEC12> arf 2:1 arf_file.pha
```

Source numbers do not need to be entered in consecutive order for a given spectrum, and gaps in numbering are allowed. Please see the individual **model** and **response** entries in the "XSPEC Commands" section for more information and examples.

3.9 Fitting Commands

The basic fit command is called **fit**. This command performs a minimization using the currently selected algorithm (default: Levenberg-Marquadt). **fit** takes arguments that are passed to the fitting method: by default, these are the number of iterations to execute before asking the user whether to continue, and the numerical convergence criterion.

A systematic model uncertainty can be included using the **systematic** command. The **error** or **uncertain** command calculates error bounds for one interesting parameter for the specified parameters and confidence levels. To produce multi-dimensional errors the **steppar** command is used to generate a fit-statistic grid. Two-dimensional grids may be expressed as contour plots (using **plot contour**). The model normalization can be set using the **renorm** command. The normalization of the correction file background can be set with **cornorm. ftest** and the Tcl script **simftest** can be used to calculate F-test probabilities.

Markov Chain Monte Carlo runs can be performed using the **chain** command with a useful Tcl script **rescalecov** to rescale the proposal distribution covariance. The results can be analyzed using the **margin** command.

3.9.1 What to do when you have small numbers of counts

The χ^2 statistic assumes that all the spectral channels are Gaussian distributed and that the estimate for the variance is uncorrelated with the observed counts. If there are small numbers of counts in a channel these will not be true. An alternative statistic, the C-statistic, should be used in this case. The C-statistic now in use does provide a goodness-of-fit if there are enough counts and this can be checked using the **goodness** command which uses Monte Carlo methods. The C-statistic can also provide confidence intervals in exactly the same way as χ^2

To use, give the command

```
XSPEC12> statistic cstat
```

and then use the **fit** and **error** commands as usual. An alternative approach is to continue using the χ^2 statistic but change the weighting to provide a better estimate of the variance in the small number limit. This can be done using the **weight gehrels** or **weight churazov** commands. The latter is to be preferred.

3.9.2 Binning and Grouping data

Often one does not want to use the full resolution of a spectrum, either because the channels over-sample the spectral resolution or because the S/N is low. XSPEC and the associated programs provide a number of ways of handling this. Firstly, the XSPEC command **setplot rebin** can be used to add channels together in the plot. It is important to realize that this effects only the plot and not the data being fitted.

Two FTOOLS are available to bin and group data for fitting purposes. RBNPHA bins up the data in a non-reversible manner and should only be used to ensure that the number of bins in the spectrum is the same as that in the response. GRPPHA is the tool of choice for grouping the data to get adequate S/N or number of counts in each channel. GRPPHA does not actually add together channels, but instead sets a flag which is read by XSPEC and causes XSPEC to sum the appropriate channels. If a data file is read with some grouping then XSPEC will apply the same operation to any background or response files used.

3.10 Plotting Commands

XSPEC plotting is currently performed using the PLT interface. There are two basic commands: **plot** and **iplot**. The **plot** command makes a plot and returns the user to the XSPEC prompt, while the **iplot** command leaves the user in the interactive plotting interface, thus allowing the user to edit the plot. A variety of different quantities may be plotted, including the data and the current model; the integrated counts; the fit residuals; the ratio of data to model; the contributions to the fit statistic; the theoretical model; the unfolded (incident) spectrum; the detector efficiency; and the fit-statistic contours. All data plots can have an x-axis of channels, energy, or wavelength, which are specified with **setplot channel**, **setplot energy**, **setplot wavelength** respectively. The plotting device to be used is set using **setplot device** or **cpd**. Separate spectra may be added together and channels binned up (for plotting purposes only) using **setplot group** (and ungrouped with **setplot ungroup**) and **setplot rebin**. There is an option to plot individual

additive model components on data plots, this option is enabled by **setplot add** and disabled by **setplot noadd**. Line IDs can be plotted using **setplot id** and turned off by **setplot noid**. A stack of PLT commands can be created and manipulated with **setplot command**, **setplot delete**, and **setplot list**. This command stack then is applied to every plot.

PLT is built on top of the PGPLOT package, which comes with a standard set of device drivers. Any machine running X-windows should support **/xs** and **/xw,** while xterm windows should support **/xt**. PGPLOT supports monochrome and color postscript and both landscape and portrait orientation with the drivers **/ps**, **/cps**, **/vps**, and **/vcps**.

The easiest way to make a hardcopy of an XSPEC plot is to use

```
XSPEC12> iplot
```

command and then at the PLT prompt to enter

```
PLT> hard /ps
```

This will make a file called **pgplot.ps** which can be printed. Alternatively, the sequence

```
XSPEC12> cpd  <filename>/ps
XSPEC12> … plot commands …
XSPEC12> cpd none
```

will place the plots in a PostScript file <filename>.

3.11 Setting Commands

The fit statistics available within XSPEC are the χ^2 and C statistics: the **statistic** command specifies which one is to be used. Other fit-minimization algorithms are available, and can be selected using the **method** command. The various fit methods require first and in some cases second derivatives of the statistic with respect to the parameters. By default XSPEC calculates these analytically, using an approximation for the second derivatives. This may be changed by setting the USE_NUMERICAL_DIFFERENTIATION flag in the user's startup Xspec.init file. The weighting algorithm used to calculate χ^2 can be altered by the **weight** command.

Other setting commands modify:

cosmological parameters used to calculate luminosity **(cosmo)**

solar abundances for 18 elements **(abund)**

photoionization cross-sections **(xsect)**

The **xset** command can be used as an interface for **abund**, **cosmo**, **method**, **statistic**, and **xsect**. Additionally, **xset** may set string expressions that are used by models, for example the path to, and version number of APEC atomic line calculations, or the coordinate system for surface brightness calculations used in the **xmmpsf** mixing model.

3.12 Breaking With Ctrl-C

Ctrl-C can be used to break out of the **data**, **chain**, **error**, **fit**, and **steppar** commands. If a Ctrl-C is entered elsewhere, it will have no effect.

When a break is entered during the fitting commands (**error**, **fit**, and **steppar**), the fit will proceed until the end of the current fit iteration (ie. current lambda value when using Levenberg-Marquardt) before breaking. This is to ensure the program remains in a stable well-defined state. Therefore on slower machines, a user may notice a slight delay before the program actually breaks. Ctrl-C breaking is currently only implemented for the Levenberg-Marquardt fitting method.

Breaking is implemented for the data command primarily for users who load a large number of Type-II spectra with one data command. So if you enter

```
XSPEC12> data my_data{1-1000}
```

and decide it is taking too long to load, you can break out at any time. However, if you do choose to break, all spectra loaded from that particular data set will be lost. For example, if the command below is entered and a Ctrl-C is sent while the spectra from my_data2 are loading, the 50 spectra from my_data1 will be retained while none will be from my_data2:

```
XSPEC12> data my_data1{1-50} mydata2{1-50}
```

3.13 Customizing XSPEC

The XSPEC environment can be customized using two separate files, both of which are searched for in the directory

$HOME/.xspec

The first file, `Xspec.init` contains a number of settings that control items in XSPEC. An abridged version of this file is reproduced below.

```
#  XSPEC Initial settings file. 07/2009
#  Valid setting lines consist of two strings  in the format Key: Value
#  leading and trailing blanks are ignored for the key, leading
blanks/tabs ignored for
#  the value. Invalid settings (no colon) are ignored, keys valid in
format but not
#  implemented are simply read but not used.
#
#
#       Do not modify above this line
################################################
#
#  User default local model directory
#  example code may be found in the source tree at:
#  ${PATH_TO_SRC}/src/XSModel/Model/LocalModelTemplate
```

```
#LOCAL_MODEL_DIRECTORY:  /path/to/your/local/model/dir
################################################
#
#  options and commands for displaying helpfiles
#
   USE_ONLINE_HELP:   true

   # Recognized local help formats: html pdf
   # This is ignored when using online help
   LOCAL_HELP_FORMAT: html

   # Recommended command for Adobe Acrobat version 7 and later:
   # PDF_COMMAND:  acroread  -openInNewWindow -tempFileTitle

   # Recommended command for Adobe Acrobat prior to version 7:
   # PDF_COMMAND:  acroread  -useFrontEndProgram -tempFileTitle

   # Recommended command for Mac PDF viewing
   PDF_COMMAND:  open

   # Recommended command for Cygwin PDF viewing
   # PDF_COMMAND:  xpdf -q

   HTML_COMMAND:   open
################################################
#
#  setting for GUI mode. The code requires that the GUI setting
#  starts with a 't' (case-insensitive) otherwise GUI mode is false
#  and the command line mode is used.
#
GUI:   false
#
#  user-definable setting for the dummy response. Arguments required
#  begin-range end-range, number of bins, logarithmic/linear. Defaults
#  are {0.1,100,200,log} respectively. Setting for bin type must be
"linear"
#  if linear bins are to be created.
#
```

```
DUMMY:  0.1   50.  50  log
#
# Chatter Level: Console chatter level then log chatter level.
Currently (4/2001)
# logging has not been reimplemented.
#
CHAT: 10 10
#
# photo absorption cross section table setting.
# possible values are vern, bcmc, obmc.
XSECT:  bcmc
#
# solar abundance table indicator. Hard coded solar abundance vector.
Choices are
#  'feld'  Feldman, U., 1992. Physica Scripta, 46, 202.
#  'angr' is from Anders, E. & Grevesse, N., 1989. Geochimica and
Cosmochimica Acta 53, 197.
#  'aneb' is from Anders, E. & Ebihara, 1982.  Geochimica and
Cosmochimica Acta 46, 2363.
#  'file' is from a file read in by the user, but is not yet
implemented (4/2001)
#
ABUND: angr
#
# fitting method  (leven | anneal ...)
#
METHOD: leven
#
#  statistic to be minimized (chi | cstat)
#
STATISTIC: chi
#
#  weighting technique (standard | gehrels | churazov | model )
#
WEIGHT: standard
#
# If true, fitting algorithm will calculate parameter derivatives
# numerically.  If false, a faster analytic expression will be used,
# if applicable to the current fitting statistic.
```

```
#
USE_NUMERICAL_DIFFERENTIATION: false
#
#  cosmology parameters ( H0, q0, lambda0 )
#
COSMO:  70. .0 .73
#
#
#  Default graphics package (PLT is currently the only option).
#
GRAPH:  plt
#
#  Default plotting device (e.g. for PGPLOT)
#
PLOTDEVICE:    /null
#
# Y-axis plotting units when in setplot wave mode (angstrom, hz)
#
WAVE_PLOT_UNITS:  hz
#
#  User scripting directory
#
USER_SCRIPT_DIRECTORY:  $HOME/.xspec
```

A copy of this file is placed in the `$HOME/.xspec` directory on XSPEC12's first start-up or when it is not found. After this users can modify settings such as default cosmology or the energy range for dummy response for their own requirements.

This is also the place where users can select if they want to view PDF help files from the XSPEC distribution or HTML either locally or from the HEASARC site. Setting USE_ONLINE_HELP to true uses the remote HTML files while false will use either PDF or HTML local files depending on the value of LOCAL_HELP_FORMAT.

The PDF_COMMAND and HTML_COMMAND entries determine which applications are run for the two viewing cases. The HTML_COMMAND value should typically just be the name of a web browser, or "open" for Mac OS X users. The default settings for the PDF_COMMAND entry are what work best for launching Adobe Acrobat Reader 7.0.x on Linux/Unix systems. For those launching earlier versions, the "-openInNewWindow" flag should be replaced with "-useFrontEndProgram". For Mac users, again we recommend the entire entry simply be replaced with "open".

The second file that is searched for is the xspec.rc file. This contains users' own customizations, for example Tcl or XSPEC command abbreviations, packages to be

loaded on startup, or Tcl scripts containing procedures that are to be executed as commands. Please consult **Appendix A** and references/links therein for details of Tcl commands and scripting.

3.13.1 Customizing system-wide

When an XSPEC build is intended for many users across a system, it is also possible for the installer (or whoever has write access to the distribution and installation areas) to globally customize XSPEC. This is done through the file global_customize.tcl, located in the …/Xspec/src/scripts directory. (This was done in the xspec.tcl file prior to v12.2.1) Any of the customizations mentioned above for the individual's own xspec.rc file can also be placed in the global_customize.tcl file. After making the additions, run "hmake install" out of the …/Xspec/src/scripts directory in order to copy the modified global_customize.tcl file to the installation area. This additional code will be executed for all users upon startup, BEFORE any of their own customizations in their xspec.rc files.

4. Walks through XSPEC

4.1 Introduction

This chapter demonstrates the use of XSPEC. The brief discussion of data and response files is followed by fully worked examples using real data that include all the screen input and output with a variety of plots. The topics covered are as follows: defining models, fitting data, determining errors, fitting more than one set of data simultaneously, simulating data, and producing plots.

4.1.1 Brief Discussion of XSPEC Files

At least two files are necessary for use with XSPEC: a data file and a response file. In some cases, a file containing background may also be used, and, in rare cases, a *correction* file is needed to adjust the background during fitting. If the response is split between an rmf and an arf then an ancillary response file is also required. However, most of the time the user need only specify the data file, as the names and locations of the correct response and background files should be written in the header of the data file by whatever program created the files.

4.2 Fitting Models to Data: An Example from EXOSAT

The 6s X-ray pulsar 1E1048.1–5937 was observed by *EXOSAT* in June 1985 for 20 ks. In this example, we'll conduct a general investigation of the spectrum from the Medium Energy (ME) instrument, i.e. follow the same sort of steps as the original investigators (Seward, Charles & Smale, 1986). The ME spectrum and corresponding response matrix were obtained from the HEASARC On-line service. Once installed, XSPEC is invoked by typing

```
%xspec
```

as in this example:

%xspec

```
                        XSPEC version: 12.2.1
                Build Date/Time: Wed Nov 2 16:16:52 2005

XSPEC12>data s54405.pha

1 spectrum in use

Source File: s54405.pha
Net count rate (cts/s) for Spectrum:1  3.783  +/- 0.1367
 Assigned to Data Group 1 and Plot Group 1
 Using Response (RMF) File    s54405.rsp
```

The **data** command tells the program to read the data as well as the response file that is named in the header of the data file. In general, XSPEC commands can be truncated, provided they remain unambiguous. Since the default extension of a data file is `.pha`, and the abbreviation of **data** to the first two letters is unambiguous, the above command can be abbreviated to **da** `s54405`, if desired. To obtain help on the **data** command, or on any other command, type **help** `command` followed by the name of the command.

One of the first things most users will want to do at this stage—even before fitting models—is to look at their data. The plotting device should be set first, with the command **cpd** (*change plotting device*). Here, we use the pgplot X-Window server, `/xw`.

```
XSPEC12> cpd /xw
```

There are more than 50 different things that can be plotted, all related in some way to the data, the model, the fit and the instrument. To see them, type:

```
XSPEC12> plot ?

plot data/models/fits etc
Syntax: primary plot commands:
  chisq    contour  counts   data     delchi
  emodel   eemodel  efficiency   eufspec  eeufspec
  foldmodel  icounts  insensitivity  delchi   lcounts
  model    ratio    residuals  sensitivity  sum
  ufspec
  secondary options (2-panel data plots - use with data, ldata, counts, lcounts,
icounts):
  chisq    delchi   ratio    residuals
```

The most fundamental is the data plotted against instrument channel (**data**); next most fundamental, and more informative, is the data plotted against channel energy. To do this plot, use the XSPEC command **setplot** `energy`. Figure A shows the result of the commands:

```
XSPEC12> setplot energy
XSPEC12> plot data
```

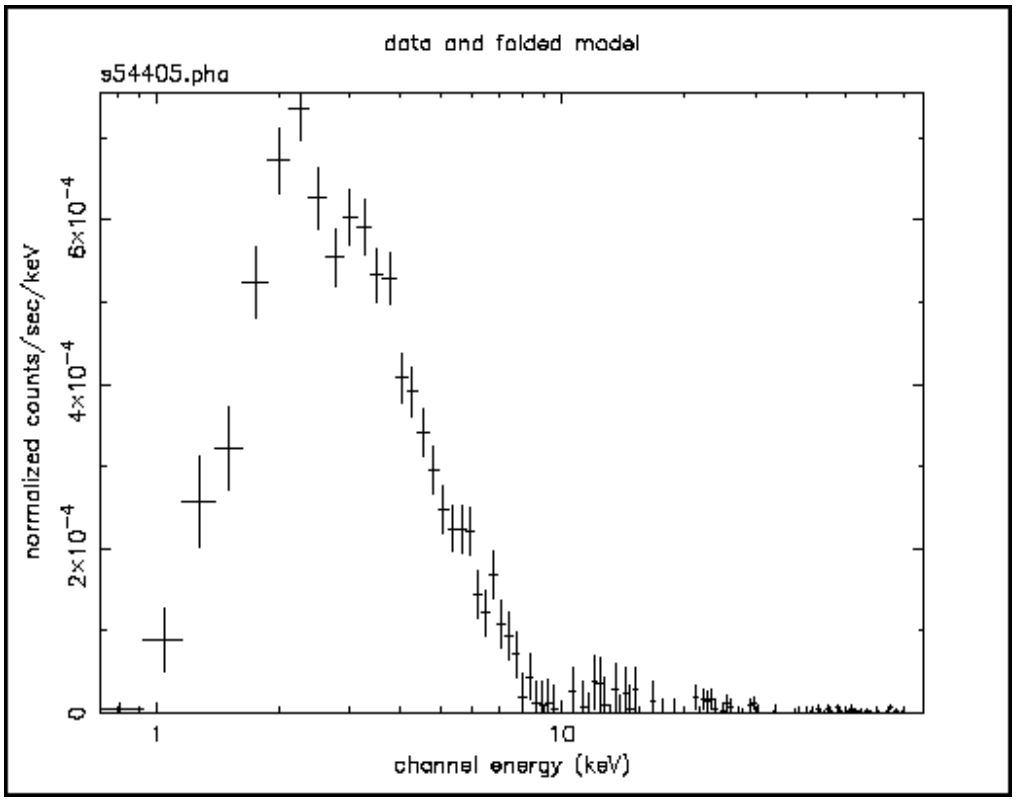


Figure A: The result of the command plot data when the data file in question is the EXOSAT ME spectrum of the 6s X-ray pulsar 1E1048.1--5937 available from the HEASARC on-line service

People familiar with *EXOSAT* ME data will recognize the spectrum to be soft, absorbed and without an obvious bright iron emission line. We are now ready to fit the data with a model. Models in XSPEC are specified using the **model** command, followed by an algebraic expression of a combination of model components. There are two basic kinds of model components: *additive,* which represent X-Ray sources of different kinds. After being convolved with the instrument response, the components prescribe the number of counts per energy bin (e.g., a bremsstrahlung continuum); and *multiplicative* models components, which represent phenomena that modify the observed X-Radiation (e.g. reddening or an absorption edge). They apply an energy-dependent multiplicative factor to the source radiation before the result is convolved with the instrumental response.

More generally, XSPEC allows three types of modifying components: convolutions and mixing models in addition to the multiplicative type. Since there must be a source, there must be least one additive component in a model, but there is no restriction on the number of modifying components. To see what components are available, type **model** `?`:

```
XSPEC12>model
 Additive Models:
apec        bbody       bbodyrad    bexrav      bexriv      bknpower
bmc         bremss      c6mekl      c6pmekl     c6vmekl     cemekl
cevmkl      cflow       compLS      compST      compTT      compbb
```

```
cutoffpl    disk        diskbb      diskline    diskm       disko
diskpn      equil       gaussian    gnei        grad        grbm
laor        lorentz     meka        mekal       mkcflow     nei
npshock     nteea       pegpwrlw    pexrav      pexriv      plcabs
posm        powerlaw    pshock      raymond     redge       refsch
sedov       srcut       sresc       step        vapec       vbremss
vequil      vgnei       vmcflow     vmeka       vmekal      vnei
vnpshock    vpshock     vraymond    vsedov      zbbody      zbremss
zgauss      zpowerlw

 Multiplicative Models:
SSS_ice     TBabs       TBgrain     TBvarabs    absori      cabs
constant    cyclabs     dust        edge        expabs      expfac
highecut    hrefl       notch       pcfabs      phabs       plabs
redden      smedge      spline      uvred       varabs      vphabs
wabs        wndabs      xion        zTBabs      zedge       zhighect
zpcfabs     zphabs      zvarabs     zvfeabs     zvphabs     zwabs
zwndabs

 Convolution Models:
gsmooth     lsmooth     reflect

 Pile-up Models:
pileup

 Additive Models:                68
 Multiplicative Models:          37
 Convolution Models:             3
 Pile-up Models:                 1
 Total Models:                   109
```

For information about a specific component, type **help** `model` followed by the name of the component):

XSPEC12>help model raymond

Given the quality of our data, as shown by the plot, we'll choose an absorbed power law, specified as follows :

```
XSPEC12> model phabs(powerlaw)
```

Or, abbreviating unambiguously:

```
XSPEC12> mo pha(po)
```

The user is then prompted for the initial values of the parameters. Entering `<return>` or `/` in response to a prompt uses the default values. We could also have set all parameters to their default values by entering `/*` at the first prompt. As well as the parameter values themselves, users also may specify step sizes and ranges (`<value>, <delta>`, `<min>`, `<bot>`, `<top>`, and `<max values>`), but here, we'll enter the defaults:

```
XSPEC12>mo pha(po)
 Model: phabs[1]( powerlaw[2] )
Input parameter value, delta, min, bot, top, and max values for ...
Current:     1   0.001     0     0   1E+05   1E+06
phabs:nH>/*
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Model: phabs[1]( powerlaw[2] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22   1.000   +/-   0.
  2  2  2  powerlaw  PhoIndex      1.000   +/-   0.
  3  3  2  powerlaw  norm        1.000   +/-   0.
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Chi-Squared =   4.8645994E+08 using  125 PHA bins.
 Reduced chi-squared =   3987376.   for  122 degrees of freedom
 Null hypothesis probability =  0.
```

Note that most of the other numerical values in this section are have changed from those produced by earlier versions. This is because the default photoelectric absorption cross-sections have changed since XSPEC V.10. To recover identical results to earlier versions, use **xsect** `obcm`. `bcmc` is the default; see **help** `xsect` for details). The current statistic is χ^2 and is huge for the initial, default values—mostly because the power law normalization is two orders of magnitude too large. This is easily fixed using the **renorm** command.

```
XSPEC12> renorm
 Chi-Squared =   852.1660   using  125 PHA bins.
 Reduced chi-squared =   6.984967   for  122 degrees of freedom
 Null hypothesis probability =  0.
```

We are not quite ready to fit the data (and obtain a better χ^2), because not all of the 125 PHA bins should be included in the fitting: some are below the lower discriminator of the instrument and therefore do not contain valid data; some have imperfect background subtraction at the margins of the pass band; and some may not contain enough counts for χ^2 to be strictly meaningful. To find out which channels to discard (*ignore* in XSPEC terminology), users must consult mission-specific documentation, which will inform them of discriminator settings, background subtraction problems and other issues. For the mature missions in the HEASARC archives, this information already has been encoded in the headers of the spectral files as a list of "bad" channels. Simply issue the command:

```
XSPEC12> ignore bad
 Chi-Squared =   799.7109   using  85 PHA bins.
 Reduced chi-squared =   9.752572   for   82 degrees of freedom
 Null hypothesis probability =  0.
XSPEC12> setplot chan
XSPEC12> plot data
```

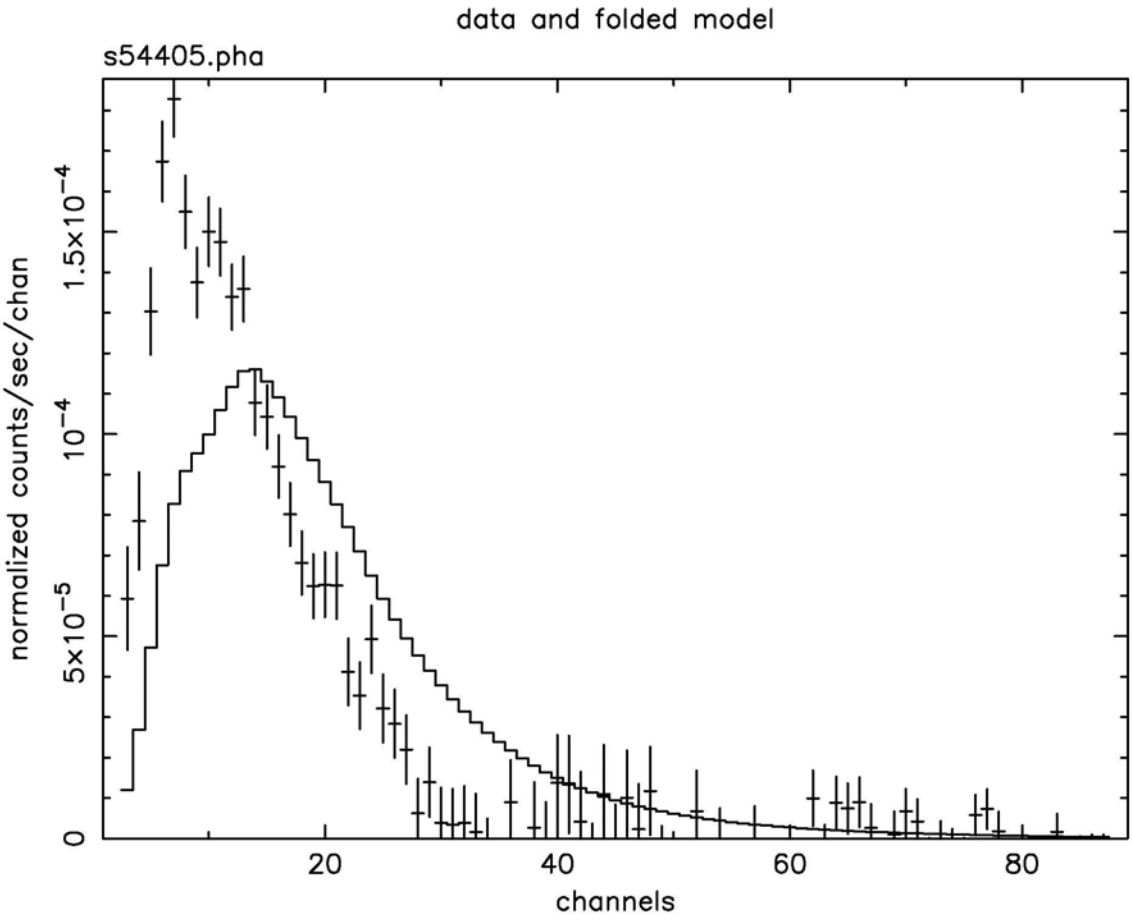


Figure B: The result of the command plot data after the command ignore bad on the EXOSAT ME spectrum 1E1048.1–5937

We can see that 40 channels are bad—but do we need to ignore any more? These channels are bad because of certain instrument properties: other channels still may need to be ignored because of the shape and brightness of the spectrum itself. Figure B shows the result of plotting the data in channels (using the commands **setplot** `channel` and **plot** `data`). We see that above about channel 33 the S/N becomes small. We also see, comparing Figure B with Figure A, which bad channels were ignored. Although visual inspection is not the most rigorous method for deciding which channels to ignore (more on this subject later), it's good enough for now, and will at least prevent us from getting grossly misleading results from the fitting. To ignore channels above 33:

```
XSPEC12> ignore 34-**
 Chi-Squared =   677.6218   using  31 PHA bins.
 Reduced chi-squared =   24.20078   for   28 degrees of freedom
 Null hypothesis probability =  0.
```

The same result can be achieved with the command **ignore** `34-125`. The inverse of **ignore** is **notice**, which has the same syntax.

We are now ready to fit the data. Fitting is initiated by the command **fit**. As the fit proceeds, the screen displays the status of the fit for each iteration until either the fit converges to the minimum χ^2, or the user is asked whether the fit is to go through another set of iterations to find the minimum. The default number of iterations is ten.

```
XSPEC12>fit
 Chi-Squared  Lvl Fit param # 1   2      3
  204.136   -3   7.9869E-02  1.564   4.4539E-03
  84.5658   -4   0.3331    2.234   1.0977E-02
  30.2511   -5   0.4422    2.174   1.1965E-02
  30.1202   -6   0.4648    2.196   1.2264E-02
  30.1189   -7   0.4624    2.195   1.2244E-02
 ------------------------------------------------------------------------
 Variances and Principal axes :
        1   2   3
 4.14E-08 | 0.00 -0.01 1.00
 8.70E-02 | -0.91 -0.41 -0.01
 2.32E-03 | -0.41 0.91 0.01
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Model: phabs[1]( powerlaw[2] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22   0.4624   +/- 0.2698
  2  2  2  powerlaw  PhoIndex      2.195   +/- 0.1288
  3  3  2  powerlaw  norm        1.2244E-02 +/- 0.2415E-02
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Chi-Squared =   30.11890   using  31 PHA bins.
 Reduced chi-squared =   1.075675   for   28 degrees of freedom
 Null hypothesis probability = 0.358
```

The fit is good: reduced χ^2 is 1.075 for 31 – 3 = 28 degrees of freedom. The null hypothesis probability is the probability of getting a value of χ^2 as large or larger than observed if the model is correct. If this probability is small then the model is not a good fit. The matrix of principal axes printed out at the end of a fit provides an indication of whether parameters are correlated (at least local to the best fit). In this example the powerlaw norm is not correlated with any other parameter while the column and powerlaw index are slightly correlated. To see the fit and the residuals, we use the command

```
XSPEC12>plot data resid
```

The result is shown in Figure C.

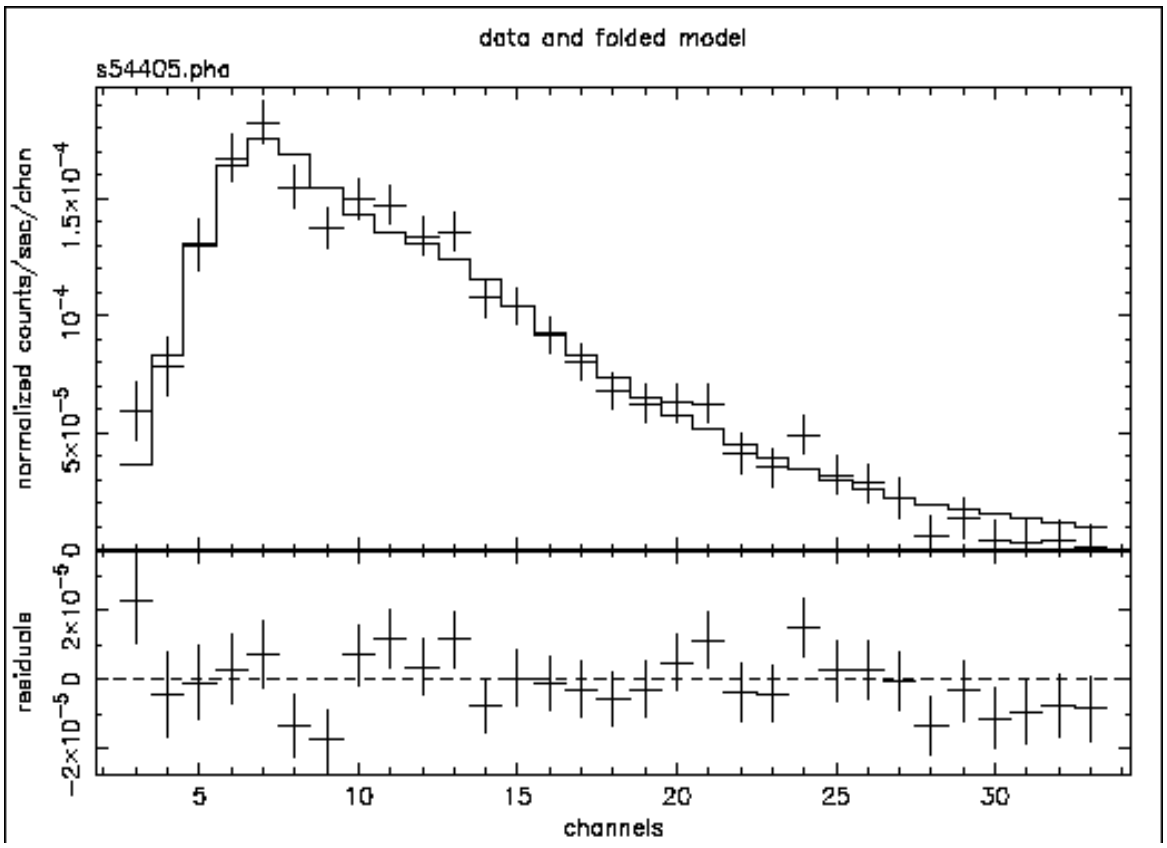


Figure C: The result of the command plot data with: the ME data file from 1E1048.1—5937; "bad" and negative channels ignored; the best-fitting absorbed power-law model; the residuals of the fit.

The screen output shows the best-fitting parameter values, as well as approximations to their errors. These errors should be regarded as indications of the uncertainties in the parameters and should *not* be quoted in publications. The true errors, i.e. the confidence ranges, are obtained using the **error** command:

```
XSPEC12>error 1 2 3
 Parameter  Confidence Range (   2.706)
   1  3.254765E-02  0.932778
   2   1.99397     2.40950
 *WARNING*:RENORM: No variable model to allow renormalization
 *WARNING*:RENORM: No variable model to allow renormalization
 *WARNING*:RENORM: No variable model to allow renormalization
 *WARNING*:RENORM: No variable model to allow renormalization
 *WARNING*:RENORM: No variable model to allow renormalization
 *WARNING*:RENORM: No variable model to allow renormalization
 *WARNING*:RENORM: No variable model to allow renormalization
 *WARNING*:RENORM: No variable model to allow renormalization
 *WARNING*:RENORM: No variable model to allow renormalization
 *WARNING*:RENORM: No variable model to allow renormalization
8.942987E-03  1.711637E-02
```

Here, the numbers 1, 2, 3 refer to the parameter numbers in the `Model par` column of the screen output. For the first parameter, the column of absorbing hydrogen atoms, the 90% confidence range is $3.3\times10^{20} < N_H < 9.3\times10^{21}\,\mathrm{cm}^{-2}$. This corresponds to an excursion in χ^2 of 2.706. The reason these "better" errors are not given automatically as part of the **fit** output is that they entail further fitting. When the model is simple, this does not require much CPU, but for complicated models the extra time can be considerable. The warning message is generated because there are no free normalizations in the model while the error is being calculated on the normalization itself. In this case, the warning may safely be ignored.

What else can we do with the fit? One thing is to derive the flux of the model. The data by themselves only give the instrument-dependent count rate. The model, on the other hand, is an estimate of the true spectrum emitted. In XSPEC, the model is defined in physical units independent of the instrument. The command flux integrates the current model over the range specified by the user:

```
XSPEC12> flux 2 10
 Model flux 3.5496E-03 photons ( 2.2492E-11 ergs)cm**-2 s**-1 ( 2.000- 10.000)
```

Here we have chosen the standard X-ray range of 2—10 keV and find that the energy flux is 2.2×10^{-11} erg cm^{-2}s^{-1} Note that **flux** will integrate only within the energy range of the current response matrix. If the model flux outside this range is desired—in effect, an extrapolation beyond the data---then the command **dummyrsp** should be used. This command sets up a dummy response that covers the range required. For example, if we want to know the flux of our model in the *ROSAT* PSPC band of 0.2—2 keV, we enter:

```
XSPEC12>dummy 0.2 2.
 Chi-Squared =   3583.779   using  31 PHA bins.
 Reduced chi-squared =   127.9921   for   28 degrees of freedom
 Null hypothesis probability =  0.
XSPEC12>flux 0.2 2.
 Model flux 4.5306E-03 photons ( 9.1030E-12 ergs)cm**-2 s**-1 ( 0.200- 2.000)
```

The energy flux, at 9.1×10^{-12} erg cm^{-2}s^{-1} is lower in this band but the photon flux is higher. To get our original response matrix back we enter:

```
XSPEC12> response
 Chi-Squared =   30.11890   using  31 PHA bins.
 Reduced chi-squared =   1.075675   for   28 degrees of freedom
 Null hypothesis probability = 0.358
```

The fit, as we've remarked, is good, and the parameters are constrained. But unless the purpose of our investigation is merely to measure a photon index, it's a good idea to check whether alternative models can fit the data just as well. We also should derive upper limits to components

such as iron emission lines and additional continua, which, although not evident in the data nor required for a good fit, are nevertheless important to constrain. First, let's try an absorbed black body:

```
XSPEC12>mo pha(bb)
 Model: phabs[1]( bbody[2] )
Input parameter value, delta, min, bot, top, and max values for ...
Current:     1   0.001     0     0   1E+05   1E+06
phabs:nH>/*
 ------------------------------------------------------------------------------
 ------------------------------------------------------------------------------
 Model: phabs[1]( bbody[2] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22   1.000   +/-   0.
  2  2  2  bbody   kT    keV    3.000   +/-   0.
  3  3  2  bbody   norm        1.000   +/-   0.
 ------------------------------------------------------------------------------
 ------------------------------------------------------------------------------
 Chi-Squared =   3.3142067E+09 using  31 PHA bins.
 Reduced chi-squared =   1.1836453E+08 for   28 degrees of freedom
 Null hypothesis probability =  0.
XSPEC12>fit
 Chi-Squared  Lvl Fit param # 1   2      3
  1420.96   0   0.2116    2.987   7.7666E-04
  1387.72   0   4.4419E-02  2.975   7.7003E-04
  1376.39   0   4.3009E-03  2.963   7.6354E-04
  1371.67   0   1.8192E-03  2.951   7.5730E-04
  1367.04   0   5.8100E-04  2.939   7.5130E-04
  1362.47   0   1.9059E-04  2.926   7.4548E-04
  1357.84   0   6.1455E-05  2.913   7.3982E-04
  1353.14   0   2.5356E-05  2.900   7.3429E-04
  1348.36   0   6.7582E-06  2.887   7.2885E-04
  1343.50   0   2.0479E-06  2.874   7.2350E-04
 Number of trials exceeded - last iteration delta =  4.861
 Continue fitting? (Y)y
 ...

  113.954   0     0.   0.8907   2.7865E-04
  113.954   -1     0.   0.8905   2.7859E-04
  113.954   4     0.   0.8905   2.7859E-04
 ------------------------------------------------------------------------------
 Variances and Principal axes :
        2   3
 2.88E-04 | -1.00 0.00
 8.45E-11 | 0.00 -1.00
 ------------------------------------------------------------------------------
 ------------------------------------------------------------------------------
 Model: phabs[1]( bbody[2] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22     0.   +/- -1.000
  2  2  2  bbody   kT    keV    0.8905   +/- 0.1696E-01
  3  3  2  bbody   norm        2.7859E-04 +/- 0.9268E-05
 ------------------------------------------------------------------------------
 ------------------------------------------------------------------------------
 Chi-Squared =   113.9542   using  31 PHA bins.
```

```
Reduced chi-squared =   4.069792   for   28 degrees of freedom
Null hypothesis probability = 2.481E-12
```

Note that when more than 10 iterations are required for convergence the user is asked whether or not to continue at the end of each set of 10. Saying *no* at these prompts is a good idea if the fit is not converging quickly. Conversely, to avoid having to keep answering the question, i.e., to increase the number of iterations before the prompting question appears, begin the fit with, say **fit** `100`. This command will put the fit through 100 iterations before pausing.

Plotting the data and residuals again with

```
XSPEC12> plot data resid
```

we obtain Figure D:

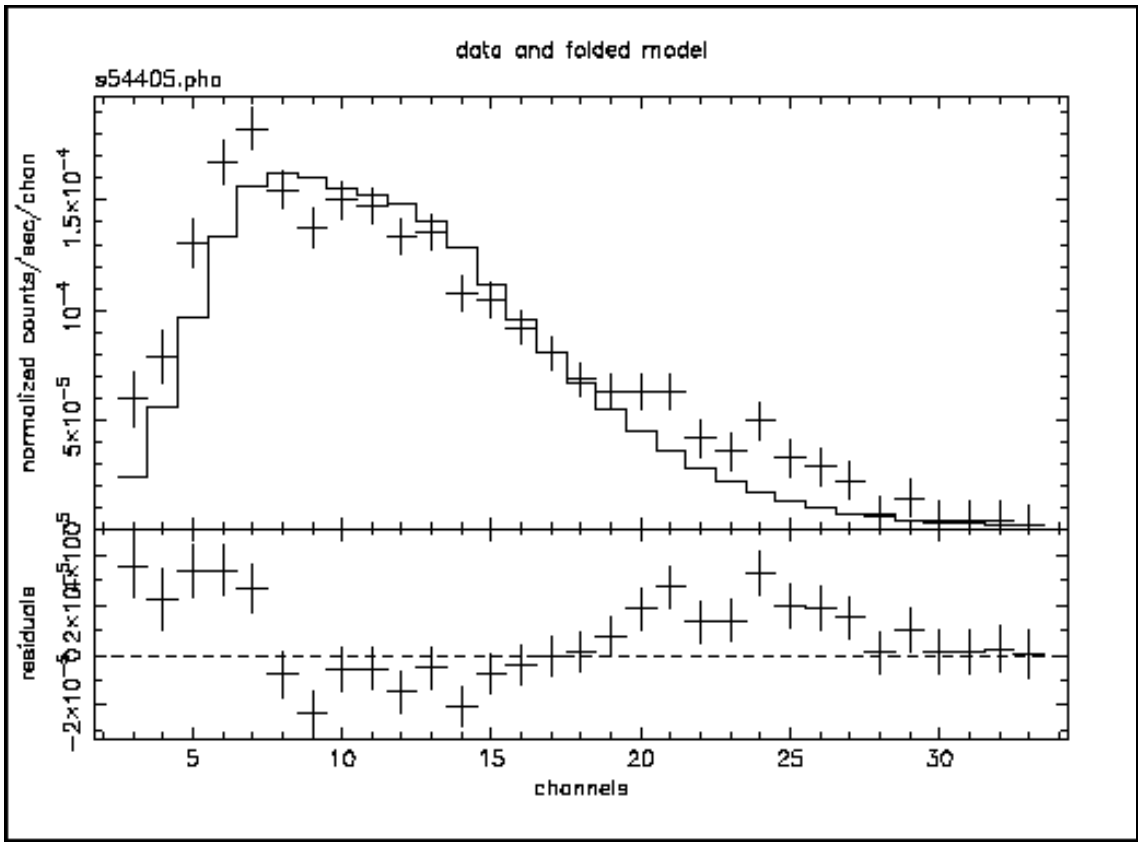


Figure D: As for Figure C, but the model is the best-fitting absorbed black body. Note the wave-like shape of the residuals which indicates how poor the fit is, i.e. that the continuum is obviously not a black body.

The black body fit is obviously not a good one. Not only is χ^2 large, but the best-fitting N_H is rather low. Inspection of the residuals confirms this: the pronounced wave-like shape is indicative of a bad choice of overall continuum (see Figure D). Let's try thermal bremsstrahlung next:

```
XSPEC12>mo pha(br)
 Model: phabs[1]( bremss[2] )
Input parameter value, delta, min, bot, top, and max values for ...
Current:     1   0.001     0     0   1E+05   1E+06
phabs:nH>/*
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Model: phabs[1]( bremss[2] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22   1.000   +/-   0.
  2  2  2  bremss   kT    keV    7.000   +/-   0.
  3  3  2  bremss   norm        1.000   +/-   0.
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Chi-Squared =   4.5311800E+07 using  31 PHA bins.
 Reduced chi-squared =   1618279.   for   28 degrees of freedom
 Null hypothesis probability =  0.
XSPEC12>fit
 Chi-Squared  Lvl Fit param # 1   2      3
  113.305   -3   0.2441    6.557   6.8962E-03
  40.4519   -4   0.1173    5.816   7.7944E-03
  36.0549   -5   4.4750E-02  5.880   7.7201E-03
  33.4168   -6   1.8882E-02  5.868   7.7476E-03
  32.6766   -7   7.8376E-03  5.864   7.7495E-03
  32.3192   -8   2.7059E-03  5.862   7.7515E-03
  32.1512   -9   2.3222E-04  5.861   7.7525E-03
  32.1471  -10   1.0881E-04  5.861   7.7523E-03
 ------------------------------------------------------------------------
 Variances and Principal axes :
        1   2   3
 2.29E-08 | 0.00 0.00 1.00
 3.18E-02 | 0.95 0.31 0.00
 8.25E-01 | 0.31 -0.95 0.00
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Model: phabs[1]( bremss[2] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22   1.0881E-04 +/- 0.3290
  2  2  2  bremss   kT    keV    5.861   +/- 0.8651
  3  3  2  bremss   norm        7.7523E-03 +/- 0.8122E-03
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Chi-Squared =   32.14705   using  31 PHA bins.
 Reduced chi-squared =   1.148109   for   28 degrees of freedom
 Null hypothesis probability = 0.269
```

Bremsstrahlung is a better fit than the black body—and is as good as the power law—although it shares the low N_H. With two good fits, the power law and the bremsstrahlung, it's time to scrutinize their parameters in more detail.

First, we reset our fit to the powerlaw (output omitted):

```
XSPEC12>mo pha(po)
```

From the *EXOSAT* database on HEASARC, we know that the target in question, 1E1048.1--5937, has a Galactic latitude of $24'$, i.e., almost on the plane of the Galaxy. In fact, the database also provides the value of the Galactic N_H based on 21-cm radio observations. At $4\times10^{22}\,\mathrm{cm}^{-2}$, it is higher than the 90 percent-confidence upper limit from the power-law fit. Perhaps, then, the power-law fit is not so good after all. What we can do is fix (**freeze** in XSPEC terminology) the value of N_H at the Galactic value and refit the power law. Although we won't get a good fit, the shape of the residuals might give us a clue to what is missing. To freeze a parameter in XSPEC, use the command **freeze** followed by the parameter number, like this:

```
XSPEC12> freeze 1
 Number of variable fit parameters =  2
```

The inverse of **freeze** is **thaw**:

```
XSPEC12> thaw 1
 Number of variable fit parameters =  3
```

Alternatively, parameters can be frozen using the **newpar** command, which allows all the quantities associated with a parameter to be changed. The second quantity, `delta`, is the step size used to calculate the derivative in the fitting, and, if set to a negative number, will cause the parameter to be frozen. In our case, we want N_H frozen at $4\times10^{22}\,\mathrm{cm}^{-2}$, so we go back to the power law best fit and do the following :

```
XSPEC12>newpar 1
Current:   0.463   0.001     0     0   1E+05   1E+06
phabs:nH>4,0
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Model: phabs[1]( powerlaw[2] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22   4.000   frozen
  2  2  2  powerlaw  PhoIndex      2.195   +/- 0.1287
  3  3  2  powerlaw  norm        1.2247E-02 +/- 0.2412E-02
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
  2 variable fit parameters
 Chi-Squared =   829.3545   using  31 PHA bins.
 Reduced chi-squared =   28.59843   for   29 degrees of freedom
 Null hypothesis probability =  0.
```

Note the useful trick of giving a value of zero for **delta** in the **newpar** command. This has the effect of changing **delta** to the negative of its current value. If the parameter is free, it will be frozen, and if frozen, thawed. The same result can be obtained by putting everything onto the command line, i.e., **newpar** `1 4, 0`, or by issuing the two commands, **newpar** `1 4` followed by **freeze** `1`. Now, if we fit and plot again, we get the following model (Fig. E).

```
XSPEC12>fit
...
 ------------------------------------------------------------------------------
 ------------------------------------------------------------------------------
 Model: phabs[1]( powerlaw[2] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs    nH     10^22   4.000   frozen
  2  2  2  powerlaw  PhoIndex      3.594   +/- 0.6867E-01
  3  3  2  powerlaw  norm        0.1161   +/- 0.9412E-02
 ------------------------------------------------------------------------------
 ------------------------------------------------------------------------------
 Chi-Squared =   125.5134   using  31 PHA bins.
 Reduced chi-squared =   4.328048   for   29 degrees of freedom
 Null hypothesis probability = 5.662E-14
 XSPEC12>plot data resid
```

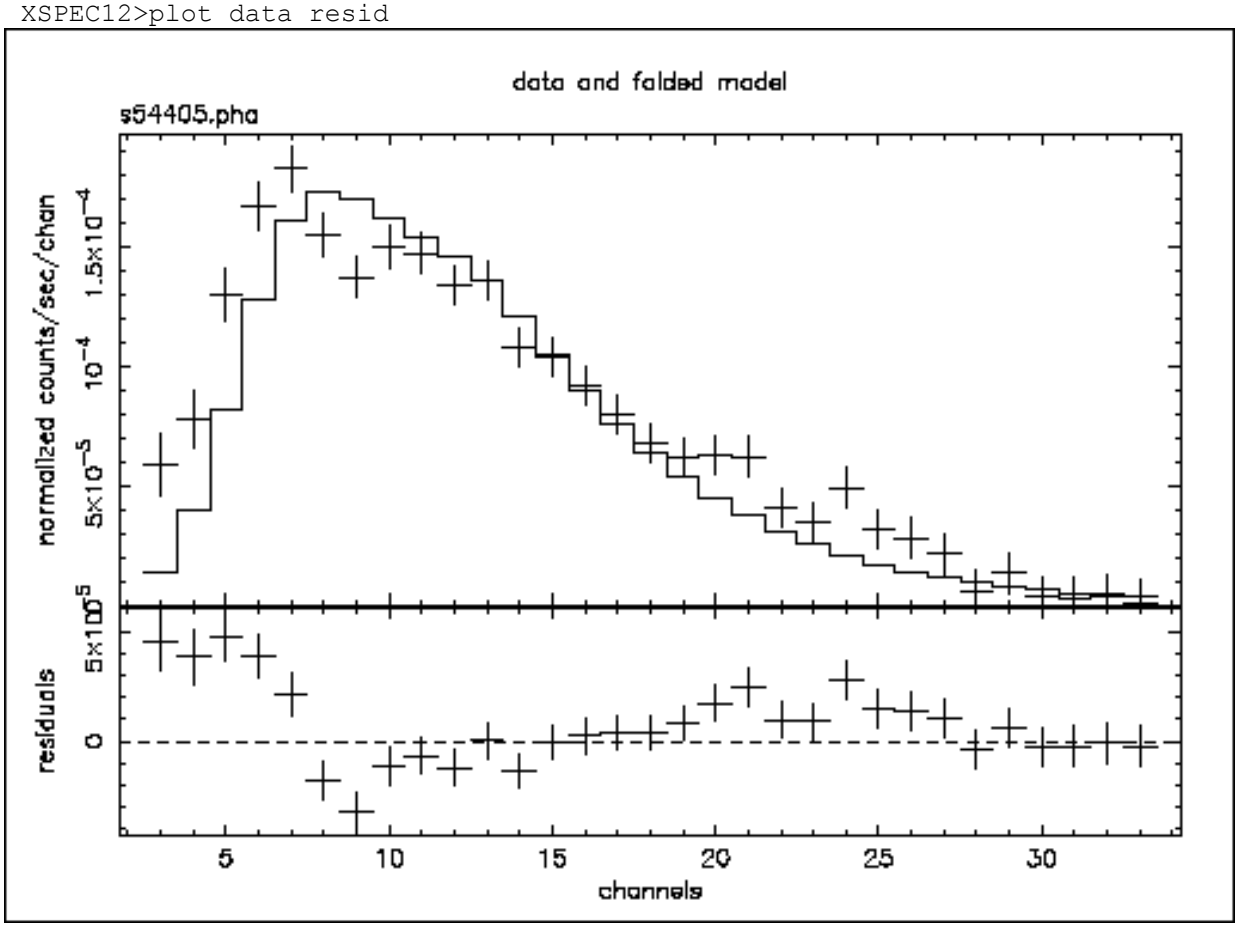


Figure E: As for Figure C & D, but the model is the best-fitting power law with the absorption fixed at the Galactic value. Under the assumptions that the absorption really is the same as the 21-cm value and that the continuum really is a power law, this plot provides some indication of what other components might be added to the model to improve the fit.

The fit is not good. In Figure E we can see why: there appears to be a surplus of softer photons, perhaps indicating a second continuum component. To investigate this possibility we can

add a component to our model. The **editmod** command lets us do this without having to respecify the model from scratch. Here, we'll add a black body component.

```
XSPEC12>editmod pha(po+bb)
 Model: phabs[1]( powerlaw[2] + bbody[3] )
Input parameter value, delta, min, bot, top, and max values for ...
Current:     3   0.01  0.0001   0.01    100    200
bbody:kT>2,0
Current:     1   0.01     0     0   1E+24   1E+24
bbody:norm>1.e-5
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Model: phabs[1]( powerlaw[2] + bbody[3] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22   4.000   frozen
  2  2  2  powerlaw  PhoIndex      3.594   +/- 0.6867E-01
  3  3  2  powerlaw  norm        0.1161   +/- 0.9412E-02
  4  4  3  bbody   kT    keV    2.000   frozen
  5  5  3  bbody   norm        1.0000E-05 +/-   0.
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Chi-Squared =   122.1538   using  31 PHA bins.
 Reduced chi-squared =   4.362635   for   28 degrees of freedom
 Null hypothesis probability = 9.963E-14
```

Notice that in specifying the initial values of the black body, we have frozen kT at 2 keV (the canonical temperature for nuclear burning on the surface of a neutron star in a low-mass X-ray binary) and started the normalization at zero. Without these measures, the fit might "lose its way". Now, if we fit, we get (not showing all the iterations this time):

```
 ------------------------------------------------------------------------
 Model: phabs[1]( powerlaw[2] + bbody[3] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22   4.000   frozen
  2  2  2  powerlaw  PhoIndex      4.932   +/- 0.1618
  3  3  2  powerlaw  norm        0.3761   +/- 0.5449E-01
  4  4  3  bbody   kT    keV    2.000   frozen
  5  5  3  bbody   norm        2.3212E-04 +/- 0.3966E-04
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Chi-Squared =   55.63374   using  31 PHA bins.
 Reduced chi-squared =   1.986919   for   28 degrees of freedom
 Null hypothesis probability = 1.425E-03
```

The fit is better than the one with just a power law *and* the fixed Galactic column, but it is still not good. Thawing the black body temperature and fitting gives us:

```
XSPEC12>thaw 4
 Number of variable fit parameters =  4
XSPEC12>fit
...
 ------------------------------------------------------------------------------
 ------------------------------------------------------------------------------
 Model: phabs[1]( powerlaw[2] + bbody[3] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs    nH     10^22   4.000    frozen
  2  2  2  powerlaw  PhoIndex      6.401   +/- 0.3873
  3  3  2  powerlaw  norm         1.086   +/- 0.3032
  4  4  3  bbody    kT     keV    1.199   +/- 0.8082E-01
  5  5  3  bbody    norm         2.6530E-04 +/- 0.3371E-04
 ------------------------------------------------------------------------------
 ------------------------------------------------------------------------------
 Chi-Squared =   37.21207   using  31 PHA bins.
 Reduced chi-squared =   1.378225   for   27 degrees of freedom
 Null hypothesis probability = 9.118E-02
```

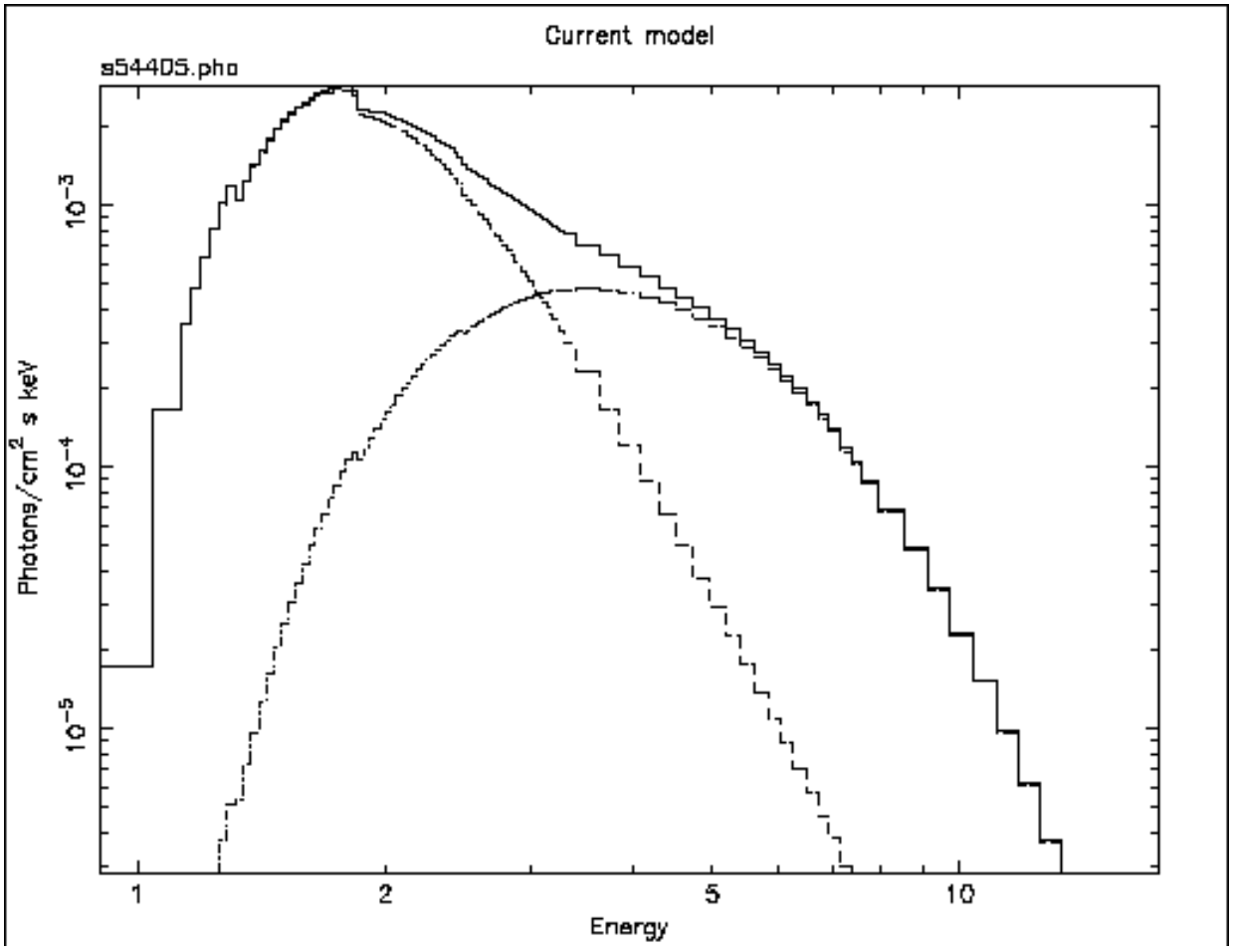


Figure F: The result of the command plot model in the case of the ME data file from 1E1048.1—5937. Here, the model is the best-fitting combination of power law, black body and fixed Galactic absorption. The three lines show the two continuum components (absorbed to the same degree) and their sum.

This, of course, is a better fit, but the photon index of the power law has ended up extremely and implausibly steep. Looking at this odd model with the command

```
XSPEC12> plot model
```

we see, in Figure F, that the black body and the power law have changed places, in that the power law provides the soft photons required by the high absorption, while the black body provides the harder photons.

We could continue to search for a plausible, well-fitting model, but the data, with their limited signal-to-noise and energy resolution, probably don't warrant it (the original investigators published only the power law fit). There is, however, one final, useful thing to do with the data: derive an upper limit to the presence of a fluorescent iron emission line. First we delete the black body component using **delcomp**:

```
XSPEC12>delcomp 3
 Model: phabs[1]( powerlaw[2] )
 Chi-Squared =   1285.487   using  31 PHA bins.
 Reduced chi-squared =   44.32712   for   29 degrees of freedom

Then we thaw N_H and refit to recover our original, best fit:

XSPEC12>thaw 1
 Number of variable fit parameters =  3
XSPEC12>fit
 Chi-Squared  Lvl Fit param # 1   2      3
  924.178   -2   5.087    5.076   0.4056
  305.507   -2   4.525    3.791   0.1249
  140.460   -2   2.930    3.367   6.5553E-02
  64.4275   -3   0.6068    2.244   1.4635E-02
  30.3738   -4   0.4837    2.201   1.2279E-02
  30.1189   -5   0.4641    2.195   1.2258E-02
  30.1189   -6   0.4637    2.195   1.2255E-02
 ------------------------------------------------------------------------
 Variances and Principal axes :
        1   2   3
 4.13E-08 | 0.00 -0.01 1.00
 8.69E-02 | -0.91 -0.41 -0.01
 2.31E-03 | -0.41 0.91 0.01
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Model: phabs[1]( powerlaw[2] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22   0.4637   +/- 0.2696
  2  2  2  powerlaw  PhoIndex      2.195   +/- 0.1287
  3  3  2  powerlaw  norm        1.2255E-02 +/- 0.2412E-02
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Chi-Squared =   30.11890   using  31 PHA bins.
 Reduced chi-squared =   1.075675   for   28 degrees of freedom
```

```
 Null hypothesis probability = 0.358
```

Now, we add a gaussian emission line of fixed energy and width:

```
XSPEC12>editmod pha(po+ga)
 Model: phabs[1]( powerlaw[2] + gaussian[3] )
Input parameter value, delta, min, bot, top, and max values for ...
Current:    6.5   0.05     0     0   1E+06   1E+06
gaussian:LineE>6.4 0
Current:    0.1   0.05     0     0    10    20
gaussian:Sigma>0.1 0
Current:     1   0.01     0     0   1E+24   1E+24
gaussian:norm>1.e-4
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Model: phabs[1]( powerlaw[2] + gaussian[3] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22   0.4637   +/- 0.2696
  2  2  2  powerlaw  PhoIndex      2.195   +/- 0.1287
  3  3  2  powerlaw  norm        1.2255E-02 +/- 0.2412E-02
  4  4  3  gaussian  LineE  keV    6.400   frozen
  5  5  3  gaussian  Sigma  keV    0.1000   frozen
  6  6  3  gaussian  norm        1.0000E-04 +/-   0.
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Chi-Squared =   32.75002   using  31 PHA bins.
 Reduced chi-squared =   1.212964   for   27 degrees of freedom
 Null hypothesis probability = 0.205
XSPEC12>fit
...
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Model: phabs[1]( powerlaw[2] + gaussian[3] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22   0.6562   +/- 0.3193
  2  2  2  powerlaw  PhoIndex      2.324   +/- 0.1700
  3  3  2  powerlaw  norm        1.4636E-02 +/- 0.3642E-02
  4  4  3  gaussian  LineE  keV    6.400   frozen
  5  5  3  gaussian  Sigma  keV    0.1000   frozen
  6  6  3  gaussian  norm        9.6462E-05 +/- 0.9542E-04
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Chi-Squared =   29.18509   using  31 PHA bins.
 Reduced chi-squared =   1.080929   for   27 degrees of freedom
 Null hypothesis probability = 0.352
```

The energy and width have to be frozen because, in the absence of an obvious line in the data, the fit would be completely unable to converge on meaningful values. Besides, our aim is to see how bright a line at 6.4 keV can be and still not ruin the fit. To do this, we fit first and then use the **error** command to derive the maximum allowable iron line normalization. We then set the normalization at this maximum value with **newpar** and, finally, derive the equivalent width using the **eqwidth** command. That is:

```
XSPEC12>err 6
 Parameter  Confidence Range (   2.706)
 Parameter pegged at hard limit     0.
 with delta ftstat=  0.9338
   6     0.    1.530722E-04
XSPEC12>new 6 1.530722E-04
  4 variable fit parameters
 Chi-Squared =   34.91923   using  31 PHA bins.
 Reduced chi-squared =   1.293305   for   27 degrees of freedom
 Null hypothesis probability = 0.141
XSPEC12>eqwidth 3
 Additive group equiv width for model 3 (gaussian): 839. eV
```

Things to note:

The true minimum value of the gaussian normalization is less than zero, but the **error** command stopped searching for a $\Delta\chi^2$ of 2.706 when the minimum value hit zero, the "hard" lower limit of the parameter. Hard limits can be adjusted with the **newpar** command, and they correspond to the quantities `min` and `max` associated with the parameter values. In fact, according to the screen output, the value of $\Delta\chi^2$ corresponding to zero normalization is 0.934.

The command **eqwidth** takes the component number as its argument.

The upper limit on the equivalent width of a 6.4 keV emission line is high (839 eV)!

4.3 Simultaneous Fitting: Examples from Einstein and Ginga

XSPEC has the very useful facility of allowing models to be fitted simultaneously to more than one data file. It is even possible to group files together and to fit different models simultaneously. Reasons for fitting in this manner include:

The same target is observed at several epochs but, although the source stays constant, the response matrix has changed. When this happens, the data files cannot be added together; they have to be fitted separately. Fitting the data files simultaneously yields tighter constraints.

The same target is observed with different instruments. The GIS and SIS on *ASCA*, for example, observe in the same direction simultaneously. As far as XSPEC is concerned, this is just like the previous case: two data files with two responses fitted simultaneously with the same model.

Different targets are observed, but the user wants to fit the same model to each data file with some parameters shared and some allowed to vary separately. For example, if you have a series of spectra from a variable AGN, you might want to fit them simultaneously with a model that has the same, common photon index but separately vary the normalization and absorption.

Other scenarios are possible---the important thing is to recognize the flexibility of XSPEC in this regard.

As an example of the first case, we'll fit two spectra derived from two separate *Einstein* Solid State Spectrometer (SSS) observations of the cooling-flow cluster Abell 496. Although the two observations were carried out on consecutive days (in August 1979), the response is different, due to the variable build-up of ice on the detector. This problem bedeviled analysis during the

mission; however, it has now been calibrated successfully and is incorporated into the response matrices associated with the spectral files in the HEASARC archive. The SSS also provides an example of how background correction files are used in XSPEC.

To fit the same model with the same set of parameters to more than one data file, simply enter the names of the data files after the **data** command:

```
XSPEC12> data sa496b.pha sa496c.pha
 Net count rate (cts/s) for file  1 0.7806  +/- 9.3808E+05( 86.9% total)
  using response (RMF) file...    sa496b.rsp
  using background file...      sa496b.bck
  using correction file...      sa496b.cor
 Net count rate (cts/s) for file  2 0.8002  +/- 9.3808E+05( 86.7% total)
  using response (RMF) file...    sa496c.rsp
  using background file...      sa496c.bck
  using correction file...      sa496c.cor
 Net correction flux for file 1=  8.4469E-04
 Net correction flux for file 2=  8.7577E-04
  2 data sets are in use
```

As the messages indicate, XSPEC also has read in the associated:

response files (`sa496b.rsp` & `sa496c.rsp`),

background files (`sa496b.bck`& `sa496c.bck`) and

correction files (`sa496b.cor` & `sa496c.cor`).

These files are all listed in the headers of the data files (`sa496b.pha` & `sa496c.pha`).

To ignore channels, the file number (1 & 2 in this example) precedes the range of channels to be ignored. Here, we wish to ignore, for both files, channels 1—15 and channels 100—128. This can be done by specifying the files one after the other with the range of ignored channels:

```
XSPEC12> ignore 1:1-15 1:100-128 2:1-15 2:100-128
 Chi-Squared =   1933.559   using  168 PHA bins.
 Reduced chi-squared =   11.79000   for  164 degrees of freedom
 Null hypothesis probability =  0.

or by specifying the range of file number with the channel range:

XSPEC12> ignore 1-2:1-15 100-128
```

In this example, we'll fit a cooling-flow model under the reasonable assumption that the small SSS field of view sees mostly just the cool gas in the middle of the cluster. We'll freeze the values of the maximum temperature (the temperature from which the gas cools) and of the abundance to the values found by instruments such as the *Ginga* LAC and the *EXOSAT* ME, which observed the entire cluster. The minimum gas temperature is frozen at 0.1 keV; the “slope” is frozen at zero (isobaric cooling) and the normalization is given an initial value of 100 solar masses per year:

```
XSPEC12>mo pha(cflow)
 Model: phabs[1]( cflow[2] )
Input parameter value, delta, min, bot, top, and max values for ...
Current:     1   0.001     0     0   1E+05   1E+06
phabs:nH>0.045
Current:     0   0.01    -5    -5     5     5
cflow:slope>0,0
Current:    0.1   0.001  0.0808  0.0808   79.9   79.9
cflow:lowT>0.1,0
Current:     4   0.001  0.0808  0.0808   79.9   79.9
cflow:highT>4,0
Current:     1   0.01     0     0     5     5
cflow:Abundanc>0.5,0
Current:     0   -0.1     0     0    100    100
cflow:Redshift>0.032
Current:     1   0.01     0     0   1E+24   1E+24
cflow:norm>100
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Model: phabs[1]( cflow[2] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22   4.5000E-02 +/-   0.
  2  2  2  cflow   slope         0.   frozen
  3  3  2  cflow   lowT   keV    0.1000   frozen
  4  4  2  cflow   highT  keV    4.000   frozen
  5  5  2  cflow   Abundanc      0.5000   frozen
  6  6  2  cflow   Redshift      3.2000E-02 frozen
  7  7  2  cflow   norm        100.0   +/-   0.
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Chi-Squared =   2740.606   using  168 PHA bins.
 Reduced chi-squared =   16.50968   for  166 degrees of freedom
 Null hypothesis probability =  0.
XSPEC12>fit
 Chi-Squared  Lvl Fit param # 1   2      3      4
         5      6      7
  414.248   -3   0.2050     0.   0.1000    4.000
       0.5000   3.2000E-02  288.5
  373.205   -4   0.2508     0.   0.1000    4.000
       0.5000   3.2000E-02  321.9
  372.649   -5   0.2566     0.   0.1000    4.000
       0.5000   3.2000E-02  325.9
  372.640   -6   0.2574     0.   0.1000    4.000
       0.5000   3.2000E-02  326.3
 ------------------------------------------------------------------------
 Variances and Principal axes :
        1   7
 3.55E-05 | -1.00 0.00
 3.52E+01 | 0.00 -1.00
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Model: phabs[1]( cflow[2] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
```

```
 1  1  1  phabs   nH    10^22   0.2574   +/- 0.9219E-02
 2  2  2  cflow   slope         0.   frozen
 3  3  2  cflow   lowT   keV    0.1000   frozen
 4  4  2  cflow   highT  keV    4.000   frozen
 5  5  2  cflow   Abundanc      0.5000   frozen
 6  6  2  cflow   Redshift      3.2000E-02 frozen
 7  7  2  cflow   norm        326.3   +/-  5.929
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Chi-Squared =   372.6400   using  168 PHA bins.
 Reduced chi-squared =   2.244819   for  166 degrees of freedom
 Null hypothesis probability = 6.535E-18
```

As we can see, χ^2 is not good, but the high statistic could be because we have yet to adjust the correction file. Correction files in XSPEC take into account detector features that cannot be completely prescribed *ab initio* and which must be fitted at the same time as the model. *Einstein* SSS spectra, for example, have a background feature the level of which varies unpredictably. Its spectral form is contained in the correction file, but its normalization is determined by fitting. This fitting is set in motion using the command **recornrm** (reset the correction-file normalization):

```
XSPEC12>reco 1
 File #   Correction
   1   0.4118 +/- 0.0673
 After correction norm adjustment 0.412 +/- 0.067
 Chi-Squared =   335.1577   using  168 PHA bins.
 Reduced chi-squared =   2.019022   for  166 degrees of freedom
 Null hypothesis probability = 1.650E-13
XSPEC12>reco 2
 File #   Correction
   2   0.4864 +/- 0.0597
 After correction norm adjustment 0.486 +/- 0.060
 Chi-Squared =   268.8205   using  168 PHA bins.
 Reduced chi-squared =   1.619400   for  166 degrees of freedom
 Null hypothesis probability = 7.552E-07
```

This process is iterative, and, in order to work must be used in tandem with fitting the model. Successive fits and recorrections are applied until the fit is stable, i.e., until further improvement in χ^2 no longer results. Of course, this procedure is only worthwhile when the model gives a reasonably good account of the data. Eventually, we end up at:

```
XSPEC12>fit
 Chi-Squared  Lvl Fit param # 1   2      3      4
         5      6      7
  224.887   -3   0.2804     0.   0.1000    4.000
       0.5000   3.2000E-02  313.0
  224.792   -4   0.2835     0.   0.1000    4.000
       0.5000   3.2000E-02  314.5
  224.791   -5   0.2837     0.   0.1000    4.000
       0.5000   3.2000E-02  314.6
 ------------------------------------------------------------------------
```

```
Variances and Principal axes :
       1   7
4.64E-05 | -1.00 0.00
3.78E+01 | 0.00 -1.00
------------------------------------------------------------------------
------------------------------------------------------------------------
Model: phabs[1]( cflow[2] )
Model Fit Model Component Parameter Unit   Value
par  par comp
 1  1  1  phabs   nH    10^22   0.2837   +/- 0.1051E-01
 2  2  2  cflow   slope         0.   frozen
 3  3  2  cflow   lowT   keV    0.1000   frozen
 4  4  2  cflow   highT  keV    4.000   frozen
 5  5  2  cflow   Abundanc      0.5000   frozen
 6  6  2  cflow   Redshift      3.2000E-02 frozen
 7  7  2  cflow   norm        314.6   +/-  6.147
------------------------------------------------------------------------
------------------------------------------------------------------------
Chi-Squared =   224.7912   using  168 PHA bins.
Reduced chi-squared =   1.354164   for  166 degrees of freedom
Null hypothesis probability = 1.616E-03
```

The final value of χ^2 is much better than the original, but is not quite acceptable. However, the current model has only two free parameters: further explorations of parameter space would undoubtedly improve the fit.

We'll leave this example and move on to look at another kind of simultaneous fitting: one where the same model is fitted to two different data files. This time, not all the parameters will be identical. The massive X-ray binary Centaurus X-3 was observed with the LAC on *Ginga* in 1989. Its flux level before eclipse was much lower than the level after eclipse. Here, we'll use XSPEC to see whether spectra from these two phases can be fitted with the same model, which differs only in the amount of absorption. This kind of fitting relies on introducing an extra dimension, the *group*, to the indexing of the data files. The files in each group share the same model but not necessarily the same parameter values, which may be shared as common to all the groups or varied separately from group to group. Although each group may contain more than one file, there is only one file in each of the two groups in this example. Groups are specified with the data command, with the group number preceding the file number, like this:

```
XSPEC12> da 1:1 losum 2:2 hisum
 Net count rate (cts/s) for file  1  140.1  +/- 0.3549
  using response (RMF) file...    ginga_lac.rsp
 Net count rate (cts/s) for file  2  1371.  +/-  3.123
  using response (RMF) file...    ginga_lac.rsp
  2 data sets are in use
```

Here, the first group makes up the file `losum.pha`, which contains the spectrum of all the low, pre-eclipse emission. The second group makes up the second file, `hisum.pha`, which contains all the high, post-eclipse emission. Note that file number is "absolute" in the sense that it is independent of group number. Thus, if there were three files in each of the two groups (`lo1.pha`, `lo2.pha`, `lo3.pha`, `hi1.pha`, `hi2.pha, and hi3.pha`, say), rather than one, the six files would be specified as **da** `1:1 lo1 1:2 lo2 1:3 lo3 2:4 hi1 2:5 hi2 2:6 hi3`. The **ignore** command works, as usual, on file number, and does not take group number into account. So, to ignore channels 1–3 and 37–48 of both files:

XSPEC12> ignore 1-2:1-3 37-48

The model we'll use at first to fit the two files is an absorbed power law with a high-energy cut-off:

XSPEC12> mo phabs * highecut (po)

After defining the model, the user is prompted for two sets of parameter values, one for the first group of data files (`losum.pha`), the other for the second group (`hisum.pha`). Here, we'll enter the absorption column of the first group as 10^{24} cm^{-2} and enter the default values for all the other parameters in the first group. Now, when it comes to the second group of parameters, we enter a column of 10^{22} cm^{-2} and then enter defaults for the other parameters. The rule being applied here is as follows: to tie parameters in the second group to their equivalents in the first group, take the default when entering the second-group parameters; to allow parameters in the second group to vary independently of their equivalents in the first group, enter different values explicitly:

```
XSPEC12>mo phabs*highecut(po)
 Model: phabs[1]*highecut[2]( powerlaw[3] )
Input parameter value, delta, min, bot, top, and max values for ...
Current:     1   0.001     0     0   1E+05   1E+06
DataGroup 1:phabs:nH>100
Current:     10   0.01  0.0001   0.01   1E+06   1E+06
DataGroup 1:highecut:cutoffE>/
Current:     15   0.01  0.0001   0.01   1E+06   1E+06
DataGroup 1:highecut:foldE>/
Current:     1   0.01    -3    -2     9    10
DataGroup 1:powerlaw:PhoIndex>/
Current:     1   0.01     0     0   1E+24   1E+24
DataGroup 1:powerlaw:norm>/
Current:    100   0.001     0     0   1E+05   1E+06
DataGroup 2:phabs:nH>1
Current:     10   0.01  0.0001   0.01   1E+06   1E+06
DataGroup 2:highecut:cutoffE>/*
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Model: phabs[1]*highecut[2]( powerlaw[3] )
```

```
 Model Fit Model Component Parameter Unit   Value          Data
 par  par comp                              group
  1  1  1  phabs   nH    10^22   100.0   +/-   0.    1
  2  2  2  highecut  cutoffE keV    10.00   +/-   0.    1
  3  3  2  highecut  foldE  keV    15.00   +/-   0.    1
  4  4  3  powerlaw  PhoIndex      1.000   +/-   0.    1
  5  5  3  powerlaw  norm        1.000   +/-   0.    1
  6  6  4  phabs   nH    10^22   1.000   +/-   0.    2
  7  2  5  highecut  cutoffE keV    10.00   = par  2     2
  8  3  5  highecut  foldE  keV    15.00   = par  3     2
  9  4  6  powerlaw  PhoIndex      1.000   = par  4     2
  10  5  6  powerlaw  norm        1.000   = par  5     2
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Chi-Squared =   2.0263934E+07 using  66 PHA bins.
 Reduced chi-squared =   337732.2   for   60 degrees of freedom
 Null hypothesis probability =  0.
```

Notice how the summary of the model, displayed immediately above, is different now that we have two groups, as opposed to one (as in all the previous examples). We can see that of the 10 model parameters, 6 are free (i.e., 4 of the second group parameters are tied to their equivalents in the first group). Fitting this model results in a huge χ^2 (not shown here), because our assumption that only a change in absorption can account for the spectral variation before and after eclipse is clearly wrong. Perhaps scattering also plays a role in reducing the flux before eclipse. This could be modeled (simply at first) by allowing the normalization of the power law to be smaller before eclipse than after eclipse. To decouple tied parameters, we change the parameter value in the second group to a value—any value—different from that in the first group (changing the value in the first group has the effect of changing both without decoupling). As usual, the **newpar** command is used:

```
XSPEC12>newpar 10 1
  7 variable fit parameters
 Chi-Squared =   2.0263934E+07 using  66 PHA bins.
 Reduced chi-squared =   343456.5   for   59 degrees of freedom
 Null hypothesis probability =  0.
XSPEC12>fit
...
 ------------------------------------------------------------------------
 Model: phabs[1]*highecut[2]( powerlaw[3] )
 Model Fit Model Component Parameter Unit   Value          Data
 par  par comp                              group
  1  1  1  phabs   nH    10^22   20.23   +/- 0.1823    1
  2  2  2  highecut  cutoffE keV    14.68   +/- 0.5552E-01  1
  3  3  2  highecut  foldE  keV    7.430   +/- 0.8945E-01  1
  4  4  3  powerlaw  PhoIndex      1.187   +/- 0.6505E-02  1
  5  5  3  powerlaw  norm        5.8958E-02 +/- 0.9334E-03  1
  6  6  4  phabs   nH    10^22   1.270   +/- 0.3762E-01  2
  7  2  5  highecut  cutoffE keV    14.68   = par  2     2
  8  3  5  highecut  foldE  keV    7.430   = par  3     2
  9  4  6  powerlaw  PhoIndex      1.187   = par  4     2
  10  7  6  powerlaw  norm        0.3123   +/- 0.4513E-02  2
```

```
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
Chi-Squared =   15424.73   using  66 PHA bins.
Reduced chi-squared =   261.4362   for   59 degrees of freedom
Null hypothesis probability =  0.
```

After fitting, this decoupling reduces χ^2 by a factor of six to 15,478, but this is still too high. Indeed, this simple attempt to account for the spectral variability in terms of "blanket" cold absorption and scattering does not work. More sophisticated models, involving additional components and partial absorption, should be investigated.

4.4 Using XSPEC to Simulate Data: an Example from ASCA

In several cases, analyzing simulated data is a powerful tool to demonstrate feasibility. For example:

To support an observing proposal. That is, to demonstrate what constraints a proposed observation would yield.

To support a hardware proposal. If a response matrix is generated, it can be used to demonstrate what kind of science could be done with a new instrument.

To support a theoretical paper. A theorist could write a paper describing a model, and then show how these model spectra would appear when observed. This, of course, is very like the first case.

Here, we'll use XSPEC to see how an *ASCA* observation of the elliptical galaxy NGC 4472 can constrain the condition of the hot gas. The first step is to define a model on which to base the simulation. The way XSPEC creates simulated data is to take the current model, convolve it with the current response matrix, while adding noise appropriate to the integration time specified. Once created, the simulated data can be analyzed in the same way as real data to derive confidence limits.

We begin by looking in the literature for the best estimate of the NGC 4472 spectrum. *BBXRT* observed the galaxy in 1990 and the results were published in Serlemitsos et al., (1993). They found a flux in the 0.5–4.5 keV range of 6.7×10^{-12} erg cm$^{-2}s^{-1}$, a temperature range of 0.74 < kT < 0.98, an abundance range (as a fraction of solar) of 0.09 < A < 0.46 and a column range of $5\times10^{20} < N_H < 3.7\times10^{21} cm^{-2}$. A Raymond-Smith spectral model was found to give a good fit. We specify this model at first with the median parameter values, except for the normalization of the Raymond-Smith, which we leave at its default value of unity at first (but adjust later):

```
XSPEC12>mo pha(ray)
 Model: phabs[1]( raymond[2] )
Input parameter value, delta, min, bot, top, and max values for ...
Current:     1   0.001     0     0   1E+05   1E+06
phabs:nH>0.21
Current:     1   0.01   0.008   0.008    64    64
raymond:kT>0.86
Current:     1  -0.001     0     0     5     5
raymond:Abundanc>0.27
Current:     0  -0.001     0     0     2     2
raymond:Redshift>/*
 ------------------------------------------------------------------------
```

```
------------------------------------------------------------------------
Model: phabs[1]( raymond[2] )
Model Fit Model Component Parameter Unit   Value
par  par comp
 1  1  1  phabs   nH    10^22   0.2100   +/-   0.
 2  2  2  raymond  kT    keV    0.8600   +/-   0.
 3  3  2  raymond  Abundanc      0.2700   frozen
 4  4  2  raymond  Redshift        0.   frozen
 5  5  2  raymond  norm        1.000   +/-   0.
------------------------------------------------------------------------
------------------------------------------------------------------------
```

We now can derive the correct normalization by using the commands **dummyrsp**, **flux** and **newpar**. That is, we'll determine the flux of the model with the normalization of unity (this requires a response matrix to cover the *BBXRT* band—we use a dummy response here). We then work out the new normalization and reset it:

```
XSPEC12> dummy 0.5 4.5
XSPEC12>flux 0.5 4.5
 Model flux 0.2802   photons ( 4.9626E-10 ergs)cm**-2 s**-1 ( 0.500- 4.500)
XSPEC12> newpar 5 0.014
  3 variable fit parameters
XSPEC12>flux
 Model flux 3.9235E-03 photons ( 6.9476E-12 ergs)cm**-2 s**-1 ( 0.500- 4.500)
```

Here, we have changed the value of the normalization (the fifth parameter) from 1 to $6.7\times10^{-12}/4.78\times10^{-10}=0.014$ to give the flux observed by *BBXRT* (6.7×10^{-12} erg cm$^{-2}s^{-1}$ in the energy range 0.5–4.5).

The simulation is initiated with the command **fakeit**. If the argument `none` is given, the user will be prompted for the name of the response matrix. If no argument is given, the current response will be used:

```
XSPEC12>fakeit none
For fake data, file #1 needs response file: s0c1g0234p40e1_512_1av0_8i
       ... and ancillary response file: none
```

There then follows a series of prompts asking the user to specify whether he or she wants counting statistics (yes!), the name of the fake data (file `ngc4472_sis.fak` in our example), and the integration time T (40,000 seconds – `cornorm` can be left at its default value).

```
Use counting statistics in creating fake data? (y) /
Input optional fake file prefix (max 4 chars): /
 Fake data filename (s0c1g0234p40e1_512_1av0_8i.fak) [/ to use default]:
ngc4472_sis.fak
 T, cornorm (1, 0): 40000
 Net count rate (cts/s) for file  1 0.3563  +/- 3.0221E-03
```

```
 using response (RMF) file...    s0c1g0234p40e1_512_1av0_8i.rsp
 Chi-Squared =   188.6545   using  512 PHA bins.
 Reduced chi-squared =   0.3706375   for  509 degrees of freedom
 Null hypothesis probability = 1.00
```

We now have created a file containing a simulated spectrum of NGC 4472. As is usual before fitting, we need to check which channels to ignore. This time, we'll examine the actual numbers of counts in each channel and reject those that have fewer than 20 per channel. We use **iplot** `counts` and see that our criterion requires us to ignore channels 1–15 and 76–512:

```
XSPEC12>ignore 1-15 76-**
 Chi-Squared =   63.30437   using  60 PHA bins.
 Reduced chi-squared =   1.110603   for   57 degrees of freedom
 Null hypothesis probability = 0.264
```

As expected, χ^2 is reasonable even before fitting because the model and the data have the same shape. But the point of this simulation is to determine confidence ranges. First, we thaw the value of the abundance (fixed by default), fit and then use the **error** command:

```
XSPEC12> thaw 3
 Number of variable fit parameters =  4
XSPEC12>fit
 Chi-Squared  Lvl Fit param # 1   2      3      4
         5
  55.3176   -3   0.2309   0.8569   0.2772     0.
       1.4322E-02
  55.2946   -4   0.2320   0.8565   0.2784     0.
       1.4322E-02
  55.2945   -5   0.2321   0.8565   0.2784     0.
       1.4322E-02
 ------------------------------------------------------------------------
 Variances and Principal axes :
        1   2   3   5
 1.51E-08 | -0.03 -0.01 0.03 1.00
 1.02E-05 | 0.39 0.91 -0.11 0.03
 9.98E-05 | -0.91 0.40 0.11 -0.03
 2.32E-04 | -0.15 -0.06 -0.99 0.03
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Model: phabs[1]( raymond[2] )
 Model Fit Model Component Parameter Unit   Value
 par  par comp
  1  1  1  phabs   nH    10^22   0.2321   +/- 0.9426E-02
  2  2  2  raymond  kT    keV    0.8565   +/- 0.5048E-02
  3  3  2  raymond  Abundanc      0.2784   +/- 0.1510E-01
  4  4  2  raymond  Redshift        0.   frozen
  5  5  2  raymond  norm        1.4322E-02 +/- 0.5423E-03
 ------------------------------------------------------------------------
 ------------------------------------------------------------------------
 Chi-Squared =   55.29454   using  60 PHA bins.
```

```
 Reduced chi-squared =   0.9874024   for   56 degrees of freedom
 Null hypothesis probability = 0.502
XSPEC12>err 1 2 3
 Parameter  Confidence Range (   2.706)
   1  0.217009    0.248102
   2  0.847909    0.864666
   3  0.254807    0.304992
```

These confidence ranges show that an *ASCA* observation would definitely constrain the parameters, especially the column and abundance, more tightly than the original *BBXRT* observation. Of course, whether these constraints are sufficient depends on the theories being tested. When producing and analyzing simulated data, it is crucial to keep in mind the purpose of the proposed observation, for the potential parameter space that can be covered with simulations is almost limitless.

4.5 Producing Plots: Modifying the Defaults

The final results of using XSPEC are usually one or more tables containing confidence ranges and fit statistics, and one or more plots showing the fits themselves. So far, all the plots shown have the default settings, but it is possible to edit plots to get closer to the appearance what you want.

The plotting package used by XSPEC is PGPLOT, which is comprised of a library of low-level tasks. At a higher level is QDP/PLT, the interactive program that forms the interface between the XSPEC user and PGPLOT. QDP/PLT has its own manual; it also comes with on-line help. Here, we show how to make some of the most common modifications to plots.

To initiate interactive plotting in XSPEC, use the command **iplot** instead of the usual **plot**. In this example, we'll take the simulated *ASCA* SIS spectrum of the previous section and make the following modifications to the **data** plot:

Change the aspect ratio

Change the labels

Rescale the x-axis and y-axis

Change the y-axis to be a logarithmic scale

Thicken the lines and make the characters smaller to make the hardcopy look better

Produce a postscript file

After the **iplot** command, the plot itself appears, followed by the QDP/PLT prompt:

XSPEC12> **setplot** energy

XSPEC12> **iplot** data

PLT>

The first thing we'll do is change the aspect ratio of the box that contains the plot (*viewport* in QDP terminology). The viewport is defined by the coordinates of the lower left and upper right corners of the page, normalized so that the width and height of the page are unity. The labels fall outside the viewport, so if the full viewport were specified, only the plot would appear. The default box has a viewport with corners at (0.1, 0.1) and (0.9, 0.9). For our purposes, we want a viewport with corners at (0.2, 0.2) and (0.8, 0.7): with this size and shape, the hardcopy will fit nicely on the page and not have to be reduced for photocopying. To change the viewport, use the command *viewport* followed by the coordinates:

```
PLT> viewport 0.2 0.2 0.8 0.7
```

Next we want to change two of the labels: the label at the top, which currently says only *data*, and the label that specifies the filename. This change is a straightforward one using the `label` command, which takes as arguments a location description and the text string:

```
PLT> label top Simulated Spectrum of NGC 4472
PLT> label file ASCA SIS
```

Other location descriptors are available, including `x` and `y` for the x-axis and y-axis, respectively. To get help on a QDP command, type `help` followed by the name of the command at the `PLT>` prompt. Note that QDP commands can be abbreviated, just like XSPEC commands. To see the results of changing the viewport and the labels, just enter the command `plot`:

```
PLT> plot
```

The two changes we want to make next are to rescale the axes and to change the y-axis to a logarithmic scale. The commands for these changes also are straightforward: the `rescale` command takes the minimum and maximum values as its arguments, while the `log` command takes `x` or `y` as arguments:

```
PLT> rescale x 0.4 2.5
PLT> rescale y 0.01 1
PLT> log y
PLT> plot
```

To revert to a linear scale, use the command `log off y`. All that is left to change are the thickness of the lines (the default, least for postscript files that are turned into hardcopies, is too fine) and the size of the characters (we want slightly smaller characters). The `lwidth` command does the former: it takes a width as its argument: the default is 1: we'll reset it to 3. The `csize` command does the latter, taking a normalization as its argument. One (1) will not change the size, a number less than one will reduce it and a number bigger than one will increase it.

```
PLT> lwidth 3
```

```
PLT> csize 0.8
PLT> plot
```

Finally, to produce a postscript file that we can print, we use the

```
PLT> hardcopy ngc4472_sis.ps/ps
PLT> quit
```

Here, we have given the file the name **`ngc4472_sis.ps.`** It will be written into the current directory. The suffix **`ps`** tells the program to produce a postscript file. The quit command returns us to the `XSPEC12>` prompt.

The result of all this manipulation is shown proudly in Figure G.

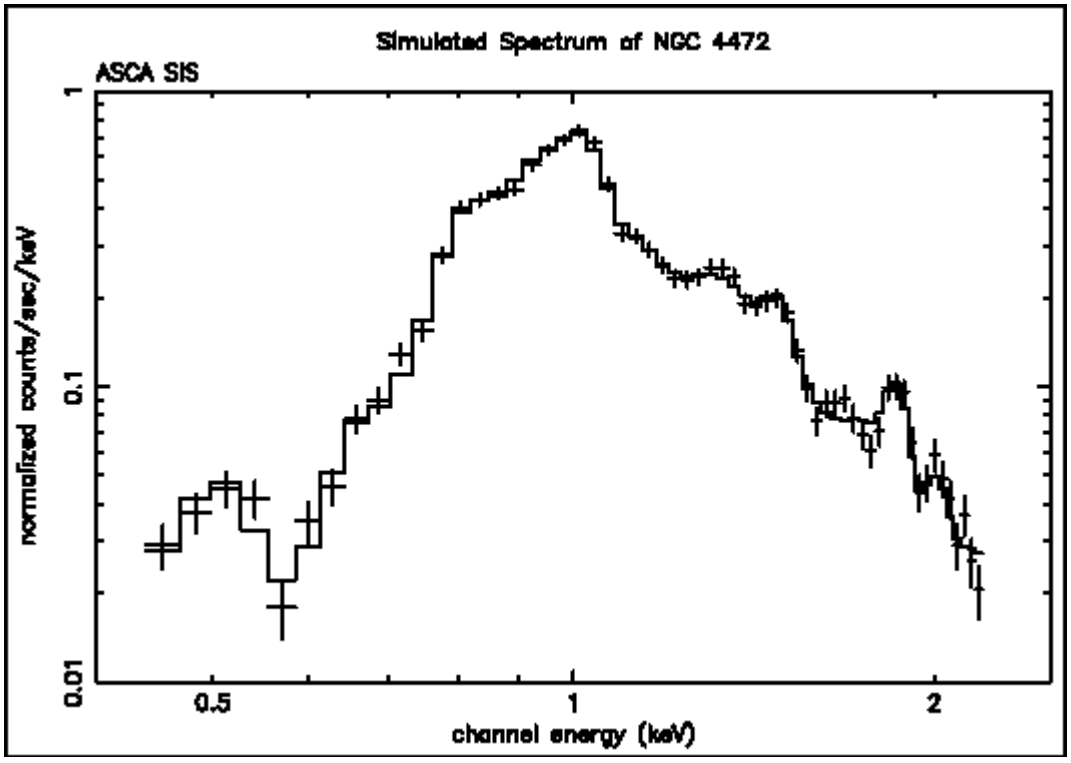


Figure G: A simulated ASCA SIS spectrum of NGC 4472 produced to show how a plot can be modified by the user.

4.6 INTEGRAL/SPI

4.6.1 A Walk Through Example

Consider an observation of the Crab, for which a (standard) 5°×5°dithering observation strategy was employed. Since the Crab (pulsar and nebular components are of course un-resolvable at INTEGRAL's spatial resolution) is by far the brightest source in it immediate region of the sky, and its position is precisely known, we can opt not to perform SPI or IBIS imaging analysis prior to XSPEC analysis. We thus run the standard INTEGRAL/SPI analysis chain on detectors 0-18 up to the SPIHIST level for (or BIN_I level in the terminology of the INTEGRAL documentation),

selecting the "PHA" output option. We then run SPIARF, providing the name of the PHA-II file just created, and selecting the "update" option in the spiarf.par parameter file (you should refer to the SPIARF documentation prior to this step if it is unfamiliar). The celestial coordinates for the Crab are provided in decimal degrees (RA,Dec = 83.63,22.01) interactively or by editing the parameter file. This may take a few minutes, depending on the speed of your computer and the length of your observation. Once completed, SPIARF must be run one more time, setting the "bkg_resp" option to "y"; this creates the response matrices to be applied to the background model, and updates the PHA-II response database table accordingly. Then SPIRMF, which interpolates the template RMFs to the users desired spectral binning, also writes information to the PHA response database table to be used by XSPEC. Finally, you should run SPIBKG_INIT, which will construct a set of bbackground spectral templates to initialize the SPI background model currently installed in XSPEC (read the FTOOLS help for that utility carefully your first time). You are now ready to run XSPEC; a sample session might look like this (some repetitive output has been suppressed):

```
%
% xspec

                XSPEC version: 12.2.1
        Build Date/Time: Wed Nov 2 17:14:21 2005

XSPEC12>package require Integral 1.0
1.0
XSPEC12>data ./myDataDir/rev0044_crab.pha{1-19}

19 spectra  in use

RMF # 1
 Using Response (RMF) File            resp/comp1_100x100.rmf
RMF # 2
 Using Response (RMF) File            resp/comp2_100x100.rmf
RMF # 3
 Using Response (RMF) File            resp/comp3_100x100.rmf

Using Multiple Sources

For Source # 1
 Using Auxiliary Response (ARF) Files
     resp/rev0044_100ch_crab_cmp1.arf.fits
     resp/rev0044_100ch_crab_cmp2.arf.fits
     resp/rev0044_100ch_crab_cmp3.arf.fits
```

```
For Source # 2
 Using Auxiliary Response (ARF) Files
     resp/rev0044_100ch_bkg_cmp1.arf.fits
     resp/rev0044_100ch_bkg_cmp2.arf.fits
     resp/rev0044_100ch_bkg_cmp3.arf.fits

Source File: ./myDataDir/rev0044_crab.pha{1}
Net count rate (cts/s) for Spectrum No. 1    3.7011e+01   +/- 1.2119e-01
 Assigned to Data Group No. : 1
 Assigned to Plot Group No. : 1

Source File: ./myDataDir/rev0044_crab.pha{2}
Net count rate (cts/s) for Spectrum No. 2    3.7309e+01   +/- 1.2167e-01
 Assigned to Data Group No. : 1
 Assigned to Plot Group No. : 2
...
Source File: ./myDataDir/rev0044_crab.pha{19}
Net count rate (cts/s) for Spectrum No. 19   3.6913e+01   +/- 1.2103e-01
 Assigned to Data Group No. : 1
 Assigned to Plot Group No. : 19

XSPEC12>mo 1:crab po

Input parameter value, delta, min, bot, top, and max values for ...
    1    PhoIndex              1.0000E+00         1.0000E-02     -3.0000E+00
-2.0000E+00      9.0000E+00      1.0000E+01
crab::powerlaw:PhoIndex>2.11 0.01 1.5 1.6 2.5 2.6
    2        norm              1.0000E+00         1.0000E-02      0.0000E+00
0.0000E+00      1.0000E+24      1.0000E+24
crab::powerlaw:norm>8. 0.1 1. 2. 18. 20.
 …
 XSPEC12>mo 2:bkg spibkg5

Input parameter value, delta, min, bot, top, and max values for ...
    1       Par_1              0.0000E+00         1.0000E-02     -2.0000E-01
-1.5000E-01      1.5000E-01      2.0000E-01
bkg::spibkg5:Par_1>/*
 …
```

```
XSPEC12>ign 1-19:68-80
...
XSPEC12>ign 1-19:90-100
...
XSPEC12>fit
Number of trials and critical delta: 10  1.0000000E-02
 ...
========================================================================
Model bkg:spibkg5 Source No.: 2   Active/On
Model Component Name:  spibkg5  Number:    1
  N          Name       Unit       Value                 Sigma
    1       Par_1              9.0650E-03       +/-     2.8651E-03
    2       Par_2              1.6174E-02       +/-     3.4778E-03
  …
   25      Par_25             -1.9537E-02       +/-     6.1429E-03
   26        norm              9.7286E-01       +/-     1.3527E-03
------------------------------------------------------------------------

========================================================================
Model crab:powerlaw Source No.: 1   Active/On
Model Component Name: powerlaw  Number:    1
  N          Name       Unit       Value                 Sigma
    1    PhoIndex             2.1163E+00       +/-     1.8946E-02
    2        norm             1.1390E+01       +/-     8.1414E-01
------------------------------------------------------------------------

 Chi-Squared =  1.8993005E+03 using 1463 PHA bins.
 Reduced chi-squared =  1.3235544E+00 for   1435 degrees of freedom
 Null hypothesis probability =  1.5268098E-15
XSPEC12>
```

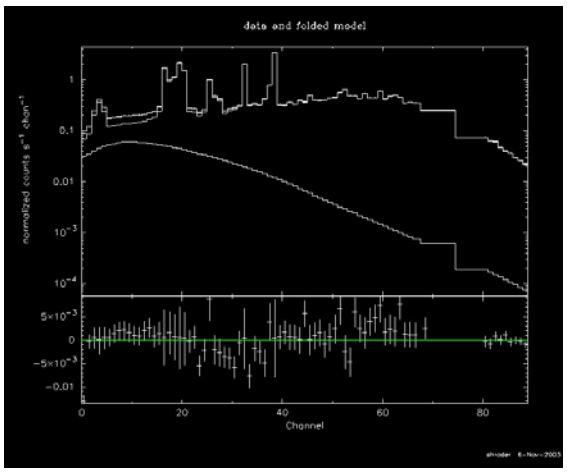
Note that the syntax used for the data statement (appended curly bracket, specifying use of spectra 1-19), and the separate model commands, which are indexed and named (in this case simply "crab" for the source of interest and "bkg" for the background model, "spibkg_lo". These commands are described in detail elsewhere in this document, as are the the spibkg_lo, spibkg_med

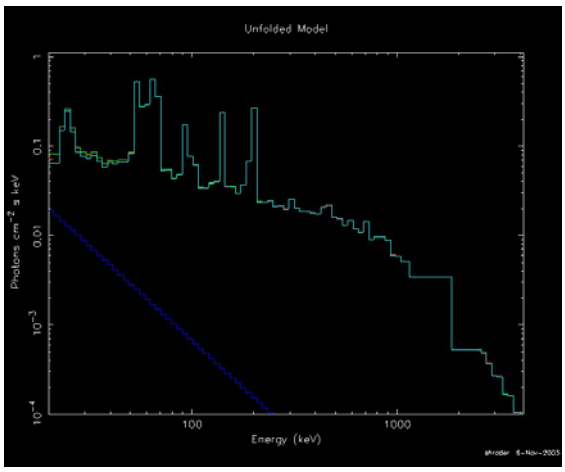
and spibkg_hi models. In this case, 100 logarithmically-spaced energy bins spanning the nominal 20-8000 keV band of the SPI instrument were used.

In this example, only one dither-point was used to solve for the Crab spectrum, and the background. The simple assumption of a single background spectrum (i.e. no detector-to-detector variations) was assumed. In general, and particularly for fainter sources, a much larger number of spectra will be needed for a solution (and even for the Crab, the quality of the fit, and the accuracy of the inferred parameters can be improved). Also, detector-to-detector and/or time (i.e. pointing-to-pointing) variations will need to be considered. This can be accomplished using the data-grouping feature of XSPEC, which will be described subsequently. Also notice that channels between about 70 and 80 were ignored; this is because there are detector electronic effects contaminating the single-event data for energies from ~1250-1400 keV (refer to the **SPI data analysis manual** for additional discussion), and that there are a lot of (scientifically uninteresting) background model parameters. Also, the highest energies were ignored, since the source flux becomes insignificant relative to the background.

Some results are illustrated below. These plots were generated with the sequence of commands:

```
XPSEC> setplot group 1-19
XSPEC12> plot ldata res
...
XSPEC12> plot ufspec
```





Note that without the "setplot group" command, XSPEC would plot 19 sets of spectral data, models and residuals. The can become confusing, especially as the number of spectra included in an analysis becomes much larger than 19! On the other hand, it can be useful to divide the data into subsets for plotting purposes, e.g. setplot group 1-6 7-12 13-19, to get an idea of relative shadowing

effects of the coded-mask. The left hand plot illustrates the source model, the background model, the total model (i.e. source + background), and the data (here in count rates per channel). The right hand plot illustrates the "unfolded model" (blue, power-law curve), the summed model, and the data as a photon flux. A possible source of confusion is the similarity of the background model curves plotted in theses two separate representations. The explanation is that the background, which is dominated by instrumental contributions, is modeled in detector count space (i.e. the background response matrix has unit effective area. Thus, to be strictly correct, the right-hand plot is a hybrid of the photon source model and the detector-rate background model. We further note that at the present time, XSPEC does not have the capability to plot (or store and manipulate) the background subtracted data. This is a feature under consideration for a future release.

If we had chosen a observation containing more than a single source, the procedure would have been similar, except that the sequence of model commands would be extended, e.g.

```
XSPEC12>data  ./MyDataDir/GCDE_aug_03.pha{1-475}
…
XSPEC12> model 1:1e1740 po
…
XSPEC12> model 2:gx1_4 po
…
XSPEC12> model 3:bkg spibkg_lo
…
```

Here data from the Galactic Center deep exposure campaign were loaded, and two sources are sought. In this case, a much larger number of spectra were loaded (475 spectra corresponds to one full 5×5 dither using all 19 detectors.

In this case, the simple approach of applying constant background (i.e. no detector-to-detector or pointing-to-pointing variation) to the full data set is likely to be a poor approximation. A more realistic approach would be to use the XSPEC grouping capability to handle such variations in the background solution. This can be accomplished in the usual manner (refer to the description of the grouping command in this document), however, it can become tedious in terms of the required command line inputs. For example, to establish a separate data group for each detector for a long (e.g. 5×5 dither) observations, a sequence of commands such as this would be required:

```
XSPEC12> data   1:1        ./MyDataDir/rev0044_Crab.pha.fits{1}
XSPEC12> data   2:2        ./MyDataDir/rev0044_Crab.pha.fits{2}
XSPEC12> data   3:3        ./MyDataDir/rev0044_Crab.pha.fits{3}
 ...
XSPEC12> data   19:19       ./MyDataDir/rev0044_Crab.pha.fits{19}
```

```
XSPEC12> data   1:20        ./MyDataDir/rev0044_Crab.pha.fits{20}
XSPEC12> data   2:21        ./MyDataDir/rev0044_Crab.pha.fits{21}
XSPEC12> data   3:22        ./MyDataDir/rev0044_Crab.pha.fits{22}
 ...
XSPEC12> data   19:38      ./MyDataDir/rev0044_Crab.pha.fits{38}
XSPEC12> data   1:39        /MyDataDir/rev0044_Crab.pha.fits{39}
XSPEC12> data   2:40        ./MyDataDir/rev0044_Crab.pha.fits{40}
XSPEC12> data   3:41        ./MyDataDir/rev0044_Crab.pha.fits{41}
 ...
XSPEC12> data   18:474       ./MyDataDir/rev0044_Crab.pha.fits{474}
XSPEC12> data   19:475       ./MyDataDir/rev0044_Crab.pha.fits{475}
```

One might then for example, make a first cut attempt by fitting a constant background. Then, as a next step, one might allow the normalization terms of the background model to vary over the groups (i.e. over the detector plane). This is accomplished with the "untie" command, using the following sequence:

```
XSPEC12>  untie   bkg:52
XSPEC12>  untie   bkg:78
XSPEC12>  untie   bkg:104
XSPEC12>  untie   bkg:130
XSPEC12>  untie   bkg:156
XSPEC12>  untie   bkg:182
XSPEC12>  untie   bkg:208
XSPEC12>  untie   bkg:234
XSPEC12>  untie   bkg:260
XSPEC12>  untie   bkg:286
XSPEC12>  untie   bkg:312
XSPEC12>  untie   bkg:338
XSPEC12>  untie   bkg:364
XSPEC12>  untie   bkg:390
XSPEC12>  untie   bkg:416
XSPEC12>  untie   bkg:442
XSPEC12>  untie   bkg:468
XSPEC12>  untie   bkg:487
```

Note that use of the "bkg" identifier, which associates the parameters index with the background model. The specific sequence of numbers use here requires some explanation; the

particular background model employed has 25 parameters (which simply correspond in rank order to the 25 most variable individual bins), and a normalization term, i.e. parameter 26. Thus, the normalization for the second detector group is parameter 52, for the third parameter 78, and so on. Similar command sequences can be used to untie additional background model parameters. Supposing that we did this and refitted the data. We then might, for example wish to go back and freeze the individual normalization terms with the freeze command:

```
XSPEC12>  freeze  bkg:26
XSPEC12>  freeze  bkg:52
 …
XSPEC12>  freeze  bkg:487
```

By now though, you probably get the idea that this all requires an unreasonable amount of command-line input. To circumvent this problem, a number of INTEGRAL/SPI specific "tcl" scripts are available which greatly streamline this process.

4.6.2 INTEGRAL Specific Command Line Scripts

SPIdata

The SPIdata procedure, which when installed can be treated as an XSPEC command, greatly facilitates the data initialization step. For example, the command

```
XSPEC12>  SPIdata  ./MyData/Dir/rev0044_crab.pha 475 det Y
```

Opens the Crab observation spectral data file, reads the 475 spectra into memory, grouping them by detector. The "Y" then indicates that, yes, I wish to ignore the spectral data channels corresponding to the known detector-electronic noise contamination (this is the default). Instead of "det" as the grouping option I could have selected "time" to group by time (quantized into dither-pointing intervals). A "-" lead to the data being initialzed into a single group. The command:

```
XSPEC12>  SPIdata  ./MyData/Dir/rev0044_crab.pha 475
```

Reads the 475 spectra into a single data group, and ignores the undesirable channels. If you forget all this, the command

```
XSPEC12>  SPIdata  -h
```

will remind you. The scripts SPIuntie, and SPIfreeze have similar command-line syntax.

SPIuntie and SPIfreeze

```
XSPEC12>  SPIuntie bkg 475 19 -1
```

The SPIuntie command script will accomplish the same result as the sequence of "untie" commands in the INTEGRAL/SPI example presented in this document. In that case, we had loaded 475 spectra associated with a single 5×5-dither pattern centered on the Crab nebula. The spectra were grouped by detector, which is a common approach to SPI analysis given the known detector-to-detector variations in the background rates. Suppose after an initial fitting pass, for which we assumed a single background spectrum, we know wish to untie the individual data group (i.e. detector) background models. This can be accomplished by issuing 25 "untie" commands as previously noted, or in a single command line using the SPIuntie command:

```
XSPEC12> SPIuntie bkg 475 19 -1

untie bkg:52

 Chi-Squared =  1.2030200E+04 using 1615 PHA bins.
 Reduced chi-squared =  7.5852458E+00 for   1586 degrees of freedom
 Null hypothesis probability =  0.0000000E+00

 untie bkg:78

 Chi-Squared =  1.2030200E+04 using 1615 PHA bins.
 Reduced chi-squared =  7.5900314E+00 for   1585 degrees of freedom
 Null hypothesis probability =  0.0000000E+00

 untie bkg:104
 renorm: no renormalization necessary

 Chi-Squared =  1.2030200E+04 using 1615 PHA bins.
 Reduced chi-squared =  7.5948231E+00 for   1584 degrees of freedom
 Null hypothesis probability =  0.0000000E+00
…
```

One might then make a second pass at fitting the data, hopefully leading to improved statistics. Subsequently, additional background model parameters could be untied using the SPIuntie procedure as well. For example, to untie three additional parameters over the full data set[2], the command syntax is:

```
XSPEC12> SPIuntie bkg 475 19 1 3
…
```

This will untie the first 3 parameters of the background model identified by "bkg", i.e. equivalent to issuing (475-1)×3 individual untie commands. Note that you can always be reminded of the command-line argument definitions by typing "SPIuntie -h" at the XSPEC prompt.

Suppose now that you are satisfied with the relative background normalization terms, and wish to freeze them at their current values for subsequent fitting passes. This could be accomplished using the SPIfreeze command script:

```
XSPEC12> SPIfreeze bkg 475 -1
XSPEC12>SPIfreeze bkg 19 1 -1
freeze bkg:52 1

 Chi-Squared =  6.6232600E+05 using 1805 PHA bins.
 Reduced chi-squared =  3.7589444E+02 for   1762 degrees of freedom
 Null hypothesis probability =  0.0000000E+00

freeze bkg:78

 Chi-Squared =  6.5791894E+05 using 1805 PHA bins.
 Reduced chi-squared =  3.7318148E+02 for   1763 degrees of freedom
 Null hypothesis probability =  0.0000000E+00

 …
```

[2] Note that the current SPI background models, which are documented elsewhere, are designed so that the parameter list is hierarchically ordered in terms of decreasing criticality. Thus, freeing the first parameter is likely to have the most significant impact on the statistics, the second parameter, the next most significant, and so on.

As with the SPIuntie command script, typing "SPIfreeze -h" at the XSPEC prompt will scroll the command-line definitions to your screen.

5. XSPEC commands

5.1 Summary of Commands

The following is a list of the commands available in XSPEC, together with a brief description of the purpose of each. The commands have been categorized under six headings: Control, Data, Fit, Model, Plot, Script, and Setting. The Control commands contain the interface with the operating system: they cause commands to be executed, or user input written to disk, or control how much is output. The Data commands manipulate the data being analyzed, by reading data into the program or replacing spectra or their ancillary detector, background, correction, or efficiency (auxiliary response) arrays. Additionally data commands control the channels under analysis. The fit commands invoke the fitting routines, modify their behavior by interchanging fitting algorithms or statistics in use, fixing parameters, or perform statistical testing. The Model commands create or manipulate the model, adding or editing components, modifying parameters, or alternatively performing analytical calculations from a model. The Plot commands deal with all aspects of plotting. The scripts are auto-loaded Tcl scripts that can be used in the same ways as commands. Finally the Setting commands sets variables that affect theoretical models.

Command	Category	Description
abund	SETTING	Set the abundance table.
addcomp	MODEL	Add a component to the model.
addline	MODEL	Add lines to a model
arf	DATA	Read an auxiliary response file.
autosave	CONTROL	Periodically save the XSPEC status.
backgrnd	DATA	Reset the files to be used for background subtraction.
bayes	FIT	Set up for Bayesian inference.
chain	FIT	Run a Monte Carlo Markov Chain.
chatter	CONTROL	Control the verbosity of XSPEC.
corfile	DATA	Reset the files to be used for background correction.
cornorm	DATA	Reset the normalization to be used in correcting the background.
cosmo	SETTING	Set H_0, q_0, and Λ_0

Command	Category	Description
cpd	PLOT	Alias for **setplot** `device`.
data	DATA	Input one or more PHA data files.
delcomp	MODEL	Delete a component from the model.
diagrsp	DATA	Diagonalize the current response for an ideal response.
dummyrsp	MODEL	Create a dummy response, covering a given energy range.
editmod	MODEL	Add, delete, or replace one component in the model.
energies	MODEL	Specify new energy binning for model fluxes.
eqwidth	MODEL	Calculate a model component's equivalent width.
error (rerror)	FIT	Determine a single parameter confidence region. rerror is for response parameters.
exec	CONTROL	Execute a shell command from within XSPEC.
exit	CONTROL	Wind up any hardcopy plots and exit from XSPEC.
extend	MODEL	This is now obsolete. See **energies** command.
fakeit	DATA	Produce simulated data files for sensitivity studies.
fit	FIT	Find the best fit model parameters.
flux	MODEL	Calculate the current model's flux over an energy range.
freeze (rfreeze)	FIT	Do not allow a model parameter to vary during the fit. rfreeze is for response parameters.
ftest	FIT	Calculate the F-statistic between two model fits
gain	MODEL	Perform a simple modification of the response gain.

Command	Category	Description
goodness	FIT	Monte Carlo calculation of goodness-of-fit.
hardcopy	PLOT	Spool the current plot to the printer.
help	CONTROL	Obtain help on XSPEC commands.
identify	MODEL	List possible lines in the specified energy range.
ignore	DATA	Ignore a range of PHA channels in future fit operations.
improve	FIT	Try to find a new minimum.
initpackage	MODEL	Compile, build, and initialize a package of local models.
iplot	PLOT	As plot command but interactive using PLT.
lmod	MODEL	Load a package of local models.
log	CONTROL	Open the log file to save output.
lrt	SCRIPT	Likelihood ratio test between two models.
lumin	MODEL	Calculate the current model's luminosity over a given rest frame energy range and redshift.
margin	FIT	MCMC probability distribution.
mdefine	MODEL	Define a simple model using an arithmetic expression.
method	SETTING	Set the minimization method.
model (rmodel)	MODEL	Define the model to be used when fitting the data.
modid	MODEL	Guess line IDs in the model.
multifake	SCRIPT	Perform many iterations of fakeit and save the results in a FITS file.
newpar (rnewpar)	MODEL	Modify the model parameters (use rnewpar for response parameters).
notice	DATA	Restore a range of PHA channels for future

Command	Category	Description
		operations.
plot	PLOT	Plot various information on the current plot device.
query	CONTROL	Switch on/off prompt to continue fitting.
quit	CONTROL	An alias for **exit**
renorm	FIT	Adjust the model norms, and/or control automatic renorming.
rescalecov	SCRIPT	Rescale the covariance matrix used in the proposal chain command.
response	DATA	Reset the files used to determine the detector responses.
save	CONTROL	Save aspects of the current state to a command file.
script	CONTROL	Open the script file to save all commands input.
setplot	PLOT	Modify the plot device and other values used by the plot routines.
show	CONTROL	Display current file and model information.
simftest	SCRIPT	Generate simulated datasets to estimate the F-test probability for adding a model component.
source	CONTROL	Execute a script file.
statistic	SETTING	Change the fit statistic in use.
steppar	FIT	Step through a range of parameter values; perform a fit at each step.
syscall	CONTROL	Run a shell command.
systematic	MODEL	Set the model systematic error.
tclout	CONTROL	write xspec data to a tcl variable
tcloutr	CONTROL	tclout with return value
thaw (rthaw)	FIT	Allow a model parameter to vary during the fit.

Command	Category	Description
		rthaw is for response parameters.
thleqw	MODEL	Calculates expected fluorescent line equivalent width.
time	CONTROL	Display elapsed time and other statistical information.
uncertain	FIT	Alias for error
untie (runtie)	MODEL	Untie linked parameters. runtie is for response parameters.
version	CONTROL	Print XSPEC version and build date/time
weight	FIT	Change the weighting function used for chi-squared fits.
writefits	SCRIPT	Write information about the current fit and errors to a FITS file.
xsect	SETTING	Change the photoelectric absorption cross-sections in use.
xset	SETTING	Modify a number of XSPEC internal switches

5.2 Description of Syntax

The individual commands are treated in alphabetical order in the following section. The novice would be well-served by reading the treatments of the **data**, **model**, **newpar**, and **fit** commands, in that order, then the other commands as needed. The write-up for each command includes a brief description of the purpose, an outline of the correct syntax, a more detailed discussion of the command assumptions and purpose, and a series of examples. Some commands have one or more subcommands that are similarly described following the command.

In the command description, the syntax uses the following conventions.

`<arg>`	an argument to the command
`<arg c> =:: <arg a> <arg b>`	defines <arg c> as <arga> followed by <argb>
`<arg>...`	a repeated string of arguments of the same type
`[<arg>]`	is an optional argument
`<arg a> | <arg b>`	indicates a choice between an argument of<arg a> or <arg b>

Exceptional responses to the command prompt are :

empty line or line containing only spaces and tab characters	nothing performed, prompt repeated
/	any remaining arguments will have the values given on the last invocation of the command
<EOF> (Ctrl-D on Unix)	same as quit
/*	skip input and return to prompt. Defaults for prompted values will be used.
?, ?command, command ?	Print list of commands, or summary help for a single command

5.3 Control Commands

5.3.1 autosave: set frequency of saving commands

Set or disable autosave, which saves the XSPEC environment to a file periodically.

Syntax: **autosave** <option>

where <option> is either off or a non-zero positive integer N. If the option is off, then auto-saving is disabled.If the option is N, the XSPEC environment is saved every N commands. The saving of the environment is equivalent to the command

```
XSPEC12>save all xautosav.xcm .,
```

i.e. both the file and model information is saved to the file xautosav.xcm, placed in the directory ~/.xspec/cache. Thus in case of an unexpected crash, the state of XSPEC before the crash can be restored by running @xautosav.xcm. The default value for the auto-save option is 1.

5.3.2 chatter: set verboseness level

Control the verbosity of XSPEC.

Syntax: **chatter** <chatter level> <log chatter>

where <chatter level> and <log chatter> are integer values.The initial value for each argument is 10. Higher values will encourage XSPEC to tell the user more, lower values tell the user less, or make XSPEC "quieter." <chatter level> applies to the terminal output, while <log chatter> controls the verbosity in the log file. Currently, the maximum chattiness is 25.Values below five should be avoided, as they tend to make XSPEC far too obscure.Some commands may temporarily modify the chattiness, such as the **error** command. A chattiness of 25 will generate a lot of debug output.

Examples:

```
XSPEC12> chatter 10
// Set the terminal chattiness to 10, same as the initial value.
XSPEC12> chatter ,0
//Set the chattiness for the log file to very low.
```

```
//This setting essentially disables the log file output.
XSPEC12> chatter 5
//Make XSPEC very quiet.
XSPEC12> chatter 10 25
// Restore the terminal chattiness to the initial level,
// while in the log file XSPEC will tell all
// (particularly when new data files are read in)
```

5.3.3 exit, quit: exit program

The command to end the current XSPEC run.

Syntax: **exit**

After an `exit`, the current plot files are closed.An <EOF> will have an identical result.

5.3.4 help: display manual or help for a specific command/theoretical model component

Obtain help on the XSPEC commands, their syntax, and examples of their use.

Syntax: **help** `[<topic list>]`

On the first invocation of the help command, an instance of a pdf file reader (by default Adobe Acrobat Reader) is started (a shortly delay may ensue), or the XSPEC manual is accessed online. Please see the subsection "Customizing XSPEC" in the XSPEC Overview section for details on how to control this behavior. The Acrobat reader must be in the user's path. If this default is used, then subsequent calls to help will use this instance to display other help pages. help without arguments displays the XSPEC manual, with a bookmark index that allows random access to the help system, or in the online mode will open to the XSPEC manual homepage.

The design allows for users to add help files for local models and scripts to the help system if they are placed in the help search path.

Examples:

```
XSPEC12> help
//show the entire manual.
XSPEC12> help fit
//Go to the help text for the fit command.
XSPEC12> help model pow
//Go to the help text for the powerlaw model. (Entering just "XSPEC12> model"
will produce a scrolled-text list of all available model components.)
XSPEC12> help appendices
//show the manual appendices (which document the user interface, the Cash
statistic, how to add models to XSPEC, a summary of PLT commands, and
associated FTOOLS and other programs for manipulating data).
XSPEC12>help appendix local
//show the appendix describing how to add local models
```

Help also displays the following information as scrolling text:

```
XSPEC12> help ?
//Show a list of all available commands.
```

```
XSPEC12> help ??
//Show a brief summary and usage syntax of all available commands.
XSPEC12> <command> ?
// Show brief summary and syntax of <command>.
```

5.3.5 log: log the session output

Open a log file.

Syntax: **log** `[STAMP] <log file>`

where `<log file>` is the name of the file to be opened (default extension is `.log`).If no arguments are on the line, then the default file name is `xspec.log`. If `<log file>` matches the string `none`, then the current log file is closed. If the string `STAMP` is given as an argument then the log filename will include a data and time stamp. If `<log file>` has no suffix then the stamp is appended to the name and a `.log` suffix added. To change the chattiness level for the log file (ie. the amount ofinformation written to the log file) use the `chatter` command. The default chatter level for the log file is 10.

Examples:

```
XSPEC12> log
//Turn on the log file (default xspec.log).}
XSPEC12> log none
//Close the log file.
XSPEC12> log mylog
//Open the log file (mylog.log)
XSPEC12> chatter ,, 12
```

//Set the log file chattiness to 12.

5.3.6 query: set a default answer for prompts in scripts

Switch on/off the continue fitting questions.

Syntax: **query** `<option>`

where `<option>` is `yes`, `no`, or `on`. If `on` then the continue fitting question in **fit**, **steppar**, and **error** will be asked when the number of trials is exceeded. Also, when the number of trials to find the error is exceeded a question will be asked. For either of the other two options the questions will not be asked but the answer will be assumed to be yes or no depending on the value set. To ensure that fitting continues without any questions being asked use the command

XSPEC12> query yes

5.3.7 save: save the current session commands

Save aspects of the current state to a command file.

Syntax: **save** `<option> <filename>`

If no <filename> is given, then the file savexspec.xcm is created. If you don't give the extension to the file name the default is .xcm. The values of <option> allowed are model, files, and all. The model option writes out commands to recreate the current model and parameter values; the files option writes out commands to read-in the current spectra, and the all option does both of the above. The default option is model. To recover the saved context use the command

```
XSPEC12>@filename
Examples:
XSPEC12> save model fname
// Write out model commands to the file fname.xcm
XSPEC12> save
// Same as above, but save into file savexspec.xcm.
XSPEC12> save files fname
// Write out data file commands.
```

5.3.8 script: write commands to a script file

Open a script file.

Syntax: **script** <script file>

where <script file> is the name of the file to be opened (default extension is .xcm).If no arguments are on the line, then the default file name is xspec.xcm.If <script file> matches the string none, then the current script file is closed. The script file saves all commands that are input. This command is useful for users who use the same set of commands repeatedly. Once a script file is written and saved, the user then can re-run the same set of commands on other data by

```
XSPEC12> source <script file>
```

Examples:

```
XSPEC12> script
// Turn on the script file (default xspec.xcm)
XSPEC12> script none
// Close the script file.
XSPEC12> script myscript
// Open the script file (myscript.xcm)
```

5.3.9 show: output current program state

List selected information to the user's terminal (and the log file, if open).

Syntax: **show** [<selection>]

where <selection> is a key word to select the information to be printed. If omitted, it is the information last asked for. Initially, the default selection is all. (Note: to better integrate the

usage of OGIP type-II files, much of the information given by “show files” in previous versions is now displayed by “show data.”)

Selections are:

```
XSPEC12> show abund
//show current solar abundance table

XSPEC12> show all
//All the information

XSPEC12> show allfile
// All file information = files + noticed + rates

XSPEC12> show control
// XSPEC control information

XSPEC12> show data
// File names, associated coefficients, and net count rates,
// displayed in order of spectrum number.  For higher chatter,
// also displays grouping map.

XSPEC12> show free
// Free parameters

XSPEC12> show files
// Equivalent to “show data” but displayed in order of file name.

XSPEC12> show fit
//Fit information

XSPEC12> show model
//The model specification

XSPEC12> show noticed
//Channel ranges noticed for each file.

XSPEC12> show parameters
//All current parameter values (including gain parameters, if any).

XSPEC12> show parameters <par range>
// Show subset of all model parameters given by <par range>,
// e.g. show parameters 1,3,5-8

XSPEC12> show pha
// Current data, error and model values for each channel.

XSPEC12> show plot
//Current plot settings from setplot command, includes rebinning info.


XSPEC12> show rates
//Folded model, correction rates for each file.

XSPEC12> show response
//show responses loaded
```

```
XSPEC12> show rparameters
// All current gain (response) parameters

XSPEC12> show rparameters <par range>
// Show subset of all gain (response) parameters

XSPEC12> show xsect
//show description of cross-section table
```

5.3.10 syscall: execute a shell command

Execute command in a shell.

Syntax: **syscall**{[<shell command>]>

This command executes its arguments by passing them to the users current shell for execution. Thus file name globbing (*i.e.* wildcard expansion) are performed on the command before execution. This is in contrast to the exec command, which executes commands directly, without first passing them on to a shell.

If no arguments are given, then the command will start an interactive subshell.

5.3.11 tclout: create tcl variables from current state

Write internal xspec data to a tcl variable. This facility allows the manipulation of xspec data by tcl scripts, so that one can, for example, extract data from xspec runs and store in output files, format xspec output data as desired, use independent plotting software, etc.

Syntax: **tclout** `<option> [<par1>] [<par2>] [<par3>]>`

tclout creates the tcl variable `$xspec_tclout`, which can then of course be set to any named variable. The allowed values of <option> are :

?	Show the valid options. Does not set `$xspec_tclout`.
areascal n <s|b>	Writes a string of blank separated values giving the AREASCAL values for spectrum n. If no second argument is given or it is "s" then the values are from the source file, if "b" from the background file.
arf n	The auxiliary response filename(s) for spectrum n.
backgrnd n	Background filename for spectrum n
backscal n <s|b>	Same as areascal option but for BACKSCAL value.
chatter	Current xspec chatter level.

compinfo [<mod>:]n [<groupn>]	Name, 1st parameter number and number of parameters of model component n, belonging to model w/ optional name <mod> and optional datagroup <groupn>.
cosmo	Writes a blank separated string containing the Hubble constant (H0), the deceleration parameter (q0), and the cosmological constant (Lambda0). Note that if Lambda0 is non-zero the Universe is assumed to be flat and the value of q0 should be ignored.
covariance [m, n]	Element (m,n) from the covariance matrix of the most recent fit. If no indices are specified, then entire covariance matrix is retrieved.
datagrp [n]	Data group number for spectrum *n*. If no *n* is given, outputs the total number of data groups.
datasets	Number of datasets.
dof	Degrees of freedom in fit, and the number of channels.
energies [n]	Writes a string of blank separated values giving the energies for spectrum n on which the model is calculated. If n is not specified or is 0, it will output the energies of the default dummy response matrix.
eqwidth n	Last equivalent width calculated for spectrum *n*.
error [<mod>:]n	Writes last confidence region calculated for parameter *n* of model with optional name <mod>, and a string listing any errors that occurred during the calculation. The string comprises nine letters, the letter is T or F depending on whether or not an error occurred. The 9 possible errors are: 1. new minimum found 2. non-monotonicity detected 3. minimization may have run into problem 4. hit hard lower limit 5. hit hard upper limit 6. parameter was frozen 7. search failed in –ve direction

	8. search failed in +ve direction 9. reduced chi-squared too high So for example an error string of "FFFFFFFFT" indicates the calculation failed because the reduced chi-squared was too high.
expos n <s|b>	Same as areascal option but for EXPOSURE value.
filename n	Filename corresponding to spectrum n.
flux [n]	Last model flux or luminosity calculated for spectrum *n*. Writes a string of 6 values: val errLow errHigh (in ergs/cm^2) val errLow errHigh (in photons). Error values are .0 if flux was not run with "err" option.
ftest	The result of the last ftest command.
gain [<sourceNum>:] <specNum> slope | offset	For gain fit parameters, value,delta,min,low,high,max for the slope or offset parameter belonging to the [<sourceNum>:]<specNum> response. For nonfit gain parameters, only the value is returned.
goodness	The percentage of realizations from the last goodness command with statistic value less than the best-fit statistic using the data.
idline e d	Possible line IDs within the range [e-d, e+d].
lumin [n]	Last model luminosity calculated for spectrum *n*. Same output format as flux option.
model	Description of current model(s).
modcomp [<mod>]	Number of components in model (with optional model name).
modpar [<mod>]	Number of model parameters (with optional model name).
modval [<specNum>[<mod]]	Write to Tcl the last calculated model values for the specified spectrum and optional model name. Writes a string of blank separated numbers. Note that the output is in units of photons/cm^2/s/bin.
noticed [<n>]	Range (low,high) of noticed channels for spectrum n.

noticed energy [<n>]	The noticed energies for spectrum n.
param [<mod>:]n	(value,delta,min,low,high,max) for model parameter n.
peakrsid n [lo, hi]	Energies and strengths of the peak residuals (+ve and –ve) for the spectrum n. Optional arguments lo, hi specify an energy range in which to search.
pinfo [<mod>:]n	Parameter name and unit for parameter n of model with optional name.
plink [<mod>:]n	Information on parameter linking for parameter n. This is in the form true/false (T or F) for linked/not linked, followed by the multiplicative factor and additive constants if linked.
plot <option> <array> [<plot group n>]	Write a string of blank separated values for the array. <option> is one of the valid arguments for the plot or iplot commands. <array> is one of x, xerr, y, yerr, or model. xerr and yerr output the 1-sigma error bars generated for plots with errors. The model array is for the convolved model in data and ldata plots. For contour plots this command just dumps the steppar results. The command does not work for genetic plot options.
plotgrp	Number of plot groups.
query	The setting of the query option.
rate <n | all>	Count rate, uncertainty and the model rate for the specified spectrum n, or for the sum over all spectra.
response n	Response filename(s) for the spectrum n.
sigma [<modelName>:]n	The sigma uncertainty value for parameter n. If n is not a variable parameter or fit was unable to calculate sigma, -1.0 is returned.
simpars	Creates a list of parameter values by drawing from a multivariate Normal distribution based on the covariance matrix from the last fit. This is the same mechanism that is used to get the errors on fluxes and luminosities, and to run the goodness command.

solab	Solar abundance table values.
stat	Value of statistic.
statmethod	The name of the stat method currently in use.
steppar statistic | delstat | [<modName>:]<parNum>	The statistic and delstat options return the statistic or delta-statistic column respectively from the most recent steppar run. Otherwise, the parameter column indicated by <parNum> is returned. Note that for multi-dimensional steppars the returned parameter column will contain duplicate values, in the same order as they originally appeared on the screen during the steppar run.
varpar	Number of variable fit parameters.
weight	Name of the current weighting function.
xflt n	XFLT#### keywords for spectrum n.

Examples:

```
XSPEC12>data file1
XSPEC12> model pha(po)
...
XSPEC12> fit
...
XSPEC12>tclout stat
XSPEC12>scan $xspec_tclout "%f" chistat
XSPEC12>tclout param 1
XSPEC12>scan $xspec_tclout "%f"par2
XSPEC12>tclout param 2
XSPEC12>scan $xspec_tclout "%f"par3
XSPEC12>tclout param 3
```

In this example, scan is a tcl command that does a formatted read of the variable `$xspec_tclout`. It reads the first floating point number into the variable given by the last argument on the line.This sequence creates a simple model, fits it, and then writes the χ^2 statistic and the three parameters to tcl variables `$chistat`, `$par1`, `$par2`, and `$par3`. These can now be manipulated in any way permitted by tcl.

5.3.12 tcloutr: tclout with return value

Syntax: **tcoutr** <option> [<par1>] [<par2>] [<par3>]>

tcloutr is identical to the **tclout** command except that it also provides what is stored in `$xspec_tclout` as a return value. Therefore it can be used in tcl scripts like this:

```
set var1 [tcloutr energies 1]
```

tcloutr may produce quite a lot of unwanted screen output, which can be avoided by using **tclout**.

5.3.13 time: print execution time

Get some information about the program run time.

Syntax: time

The time command prints out elapses CPU time attributed to the user and to the system. Two output lines are given, one for user/system time since the time command was last called, and one for time elapsed since the program started.

5.3.14 undo: undo the previous command

Undo the affects of the previously entered xspec command.

Syntax: undo

New for xspec version 12, the undo command will restore the state of the xspec session prior to the most recently entered command. The current implementation does not allow restoration to more than one command back, so calling undo repeatedly will have no effect. Also, a plot command cannot be undone.

5.3.15 version: print the version string

Syntax: version

version prints out the information about version number and build date and time (not current date, time) displayed when XSPEC is started.

5.4 Data Commands

5.4.1 arf: change the efficiency file for a given response

Read in one or more auxiliary response files (ARF). An ARF gives area versus energy and is used to modify the response matrix for a spectrum. The file must be in the OGIP standard format.

Syntax: **arf** `[ <filespec>...]`

where `<filespec> =:: [`[source #:]`<spectrum num>] <filename>`[{ranges}]`...` and where <spectrum num> is the spectrum number for the first <filename> specified, <spectrum num> plus one is the spectrum number for the next file (or next entry in {ranges} specifier for Type II multi-ARF files), and so on. <filename> is the name of the auxiliary response file to be used with the associated spectrum. The optional source number defaults to 1, and for ARFs stored in OGIP Type II files, {ranges} specifies the row numbers of the desired ARF(s). See the **data** command for allowed range specification.

If no `<spectrum num>` is given in the first `<filespec>` it is assumed to be 1. If no file specifications are entered, then none of the spectrum responses are modified.An error message is printed if the spectrum number is greater than the current number of spectra (as determined from the last use of the **data** command).A file name `none` indicates that no auxiliary response is to be used for that spectrum. If a file is not found or cannot be opened for input, then the user is prompted for a replacement auxiliary response file.An `<EOF>` at this point is equivalent to `none`. See the **data** command forways to completely remove the dataset from consideration.

Note: The ARF command is currently not implemented for data formats which use multiple RMFs per spectrum, such as Integral/SPI data.

Examples:

It is assumed that there are currently three spectra:

```
XSPEC> arf a,b,c
// New files for the auxiliary response are given for all three
spectra.
XSPEC> arf 2 none
// No auxiliary response will be used for the second spectrum.
XSPEC> arf ,d.fits
// d.fits becomes the auxiliary response for the second spectrum.
XSPEC> arf 2 e.fits{3-4}
// Rows 3 and 4 of multi-ARF file e.fits become the auxiliary responses
for the second and third spectra.
XSPEC> arf 2:1 f.fits
// f.fits becomes the auxiliary response for the second source of
spectrum 1.
```

5.4.2 backgrnd: change the background file for a given spectrum

Modify one or more of the files used in background subtraction.

Syntax: **backgrnd** [<filespec>...]

backgrnd <spectrum number> none

where <filespec> =:: [<spectrum num>] <filename>... and where <filename> is the name of the PHA file to be used for background subtraction. The numbering scheme is as described for the **data** command, except that the <spectrum num> must have previously been loaded.

An error message is printed if <spectrum num> is greater than the current number of spectra (as determined from the last use of the data command. **backgrnd** <n> none indicates that no background subtraction is to be performed for that spectrum. If a file is not found or cannot be opened for input, then the user is prompted for a replacement background file(an <EOF> at this point is equivalent to **backgrnd** <spectrum number> none). The current ignore status for channels is not affected by the bkgrnd command. (See the **ignore** and **notice** commands). Finally, any grouping specification will be overridden by the grouping in the source spectral file so that the source and background are binned in the same way.

The format of the background file must match that of the spectrum file: for this purpose OGIP Type I and II are considered to be the same format.

For details of how to remove spectra see the **data** command documentation.

Examples:

Suppose there are currently three spectra. Then

```
XSPEC12> backgrnd a,b,c
// New files for background subtraction are given for all
// three spectra.
XSPEC12> backgrnd 2 none
// No background subtraction will be done for the second spectrum.
XSPEC12> backgrnd ,d
// d.pha becomes the background for the second spectrum.
XSPEC12> backgrnd 2 e{4-5}
// Rows 4 and 5 of Type II file e.pha become the background for
// the second and third spectrum respectively.
```

5.4.3 corfile: change the correction file for a given spectrum

Reset the files used for background correction.

Syntax: **corfile** [<filespec>...]

where <filespec> is the same as for the **backgrnd** command. The correction file can be associated with a spectrum to further adjust the count rates. It is a PHA file whose count rate is multiplied by the current associated correction norm (see the **cornorm** and **recornrm** command) and then subtracted from the input uncorrected data. The correction norm is not changed by running the corfile command. Default values for the correction file and norm are included in the data PHA file.Unlike the background file, the correction data does NOT contribute to the measurement error. A file name of none

is equivalent to no correction file used.If an input file can not be opened or found, an error message is printed and the user prompted for a replacement.As with the **backgrnd** command, the correction file is checked against the associated spectrum for number of channels, grouping status, and detector ID. The current ignore status for channels is not affected by the **corfile** command. Note that correction files have the same format as the PHA files used by the **data** command.

Examples:

It is assumed that there are currently three spectra:

```
XSPEC12> corfile a,b,c
// New correction files are used for all three spectra.>
XSPEC12> corfile 2 none
// No correction will be done for the second spectrum.}
XSPEC12> corfile ,d
// The 2nd file now uses d.pha as its correction.
XSPEC12> corfile 2 e{4-5}
// Rows 4 and 5 of Type II file e.pha becom the correction files for
the second
// and third spectrum respectively.
```

5.4.4 cornorm: change the normalization of the correction file

Reset the normalization used in correcting the background.

Syntax: **cornorm** `[[ <spectrum range>...] [ <cornorm>]]...`

where `<spectrum range>` =:: `<first spectrum no.> - <last spectrum no.>` s a range of spectra to which the correction is to be applied and `<cornorm>` is the value to be used for the normalization. A decimal point (.) is used to distinguish a correction norm from a single spectrum `<spectrum range>`. If no correction norm is given, then the last value input is used (the initial value is one (1)). If no range is given, then the last single range input is modified. (See the `corfile` command.)

Examples:

Assume that there are four spectra, all with associated correction files already defined, either by default in their PHA file, or explicitly by using the `corfile` command.

```
XSPEC12> cornorm 1-4 1.
//The correction norm for all four is set to 1.0
XSPEC12> cornorm 0. 1-2 0.3
//The correction norm for the last input range (which was 1-4)
// is set to 0., then files 1 and 2 are reset to 0.3.
XSPEC12> cornorm 4
//file 4 has the correction also set to 0.3.
XSPEC12> cornorm 1 4 -.3
//files 1 and 4 are set to -.3.
XSPEC12> cornorm .7
//file 4 (as the last input single range) is set to 0.7.
```

5.4.5 data: read data, background, and responses

Input one or more spectra, together with their associated (background, response) files.

Syntax: **data** <file spec1>[,…] [<file spec2>…] [/]

data none

data <spectrum #> none

where the file specification is

```
      <filespec> =:: [[  <data group #:>] <spectrum #>]
<filename>[{ranges}]
```

If a particular file is not found or cannot be opened for input for some reason, then the user is prompted for a replacement file name. An `<EOF>` at this point is equivalent to typing `none`. The default extension for all files is `.pha`, so all other extensions, (e.g. `.fak`) must be entered explicitly.The default directory is the current user directory when XSPEC is invoked. When a new file is input, by default all its PHA channels are considered good channels for fitting and plotting purposes (see the `ignore` and `notice` commands).

XSPEC's "native" data format is the OGIP standard. The standard specifies the representation of spectrum and all related datasets. XSPEC12 is explicitly designed to be able to work with other data formats as required: for example, the Integral/SPI spectral data format, although based on OGIP TypeII, deviates slightly. This was necessary because 3 response/arf pairs are required per spectrum. XSPEC12 has the ability to specify how response and other data are stored on disk, composed, and combined within the spectral fitting problem by adding new data modules at run-time. In XSPEC12, unlike XSPEC11, the channels that are ignored are a property of the spectrum, and therefore must be reset when the spectrum is replaced by another.

If the file contains multiple spectra, such as an OGIP Type II PHA file, then the desired spectrum can be specified by appending `{ranges}` to the end of the filename, where `n` is the row number of the spectrum in the file.

XSPEC12 allows any combination of multiple ranges in the parentheses delimited by commas. The wildcard characters `*`and `**` may also be used. A `**` on either side of a hyphen indicates either the first or last row in the file, based on whether it is to the left or right of the hyphen. (If a `*` is entered on the left or right side of a hyphen, it is substituted by the most recently entered left or right value respectively.) All rows in the file may be selected simply with a single `*` or `**` between the brackets with no hyphen. Examples:

```
XSPEC12> data pha2data{1,3,5-8,14-26,75-**}
      //  In addition to the various specified rows between 1 and 26,
      //  also load rows 75 through the end of the file.
XSPEC12> data pha2data{*}
      //  Select all rows in the file.
```

For files with multiple spectra the data may either specify a header keyword specifying the response, auxiliary response, background and correction files, or these may be string-valued columns specifying a different filename per row.

Consult the **http://heasarc.gsfc.nasa.gov/docs/software/ftools** package documentation for details of how to modify the file.

The individual spectral data files are created outside of XSPEC by detector-specific software. They are organized as `XSPEC data` files, but often referred to as PHA files. Whatever its format, the PHA file contains such information as integration time, detector effective area, and a scaling factor (`BACKSCAL` in the OGIP standard) that estimates the expected size of the internal background. The data file also contains the names of the default files to be used for background subtraction and for the detector sensitivity versus incident photon energy (the response and arf files). A data file has the total observed counts for a number of channels and a factor for the size of any systematic error. Each channel is converted to a count rate per unit area (assumed cm^{-2}). The default background file is used for background subtraction. An error term is calculated using Poisson statistics and any systematic error indicated in the file[3]

spectrum numbering

Multiple `filespec` clauses can be input on a single data command, or also on multiple data command. Within XSPEC, each set of data is referred to by its associated spectrum number. `<spectrum #>`, as determined by the following rules. For convenience, we denote the number of spectra that have been previously read in by data command as N_s

Spectra in XSPEC are numbered sequentially from 1.

If no spectrum number is specified by the user, the spectrum in the first filename specified is assigned to 1. If spectra have already been loaded at this point, they will be replaced, deleted, or added to depending on the command. For example, if there are 3 spectra loaded ($N_s = 3$) and the user types

XSPEC12> data multidatafile{1-2}

then spectra 1 and 2 will be replaced and 3 deleted. The command

XSPEC12> data multidatafile{1-4}

will replace all three spectra and add the fourth.

If the user specifies a “load point”, i.e. the first spectrum number to be created by the new command, i.e.

XSPEC12> data 3 multidatafile{1-4}

---

[3] For OGIP files, any FITS NULL values will be converted to the value `1.E-32`. This should have no practical effect because any channels with NULL values will presumably be marked as bad or otherwise ignored.

then that load point may not exceed $N_s + 1$. If it does, XSPEC will correct the number and issue a warning.

A skipped-over argument can be effected by a comma, for example

XSPEC12> data 3 spectrum1, , spectrum2

indicates that the spectrum for that position, as input in an earlier invocation of data, will continue to be used (in this example, spectrum 3 is replaced, 4 is left untouched, and 5 is either replaced or added. Any spectra with numbers great than 5 are removed.

If the filename input is `none`, that spectrum is removed, and so are any higher-number spectra unless `none` is terminated with a / character. For example:

XSPEC12> data 3 none

removes all spectra numbered 3 or higher,

XSPEC12>data 3 none/

removes only spectrum 3 and renumbers the rest.

The data command determines the current total number N_T of spectra: either N_T spectra are implied by the command line, or the highest spectrum number added (after XSPEC has made corrections as mentioned above) is N_T This is true UNLESS a / character terminates the data command.

If the line is terminated by a slash (/), then the current number of spectra is the previous total number of datsets N_s or the number as determined from the command line, whichever is greater.

The command

XSPEC12> data

by itself prints the one-line help summary, as does

XSPEC12> data ?

data groups

XSPEC allows the user to specify separate data groups for different spectra. Each data group has its own set of parameters for the defined model. These parameters can be either independent from data group to data group, or they can be linked across data groups using the standard XSPEC syntax (see the newpar command). This facility can be used for, say, analyzing extended sources.

Note that the data group number *precedes* the spectrum number: in the example

XSPEC12> data 2:3 spectrum4

which assumes that at least two spectra are already present, the data group number is 2 and the spectrum number is 3.

XSPEC will not allow the data group number to exceed the spectrum number: for example

XSPEC12> data 3:2 spectrum4

is invalid. XSPEC will correct this and issue a warning.

More Examples:

XSPEC12> data a

//The file a.pha is read in as the first (and only) spectrum.

XSPEC12> data ,b

//b.pha becomes the second spectrum, the first spectrum is

// unmodified (i.e. it is still a.pha)

XSPEC12> data c 3 d,e,f

//c.pha replaces a.pha as the first spectrum;d.pha, e.pha, and

// f.pha provide the, third, fourth, and fifth spectra.

XSPEC12> data g/

//g.pha replaces c.pha as the first spectrum; the slash (/)

// indicates that the 2nd through the 5th spectra remain as before.

XSPEC12> data 2 none/

//the string none indicates that the 2nd spectrum (b.pha) is to be

// totally removed. The current total number of datasets thus becomes

// one less (4).The current spectra are g.pha,d.pha, e.pha,

// and f.pha.

XSPEC12> data h,,

//The current total number of spectra becomes 2, the current data

// sets are from h.pha and d.pha.

XSPEC12> data

//There is no change in the data status.

XSPEC12> data 1

//The number of spectra is set explicitly to one, that being from

// h.pha.

XSPEC12> data 1:1 a 2:2 b 3:3 c

//Read a.PHA into data group 1, b.pha into data group 2, and c.pha

//into data group 3

XSPEC12> data 1:1 a 1:2 b 2:3 c

//Read a.pha and b.pha into data group 1, and c.pha into data group 2

XSPEC12> data a{3}

// Read the third spectrum in the file a.pha.

5.4.6 diagrsp: set a 'perfect' response for a spectrum

Diagonalize the current response matrix for ideal response.

Syntax: **diagrsp**

This command diagonalizes the current response matrix. The response matrix is set so that the channel values are mapped directly into the corresponding energy ranges, based on the channel energies and energy response range of the current response matrix.

This command is very similar to running dummyrsp in mode 1, with two important differences. Unlike dummyrsp, usage of this command requires that an actual response is currently loaded. It takes its energy range and channel binning information from this currently loaded response rather than user input parameters. Secondly, this does not change the effeciency (ie. effective area) as a function of energy stored for the current detector. Invoking this command will simulate a detector with perfect spectral resolution. If you wish to simulate a detector with perfect resolution AND perfect efficiency, use the `dummyrsp` command.

The previous response matrices can be reimplemented with the `response` command, with no arguments. Any use of the `data` and `notice` commands will replace the dummy diagonal response with the correct set of matrices.

5.4.7 fakeit: simulate observations of theoretical models

Produce PHA files with simulated data.

Syntax: **fakeit** `[<file spec>...]`

where `<file spec>` =:: `[ <file number>] <file name>[{ranges}]...` is similar to the syntax used in the **backgrnd**, **corfile**, and **response** command. The **fakeit** command is used to create a number of artificial PHA files, where the current model is folded through response curves and then added to a background file. Poisson statistics can be included optionally. The integration time and correction norm are requested for each file. The file names input as arguments are PHA files to be used as background. A faked spectrum will be produced for EVERY spectrum currently loaded (if any), and additional faked spectra are produced up to the maximum number as indicated by the command line arguments. If the argument line is empty, then it is assumed that the

number of **fakeit** spectra produced is equal to the current number of loaded spectra. See the examples below for a clearer description.

If a faked spectrum is based on a currently loaded spectrum, then by default the background, response, correction file, and numerical information are taken from the currently-defined data, unless a background file is specified on the command line in which case it becomes the background. If `none` is given as an argument, then the user is prompted for the response file to be used and the default numerical data is set to 1., except the correction norm, which is set to zero.

With XSPEC12, it is now possible to produce fake spectra output in OGIP Type II format. It is also possible to enter in Type II file information (for background, arf, corfile) simply by adding a row specifier in curly brackets to the file name (see examples below). Type II file information can be entered even if the fake output is to be in Type I format, and vice versa. See the discussion below on Type I vs. Type II output for a detailed description. When prompted for exposure time and corrscale however, the values entered will apply to all the spectra in a type II file. At present, it is not possible to specify different exposure time and corrscale values for each of the spectra in a type II faked output file.

For each output file, the user will be prompted for a PHA file name. If a background file is in use then this command will also fake a new background for each faked PHA file. Background files are given the same names as faked PHA files but with `_bkg` appended to the end of the stem.

After the PHA files are created, they are read in automatically as the current datafiles. The ignore status is completely reset.

Type I vs. Type II Output:

With the addition of OGIP type II file handling capabilities, the possible options for the fakeit output format grows more complex. Backwards compatibility is maintained though, so any fakeit commands used with type I files in previous versions of Xspec will still work the same, placing all the output in type I files. Fakeit determines whether to place its fake spectra and background data into type I or type II files based on the following rules:

The simplest case is for fake spectra that are based on currently loaded spectra. Fakeit will then just use the format of the currently existing files for its output, for both the PHA spectra and background spectra if applicable. For example: Assume 3 spectra are currently loaded, spectrum 1 from file typeIdata.pha and spectra 2 and 3 from file `typeIIdata.pha`. Then,

```
XSPEC12> fakeit
```

will produce 3 fake spectra in 2 output files with names prompted from the user. The first file will be type I, the second containing 2 spectra in type II. The same is true for any background files produced.

If the user asks for more fake spectra to be created than the number of spectra currently loaded, for example by typing the following when the same 3 spectra above described are loaded:

```
XSPEC12> fakeit 5
```

then fake spectra 1-3 will be placed in the two files as before. For the additional fake spectra (4 and 5), fakeit uses the following rule: If any of the originally loaded spectra were in a type II file, then all of the additional fake spectra will be placed in 1 type II file. Otherwise, they will each be placed in a separate type I file. In this example, since a type II file was originally loaded (typeIIdata.pha) when fakeit was called, spectra 4 and 5 will be placed together in a type II output file, in addition to the type I and type II files for the first 3 fake spectra.

For cases where fakeit is used and there is no currently loaded spectra, it will produce output in type I format UNLESS either of the following situations exist: 1. The user has entered any type II background files on the command line, indicated by row specifiers in brackets. 2. The format of the FIRST response file used clearly belongs to a format associated with type II data, such as with SPI/Integral with its multiple RMF format (see section on SPI/Integral usage).

Overall, though the method of determining output format for additional spectra may seem quite complicated, it can be easily summed up: Fakeit will place all additional spectra and backgrounds (ie. those not based on already loaded data) in type I output files, UNLESS it detects ANY evidence of type II file usage amongst the user specified input, in which case it will produce type II output.

Note For SPI/Integral Format:

Since the SPI/Integral format builds its responses from a combination of multiple RMFs and ARFs, it must use a different scheme than the OGIP type I and II formats for storing RMF and ARF file location information. This information is stored in a FITS extension, named "RESPFILE_DB" , added to the PHA file. Therefore, when fakeit prompts the user for the location of the response file, simply enter the name of a FITS file which contains a RESPFILE_DB extension pointing to the RMFs and ARFs to be applied. When prompted for an ARF name, enter nothing.

The prompts will only appear for the first spectrum in the data set, and the ARFs will be assigned row by row 1 to 1 with the spectra. For example, if no data is currently loaded, to create 3 fake SPI spectra from the RMFs and ARFs named in the RESPFILE_DB extension of the file "realSpiData.pha":

```
XSPEC12> fakeit 3
      // ...(various prompts will follow)...
For fake spectrum #1 response file is needed:  realSpiData.pha
      // ...and ancillary file:  <Ret>
      // ...(more fakeit prompts)...
```

This will create 3 fake spectra, each making use of the same RMFs/ARFs, spectrum 1 using the first row of the ARFs, spectrum 2 using the second etc.

*** CAUTION – SPI/Integral ***

As currently implemented, the RESPFILE_DB method of storing ARF locations does not retain specific row information. The assumption is that the rows in the ARF correspond 1 to 1 with the rows in the spectral data extension. Therefore, much

confusion can arise when the row numbers of the loaded spectra do not match that of the fake spectra. For example:

```
XSPEC12> data my_spi_data.pha{3-4}
      // my_spi_data.pha contains a RESPFILE_DB table pointing to
arf1.fits,
      // arf2.fit, arf3.fits.
      // ...(fit to some model(s))...
XSPEC12> fakeit
```

This will produce 2 fake spectra generated from the model*response operation, where the model has parameters based on a fit to the original spectra in rows 3 and 4 of my_spi_data.pha, which used ROWS 3 AND 4 of the 3 arf files for their own responses. However, the responses used above to generate the 2 fake spectra will use ROWS 1 AND 2 of the 3 arf files. This is necessary since the fake spectra will be placed in rows 1 and 2 of their fakeit output file.

Examples:

Type I files:

For each of these examples, assume 3 spectra are currently loaded, each in its own type I file, and that the second spectrum has a background file.

```
XSPEC12> fakeit
```

This will produce 3 fake spectra each in its own type I output file, and the user will be prompted for the file names. The response file information will come from each of the original spectra. If any response information is invalid, the user will then be prompted. A fake background file will be produced for the second spectrum.

```
XSPEC12> fakeit 4
```

Produces 4 fake spectra, the first 3 created as in the previous example. The fourth will be created with no background spectrum, and this user is prompted for response information.

```
XSPEC12> fakeit backa,,none 4
```

Produces 4 fake spectra. For the first spectrum, a fake background file will be generated from the file backa. The second uses its own background file as before. The third fake spectra will no longer use the response information from loaded spectrum 3, the user will be prompted instead, and its default numerical data will be reset to 1. The fourth spectrum will be created as in the previous example.

If no data is currently loaded:

```
XSPEC12> fakeit 2
```

Produces 2 fake spectra in separate type I files, unless the first user entered response file belongs to a format that is explicitly type II (ie. SPI/Integral).

Type II files:

Assume four spectra with no backgrounds have been loaded from one type II file:

```
XSPEC12> data original_type2_data.pha{5-8}
```

Then, after model(s) have been entered and a fit:

```
XSPEC12> fakeit
```

This will produce 4 fake spectra in rows 1 to 4 of one type II output file, with responses and arfs taken from the columns of original_type2_data.pha.

```
XSPEC12> fakeit ,,backb{1-3}
```

This produces 5 fake spectra in two type II output files, and 3 fake background spectra also placed in two type II output files:

The first 4 fake spectra are placed in one output file since that is how the 4 spectra they were based on were originally organized. The default numerical data for this file are taken from the original spectra. Fake spectra 3 and 4 now have backgrounds, based on backb{1} and backb{2} respectively. These will generate 2 fake background spectra, placed in rows 3 and 4 of the first output fake background file. Rows 1 and 2 of this file will just consist of zeros since the first 2 spectra have no backgrounds.

The fifth fake spectrum will be placed in the second type II PHA file. Response and numerical data will not be based on the existing loaded spectra. A fake background will be generated from backb{3} and placed in row 1 of the second type II fake background file.

Now assume no data is currently loaded:

```
XSPEC12> fakeit 2 backb{1}
```

2 fake spectra in one type II output file are produced, as is a corresponding fake background file with 2 rows. The fact that the user has entered a type II background file on the command line tells fakeit to produce type II output. The first fake spectrum will have no associated background, so row 1 in the fake background file will be all zeros. Row 2 will consist of the fake background generated from backb{1}.

5.4.8 ignore: ignore detector channels

Ignore data channels.(See also **notice**.)

Syntax: **ignore** `<range1> [ <range2>] ... [ <rangeN>]`

ignore `bad`

where

`<rangeI> =:: <spectrum range>: <channel range> | <channel range>.`

If no `<spectrum range>` is given, then the previous range is used (the initial default range is file one (1) only). The form of `<spectrum range>` is

<spectrum range> =::<init spectrum> – <last spectrum> | <spectrum>

where `<init spectrum>`, `<last spectrum>`, and `<spectrum>` are spectrum numbers, in the order that they were input with the `data` command. The form of channel range is

<channel range> =:: <initial channel> — <last channel> | <channel>

If integers are given for the channel ranges then channels will be used while if reals are given then energies (or wavelenths if`setplot wave` has been specified). If only the last channel is indicated, then a default value of one (1) is used for the initial channel. Channels remain ignored until they are explicitly noticed with the `notice` command, or if a spectrum is replaced.

Examples:

Assume that 4 spectra have been read in, the first 2 with 100 channels and the last 2 with 50 channels.

XSPEC12> ignore **:1-10

//The first 10 channels of all 4 spectra are ignored

XSPEC12> ignore 80–**

//An attempt will be made to ignore channels `≥80` in all four data

// sets (as that was the last spectrum range specified). As a result,

// only channels 80-100 will be ignored for spectra 1 and 2.

// No change will occur for spectra 3 and 4, as they have no

// channels greater than 50.

XSPEC12> ign 4:1-20 3:30-40 45–**

//Channels 11-20 for spectrum 4 are ignored (1-10 were ignored already)

// while channels 30-40 and 45-50 of spectrum 3 are ignored.

XSPEC12> ignore 1:1-5

//No channels are ignored, as these were ignored at the beginning.

XSPEC12> ignore 2:1.-5.

//Ignore all channels between 1 and 5 keV in the second dataset

5.4.9 notice: notice data channels

Notice data channels.(See also **ignore**.)

Syntax: **notice**`<range1> <range2> ... <rangeN>`

notice all

where

`<rangeI> =:: <spectrum range>: <channel range> | <channel range>.`

If no `<spectrum range>` is given, then the previous range is used (the initial default range is file one (1) only). The form of `<spectrum range>` is

<spectrum range> =::<init spectrum> – <last spectrum> | <spectrum>

where <init spectrum>, <last spectrum>, and <spectrum> are spectrum numbers, in the order that they were input with the data command. The form of channel range is

<channel range> =:: <initial channel> — <last channel> | <channel>

If <channel range> are integers then channels will be used or if reals then energies (or wavelengths if setplot wave has beenspecified). If only the last channel is indicated, then a default value of 1 is used for the initial channel. Channels remain noticed until they are explicitly ignored with the ignore command. When a spectrum is replaced by another spectrum, all input channels automatically are noticed.

XSPEC12> **notice** all

resets all the channels to 'noticed'.

Examples:

Assume that 4 spectra have been read in, the first 2 having 100 channels and the last 2 having 50 channels.Assume also that channels 1–10 of all four spectra are ignored and that channels 80–100 of spectra 1 and 2 are ignored.

In XSPEC12, **notice** does not force the detector response to be reread (see RESPONSE DESCRIPTION).

XSPEC12> notice **:1—10

//The first 10 channels of all 4 spectra are noticed.

XSPEC12> notice 80—**

//an attempt will be made to notice channels ≥80 in all 4 spectra

// (as that was the last spectrum range specified) but the result is that

// only channels 80–100 will be noticed for spectra 1 and 2, with no

// change for spectra 3 and 4 as they have no channels greater than 50.

XSPEC12> notice 1:1—5

//No channels are noticed, as these channels were noticed

//in the beginning.

5.4.10 response: change the detector response for a spectrum

Modify one or more of the matrices used to describe the response(s) of the associated spectrum to incident X-rays.

Syntax: **response** [<filespec>...]

response [<source num>:]<spectrum num> none

where

```
<filespec> =:: [[<source num>:]<spectrum num>] <file name>...,
```

and <file name> is the name of the response file to be used for the response of the associated spectrum. If <file name> ends in a {n} specifier then the nth response will be read from the file. <spectrum num> is the spectrum number for the first file name in the specification, and follows similar rules as described in the **data** command description. An important difference however is that the response command may only be used to modify the response of a previously loaded spectrum: an error message is printed if the <spectrum num> is greater than the current number of spectra (as determined from the last use of the **data** command).

An optional <source num> may be specified to attach additional responses to a spectrum, and should be paired with <spectrum num> separated by a ':'. This allows the user to assign multiple models, each with their own response file, to a particular spectrum. See the **model** command for more information. If no <source num> is specified, it always defaults to 1. Source numbers do not need to be assigned consecutively to a spectrum, and gaps in numbering are allowed. The additional response may be removed with a **response** <source num>:<spectrum num> none command. Both the **show data** and **show response** commands will display current information regarding the response(s) to spectrum assignments.

A file name none indicates that no response is to be used for that spectrum. This situation means that any incident spectrum will produce no counts for those particular channels. If a file is not found or cannot be opened for input, then the user is prompted for a replacement response file. An <EOF> at this point is equivalent to using none as the response. See the **data** command for ways to totally remove the spectrum from consideration. The user is also prompted for a replacement if the response file has a different number of PHA channels than the associated spectrum. A warning will be printed out if the response detector ID is different from the associated spectrum's. The current ignore status for channels is not affected by the command. (See the **ignore** and **notice** commands).

Examples:

It is assumed that there are currently three spectra:

Single source usage:

```
XSPEC12> response a,b,c          // New files for the response are given for all three files.
XSPEC12> response 2 none         // No response will be used for the second file.
XSPEC12> response ,d{2}          // The second response in d becomes the response for
                                 //the second file.
```

Multiple source usage:

```
XSPEC12> response 2:1 e          // A second source with response e.pha is now added to
                                 // the first spectrum.  A second model can be assigned
                                 // to this source.
XSPEC12> response 2:2 f  3:2 g   // A second and third source is assigned to spectrum 2.
XSPEC12>  response 2:2 none      // The second source is now removed from spectrum 2.
```

5.5 Fit Commands

5.5.1 bayes: set up for Bayesian inference

Syntax: **bayes** [<option> | <mod par #>] {<prior type> <hyperparameters>}

where <opton> =:: [off | on | cons]. If a parameter number is given as the first argument then this command sets up the prior for the specified model parameter. The supported priors are `cons' and `exp'. The cons prior requires no hyperparameters and the exp prior requires a hyperparameter giving the exponential decay scale. The log prior for the exp case is taken to be -param/hparam - log(hparam), where param is the fit parameter value and hparam the hyperparameter. If the first argument to the `bayes' command is not a parameter number then one of the options 'off', 'on', 'cons' is used. The first two turn Bayesian inference off or on, while 'cons' turns Bayesian inference on and gives all parameters a constant prior.

5.5.2 chain: run a Monte Carlo Markov Chain.

Syntax: **chain** [burn <length>] [clear] [filetype fits|ascii] [info] [length <length>] [load <filename>] [proposal [<distr> <source>]|[<user-defined>]] [rand on|off] [run [>]<filename>] [stat <par num>] [temperature <value>] [unload <range>]

Beginning with v12.4.0, the default is to write the chain to a FITS file. Text file output may be selected with the filetype option.

If the proposal source is set to use the fit correlation matrix (the default), you must perform a fit before running any chains.

burn <length>	Specifies that the first <length> steps should be thrown away prior to storing the chain.
clear	Does a reset and removes all chains from the list.
filetype fits|ascii	Chooses the format of the output chain file. fits (the default) writes the chain to a binary table in a FITS file. ascii writes the chain to a simple text file.

Either format is readable when using the `load` command.

`info` — Prints out information on the current chains.

`length <length>` — Sets the length for new chains.

`load <filename>` — Loads a chain which has been run earlier, stored in file given by `<filename>`.

`proposal <distr> <source>` — Selects the proposal distribution and source of covariance information to be used when running new chains. The default is `proposal gaussian fit`. Currently implemented `<distr>` options are: `gaussian` and `cauchy`. `<source>` options are:

- `chain` — Covariance is taken from the currently loaded chains.
- `diagonal <values>` — The values of a diagonal covariance matrix are entered directly on the command line, separated by commas and/or spaces: `C_11 C_22 ... C_nn`.
- `<filename>` — Covariance is read in from a user-specified text file. The file must contain the values of an NxN matrix where N is the current number of freely varying parameters. The values of each matrix row should be entered on one line with whitespace separation. Since this matrix is always symmetrical, values above the diagonal may be omitted. For example a 2x2 matrix could be entered as:

0.98

0.15 0.96

`fit` — Covariance is taken from the correlation information produced by the current fit.

`matrix <values>` — The lower half and diagonal of a symmetrical square covariance matrix are entered directly on the command line, separated by commas and/or spaces: `C_11 C_21 C_22 C_31 C_32 C_33 ... C_nn`

Typing `chain proposal` with no other arguments will show a list of all available proposal options.

For an alternative to XSPEC's `<distr> <source>` proposal options, the user may instead want to provide their own custom randomization algorithm. This can be done by writing their own C++ class(es) derived from an XSPEC randomizer base class. The custom class is added at runtime using the same **initpackage/lmod** command sequence as for local models, and is specified by `proposal <name>` where `<name>` is the unique name attribute the user provides for their class. Please see Appendix G for more information on writing a custom randomizing class, and **initpackage** for building and loading it.

`rand on|off` — Specifies whether the chain start point will be randomized, or taken from the current parameters.

`recalc` — A deprecated option that performs the equivalent of `proposal gaussian chain`.

`run [>]<filename>` — Runs a new chain written to the specified file, or append to an already loaded file if the ">" character preceeds the filename. The chain is written to the file as it runs so its performance can be monitored by examining the file.

For high-chatter settings, additional information is printed to the screen. A long run may be interrupted with Ctrl-C, in which case the chain file will still exist but will not be automatically loaded. If appending to a file, the current `filetype` setting must match the format of the file or XSPEC will prevent it.

`stat [<modName>:]<parIdx>`

Writes out statistical information on a particular parameter of the chain, specified by the parameter index number (with optional model name). The information displayed is:

line1: The mean of the parameter over each chain file.

line2: The parameter mean over all chain files and the variance between chain means.

line3: The variance within the chains.

line4: The Rubin-Gelman convergence criterion.

line5: The fraction of repeats, defined as the number of lines in the chain file for which all parameter values are identical to the previous line, divided by the number of lines in the file.

`temperature <value>`

Sets the temperature parameter used in the Metropolis-Hastings algorithm for the proposal acceptance or rejection. The default value is 1.0 and zero or negative values are forbidden. By using the `run` append option, it is possible for different sections of the chain file to use different temperatures. The

	temperatures and the line numbers to which they apply are stored in the header of the FITS format chain files, or in the metadata section at the top of the ASCII text format files.
`unload <range>`	Removes the chains specified by `<range>` from the list in xspec. Note that this does NOT delete the chain files.

All loaded chains must contain the same fit parameters. xspec will prevent the loading of a chain with a different number of parameters from the currently loaded chains.

Examples:

```
XSPEC12>chain length 100
//Sets length of chains produced by the run command to 100.
XSPEC12>chain run chain_file1.out
//Runs a chain based on current valid fit parameters, output to
//chain_file1.out
XSPEC12>chain run >chain_file1.out
//Appends another run of length 100 to the end of chain_file1.out
XSPEC12>chain load chain_old.out
//Loads a pre-existing chain file, the result of an earlier run
//command.  Warning is issued if not the same length as
//chain_file1.out
XSPEC12>chain stat 3
//Prints statistical information on the 3rd parameter of the chain.
XSPEC12>chain proposal gaussian myfile.txt
//New chain proposals will be a normal distribution using
//covariance values stored in myfile.txt rather than fit
//correlation matrix.
XSPEC12>chain prop gauss diag .1 .001 .0001
// New chain proposals will be a normal distribution using a 3x3
// diagonal covariance matrix with the values from the
// command line.
```

```
XSPEC12>chain temperature .8
// Sets the Metropolis-Hastings temperature value to .8 for
// future chain runs, replacing the default 1.0.
XSPEC12>chain clear
```

//Removes the 2 loaded chains from xspec's chain list.

5.5.3 error, uncertain: determine confidence intervals of a fit

Determine the confidence region for a model parameter.

Syntax: **error** `[[stopat <ntrial> <toler>] [maximum <redchi>] [ <delta fit statistic>] [ <model param range>...]]`

where

<model param range> =:: [<modelName:>]<first param>-- <last param>

determines the ranges of parameters to be examined, and `<delta fit statistic>` (distinguished from the model parameter indices by the inclusion of a decimal point), is the change in fit statistic used.

For response parameters (see **gain** command), use **rerror** with identical syntax except:

<response param range> =:: [<sourceNum:>]<first param>-- <last param>

Each indicated parameter is varied, within its allowed hard limits, until the value of the fit statistic, minimized by allowing all the other non-frozen parameters to vary, is equal to the last value of fit statistic determined by the `fit` command plus the indicated `<delta fit statistic>`, to within an absolute (not fractional) tolerance of `<toler>`. Note that before the **error** command is executed, the data must be fitted. The initial default values are the range 1—1 and the `<delta fit statistic>` of 2.706, equivalent to the 90% confidence region for a single interesting parameter. The number of trials and the tolerance for determining when the critical fit statistic is reached can be modified by preceeding them with the `stopat` keyword. Initially, the values are 20 trials with a tolerance of 0.01 in fit statistic.

If a new minimum is found in the course of finding the error, then the calculation is aborted and control returned to the user. The `maximum` keyword ensures that **error** will not be run if the reduced chi-squared of the best fit exceeds `<redchi>`. The default value for `<redchi>` is 2.0.

Since there are very many scenarios which may cause an **error** calculation to fail, it is highly recommended that you check the results by viewing the 9-letter error string, which is part of the output from the **tclout error** command (see **tclout** for a description of the error string). If everything went well, the error string should be "FFFFFFFFF".

Examples:

Assume that the current model has four model parameters.

XSPEC12> error 1-4

//Estimate the 90% confidence ranges for each parameter.

XSPEC12> error 9.0

//Estimate the confidence range for parameters 1-4 with delta fit

// statistic = 9.0, equivalent to the 3 sigma range.

XSPEC12> error 2.706 1 3 1. 2

//Estimate the 90% ranges for parameters 1 and 3, and the 1. sigma

// range for parameter 2.

XSPEC12> error 4

//Estimate the 1. sigma range for parameter 4.

XSPEC12> error stop 20,,3

//Estimate the 1-sigma range for parameter 3 after resetting the number

// of trials to 20.Note that the tolerance field had to be included

//(or at least skipped over).

5.5.4 fit: fit data

Find the best fit model parameters for the current data by minimizing the current statistic.

Syntax: **fit** `<fit method parameters>`

The arguments to fit depend on the fitting method currently in use. See the **method** command for details (and for the usage of the USE_NUMERICAL_DIFFERENTIATION option in the user's startup Xspec.init file). Output from the fit command also depends on the fitting method currently in use.

Examples:

Using the Levenberg-Marquardt algorithm, the parameters accepted are the maximum `<number of iterations>` before the user is prompted, and the `<critical delta>`, which is the (absolute, not fractional) change in the statistic between iterations less than which the fit is deemed to have converged. If `<number of iterations>` or `<critical delta>` is entered through the **fit** command, it also becomes the future default value for the currently loaded fit **method** (ie. Levenberg-Marquardt).

XSPEC12> fit

// Fit with the default number of iterations and critical delta

// chi-squared.

XSPEC12> fit 60

// Fit with 60 as the number of iterations.

XSPEC12> fit 50 1.e-3

// Fit with 1.e-3 as the critical delta.

5.5.5 freeze: set parameters as fixed

Do not allow indicated model parameters to vary. (See also **thaw**.)

Syntax: **freeze** [<param range>...]

where

<param range =:: [modelName:] <param#> | <param#> – <param#>.

For response parameters (see **gain** command):

rfreeze [<param range>...]

where

<param range =:: [source number:] <param#> | <param#> – <param#>.

The indicated model parameter or range of model parameters will be marked so they cannot be varied by the `fit` command. By default,the range will be the last range input by either a **freeze** or **thaw** command.

Examples:

Currently there are six parameters, initially all unfrozen.

XSPEC12> freeze 2

//Parameter 2 is frozen

XSPEC12> freeze 4-6

//Parameters 4, 5, and 6 are frozen.

XSPEC12> thaw 2 3-5

//Parameters 2, 4, and 5 are thawed, parameter 3 is unaffected.

XSPEC12> freeze

//Parameters 3,4,5 are frozen (the last range input by a freeze

//or thaw command).

XSPEC12> rfreeze 4-6

//Response parameters 4, 5, and 6 are frozen.

5.5.6 ftest: calculate the F-statistic from two χ2 values

Calculate the F-statistic and its probability given new and old values of χ^2 and number of degrees of freedom (DOF).

Syntax: **ftest** chisq2 dof2 chisq1 dof1

The new χ^2 and DOF, chisq2 and dof2, should come from adding an extra model component to (or thawing a frozen parameter of) the model which gave chisq1 and dof1.If the F-test probability is low then it is reasonable to add the extra model component. WARNING : it is not correct to use the F-test statistic to test for the presence of a line (see Protassov et al astro-ph/0201457).

5.5.7 goodness: perform a goodness of fit Monte-Carlo simulation

Perform a Monte Carlo calculation of the goodness-of-fit.

Syntax: **goodness** `[ <# of realizations>] [sim | nosim]`

This command simulates `<# of realizations>` spectra based on the model and writes out the percentage of these simulations with the fit statistic less than that for the data. If the observed spectrum was produced by the model then this number should be around 50%. This command only works if the sole source of variance in the data is counting statistics. The `sim|nosim` switch determines whether each simulation will use parameter values drawn from a Gaussian distribution centered on the best fit with sigma from the covariance matrix. The `sim` switch turns on this option, `nosim` turns it off in which case all simulations are drawn from the best-fit model. The default starting setting is `nosim`.

5.5.8 improve: try to find a new minimum

Syntax: **improve**

This command runs the MINUIT improve command which attempts to find a new local minimum in the vicinity of the current minimum. This gives some global minimization capability.

5.5.9 margin: MCMC probability distribution.

Use the currently loaded MCMC chains to calculate a multi-dimensional probability distribution.

Syntax: **margin** `<step spec.> [<step spec.> ...]`

where `<step spec.> ::= [{LOG or NOLOG}] [<model name>:]<fit param index> <low value> <high value> <no. steps>`. The indicated fit parameter is stepped from '<low value>' to '<high value>' in '<no. steps>+1' trials. The stepping is either linear or log. Initially, the stepping is linear but this can be changed by the optional string 'log' before the fit parameter index. 'nolog' will force the stepping to be returned to the linear form. The number of steps is set initially to ten. The results of the most recently run margin command may be examined with **plot**

margin (for 1-D and 2-D distributions only). This command does not require that spectral data files are loaded, or that a valid fit must exist.

Examples:

Assuming chain(s) are loaded consisting of 4 parameters.

```
XSPEC12>margin 1 10.0 12.0 20 log 3 1.0 10.0 5

//Calculate a 2-D probability distribution of parameter 1 from 10.0-12.0 in 20
linear bins, and parameter 3 from 1.0-10.0 in 5 logarithmic bins.

XSPEC12>margin 2 10.0 100.0 10 nolog 4 20. 30. 10

//Now calculate for parameter 2 in 10 log bins and parameter 4 in 10 linear
bins.
```

5.5.10 renorm: renormalize model to minimize statistic with current parameters

Renormalize model, or change renorm conditions.

Syntax: **renorm** `[AUTO | NONE | PREFIT]`

The renorm command will adjust the normalizations of the model by a single multiplication factor, which is chosen to minimize the fit statistic.Such a renorm will be performed explicitly whenever the command is used without a key-word, or during certain XSPEC commands, as determined by the following key-words:

AUTO – Renormalize after a **model** or **newpar** command, and at the beginning of a fit

PREFIT – Renormalize only at the beginning of a fit

NONE – Perform no automatic renormalizations, i.e., only perform them when a renorm command is given explicitly.

5.5.11 steppar: generate the statistic "surface" for 1 or more parameters

Perform a fit while stepping the value of a parameter through a given range. Useful for determining confidence ranges in situations where greater control is needed than given with the error command.

Syntax: **steppar** `<step spec> [ <step spec>...]`

where

<step spec> ::= [<log | nolog>] [<current | best>]

[<modelName>:]<param index> <low value> <high value> <# steps>

The parameter is stepped from <low value> to <high value> in <# steps> plus one trials. The stepping is either linear or log. Initially, the stepping is linear but it can be changed by the optional string log before the parameter index. nolog will force the stepping to be returned to the linear form. If more than one parameter is entered, then <# steps> must be entered for each one except the last.

To perform a steppar run on **gain** (or response) parameters, the optional [<modelName>:] specifier is replaced by an optional [<sourceNumber>:] specifier, and the letter 'r' needs to be attached as a prefix to the <parameter index>. For example:

```
steppar 2:r3 1.5 2. 10
```

will step the third response parameter belonging to source number 2.

The number of steps is set initially to 10. At each value, the parameter is frozen, a fit performed, and the resulting value of chi-squared given. If best is given as an argument then the non-stepped parameters are reset to the best-fit values at each grid point. Alternatively, if current is given as an argument then the non-stepped parameters are started at their values after the last grid point (the default).

If multiple <step spec> are given for different parameters, then a raster scan of the parameter ranges is performed. At the end of the set, the parameters and chi-squared are restored to the values they had initially.

If the model is in a best-fit state when a **steppar** run is started and a new best fit is found during the run, the user will be prompted at the end of the run to determine if they wish to accept the new best-fit values for their parameters. This prompting can be disabled by the setting of the **query** flag.

Examples:

Assume that the current model has four parameters:

```
XSPEC12> steppar 3 1.5 2.5
      //Step parameter 3 from 1.5 to 2.5 in steps of .1.
XSPEC12> steppar log
      //Repeat the above, only use multiplicative steps of 1.0524.
XSPEC12> step nolog 2 -.2 .2 20
      //Step parameter 2 linearly from -.2 to .2 in steps of 0.02.
```

5.5.12 thaw: allow fixed parameters to vary.

Allow indicated parameters to vary. (See also freeze).

Syntax: **thaw**{[<param range>...]}

where

```
<param range> =:: [modelName:]<param #> | <param #>-- <param #>
```

For response parameters (see **gain** command):

rthaw {[<param range>...]}

where

```
<param range> =:: [sourceNum:]<param #> | <param #>-- <param #>
```

The indicated parameter, or range of parameters, will be marked as variable by the fitting commands and treated as a fitting parameter in subsequent fits. By default, the range will be the last range input by either a **freeze** or **thaw** command. See the **freeze** examples for an example of the use of the thaw command.

5.5.13 weight: change weighting used in computing statistic

Change the weighting function used in the calculation of chi-squared.

Syntax: **weight** `[standard | gehrels | churazov | model ]`

Standard weighting uses $\sqrt{N}$ or the statistical error given in the input spectrum. *Gehrels weighting* uses $1+\sqrt{N+0.75}$, a better approximation when N is small (Gehrels, N. 1986, ApJ 303, 336). *Churazov weighting* uses the suggestion of Churazov et al. (1996, ApJ 471, 673) to estimate the weight for a given channel by averaging the counts in surrounding channels. *Model weighting* uses the value of the model, not the data, to estimate the weight.

5.6 Model Commands

Overview of XSPEC12 Changes: In XSPEC12 several models can exist simultaneously, unlike XSPEC11. Different models are distinguished by name, which is a character string assigned by the user. The purpose of this is to allow an intuitive syntax for creating multiple models simultaneously fit to data, assigned to a corresponding number of sources. The familiar XSPEC11 syntax is, however, fully supported by assigning an internal symbol name.

For example, INTEGRAL/SPI data is modeled using 2 or more sources, one assigned to the background, and one or more assigned to objects resolved by the coded mask.

```
XSPEC12>data rev_001234{1-19}
…
XSPEC12>model 1:source1 phabs(cutoffpl)
XSPEC12>model 2:source2 phabs(powerlaw)
XSPEC12>model 3:bkg  spibk
…
```

Note that a source number must precede the name to avoid confusion with model expressions. The “normal” case, fitting to a single source, corresponds to source 1.

In the initial release, only SPI data which has a modified data format identifying the multiple responses can be used this way[4].

When the fit command is given the parameters of the model will be labeled source1:1, source1:2,…source2:1, source2:2,…bkg:1, bkg:2, etc.

Another use for multiple models is to name a model, fit with it, and then mark it as "inactive," i.e. not fit to data. A second model may then be defined and fit to the data, and afterward be interchanged. This is designed to allow the user to compare the fits from competing models without recalculation.

Apart from the removal of the pre-XSPEC10 model expression format, which was previously declared deprecated and is now no longer recognized, this new functionality provides a proper superset of the XSPEC11 syntax. The command

```
XSPEC12> model wa(po)
```

Creates a "default" model which takes an internal (hidden) symbol as a name. Its parameters are sequenced from 1 as in XSPEC11.

Another enhancement is in the newpar command. XSPEC12's expression analyzer developed for parsing model expressions is also used for parameter links. Thus newpar link expressions can be polynomials in multiple parameters, such as

XSPEC12> newpar par1 = par2*par2

or

XSPEC12> newpar par1 = 0.5*par3 + 1.5*par4

In sum, most of the syntax enhancements added to XSPEC12 support the presence of multiple models. The need to identify parameters of different models uniquely requires that their name and number be specified, which requires enhancements in the syntax not only in the model-related commands **model**, **addcomp**, **delcomp**, and **editmod** but also the parameter-related commands **newpar**, **freeze**, **thaw**, **untie**, **steppar**, and **error**. However, if the model is not named, all of these commands can be used identically as in XSPEC11.

5.6.1 addcomp: add component to a model

Add a component to the model.

Syntax: **addcomp** [modelName:]n <comp>

[4] In the initial release, only SPI data which has a modified data format identifying the multiple responses can be used this way. It is intended, in the full release, that all data may be fit this way using the same technique to implement background models

where `n` is the component number *before* which the new component is to be inserted, and <comp> is the name of the new component. Components are numbered in sequence in order of appearance in the expression entered. The new component is regarded as an operator on the component added if it is not additive.

The optional modelName qualifier allows the user to address a named model.

The user is prompted for parameter values for the component. If there are *m* components in the current model, then acceptable values for the component number added are *1* to *m+1*.

XSPEC detects the type of the model (additive, multiplicative etc), checks the correctness of the syntax of the output model, and adds the component if the resulting models obeys the syntax rules documented in the **model** command.

Thus,

```
XSPEC12> mo  wa(po)
```

Followed by

```
XSPEC12> addcomp 2 bb
```

Yields the model achieved by

```
XSPEC12> mo  wa(bb + po)
```

See also delcomp (delete component by number).

Other Examples will serve to clarify addcomp's behavior.

Suppose that the current model specification is

```
ga+po
```

which using the **show** command would yield the description

model = gaussian[1] + powerlaw[2]

The comments give the model expression following the entry of **addcomp** and **delcomp** commands:

```
XSPEC12> addcomp 2 wab
      //gaussian[1]+wabs[2](powerlaw[3])
XSPEC12> addcomp 4 pha
      //(gaussian[1]+wabs[2](powerlaw[3]))phabs[4]}
XSPEC12> delcomp 1
      //(wabs[1](powerlaw[2]))phabs[3]}
XSPEC12> addcomp 2 zg
      //(wabs[1](zgauss[2]+powerlaw[3]))phabs[4]}
XSPEC12> delcomp 3
//(wabs[1](zgauss[2]))phabs[3]

XSPEC12> mo wa(po)
XSPEC12> addcomp 1 ga
```

```
// gauss[1] + wabs[2]*powerlaw[3]
XSPEC12> delcomp 1
XSPEC12> addcomp 1 pha
// phabs[1]*wabs[2]*powerlaw[3]

XSPEC12>mo wabs(po)
XSPEC12> addcomp 3 bb
// wabs[1]*powerlaw[2] + bbody[3]
XSPEC12> delcomp 1
XSPEC12> addcomp 3 pha
// wabs[1]*powerlaw[2]*pha[3]
XSPEC12> addcomp 3 po
// ERROR: po (additive) is interpreted as being added to the multiplicative
// model pha[3], which is a context error.

For multiply nested models…
XSPEC12> mo wa(po + pha(bb + ga))
XSPEC12> addcomp 6 po
// wabs[1](powerlaw[2] + phabs[3](bbody[4] + ga[5]) + powerlaw[6])
XSPEC12> addcomp 5 peg
// wabs[1](powerlaw[2] + phabs[3](bbody[4] + pegpwlw[5] ga[6]) + powerlaw[7])
XSPEC12> addcomp 7 wa
// wabs[1](powerlaw[2] + phabs[3](bbody[4] + pegpwlw[5] ga[6]) +
wabs[7]*powerlaw[8])
```

5.6.2 addline: add spectral lines to a model

Tcl script to add one or more lines to the current model in an optimum fashion.

Syntax: addline `[<nlines>] [<modeltype>] [{fit|nofit}]`

`<nlines>` additional lines are added one at a time. Line energies are set to that of the largest residual between the data and the model. For each line a fit is performed with the line width and normalization as the only free parameters. The default option is one gaussian line. The other <modeltype> that can be used is lorentz. If no third argument is given then the sigma and normalization of each line are fit. If ``nofit'' is specified then the fit is not performed but if ``fit'' is specified then all free parameters are fit.

addline currently will only work with the default model (i.e. not for named models).

5.6.3 delcomp: delete a model component

Delete one or more components from the current model.

Syntax: **delcomp** [modelName:]`<comp num range>`

where

<comp num range>

is range of positions in the model specification of the components to be deleted.

Examples:

Suppose that the current model specification is

```
wa(po+ga+ga).
```

Then

```
XSPEC12> delcomp 3-4
      //Changes the model to wa(po)
XSPEC12> delcomp 1
      //Changes the model to po
```

5.6.4 dummyrsp: create and assign dummy response

Create a "dummy" response, covering a given energy range.

Syntax: **dummyrsp** `[ <low Energy> [ <high Energy> [ <# of ranges>[ <log or linear> [ <channel offset> [ <channel width> [<source_Num:spec_Num>]]]]]]`

This command creates a dummy response matrix based on the given command line arguments, which will either temporarily supersede the current response matrix, or create a response matrix if one is not currently present. There are two main uses for this command: to do a "quick and dirty" analysis of uncalibrated data (mode 1), and to examine the behaviour of the current model outside the range of the data's energy response (mode 2). Note that mode 2 usage has now been rendered redundant by the more flexible **energies** command.

All parameters are optional. The initial default values for the arguments are 0.01 keV, 100 keV, 200 logarithmic energy steps, 0.0 channel offset, and 0.0 channel width. The default values of the first 5 parameters will be modified each time the parameter is explicitly entered. The channel width parameter however always defaults to 0.0 which indicates mode 2 operation, described below.

In addition to the 6 optional parameters allowed for versions 11.x and earlier, a seventh optional parameter has been added allowing the user to apply the dummy response to just one particular source of a spectrum. It consists of two integers for (1-based) source number and spectrum number, separated by a colon. Either both integers should be entered, or they should be left out entirely. ie. A dummy response is either made for EVERY source in every spectrum, or just 1 source in 1 spectrum. This parameter always defaults to all sources and all spectra.

For mode 1 usage, simply enter a non-zero value for the channel width. In this instance, one has a spectrum for which typically no response matrix is currently available. This command will create a diagonal response matrix with perfect efficiency, allowing for the differences in binning between the photon energies and the detector channel energies (see example below). The response matrix will range in energy from `<low Energy>` to `<high Energy>`, using `<# of ranges>` as the number of steps into which the range is logarithmically or linearly divided. The detector channels are assigned to have widths of energy `<channel width>` (specified in keV),

the lower bound of the first channel starting at an energy of `<channel offset>`. Then the data can be fit to models, etc., under conditions that assume a perfect detector response.

For mode 2 usage (channel width = 0.0), one can use this command to examine the current model outside the range of the energy response of the detector. When examining several aspects of the current model, such as plotting it or determining flux, XSPEC uses the current evaluation array. This, in turn, is defined by the current response files being used, which depend on the various detectors. For example, low energy datasets (such as those from the *EXOSAT* LEs) may have responses covering 0.05 to 2 keV, while non-imaging proportional counters can span the range from 1 to 30 keV. If the user wishes to examine the behavior of the model outside of the current range, then he or she temporarily must create a dummy response file that will cause the model to be evaluated from `<low energy>` to `<high energy>`, using `<# of ranges>` as the number of steps into which the range is logarithmically or linearly divided. If one wishes only to set the energy response range, than the `<channel width>` argument may be omitted. In this case, or in the case where no data file has been read in, all entries of the dummy response matrix are set to zero. Under these circumstances the dummyrsp has no physically correct way of mapping the model into the data PHA channels, so the user should not try to fit–or plot–the data while the dummyrsp is active in this mode. Also, data need not even be loaded when calling this command in mode 2.

The previous response matrices can be reimplemented with the `response` command, with no arguments. Any use of the `data` and `notice` commands will replace the dummy response with a correct set of matrices, or with no response matrix if none was originally present.

Examples:

```
XSPEC12> dummyrsp
      //Create the dummy response for all spectra and sources with the
      //default limits, initially .01, 100, and 200 bins.
XSPEC12> dummyrsp .001 1
      //Create a dummy response with 200 bins that cover the range from
      //0.001 to 1 keV.
XSPEC12> dummyrsp ,,,500
      //The same range, but now with 500 bins.
XSPEC12> dummyrsp ,,,,lin
      //The same range, but now with linearly spaced bins.
XSPEC12> dummyrsp ,,,,,0.1
      //The same range, but now create a diagonal response matrix, with
      //channel widths of 0.1 keV.
XSPEC12> response
      //Restore any previous correct responses.
```

Example dummy response matrix:

Assume a spectrum with 4 channels, then

```
XSPEC12> dummyrsp .0 30.0 3 lin 5.0 8.0
```

will produce the following response:

Energies	Detector channel energies			
	5.0 – 13.0	13.0 – 21.0	21.0 – 29.0	29.0 – 37.0
0.0 – 10.0	0.5	0	0	0
10.0 – 20.0	0.3	0.7	0	0
20.0 – 30.0	0	0.1	0.8	0.1

5.6.5 editmod: edit a model component

Add, delete, or replace one component in the current model.

Syntax: **editmod** `[ <delimiter>] <component1> <delimiter> <component2> <delimiter> ... <componentN> [ <delimiter>]`

where

`<delimiter>`

is some combination of `(`,`+`,`*`,and`)`, and `<componentJ>` is one of the models known to XSPEC.

The arguments for this command should specify a new model, with thesame syntax as the previous model, except for one component whichmay be either added, deleted, or changed to a different component type. XSPEC then compares the entered model with the current model,determines which component is to be modified (prompting the user if necessary to resolve ambiguities) and then modifies the model,prompting the user for any new parameter values which may be needed.

Examples:

```
XSPEC12> mo wabs(po)
XSPEC12> ed wabs(po+ga)
      //This command will add the component gauss to model
      // in the specified place and prompt the user for its initial
      // parameters.
XSPEC12> mo wabs(po+zg)
XSPEC12> ed po+zg
      //This command will delete the component wabs from the
      //model, leaving the other components and their current
      //parameter values unchanged
XSPEC12> mo wabs(po+po)
XSPEC12> ed wabs(po)
      //Here an ambiguity exists as to which component to delete.
      //In this case XSPEC will print out  the current model,
      //showing the component number for each component, and then
      //prompt the user for which component he wants deleted.
XSPEC12> mo wabs(po+ga)
XSPEC12> ed wabs(po+zg)
      //The component gauss will be replaced by the component zgauss,
      //and the user will be prompted for parameter values for the new
```

```
// component
```

5.6.6 energies: specify new energy binning for model fluxes

Supply an energy-binning array to be used in model evaluations in place of their associated response energies. The calculated model spectra are then interpolated onto the response energy arrays before multiplying by the response matrix. This command replaces and enhances the **extend** command from earlier versions.

Syntax: **energies** <range specifier> [<additional range specifiers>…]

energies <input ascii file>

energies extend <extension specifier>

energies reset

where the first <range specifier> ::= <low E> <high E> <nBins> log | lin

<additional range specifiers> ::= <high E> <nBins> log | lin

<extension specifier> ::= low | high <energy> <nBins> log | lin

All energies are in keV. Multiple ranges may be specified to allow for varied binning in different segments of the array, but note that no gaps are allowed in the overall array. Therefore only the first range specifier accepts a <low E> parameter. Additional ranges will automatically begin at the <high E> value of the previous range.

The extend option provides the same behavior as the old **extend** command. Models will use associated response energy arrays, with an additional low and/or high array extension. <energy> is the value to which the array is extended, using <nBins> additional log or linear bins.

With the <input ascii file> option, the user can instead supply a customized energy array from a text file. The format requirements are simply that the bin values must appear 1 to a line and in ascending sorted order. Blank lines are allowed and so are comments, which must be preceded by a '#'. A simple example:

```
# myEnergyBinning.txt
.1
1.0
10.   # now some linear bins
15.
20.
25.
```

which would actually produce the same energy array as:

```
energies .1 10. 2 log  25. 3 lin
```

Once an energy array is specified, it will apply to all models, and will be used in place of any response energy array (from actual or dummy responses) for calculating and binning the model flux. It will also apply to any models that are created after it is specified. To turn off this behavior and return all models back to using their response energies, simply type "energies reset".

Similarly, an array extension created by the "extend" option will continue to be applied to all models until it is either overwritten by another extension, replaced by a new **energies** array, or removed with the "reset" option. This allows both low and high extensions to exist together.

When a custom-energy binned model flux array needs to be multiplied by a response matrix, xspec will temporarily rebin the flux array to match up with the response energy binning. This is done by simply scaling the flux by the fractional overlap between the custom and response bins. If there is no overlap between the custom and response energies, then the response will be multiplied by zero.

The **energies** command saves the most recently entered range and extension specifiers to be used as default values the next time it is called. The initial default range specifier is 1 range with <low E> = .1, <high E> = 10., <nBins> = 1000, and `lin`. The initial default extension specifier is `high` with <energy> = 100., <nBins> = 200, and `log`.

Examples:

```
XSPEC12> energies ,50,,log
      // Creates an array from .1 to 50. of 1000 logarithmic bins.
XSPEC12> energies ,,,,100. 5 lin
      // Modifies previous array by adding 5 linear bins from 50. to 100.
XSPEC12> energies ,,,,200.
      // The 2nd range is now 50. to 200. in 5 linear bins.
XSPEC12> energies 1.,,100
      // Array is now just 1 range, 1. to 50. in 100 logarithmic bins.
XSPEC12> energies myFile.txt
      // Array is replaced with values stored in myFile.txt
XSPEC12> energies extend ,75.,,lin
      // Models will go back to using response energies, but with an
      // extension of the high end to 75. keV in 100 additional linear bins.
XSPEC12> energies extend low .01
      // Add a low-end extension to .01 keV with 100 new linear bins.
XSPEC12> energies reset
      // All models will go back to using the original energy arrays
      // from responses.
```

5.6.7 eqwidth: determine equivalent width

Determine the equivalent width of a model component.

Syntax: **eqwidth** `[[RANGE <frac range>] <[model name:]model component number>] [err <number> <level> | noerr]`

The command calculates the integrated photon flux produced by an additive model component (combined with its multiplicative and/or convolution pre-factors) (FLUX), the location of the peak of the photon spectrum (E), and the flux (photons per keV) at that energy of the continuum (CONTIN). The equivalent width is then defined as {EW = FLUX / CONTIN} in units of keV. New for version 12: the continuum is defined to be the contribution from all other components of the model.

There are certain models with a lot of structure where, were they the continuum, it might be inappropriate to estimate the continuum flux at a single energy. The continuum model is integrated (from E(1−<frac range)> to E(1+<frac range)>. The initial value of <frac range> is 0.05 and it can changed using the RANGE keyword.

The err/noerr switch sets whether errors will be estimated on the equivalent width. The error algorithm is to draw parameter values from the distribution and calculate an equivalent width. <number> of sets of parameter values will be drawn. The resulting equivalent widths are ordered and the central <level> percent selected to give the error range. The parameter values distribution is assumed to be a multivariate Gaussian centered on the best-fit parameters with sigmas from the covariance matrix. This is only an approximation in the case that fit statistic space is not quadratic.

Examples:

The current model is assumed to be $M_1(A_1+A_2+A_3+A_4+M_2(A_5))$, where the M_x models are multiplicative and the A_x models are additive.

```
XSPEC12> eqwidth 3
      // Calculate the total flux of component M1A2 (the third
      // component of the model with its multiplicative pre-factor)
      // and find its peak energy (E). The continuum flux is
      // found by the integral flux of M1(A1+A3+A4+M2(A5)), using the
      // range of 0.95E to 1.05E to estimate the flux.
XSPEC12> eqwidth range .1 3
      // As before, but now the continuum is estimated from
      // its behavior over the range 0.9E to 1.1E.
XSPEC12> eqwidth range 0 3
      // Now the continuum at the single energy range (E)
      // will be used.
XSPEC12> eqwidth range .05 2
      // Now the component M1A1 is used as the feature, and
      // M1(A2+A3+A4+M2(A5)) are used for the continuum.  The range
      // has been reset to the original value.
XSPEC12> eqwidth 1
      // Illegal, as M1 is not an additive component.
```

5.6.8 flux: calculate fluxes

Calculate the flux of the current model between certain limits.

Syntax: **flux** [<lowEnergy> [<hiEnergy>]] [err <number> <level> | noerr]

where <lowEnergy> and <hiEnergy> are the values over which the flux is calculated.Initial default values are 2 to 10 keV.

The flux is given in units of photons cm^{-2} s^{-1} and ergs cm^{-2} s^{-1}. The energy range must be contained by the range covered by the current spectra (which determine the range over which the model is evaluated).Values outside this range will be reset automatically to the extremes. Note that

the energy values are two separate arguments, and are NOT connected by a dash. (see parameter ranges in the freeze command).

The flux will be calculated for all loaded spectra. If no spectra are loaded (or none of the loaded spectra have a response), the model is evaluated over the energy range determined by its dummy response. (In XSPEC12, models are automatically assigned default dummy responses when there is no data, so the dummyrsp command need not be given.) If more than 1 model has been loaded, whichever model the user has specified to be the active one for a given source is the one used for the flux calculation.

The results of a flux command may be retrieved by the "tclout flux <n>" command where n is the particular spectrum of interest. If the flux was calculated for the case of no loaded spectra, the results can be retrieved by "tclout flux" with the <n> argument omitted.

The `err/noerr` switch sets whether errors will be estimated on the flux. The error algorithm is to draw parameter values from the distribution and calculate a flux. `<number>` of sets of parameter values will be drawn. The resulting fluxes are ordered and the central `<level>` percent selected to give the error range. The parameter values distribution is assumed to be a multivariate Gaussian centered on the best-fit parameters with sigmas from the covariance matrix. This is only an approximation in the case that fit statistic space is not quadratic.

There is also a model component cflux which can be used to estimate fluxes and errors for part of the model. For instance, defining the model as wabs(pow + cflux(ga)) provides a fit parameter which gives the flux in the gaussian line.

Examples:

The current data have significant responses to data within 1.5 to 18 keV.

```
XSPEC12> flux
      //Calculate the current model flux over the default range.
XSPEC12> flux 6.4 7.0
      //Calculate the current flux over 6.4 to 7 keV
XSPEC12> flux 1 10
      //The flux is calculated from 1.5 keV (the lower limit of the
      //current response's sensitivity) to 10 keV.
```

5.6.9 gain: modify a response file gain

Modify a response file gain, in a particularly simple way. ***CAUTION*** This command is to be used with extreme care for investigation of the response properties. To properly fit data, the response matrix should be recalculated explicitly (outside of XSPEC) using any modified gain information derived.

The gain command has been slightly revised for XSPEC12. Previously when a user entered a gain command, it was generally interpreted to apply to an entire **model.** This new implementation clearly defines an applied gain as belonging to a particular **response**. It also offers less ambiguity for dealing with XSPEC12's multiple models scheme. So for example if 2 spectra are loaded, each in its own data group, and the user enters a **gain fit** command, under the old system they would be prompted for 2 sets of parameters since the model is applied to 2 data groups. With the new system, the user specifies which particular response (belonging to either spectrum 1 or 2) they wish to apply the gain fit to, and are then prompted for just the 1 set of gain

parameters for that response. This is more clearly demonstrated with the examples below. The new command options “gain nofit all” and “gain off” are also described below.

***** NOTE: Backwards incompatible syntax change *****

Beginning with XSPEC 12.5.1, **gain** parameters must be specified as [<sourceNum>:]<specNum> and NOT <specNum>[:<sourceNum>]. This reversal was made so that the **gain** command conforms to the [<sourceNum>:]<specNum> usage in other XSPEC commands, such as **response** and **arf**.

****

Syntax: **gain [**<sourceNum>:]<specNum> <slope> <intercept>

gain fit [[<sourceNum>:]<specNum>]

gain nofit { [[<sourceNum>:]<specNum>] | all }

gain off

The first variant of the gain command shown above will apply the gain shift specified by the <slope> and <intercept> parameters to the response belonging to spectrum <specNum>, and optionally specified <sourceNum> if the data is analyzed with multiple models. The initial default <specNum> is 1; later, the default is the number of the spectrum last modified. Initially, all responses are assumed to have nominal gains, determined implicitly by the data in the response files. This is equivalent to a <slope> of 1 and an <intercept> of zero. All responses can be reset back to this original state by entering **gain off.** Note that in this mode of usage, the slope and intercept values do NOT become variable fit parameters. They are simply fixed values used to modify the response.

The **gain fit** mode is used when the user wishes to have the slope and intercept parameters determined by the results of a fit. The <specNum> and optional <sourceNum> parameters specify to which response the fit gain values are to be applied. These may be omitted only if a single spectrum is loaded, with a single model source. Otherwise at least a spectrum number is required. The user will then be prompted for slope and intercept parameter information in the same way as model parameters are normally entered. These values are then immediately applied to the response, and will be adjusted the next time a fit is run.

Gain fit parameters belong to the more general category of **response parameters** in XSPEC, and may be modified using an equivalent set of commands to those used for regular model parameters. The command names are the same except prefixed by the letter **‘r’**:

XSPEC commands for editing/viewing model parameters	Equivalent commands for gain (or response) parameters
newpar	rnewpar
freeze	rfreeze
thaw	rthaw
untie	runtie
error	rerror
model	rmodel
show par	show par, show rpar

For example after assigning gain fit parameters to source 1 of spectrum 1 (with "gain fit 1"):

```
XSPEC12> rfreeze 1
XSPEC12> rnewpar 2 .05
XSPEC12> show rpar

Response parameters defined:
========================================================================
Source No.: 1
Rpar Spectrum Rmodel   Rpar_name  Unit   Value

   1     1    gain     slope            1.00000      frozen
   2     1    gain     offset           5.00000E-02  +/-  0.0
_____________________________________________________________________________
```

Rnewpar can also link gain parameters to one another and can adjust the hard and soft parameter limits, as newpar does for model parameters. The default gain parameter hard limits are hardcoded in XSPEC, but these can be overridden by setting GSLOP_MIN, GSLOP_MAX, GOFFS_MIN, and GOFFS_MAX keywords in the matrix extension of your response file.

The gain operation itself belongs to the category of **response functions,** which in future versions of XSPEC may be defined with **rmodel** just as regular XSPEC model functions are defined with **model**. Though gain is currently the only available response function, the following command will work:

```
// Apply gain to the response belonging to source 2 of spectrum 1
XSPEC12>rmodel 2:1 gain
```

which is equivalent to:

```
XSPEC12>gain fit 2:1
```

The **nofit** argument switches off the fitting and leaves the gain at the current values of the parameters. Unless the argument **all** is given, it is applied to a single response specified by <specNum> and optional <sourceNum>. As with gain fit, both arguments may be omitted if only a single spectrum with 1 source is loaded. When **all** is specified, fitting is switched off for the gain parameters of all responses. **gain off** will switch off fitting for all gain parameters, and will reset all of them to their nominal value.

Whenever a new response file is defined for a spectrum, the response will return to the nofit state with nominal value. The ignore and notice commands however will not affect the current gain of the response. THE GAIN COMMAND IS NOT CURRENTLY IMPLEMENTED FOR DUMMY RESPONSES.

Algorithm:

The gain command shifts the energies on which the response matrix is defined and shifts the effective area curve to match. The effective area curve stored by XSPEC is either the ARF, if one was in use, or is calculated from the RSP file as the total area in each energy range. This means that if there are sharp features in the response then these will only be handled correctly by the gain command if they are in the ARF or if no ARF is input. The new energy is calculated by E/<slope> - <intercept>.

Examples:

XSPEC12>gain 1 0.98

// The response belonging to spectrum 1 is adjusted with a slope of 0.98.

// The 1 may be omitted if only 1 spectrum (with 1 source) is loaded.

XSPEC12>gain 1,,.03

// The offset also is moved now by 0.03

XSPEC12>gain 2:4 1.1 0.1

// The response belonging to source number 2, spectrum 4, is adjusted with slope 1.1

// and offset 0.1.

XSPEC12>gain off

// The above 2 responses, and any others that have been adjusted, are reset to slope

// 1.0, offset 0.0.

XSPEC12> gain fit 3

// Variable fit parameters are created for spectrum 3 response. User will be prompted

// for starting fit parameter values of slope and offset.

XSPEC12> fit

// Best fit gain values will now be determined for and applied to spectrum 3 response.

XSPEC12> gain nofit 3

// Spectrum 3 response will retain its current gain values, but values will not be

// adjusted during future fits.

NOTE: Current gain information may be easily viewed with the **show response** command. Gain fit parameters may also be viewed with the **show par** or **show rpar** commands.

5.6.10 identify: identify spectral lines

List possible lines in the specified energy range.

Syntax: **identify** `<energy> <delta_energy> <redshift> <line_list>`

The energy range searched is `<energy>`±Δ`<energy>` (keV) in the rest frame of the source. If working in wavelength mode, as set by the **setplot** command, then the <energy> and <delta energy> parameters should be entered as wavelengths (in Angstroms). `<line list>` specifies the list of lines to be searched. The options are `bearden`, which searches the Bearden compilation of fluorescence lines (Bearden, J.A., 1967, Rev.Mod.Phys. 39, 78), `mekal`, which uses the lines from the mekal model (q.v.) and `apec`, which uses the APEC **http://cxc.harvard.edu/atomdb** line list. The `apec` option takes an additional two arguments: the temperature of the plasma (keV) and a minimum emissivity of lines to be shown. If the command **xset** has been used to set `APECROOT` then `identify` uses the `APECROOT` value to define the new atomic physics data files. See the help on the `apec` model for details.

5.6.11 initpackage: initialize a package of local models

The new **initpackage** command initializes a package of local models from their source code and from a model component description file in "model.dat" format which defines the component's name, type, function call, and its parameter names and initial settings. Further details of the file format, function and parameter specifications are given in Appendix C, **Adding Local Models To XSPEC**. **initpackage** is NOT CURRENTLY SUPPORTED on **Cygwin.** See the **static_initpackage** subsection below for the alternative local model build method for **Cygwin** users.

Syntax: **initpackage** <name> <description file> [<directory>] [-udmget]

The <name> argument names the package. For internal reasons package names must be lowercase: the initpackage command will force lower case and warn the user if the argument contains uppercase letters. Also there should be no numerals in the package name.

The <description file> argument specifies the model component description file. The third argument <directory> is optional and specifies the location of the source code. If it is not given, the value of the setting LOCAL_MODEL_DIRECTORY given in the user's Xspec.init file will be used. Finally, the <description file>, if not specified as an absolute pathname, will be read from the same directory as the source code.

Another optional argument is "-udmget", for local model libraries containing Fortran code which makes use of XSPEC's now-obsolete udmget function for dynamic memory allocation. None of the functions in XSPEC's built-in models library use udmget anymore, and the necessary xsudmget.cxx file no longer resides there. If a user still requires this code for their own local

models, they should add "-udmget" (without the quotes) at the end of the comamnd line. **initipackage** will then copy the files xsudmget.cxx and xspec.h into the user's local model directory.

initpackage performs the following tasks:

reads the model description file

writes code that will load the new component calculation functions

writes a makefile that will drive the compilation and installation of the new code

invokes the compiler and builds the library.

A separate command, **lmod**, actually loads the library.This two step process makes it easier to determine where the user is during the process if compilation failures arise. Further, if the model is complete and working correctly, only the **lmod** command need be invoked.

Initpackage can also be run as a stand-alone program outside of XSPEC. When used like this however, after initpackage has finished the user must manually run hmake to build their library. XSPEC performs this part automatically using a script file.

CYGWIN Users: static_initpackage

XSPEC dynamic libraries are not currently supported on Cygwin. Therefore local model libraries must be statically built outside of the XSPEC shell, and the xspec.exe executable must be re-linked to pick up the new library. Unlike on other platforms, local model libraries cannot be loaded at runtime with the **lmod** command. We have provided a static variation of the initpackage command for Cygwin users:

Syntax: **static_initpackage** <description file> <directory>

static_initpackage none

Unlike initpackage, this command can only be run as a stand-alone application outside of XSPEC. The <description file> argument is the same as for initpackage. The <directory> is the full path to your local model directory and is a required argument (also unlike initpackage). There is no <name> parameter since all static local model libraries will be assigned the name "static_local_mods." This command will perform similar tasks to initpackage, but for a static library build, and then will automatically re-link the XSPEC executable to pick up the new library.

The "static_initpackage none" option will restore the default (empty) static model library to the XSPEC executable. It will not remove or alter anything in the user's local model directory.

5.6.12 lmod, localmodel: load a package of local models

The new **lmod** command (**localmodel** is an alias for this command) loads a user model package Further details are given in Appendix C. This command is NOT SUPPORTED on **Cygwin**, where only statically built local model libraries are allowed. **Cygwin** users should instead consult the **static_initpackage** section of the **initpackage** help document.

Syntax: **lmod** <name> [directory]

As for **initpackage**, the <name> argument is the name of the model package being loaded, and the <directory> is the its location, defaulting to the setting of LOCAL_MODEL_DIRECTORY given in the user's Xspec.init

lmod performs the following tasks:

- loads the library corresponding to the package named <name>
- reads the model description file supplied by the **initpackage** command for the library
- adds the new model components to the list of models recognized by the model command.

Note that **lmod** requires that the user has write-access to <directory> (please see Appendix C for details).

5.6.13 lumin: calculate luminosities

Calculate the luminosity of the current model for a given redshift and rest frame energy range.

Syntax: **lumin** [<lowEnergy> [<hiEnergy>] [<redshift>] [err <number> <level> |noerr]

where <low Energy> and <hi Energy> are the rest frame energies over which the luminosity is calculated and <redshift> is the source redshift.Initial default values are 2 to 10 keV for 0 redshift. The luminosity is given in units of ergs/s. The energy range redshifted to the observed range must be contained by the range covered by the current spectra (which determine the range over which the model is evaluated). Values outside this range will be automatically reset to the extremes. Note that the energy values are two separate arguments and are NOT connected by a dash (see parameter ranges in the freeze command description).

The lumin will be calculated for all loaded spectra. If no spectra are loaded (or none of the loaded spectra have a response), the model is evaluated over the energy range determined by its dummy response. (In XSPEC12, models are automatically assigned default dummy responses when there is no data, so the dummyrsp command need not be given.) If more than 1 model has been loaded, whichever model the user has specified to be the active one for a given source is the one used for the lumin calculation.

The results of a lumin command may be retrieved by the "tclout lumin <n>" command where n is the particular spectrum of interest. If lumin was calculated for the case of no loaded spectra, the results can be retrieved by "tclout lumin" with the <n> argument omitted.

The err/noerr switch sets whether errors will be estimated on the luminosity. The error algorithm is to draw parameter values from the distribution and calculate a luminosity. <number> of sets of parameter values will be drawn. The resulting luminosities are ordered and the central <level> percent selected to give the error range. The parameter values distribution is assumed to be a multivariate Gaussian centered on the best-fit parameters with sigmas from the covariance matrix. This is only an approximation in the case that fit statistic space is not quadratic.

Examples:

The current data have significant response to data within 1 to 18 keV.

```
XSPEC> lumin,,,0.5
      //Calculate the current model luminosity over the default range for z=0.5
XSPEC> lumin 6.4 7.0
      //Calculate the current luminosity over 6.4 to 7 keV.
```

5.6.14 mdefine: Define a simple model using an arithmetic expression.

Syntax: mdefine `[name [expression [: [type] [emin emax]]]`

where 'name' = the name of the model. If "name" is a previously defined model with mdefine, the current definition will overwrite the old one, and the user is warned; if it is a built-in model, however, the user will be asked to use a different name.

'expression' = a string of arithmetic expression. Simple rules for expression:

1) The energy term, must be 'e' or 'E' in the expression. Other words, which are not numerical constants nor internal functions, are assumed to be model parameters.

2) If a convolution model varies with the location on the spectrum to be convolved, the special variable ".e" or ".E" may be used to refer to the convolution point.

3) The expression may contain spaces for better readability.

'type' = user may optionally specify the type of the model, the valid types are (add, mul, con). (Mix models are not yet implemented as of v12.5.0) Please note that the character ":" must be used to separate the options from the "expression". If "type" is not given default is add.

'emin emax' = user may also specify the minimum and maximum energy values for the model, the default values are 1.e-20 and 1.e+20, respectively.

Note that MDEFINE can also be used to display and delete previously defined models:

1) To display the name, type and expression of all previously defined models:

```
XSPEC12>mdefine
```

2) To display the name, type and expression of a previously defined model by the name, MNAME:

```
XSPEC12> mdefine MNAME
```

3) To delete a previously defined model by the name, MNAME:

```
XSPEC12> mdefine  MNAME :
```

Operators:

The following operators are recognized in an expression:

+ = plus operator
- = minus operator
* = multiplying operator
/ = dividing operator
** = exponentiation operator
^ = exponentiation operator

Functions:

The following internal functions are supported:

```
Unary Functions ..............................
```

EXP	(expr)	=	exp of a vector expression
SIN	(expr)	=	sine of vector expression in rad
SIND	(expr)	=	sine of a vector expression in degree
COS	(expr)	=	cosine of a vector expression in rad
COSD	(expr)	=	cosine of a vector expression in degree
TAN	(expr)	=	tangent of a vector expression in rad
TAND	(expr)	=	tangent of a vector expression in degree
LOG	(expr)	=	base 10 log of a vector expression
LN	(expr)	=	natural log of a vector expression
SQRT	(expr)	=	sqrt of a vector expression
ABS	(expr)	=	absolute value of a vector expression
INT	(expr)	=	integer part of a vector expression
ASIN	(expr)	=	sin^-1 of a vector expression in rad
ACOS	(expr)	=	cos^-1 of a vector expression in rad
MEAN	(expr)	=	mean value of a vector expression
DIM	(expr)	=	dimension of a vector expression
SMIN	(expr)	=	minimum value of a vector expression
SMAX	(expr)	=	maximum value of a vector expression

```
Binary Functions .............................
```

MAX	(expr1, expr2)	=	maximum of the two vector expressions
MIN	(expr1, expr2)	=	minimum of the two vector expressions

Examples:

```
XSPEC12> mdef dplaw E**p1 + f*E**p2        ! define a model named "dplaw" with
                                            3 parameters, p1, p2, f

XSPEC12> mdef junk a*e+b*log(e)/sin(e)     ! define a model named "junk" with
                                            2 parameters (a, b)

XSPEC12> mdef junk2  exp(-a*e) : mul       ! define a model named "junk2" with
                                            1 parameter, a; the option
                                            following ":" says that it will be
                                            a multiplicative model.

XSPEC12> mdef junk3  0.2+B*e : mul         ! define a model named "junk3" with
                                            1 parameter, B, options following
                                            ":" says that this will be a
                                            multiplicative model

XSPEC12> mdef bb E**2/T**4/(exp(E/T)-1)    ! try to define a blackbody model
                                            with name "bb", you get warning:
```

```
                        ***Warning: bb is a pre-defined model
                           Please use a different name for your model.

XSPEC12> mdef sg  exp(-E^2/(2*A*.E)) / sqrt(6.283*A*sqrt(.E))  :  con

                                              ! this defines a Gaussian
                                               convolution model with sigma
                                               varying with square root of
                                               energy.


XSPEC12> mdef junk2 :                         ! delete junk2

XSPEC12> mdef                                 ! display all user-defined models

-- Name ---- Type ------ Expression -----
 dplaw      add        E**p1+f*E**p2
 junk       add        a*E+b*LOG(E)/SIN(E)
 junk3      mul        a+b*E
 sg         con        EXP(-E^2/(2*A*.E))/SQRT(6.283*A*SQRT(.E))
----------------------------------------
```

5.6.15 model: define a theoretical model

Define the form of the theoretical model to be fit to the data.

model [<source num>:<name>] [<delimiter>] <component1> <delimiter> <component2> <delimiter>... <componentN> [<delimiter>]

model [?]

model [<name>|unnamed] none

model clear

model <name>|unnamed active|inactive

rmodel [<source num>:]<spec num> <response function>|none

where <delimiter> is some combination of (, +, *,), and <componentJ> is one of the model components known to XSPEC. The optional name must be preceded by a source number followed by a colon. To specifically refer to the default model use the string unnamed. Descriptions of these models may be accessed by typing help models at the prompt.

The source argument and name, if present, assign that model to be used with one of the sources found to be in the spectrum during the data pipelining. These 2 parameters allow one to simultaneously analyze multiple models, each assigned to their own responses. The model will be referred to the channel space using a response corresponding to that source number. To create a model for a source number higher than 1, a detector response must first exist for that number. See the examples below and the **response** command for more information about using multiple sources. This ability to assign multiple models both generalizes and replaces the XSPEC11 method of using '/b' to specify background models.

After the model is loaded, if there are data present the model is attached through the instrumental response to the spectra to be fitted, as in XSPEC11. Unlike XSPEC11, however, if there are no data loaded the model will be attached to a default diagonal dummy response. The parameters of that dummy response (energy range, number of flux points, linear/logarithmic intervals) can be set by the user in the Xspec.init file using the DUMMY setting. Thus any model can be plotted in energy or wavelength space as soon as it has been defined.

The model components are of various types depending on what they represent and how they combine with other models additive, multiplicative, convolution, and mixing models. Each component may have one or more parameters that can be varied during the fit (see the `newpar` command writeup).

- Additive model components are those directly associated with sources, such as power laws, thermal models, emission lines, etc. The net effect of two independent additive models is just the sum of their individual emissivities.
- Multiplicative model components do not directly produce photons, but instead modify (by an energy-dependent multiplicative parameter) the spectrum produced by one or more additive components. Examples of multiplicative models are photoelectric absorption models, edges, absorption lines, etc.
- Convolution models components modify the spectrum as a whole, acting like operators rather than simply applying bin by bin multiplication factors. An example of a convolution model is a gaussian smoothing with energy dependent width. Thus, when using convolution models, the ordering of components is in general significant (see below under **syntax rules**).
- Mixing model components implement two-dimensional transformations of model spectra. The data are divided into regions by assigning them to 2 or more datagroups, and the transformation "mixes" the flux among the regions. An example is the projct (projection) model, which assumes that the regions are 3-dimensional ellipsoidal shells in space, and projects the flux computed from the other components onto 2-dimensional elliptical annuli.

A list of all the currently installed models is given in response to the command

`model ?` (the '?' is not actually required)

(this will leave the current model in use).

The new command variants have the following uses:

model [<name>] none

removes the model of name <name> if given. Without the <name> argument, the command removes the unnamed "default" model, which is of course the XSPEC11 behavior.

model clear

removes all models

model <name>|unnamed active|inactive

makes the model named <name> active (fit to data) or inactive. Inactive models are tied to a dummy (unit diagonal) response. Making a model assigned to a given source active makes any previous model assigned to that source inactive. Note that to make the default unnamed model active or inactive refer to it by the string unnamed.

See the commands `delcomp`, `addcomp` and `editmod` for details on how to modify the current model without having to enter a completely new model.

rmodel [<source num>:]<spec num> <response function>|none

assigns or removes a response function to the response belonging to <source num> of spectrum <spec num>. Currently the only available <response function> in XSPEC is `gain`, which makes **rmodel** redundant with the **gain** command usage:

gain fit [<source num>:]<spec num>

Syntax Rules

Model components are combined in the obvious algebraic way, with + separating additive models, * separating multiplicative models, and parentheses to show which additive models the multiplicative models act on. The * need not be included next to parentheses, where it is redundant. Also, if only one additive model is being modified by one or more multiplicative models, the required brackets may be replaced by a *. In this case the additive model must be the last component in the grouping. Thus

$$M_1*(A_1+A_2) + M_2*M_3(A_3) + M_4*A_4 + A_5$$

is a valid model, where the *M*'s signify multiplicative models and the *A*'s additive models.

The old style syntax for entering models (versions 9.02 and earlier) is not supported in version 12 and will return a syntax error.

XSPEC12's recursive lexical analyzer and expression parser allows, in principle, infinite nesting depth. It has been tested to 3 levels of parentheses, although it should be said that this new behavior is a by-product of the design rather than fulfilling an important need. Thus, expressions such as

$$M_1*(A_1 + A_2*(A_3 + M_2*M_3*(A_6 + A_7))) + C_1*(A_8 + A_9*(A_{10} + M_2*A_6))$$

are supported.

The model expression is analyzed on entry and syntax errors, or undefined models, will return control to the prompt with an error message. XSPEC12's model definition algorithm treats expressions delimited by '+' signs that are not within parentheses as separate "Component Groups". The Component Group comprises a list of components of the different types, and these are in turn calculated and then combined to produce an internal "Sum Component". These Sum Components from each such component group are then added to produce the output model (note that if there is an overall component – for example, a convolution or mixing component – then all of the model will be contained inside one Component Group).

The syntax rules that are checked for are as follows:

Expression must not begin with a "*"

A "*" must be preceded and followed by words or a brace (redundant braces are removed).

A standalone component must be additive. A standalone component is defined as a single component model or a single component at the beginning (end) of the expression followed (preceded) by a "+", or in the middle of the expression delimited by 2 "+" signs.

A convolution component must not appear at the end, or followed by a closing brace.

A mixing model component must appear first in the expression and apply to all components (thus a model including a mixing component always has one Component Group.

When using convolution components, the order in which they are applied is in general significant.For example, the two models

$C_1*M_1(A_1+A_2)$ and $M_1* C_1 (A_1+A_2)$

are not necessarily equivalent (here the C's represent convolution models).The way XSPEC handles the ordering of components is by first computing the spectrum for the additive components of a given additive group (A1+A2 in the above example). It then applies all multiplicative or convolution components in the additive group from right to left in the order they appear in the model formula.

N.B. Beginning with v12.5.0, convolutions no longer have to precede the source. Parentheses may also be used to specify convolution precedence, so the following two examples are not equivalent:

$C_1*M_1(A_1+A_2)$ and $(C_1*M_1) (A_1+A_2)$

Mixing models are a special case. The mixing transformation is applied to the entire model once the combination into a single Sum Component has been executed. Note that since XSPEC12 can have multiple models applied to a given spectrum, the mixing transformation can nevertheless be applied to only one of the models being fit. This will be relevant, for example, for the case where the background is fitted by a separate model

Examples

Note that `po (= powerlaw)` and `ga (= gauss)` are additive models, and that `wabs` and `phabs` (different photoelectric absorption screens) are multiplicative models.

```
XSPEC12> model po
      // The single component po (powerlaw) is the model.
XSPEC12> model po+ga
XSPEC12> model (po+ga)wabs
XSPEC12> model phabs(po+ga)
XSPEC12> model wa(phabs(po)+ga)
XSPEC12> model wa po phabs ga //error: old syntax
XSPEC12> model wa*phabs*po
XSPEC12> model (po+po)phabs
      //Note that though the first and second components are the same
      // form, their parameters are varied separately.
XSPEC12> model phabs*wa(po)

A complex (and almost certainly unphysical) example is the following:

XSPEC12>model wa(po+pha(peg+edge(disk+bbod)))const + pla(pos+hr*step) + not*gau
```

Applying multiple models:

Assume 3 spectra are loaded, each with a single response (source 1 by default).

```
XSPEC12> model wa(po)
      // The unnamed model wa(po) will apply to all 3 spectra, accordingly
      // multiplied by each spectrum's response.
XSPEC12> response 2:2 new_resp.pha 2:3 another_new_resp.pha
      // Additional responses assigned to source number 2 for spectra 2 and 3.
XSPEC12> model 2:second_mod ga
      // The model "second_mod" will now apply to source 2, and is therefore
      // multiplied by new_resp.pha and another_new_resp.pha for spectra 2
      // and 3 respectively.
XSPEC12> model second_mod inactive
      // "second_mod" will no longer apply to spectra 2 and 3, though they
      // retain responses for source 2.
      OR
XSPEC12> response 2:2 none
XSPEC12> response 2:3 none
      // No responses exist for source number 2, second_mod is
      // rendered inactive.
```

5.6.16 modid: write out possible IDs for lines in the model.

Tcl script to write out possible IDs for gaussian or lorentzian lines in the current model.

Syntax: modid `[{<delta> | conf }`

This script runs the identify command for every gaussian or lorentzian line included in the current model. If a number is given as an argument then that is used as the delta energy for identify. If the string "conf" is given as the argument then the last calculated confidence regions are searched for possible line IDs. If no argument is given then "conf" is assumed.

5.6.17 newpar: change parameter values

Adjust one or more of the model parameters.

Syntax: **newpar** `[modelName:]<index range> [<param spec list> ]`

newpar `[modelName:]<index> = <coupling expression>`

newpar `0`

where

<param spec list> =:: <param value> <delta> <param range spec>

<param range spec> =:: <hard min> <soft min> <soft max> <hard max>

For response parameters (created with the **gain** or **rmodel** command):

rnewpar `[<sourceNum>:]<idx range> [<param spec list>]`

rnewpar `[<sourceNum>:]<index> = <coupling expression>`

The model parameters are accessed through their model parameter indices. For example, the first parameter of the first model component generally is model parameter 1, etc.The first command line argument, `<index range>`, gives the indices' parameters to be modified by the `newpar` command. The default value is the range from the previous invocation of `newpar`. The remaining arguments can be used to update the parameter specification. If the parameter specification is omitted from the command line, then the user is explicitly prompted for it. The first two arguments of the parameter specification are:

<param value>	The trial value of the parameter used initially in the fit
<delta>	The step size used in the numerical determination of the derivatives used during the fitting process. When delta is set to zero, the parameter is not adjustable during the fit. This value may be overriden for all parameters by the `xset delta` command option, which will apply a proportional rather than a fixed delta.

The four arguments of the range specification determine the range of acceptable values for the parameter. The soft limits should include the range of expected parameter behavior. Between the hard and soft limits, the parameter is made stiffer to adjustment by the minimization routine invoked by the `fit` command. The parameter is never allowed to have a value at or outside the hard limits. (One exception to this rule: the parameter can equal one of the hard limits if the soft limits have been placed outside the hard limit).

A slash (`/`) will set all the six parameter specification values (value, delta, range specification) to the previous value (default for a new model, current value if the parameter has previously been set or fit).

The sequence `/*` leaves all parameters unchanged (in the case of a new model, to be set to the default).

newpar `0`

Prints the current parameter settings.

Parameter Links

Coupling of parameters allows parameters in a model to always have the same value or to be related by an expression. The expression is a polynomial function of the other parameters

(XSPEC will reject attempts to link parameters to themselves!). Also, XSPEC12 allows parameters to be designated in their initialization file to be fixed, i.e. never variable during a fit, or to act as switches that change the mode in which a theoretical component is calculated (i.e. it may be interpolated or analytically calculated). "scale" or "switch" parameters cannot be linked to any other type of parameter, but only to other scale or switch parameters. Details of parameter types are explained in more detail in Appendix C.

The syntax for linking parameters is

```
XSPEC12> newpar  <par> =  f( par ),
```

where *f* is a polynomial in the (other) parameters with real coefficients. N.B. Integers appearing in *f* that are within the range of existing parameter numbers will be interpreted as parameters: to avoid confusion, if a real number is intended it should include a decimal point. Integers larger than the last parameter number will be interpreted as integers. Parameters of named models must have their index numbers prefixed by `[modelName:]`.

If there are multiple data groups present, then the parameters of models associated with datagroups greater than 1 ("secondary models") are coupled by default to their "primary" counterparts. For example, if there are 5 parameters in the model and 3 datagroups present, then the model command will prompt for 15 parameters. If the user types

```
XSPEC12> model <expression>
XSPEC12>/*
```

Then parameters 1-5 will be set to their values specified in the initialization ("model.dat") file. Parameters 6-15 will be linked to their counterparts, i.e. as if the user had typed

```
XSPEC12> newpar 6 = 1
XSPEC12> newpar 7 = 2
…
XSPEC12> newpar 11 = 1
```

And so on.

Examples:

The total number of model parameters for the example is four.

```
XSPEC12> newpar 2 0.1
      //The value of the second parameter is set to 0.1.
XSPEC12> newpar 3-4
      //The program will prompt for a specification for the 3rd
      // parameter (comp gives the name of the corresponding model component)
comp:param3>0.001, 0
      //which has its value set to 0.001 and its delta set to zero, fixing
      // it in later fits.The program now prompts for a specification for
      // the 4th parameter
comp:param4>21
      // which is set to 21.As there is no 5th parameter, the program
      // displays a summary and returns to command level.
XSPEC12> newpar ,,.001
      //The value of the delta of the 3rd parameter (which is the default
      // index as it was the first parameter modified in the previous
      // newpar invocation) is set to 0.001, allowing it to be adjusted
      // during any fits.
```

The total number of parameters for this example is eight.

```
XSPEC12> newpar 4 = 1
      //The value of parameter 4 is set to the value of parameter 1.
      //This has the consequence of model parameter 4 being frozen at the
      // value of parameter 1 during subsequent fitting procedures.
      // If model parameter 1 is a free parameter, then both parameters
      // 1 and 4 change their values simultaneously in the fit procedure.
XSPEC12> newpar 4 = 3/5 + 6.7
      //The value of parameter 4 is set to the value of
      // (parameter 3/ parameter 5) plus 6.7
XSPEC12> newpar 6 = 3 * .1 - 9.5
      //The value of parameter 6 is set to 0.1 times the
      // value of parameter 3 minus 9.5
XSPEC12> newpar 5 = 2 + 5.
      //The value of parameter 5 is set to the value
      // of parameter 2 plus 5.
XSPEC12> newpar 8 = 1 / 4.6
      //parameter 8 is set to parameter 1 divided by 4.6
XSPEC12> untie 6
      //Makes parameter 6 independent of parameter 3 and a free
      //parameter.
```

5.6.18 systematic: add a model-dependent systematic term to the variance

Syntax: **systematic**`[ <model systematic error>]`

Set a systematic error term on the model to be added in quadrature to that on the data when evaluating chi-squared. The default value is zero.

5.6.19 untie: unlink previously linked parameters

Untie the specified parameter from any links to other parameters.

Syntax: **untie** `<param range>`

where <param range> is of the form

```
<param range> =::  [modelName:]<param #>
```

For response parameters (see **gain** command):

runtie `<param range>`

where <param range> is of the form

```
<param range> =::  [sourceNum:]<param #>
```

Parameters previously linked together with commands such as

```
XSPEC12> newpar <param spec>
```

are unlinked. The parameter will retain its current value for the next fit.

5.7 Plot Commands

5.7.1 cpd: set current plotting device

Syntax: **cpd** `< plot device>`

cpd `<filename>`

cpd `<filename>/{ps,cps,vps,vcps}`

cpd `none`

Set current plot device. The same can be achieved with the `setplot device` command, which takes the same options. In the initial release of XSPEC12, as in previous versions, the plot device options are those allowed by the PGPLOT library.

If the second argument does not start with a '/' character, which indicates that the string represents a PGPLOT device, it is taken to be a filename for Postscript output, and the default postscript driver will be used. The default postscript driver produces a monochrome plot in landscape orientation.

The filename argument can be followed by a '/' that specifies a particular postscript driver variant. Allowable variants are: cps (color postscript), vps (monochrome portrait orientation), and vcps (color portrait orientation), as well as the default, ps.

cpd `none`

PGPLOT devices

A number of plot device types are supported in XSPEC. PGPLOT devices available on Unix machines are :

```
/GIF            Graphics Interchange Format file, landscape orientation
/VGIF           Graphics Interchange Format file, portrait orientation
/NULL           Null device, no output
/PPM            Portable Pixel Map file, landscape orientation
/VPPM           Portable Pixel Map file, portrait orientation
/PS             PostScript file, landscape orientation
/VPS            PostScript file, portrait orientation
/CPS            Colour PostScript file, landscape orientation
/VCPS           Colour PostScript file, portrait orientation
/TEK4010        Tektronix 4010 terminal
/GF             GraphOn Tek terminal emulator
/RETRO          Retrographics VT640 Tek emulator
/GTERM          Color gterm terminal emulator
/XTERM          XTERM Tek terminal emulator
/ZSTEM          ZSTEM Tek terminal emulator
```

```
/V603          Visual 603 terminal
/KRM3          Kermit 3 IBM-PC terminal emulator
/TK4100        Tektronix 4100 terminals
/VT125DEC      VT125 and other REGIS terminals
/XDISP         pgdisp or figdisp server
/XWINDOW       X window window@node:display.screen/xw
/XSERVE        An /XWINDOW window that persists for re-use
```

Closes the device. For Postscript output, it flushes the write buffer into the file and closes the file.

Note that in XSPEC12, each plot command produces a separate page in the postscript file, unlike previously where each plot overwrote the previous plot.

Example:

```
// produce a set of color postscript plots in landscape orientation
// … commands to produce a plot.
XSPEC12> cpd   dataplot.ps/cps
XSPEC12> plot data chi
XSPEC12> plot ufspec
XSPEC12> plot efficiency
XSPEC12> cpd none
```

Will produce 3 plots in the file dataplot.ps.

Note, in contrast, that the hardcopy command will print only the plot that is currently in a graphics frame.

5.7.2 hardcopy: print plot

Spool the current plot to the printer.

Syntax: **hardcopy** [<filename>] [mono | color]

This command takes whatever is the current display in you plot window, writes it to a postscript file, and then sends it to a printer using the unix `lpr` command. It will thus be printed on whatever printer `lpr` uses as your default printer. If a filename is specified, the postscript file will be saved (e.g. “hardcopy dataplot.ps color” will produce a color plot saved in the file dataplot.ps). If mono or color is not given, the hardcopy will be monochrome.

5.7.3 iplot: make a plot, and leave XSPEC in interactive plotting mode

Interactive plotting on the current plot device.

iplot <plot type>

This command works like the `plot` command (see the `plot` command description), but allows the user to change the plot and to add text to the plot interactively using the PLT package. See the Overview of PLT in the Appendices for more information.

5.7.4 plot: make a plot

Make one or more plots to the current plot device (see setplot device).

Syntax: **plot** `<plot type> [ <plot type>]`

`<plot type>` is a keyword describing the various plots allowed. Any of the options `counts`, `data`, or `ldata` can be followed by a second option, which should be one of `chisq`, `delchi`, `ratio`, `residuals`, or `none`. If one of these second options is given, then a two-pane plot is drawn with the first option in the upper pane and the second option in the lower. (see also `iplot`)

background

Plot only the background spectra (with folded model, if defined). To plot both the data and background spectra, use `plot data` with the `setplot background` option.

chain

Formerly named `plot mcmc`, plot a Monte Carlo Markov chain.

```
plot chain <par1> [<par2>]
```

Chains must be currently loaded (see `chain` command), and `<par1>` and `<par2>` are parameter identifiers of the form `[<model name>:]n` where `n` is an integer, specifying the parameter columns in the chain file to serve as the X and Y axes respectively. To select the fit-statistic column, enter '0' for the `<par>` value. If `<par2>` is omitted, `<par1>` is simply plotted against row number.

chisq

Plot contributions to chisq. The contribution is plotted +ve or –ve depending on whether the residual is +ve or –ve.

contour

Plot the results of the last `steppar` run. If this was over one parameter then a plot of statistic versus parameter value is produced while a `steppar` over two parameters results in a fit-statistic contour plot.

```
plot contour [ <min fit stat> [ <# levels> [ <levels>]]]
```

where `<min fit stat>` is the minimum fit statistic relative to which the delta fit statistic is calculated, `<# levels>` is the number of contour levels to use and `<levels> := <level1> ... <levelN>` are the contour levels in the deltafit statistic. contour will plot the fit statistic grid calculated by the last `steppar` command (which should have gridded on two

parameters). A small plus sign "+" will be drawn on the plot at the parameter values corresponding to the minimum found by the most recent fit.

The fit statistic confidence contours are often drawn based on a relatively small grid (i.e., 5x5). To understand fully what these plots are telling you, it is useful to know a couple of points concerning how the software chooses the location of the contour lines. The contour plot is drawn based only on the information contained in the sample grid. For example, if the minimum fit statistic occurs when parameter 1 equal 2.25 and you use `steppar` 1 1.0 5.0 4, then the grid values closest to the minimum are 2.0 and 3.0. This could mean that there are no grid points where delta-fit statistic is less than your lowest level (which defaults to 1.0). As a result, the lowest contour will not be drawn. This effect can be minimized by always selecting a `steppar` range that causes XSPEC to step very close to the true minima.

For the above example, using `steppar` 1 1.25 5.25 4, would have been a better selection. The location of a contour line between grid points is designated using a linear interpolation. Since the fit statistic surface is often quadratic, a linear interpolation will result in the lines being drawn inside the true location of the contour. The combination of this and the previous effect sometimes will result in the minimum found by the fit command lying outside the region enclosed by the lowest contour level.

Examples:

```
XSPEC12> steppar 2 0.5 1. 4 3 1. 2. 4
      //create a  grid for parameters 2 and 3
XSPEC12> plot contour
      //Plot out a grid with three contours with
      // delta fit statistic of 2.3, 4.61 and 9.21
XSPEC12> plot cont,,4,1.,2.3,4.61,9.21
      //same as above, but with a delta fit statistic = 1 contour.}
```

counts

Plot the data (with the folded model, if defined) with the y-axis being numbers of counts in each bin.

data

Plot the data (with the folded model, if defined).

delchi

Plot the residuals in terms of sigmas with error bars of size one.

dem

Plot the relative contributions of plasma at different temperatures for multi-temperature models. This is not very clever at the moment and only plots the last model calculated.

eemodel

Plot the current incident model spectrum in $E^2f(E)$ (Note: This is NOT the same as an "unfolded" spectrum.) or, if wavelength plotting has been set, $\lambda^2 f(\lambda)$. The contributions of the various additive components also are plotted.

eeufspec

Plot the unfolded spectrum and the model in $E^2f(E)$ or, if wavelength plotting has been set, $\lambda^2 f(\lambda)$. The contributions to the model of the various additive components are also plotted. This corresponds to the ν–f_ν plot beloved of AGN researchers. WARNING ! This plot is not model-independent and your unfolded model points will move if the model is changed.

efficien

Plot the total response efficiency versus incident photon energy.

emodel, eemodel

Plot the current incident model spectrum in $Ef(E)[E^2f(E)]$ (Note: This is NOT the same as an unfolded spectrum.) or, if wavelength plotting has been set, $\lambda f(\lambda),\lambda^2 f(\lambda)$. The contributions of the various additive components also are plotted.

eufspec, eeufspec

Plot the unfolded spectrum and the model in $Ef(E),)[E^2f(E)]$ or, if wavelength plotting has been set, $\lambda f(\lambda), \lambda^2 f(\lambda)$. The contributions to the model of the various additive components also are plotted.WARNING ! This plot is not model-independent and your unfolded model points will move if the model is changed.

icounts

Integrated counts and folded model. The integrated counts are normalized to unity.

insensitv

Plot the insensitivity of the current spectrum to changes in the incident spectra (experimental).

lcounts

Plot the data (with the folded model, if defined) with a logarithmic y-axis indicating the count spectrum

ldata

Plot the data (with the folded model, if defined) with a logarithmic y-axis.

margin

Plot the probability distribution from the results of the most recently run `margin` command. (Must be a 1-D or 2-D distribution.)

model

Plot the current incident model spectrum (Note: This is NOT the same as an unfolded spectrum.) The contributions of the various additive components also are plotted. If using a named model, the model name should be given as an additional argument.

ratio

Plot the data divided by the folded model.

residuals

Plot the data minus the folded model.

sensitvty

Plot the sensitivity of the current spectrum to changes in the incident spectra (experimental).

sum

A pretty plot of the data and residuals against both channels and energy.

ufspec

Plot the unfolded spectrum and the model. The contributions to the model of the various additive components also are plotted. WARNING ! This plot is not model-independent and your unfolded model points will move if the model is changed. The data points plotted are the model values multiplied by the ratio of the data values to the model multiplied by the response.

5.7.5 setplot: modify plotting parameters

Set one of the various plot options.

```
setplot <subcommand string>
```

where `<subcommand string>` is a keyword followed in some cases by arguments. Current settings of all **setplot** items can be viewed with **show plot**.

add

Show individual additive model components on the data plots.

The opposite is `setplot noadd`.

area, noarea

After `setplot area` is entered, `plot data` and `plot ldata` will show the data divided by the response effective area for each particular channel. `plot residuals` will necessarily also be affected by this. Usual plotting is restored by `setplot noarea`. If data is associated with more than 1 response, the response effective area is calculated by simply summing the contributions from each response.

background, nobackground

When running `plot data` or `plot ldata`, also show associated background spectra (if any).

channel

Change the x-axis on data and residual plots to channels.

command

Add a PLT command to the command list.

```
setplot command <PLT command>
```

where `<PLT command>` is any valid PLT command. very time you use `setplot command`, that command is added to the list that is passed toPLT when you use `plot` or `iplot`. The most common use of `setplot command` is to add a common label to all plots produced. You should be careful when using this command, because XSPEC does not check to see if you have entered a valid PLT command.These commands are appended to the list that XSPEC creates to generate the plot and so `setplot command` will override these values (this can either be a bug or a feature, depending on what you have done!) See also `setplot delete` and `setplot list`.

Example:

```
XSPEC12> setp co LA OT Crab {Add the label "Crab" to future plots.
```

delete

Delete a PLT command from the command list.

setplot delete <command #>

where `<command #>` is the number of a PLT command that hadbeen entered previously using `setplot command`.This command isused to delete commands from the list passed to PLT when you use the XSPEC `plot` or `iplot` commands.

Example:

```
XSPEC12> setp co LA OT Testing
      //PLT label command
XSPEC12> setp co LWidth 5
      //PLT line-width command
```

```
XSPEC12> setplot lis
      //List the PLT command stack.
1: LAbel OT Testing
2: LWidth 5
XSPEC12> setplot del 1
      //Delete the first command in the stack.
XSPEC12> setplot lis
1: LWidth 5
```

device

Set current plot device.

```
XSPEC12>setplot device   < plot device>
XSPEC12>setplot device  <filename>
XSPEC12>setplot device  <filename>/{ps,cps,vps,vcps}
XSPEC12>setplot device   none
```

If the second argument does not start with a '/' character, which indicates that the string represents a PGPLOT device, it is taken to be a filename for Postscript output, and the default postscript driver will be used. The default postscript driver produces a monochrome plot in landscape orientation.

The filename argument can be followed by a '/' that specifies a particular postscript driver variant. Allowable variants are: cps (color postscript), vps (monochrome portrait orientation), and vcps (color portrait orientation), as well as the default, ps.

Set the device used for plots.

PGPLOT devices

A number of plot device types are supported in XSPEC. PGPLOT devices available on Unix machines are :

```
/GIF           Graphics Interchange Format file, landscape orientation
/VGIF          Graphics Interchange Format file, portrait orientation
/NULL          Null device, no output
/PPM           Portable Pixel Map file, landscape orientation
/VPPM          Portable Pixel Map file, portrait orientation
/PS            PostScript file, landscape orientation
/VPS           PostScript file, portrait orientation
/CPS           Colour PostScript file, landscape orientation
/VCPS          Colour PostScript file, portrait orientation
/TEK4010       Tektronix 4010 terminal
/GF            GraphOn Tek terminal emulator
/RETRO         Retrographics VT640 Tek emulator
/GTERM         Color gterm terminal emulator
/XTERM         XTERM Tek terminal emulator
/ZSTEM         ZSTEM Tek terminal emulator
/V603          Visual 603 terminal
```

```
      /KRM3          Kermit 3 IBM-PC terminal emulator
      /TK4100        Tektronix 4100 terminals
      /VT125DEC      VT125 and other REGIS terminals
      /XDISP         pgdisp or figdisp server
      /XWINDOW       X window window@node:display.screen/xw
      /XSERVE        An /XWINDOW window that persists for re-use
```

Examples:

```
XSPEC12> setplot device /xt
      //sets the device to the xterm.
XSPEC12> setplot device none
      //closes the plot file.
```

energy

Change the x-axis on plots to energy in units of keV.

```
setplot energy
```

group

Define a range of spectra to be in the same group for plotting purposes only.

```
setplot group <spectrum range>...
```

where `<spectrum range>` is a range of contiguous spectra to be treated as a single spectrum for plotting purposes. The spectra still are fit individually. If multiple ranges are given, each range becomes a single group. Initially, all spectra read in are treated as single spectra. (See also **ungroup**.)

Examples:

Assume that there are five spectra currently read in, all of them ungrouped initially.

```
XSPEC12> setplot group 1-4
      //The first four spectra are treated as one group, with the fifth
      //spectra on its own. Thus all plots will appear to have two spectra.
XSPEC12> setplot group 1 2 3 4
      //The spectra are reset to each be in their own group.
XSPEC12> setplot group 2-3 4-5
      //Now there are three plot groups, being spectrum 1, by itself, and
      //spectra 2-3 and 4-5 as groups.
XSPEC12> setplot group 1-**
      //All the spectra are placed in a single plot group.
```

id

Switch on plotting of line IDs.

```
setplot id <temperature> <emissivity limit> <redshift>
```

The IDs are taken from the APEC line list for the temperature given by the first argument. The plot only shows those lines with emissivities above the limit set and the lines are redshifted by the amount specified. Currently theAPEC version used is 1.10. If **xset** `apecroot` has been used to reset the APEC files then setplot id uses a filename based on the value of `apecroot` as described in the documentation for the `apec` model.

list

List all the PLT commands in the command list.

```
setplot list
```

See `setplot delete` for an example of use.

noadd

Do not show individual additive model components on the data plots.

```
setplot noadd
```

The opposite is `setplot add`.

noid

Switch off plotting of line IDs.

```
setplot noid
```

The opposite is `setplot id`.

rebin

Define characteristics used in rebinning the data (for plotting purposes ONLY).

```
setplot rebin <min significance> <max # bins> <plot group> <error type>
```

In plotting the data from a spectrum (or group of spectra, see `setplot group`), adjacent bins are combined until they have a significant detection at least as large as `<min significance>` (in σ).However, no more than `<max # bins>` may be so combined. Initial values are 0. and 1, respectively. This argument effects only the presentation of the data in plots. It does not change the fitting, in particular the number of degrees of freedom. The values given are applied to all the plotted data in the plot group specified as the final argument. To change the rebinning simultaneously for all the plot groups give anegative value of the plot group.

The `<error type>` argument specifies how to calculate the error barson the new bins. The default is `quad` which sums in quadrature the errors on the original bins. `sqrt` uses $\sqrt{N}$ where N is the number of counts in the new bin, `poiss-1` uses $1+\sqrt{N+0.75}$, `poiss-2` uses $\sqrt{N-0.25}$, and

`poiss-3` is the arithmetic mean of `poiss-1` and `poiss-2`. If background is present its error is calculated by the same method then added in quadrature to the source error.

Examples:

```
XSPEC12> setplot rebin 3 5 1
      //Bins in plot group 1 are plotted that have at least 3σ,
      //or are grouped in sets of 5 bins.
XSPEC12> setplot rebin 5 5
      //The significance is increased to 5σ.
XSPEC12> setplot rebin,,10,-1
      //All plotted bins can be grouped into up to 10 bins in reaching the
      //5σ significance criterion.
XSPEC12> setplot rebin ,,,sqrt}
      //Uses √N to calculate error bars.
```

splashpage (on|off)

When set to off, the usual XSPEC version and build date information will not be printed to the screen when the first plot window is initially opened. This is intended primarily for the HERA installation of XSPEC.

ungroup

Remove previous grouping set up by setplot group, resetting all spectra to be in a distinct plot group.

wave

Change the x-axis on plots to wavelength. Units can either be in Hz or in angstroms, and are configured by the WAVE_PLOT_UNITS setting in the user's ~/.xspec/Xspec.init file (default is Hz). This command also makes ignore and notice operate in terms of wavelength rather than energies.

xlog (on | off)

Set the x-axis to logarithmic or linear respectively for energy or wavelength plots. xlog has no effect on plots in channel space (recall that the default for energy plots is logarithmic: xlog allows the user to override this setting). xlog and ylog will not work for model-related plots (eg. model, ufspec, and their variants) as their axes are always set to log scale.

ylog (on | off)

Set the y-axis to logarithmic or linear respectively for energy or wavelength plots. For plot instructions that are explicitly logarithmic (plot ldata, plot lcounts) the state of the ylog setting is ignored. xlog and ylog will not work for model-related plots (eg. model, ufspec, and their variants) as their axes are always set to log scale.

5.8 Setting Commands

5.8.1 abund: set the Solar abundances

Set the abundance table used in the plasma emission and photoelectric absorption models.

Syntax: abund `<option>`

where `<option>` is:

`angr`, from Anders E. & Grevesse N. (1989, Geochimica et Cosmochimica Acta 53, 197)

`feld`, from Feldman U.(1992, Physica Scripta 46, 202 except for elements not listed which are given grsa abundances),

`aneb`, from Anders E. & Ebihara (1982, Geochimica et Cosmochimica Acta 46, 2363),

`grsa` from Grevesse, N. & Sauval, A.J. (1998, Space Science Reviews 85, 161)

`wilm` from Wilms, Allen & McCray (2000, ApJ 542, 914 except for elements not listed which are given zero abundance)

`lodd`, from Lodders, K (2003, ApJ 591, 1220)

`file filename`, where `filename` is an ASCII file containing 30 lines with one number on each line. All abundances are number relative to H.

The tables are:

Element	angr	feld	aneb	grsa	wilm	lodd
H	1.00e+00	1.00e+00	1.00e+00	1.00e+00	1.00e+00	1.00e+00
He	9.77e-02	9.77e-02	8.01e-02	8.51e-02	9.77e-02	7.92e-02
Li	1.45e-11	1.26e-11	2.19e-09	1.26e-11	0.00	1.90e-09
Be	1.41e-11	2.51e-11	2.87e-11	2.51e-11	0.00	2.57e-11
B	3.98e-10	3.55e-10	8.82e-10	3.55e-10	0.00	6.03e-10
C	3.63e-04	3.98e-04	4.45e-04	3.31e-04	2.40e-04	2.45e-04
N	1.12e-04	1.00e-04	9.12e-05	8.32e-05	7.59e-05	6.76e-05
O	8.51e-04	8.51e-04	7.39e-04	6.76e-04	4.90e-04	4.90e-04
F	3.63e-08	3.63e-08	3.10e-08	3.63e-08	0.00	2.88e-08
Ne	1.23e-04	1.29e-04	1.38e-04	1.20e-04	8.71e-05	7.41e-05
Na	2.14e-06	2.14e-06	2.10e-06	2.14e-06	1.45e-06	1.99e-06

Mg	3.80e-05	3.80e-05	3.95e-05	3.80e-05	2.51e-05	3.55e-05
Al	2.95e-06	2.95e-06	3.12e-06	2.95e-06	2.14e-06	2.88e-06
Si	3.55e-05	3.55e-05	3.68e-05	3.35e-05	1.86e-05	3.47e-05
P	2.82e-07	2.82e-07	3.82e-07	2.82e-07	2.63e-07	2.88e-07
S	1.62e-05	1.62e-05	1.89e-05	2.14e-05	1.23e-05	1.55e-05
Cl	1.88e-07	1.88e-07	1.93e-07	3.16e-07	1.32e-07	1.82e-07
Ar	3.63e-06	4.47e-06	3.82e-06	2.51e-06	2.57e-06	3.55e-06
K	1.32e-07	1.32e-07	1.39e-07	1.32e-07	0.00	1.29e-07
Ca	2.29e-06	2.29e-06	2.25e-06	2.29e-06	1.58e-06	2.19e-06
Sc	1.26e-09	1.48e-09	1.24e-09	1.48e-09	0.00	1.17e-09
Ti	9.77e-08	1.05e-07	8.82e-08	1.05e-07	6.46e-08	8.32e-08
V	1.00e-08	1.00e-08	1.08e-08	1.00e-08	0.00	1.00e-08
Cr	4.84e-07	4.84e-07	4.93e-07	4.68e-07	3.24e-07	4.47e-07
Mn	2.45e-07	2.45e-07	3.50e-07	2.45e-07	2.19e-07	3.16e-07
Fe	4.68e-05	3.24e-05	3.31e-05	3.16e-05	2.69e-05	2.95e-05
Co	8.60e-08	8.60e-08	8.27e-08	8.32e-08	8.32e-08	8.13e-08
Ni	1.78e-06	1.78e-06	1.81e-06	1.78e-06	1.12e-06	1.66e-06
Cu	1.62e-08	1.62e-08	1.89e-08	1.62e-08	0.00	1.82e-08
Zn	3.98e-08	3.98e-08	4.63e-08	3.98e-08	0.00	4.27e-08

5.8.2 cosmo: set the cosmology

Set the cosmology used (i.e., $< H_0 >, < q_0 >$, and $< \Lambda_0 >$).

Syntax: **cosmo** < H_0 > < q_0 > < Λ_0 >

where $< H_0 >$ is the Hubble constant in km s^{-1} Mpc^{-1}, $< q_0 >$ is the deceleration parameter, and $< \Lambda_0 >$ is the cosmological constant. If the cosmological constant is non-zerothen at present XSPEC requires that the universe is flat. In this case the value of $< q_0 >$ will be ignored and XSPEC will assume that $\Omega_{matter} \geq 1 - \Lambda_0$. The default values are $< H_0 >= 50$, $< q_0 >= 0.5$, and $< \Lambda_0 >= 0$.

Examples:

```
XSPEC12> cosmo 100
      // Set <H0>= 100km s-1 Mpc-1
XSPEC12> cosmo ,0
      // Set <q0>= 0
XSPEC12> cosmo ,,0.7
      // Set a flat universe with <Λ0>= 0.7
```

.

5.8.3 method: change the fitting method

Set the minimization method.

Syntax: **method** <algorithm> [<# of trials/evaluations> [<critical delta>] [method-specific options]

where <algorithm> is the method in use and the other arguments are control values for the minimization. Their meanings are explained under the individual methods. Note that all but **leven** require the MINUIT library from CERN to be linked into XSPEC. If any of the MINUIT library methods are set, then the **error** command will use the MINUIT MINOS command to find the confidence regions.

XSPEC is required to calculate derivates of the fit statistic with respect to the model parameters for both the **leven** and **migrad** methods. **leven** further requires second derivatives. By default, XSPEC calculates these using an analytic expression which assumes that partial 2nd derivatives of the model with respect to its parameters may be ignored. This may be changed by setting the USE_NUMERICAL_DIFFERENTIATION flag to "true" in the user's startup Xspec.init initialization file. XSPEC will then calculate all derivatives numerically, which can be noticeably slower.

leven

method leven [<# of eval> [<crit delta>]]

The default XSPEC minimization method using the modified Levenberg-Marquardt based on the CURFIT routine from Bevington. <# of eval> is the number of trial vectors before the user is prompted to say whether they want to continue fitting. <crit delta> is the convergence criterion, which is the (absolute, not fractional) difference in fit statistic between successive iterations, less than which the fit is determined to have converged. <# of eval> and <crit delta> may also be changed through the **fit** command.

migrad

method migrad [<# of eval> [<crit delta>]]

The MINUIT MIGRAD method. <# of eval> is the number of function evaluations to perform before giving up and <crit delta> is the convergence criterion.

XSPEC12.0 includes version94.1 of the CERN MINUIT library – dated August 1998. The manual for the library is included with the XSPEC12 documentation and can be accessed by

```
XSPEC12>help minuit
```

When minuit is used, the output from the fitting procedure is different from xspec's normal behavior. It is written to the file mn_output.log in the current directory. For uncertainty calculations (the error command), XSPEC calls the equivalent MINUIT implementation (MNERRS).

Following the advice in section 5 of the MINUIT manual, instead of providing the full range of MINUIT methods, most of which are said to be inferior, we have chosen to give access to the robust **migrad** algorithm.

Advice

migrad uses only first derivatives of models, and part of its operation is to approximate the Hessian, or second derivative matrix. The Levenberg-Marquadt assumes that the model is twice [numerically] differentiable, and calculates the Hessian explicitly. Thus the latter is the method of choice for analytical models.

minim

method minim [<`# of evaluations`> [<`critical delta`>]]

The MINUIT MINIMIZE method, used MIGRAD unless it gets into trouble in which case it switches to SIMPLEX. <`# of evaluations`> is the number of function evaluations to perform before giving up and <`critical delta`> is the convergence criterion.

monte

method monte [<`# of evaluations`> [<`critical delta`>]]

The MINUIT SEEK method, a simple random sampling of parameter space (not recommended!). <`# of evaluations`> is the number of function evaluations to perform before giving up and <`critical delta`> is the convergence criterion.

simplex

method simplex [<`# of evaluations`> [<`critical delta`>]]

The MINUIT SIMPLEX method. <`# of evaluations`> is the number of function evaluations to perform before giving up and <`critical delta`> is the convergence criterion.

5.8.4 statistic: change the objective function (statistic) for the fit

Change the fit statistic in use.

Syntax: **statistic** `[chi | cstat | lstat]`

The options are chi-squared (chi) or C statistic (cstat) or lstat. Note that the C statistic has a couple of limitations: a) if the calculated model goes to zero in any channel then the format statistic

goes to infinity -in practice this is trapped and a large value of the statistic should result; b) the C statistic can be used to estimate parameter values and confidence regions but does not provide a goodness-of-fit. See Arnaud (2003, ApJ submitted) for further details.

5.8.5 xsect: set the photoionization cross-sections

Change the photoelectric absorption cross-sections in use.

Syntax: **xsect** `[bcmc|obcm|vern]`

The three options are: `bcmc`, from Balucinska-Church & McCammon (1992; Ap.J.400, 699) with a new He cross-section based on (1998; Ap.J. 496, 1044); `obcm`, as `bcmc` but with the old He cross-section, and, `vern`, from Verneret. al. (1996 Ap.J.). This changes the cross-sections in use for all absorption models with the exception of `wabs`.

5.8.6 xset: set variables for XSPEC models.

Modify a number of XSPEC internal switches.

Syntax: **xset** `[abund | cosmo | delta | mdatadir | method | seed | statistic | weight | xsect | <string_name> ] [ <options> | <string_value> ]`

The arguments `abund, cosmo, method, statistic, weight,` and `xsect` just run the appropriate XSPEC commands. `mdatadir` changes the directory in which XSPEC searches for model data files. You probably don't want to change this. The `seed` option requires an integer argument, which will then be used to immediately re-seed and re-initialize XSPEC's random-number generator.

The `delta` option is for setting fit delta values (see the **newpar** command) which are proportional to the current parameter value rather than fixed. For example,

```
XSPEC12> xset delta .15
```

will set each parameter fit delta to .15 * parVal. To turn proportional deltas off and restore the original fixed deltas, set `delta` to a negative value or 0.0. The current proportional delta setting can be seen with **show control**.

The `<string_name>` option can be used to pass string values to models. XSPEC maintains a database of `<string_name>`, `<string_value>` pairs created using this command. Individual model functions can then access this database. Note that xset does no checking on whether the `<string_name>` is used by any model so spelling errors will not be trapped.

To access the `<string_name>`, `<string_value>` database from within a model function use the fortran function `fgmstr`. This is defined as `character*128` and takes a single argument, the string name as a `character*128`. If the `<string_name>` has not been set then a blank string will be returned.

The current `<string_name>` options, models to which they apply and brief descriptions are given in the following table :

APECROOT	apec, vapec, bapec, bvapec, gnei, vgnei, equil, vequil, npshock, vnpshock, pshock, vpshock, sedov, vsedov, c6mekl, c6vmekl, c6pmekl, c6pvmekl, cemkl, cevmkl, mekal, vmekal, mkcflow, vmclow	Switch from default APEC input files.

APECTHERMAL	apec, vapec, bapec, bvapec, gnei, vgnei, equil, vequil, npshock, vnpshock, pshock, vpshock, sedov, vsedov, c6mekl, c6vmekl, c6pmekl, c6pvmekl, cemkl, cevmkl, mekal, vmekal, mkcflow, vmclow	Thermally broaden emission lines in APEC input files.
APECVELOCITY	apec, vapec, bapec, bvapec, gnei, vgnei, equil, vequil, npshock, vnpshock, pshock, vpshock, sedov, vsedov, c6mekl, c6vmekl, c6pmekl, c6pvmekl, cemkl, cevmkl, mekal, vmekal, mkcflow, vmclow	Velocity broaden emission lines in APEC input files.
NEIAPECROOT	gnei, vgnei, equil, vequil, npshock, vnpshock, pshock, vpshock, sedov, vsedov	Switch from default NEIAPEC input files.
NEIVERS	gnei, vgnei, equil, vequil, npshock, vnpshock, pshock, vpshock, sedov, vsedov	Switch NEIAPEC version number.
CFLOW_VERSION	mkcflow, vmclow	Switch CFLOW version number.
CFLOW_NTEMPS	mkcflow, vmclow	Switch number of temperature bins used in CFLOW model.
SUZPSF-IMAGE	suzpsf	Set image file to be used for surface brightness.
SUZPSF-RA	suzpsf	Set RA for center surface brightness map which is taken from the WMAP.
SUZPSF-DEC	suzpsf	Set Dec for center surface brightness map which is taken from the

		WMAP.
SUZPSF-MIXFACT-IFILE#	suzpsf	Set filename to read mixing factors.
SUZSF-MIXFACT-OFILE#	suzpsf	Set filename to write mixing factors.
XMMPSF-IMAGE	xmmpsf	Set image file to be used for surface brightness.
XMMPSF-RA	xmmpsf	Set RA for center surface brightness map which is taken from the WMAP.
XMMPSF-DEC	xmmpsf	Set Dec for center surface brightness map which is taken from the WMAP.
XMMPSF-MIXFACT-IFILE#	xmmpsf	Set filename to read mixing factors.
XMMPSF-MIXFACT-OFILE#	xmmpsf	Set filename to write mixing factors.
NSA_FILE	nsa	Change filename used for model data.
NSAGRAV_DIR	nsagrav	Change directory used for model data files.
NSMAX_DIR	nsmax	Change directory used for model data files.
ZXIPCF_DIR	zxipcf	Change directory used for model data files.

Examples:

```
XSPEC12> xset neivers 2.0
      // Set the NEIVERS variable to 2.0
XSPEC12> xset
```

```
      // List the current string variables
XSPEC12> xset apecroot /foo/bar/apec_v1.01
      // Set the APECROOT variable
XSPEC12> xset seed 1515151
      // Re-initialize the pseudo random-number generator
      // with the seed value 1515151
```

5.9 Tcl Scripts

The following Tcl scripts are auto-loaded when xspec starts up so can be used in the same ways as commands. Entering the name of the script without arguments will produce a short summary. The scripts themselves can be found in $HEADAS/../spectral/scripts and can be used as the starting point for more complicated scripting of xspec.

5.9.1 lrt: likelihood ratio test between two models

Tcl script to perform a likelihood ratio test between two models.

Syntax: lrt `<niter> <model0_name> <model1_name>`

`Run <niter>` simulations of datasets based on <model0_name>, calculates the likelihood ratio for <model1_name> relative to <model0_name>, and outputs the fraction of iterations with the likelihood ratio larger than that for the data.

Before running this procedure you must have created command files called <model0_name>.xcm and <model1_name>.xcm which define the two models. A good way to do this is to set up the model then use save model to make the command file.

5.9.2 multifake: perform multiple fakeit iterations and save to file.

Tcl script to perform many iterations of fakeit and save the results in a FITS file.

Syntax: multifake `<time> <niter> <outfile>`

This script runs <niter> iterations of fakeit with an exposure of <time> and writes the results to <outfile>. Before running this procedure you have read in one (and only one) dataset along with its response and optional background and arf files. You must also have defined the model.

The output file is a FITS binary table with the columns being the value fit for each parameter in each iteration. The final column is the statistic value for that iteration.

Note that if an error occurs during the fit of a faked spectrum then -999 is written for all parameters and the statistic value for that iteration.

5.9.3 rescalecov: rescale the covariance matrix.

Tcl script to rescale the entire covariance matrix used in the proposal chain command.

Syntax: rescalecov `<scale>`

Rescales the chain proposal distribution covariance matrix by the factor input as <scale>.

5.9.4 simftest: estimate the F-test probability for adding a component.

Tcl script to generate simulated datasets and use these to estimate the F-test probability for adding a model component.

Syntax: simftest `<model_comp> <niter>`

This script runs <niter> sets of simulated datasets to estimate the F-test probability for adding the additional model component number <model_comp>. Before running this script the model should be set up including the additional component to be tested. The script will create temporary files model0.xcm and model1.xcm.

5.9.5 writefits: write information about the current fit and errors to a FITS file.

Tcl script to dump a lot of useful information to a FITS file.

Syntax: writefits `<FITS filename>`

This script writes filenames, free parameter values and errors to one row of a FITS file. The error command should have been run on all the free parameters before running this script. If the FITS file already exists then a new row is appended.

6. XSPEC V12 Models

6.1 Alphabetical Summary of Models

Model	Description
absori	Ionized absorber.
acisabs	Extra absorption due to contamination on the ACIS filters.
ascac	ASCA PSF mixing model.
apec, vapec	APEC thermal plasma model.
atable	Additive table model.
bapec, bvapec	Velocity broadened APEC thermal plasma model.
bbody, zbbody	Blackbody spectrum, with redshift variant
bbodyrad	Blackbody spectrum with norm proportional to surface area.
bexrav	E-folded broken power-law reflected from neutral matter
bexriv	E-folded broken power-law reflected from ionized matter
bknpower	Broken powerlaw.
bkn2pow	Three-segment broken powerlaw.
bmc	Comptonization by relativistically moving matter.
bremss, vbremss, zbremss	Thermal bremsstrahlung, with redshift variant.
c6mekl, c6pmkl, c6vmkl, c6vpmkl	6th-order Chebyshev polynomial DEM using mekal and variants
cabs	Compton scattering (non-relativistic)
cemekl, cevmkl	Multi-temperature mekal.
cflow	Cooling flow model.
cflux	Calculate flux of other model components.
compbb	Comptonized blackbody spectrum after Nishimura et al. 1986.

Model	Description
compLS	Comptonization spectrum after Lamb and Sanford 1979.
compPS	Comptonization spectrum after Poutanen and Svenson 1986.
compST	Comptonization spectrum after Sunyaev and Titarchuk 1980.
compTT	Comptonization spectrum after Titarchuk 1994.
constant	Energy-independent multiplicative factor.
cutoffpl	Powerlaw with high energy exponential rolloff.
cyclabs	Cyclotron absorption line.
disk	Disk model.
diskbb	Multiple blackbody disk model.
diskir	Irradiated inner and outer disk.
diskline	Line emission from relativistic accretion disk.
diskm	Disk model with gas pressure viscosity.
disko	Modified blackbody disk model.
diskpbb	Accretion disk with power-law T(r)
diskpn	Accretion disk around a black hole.
dust	Dust scattering out of the beam.
edge, zedge	Absorption edge.
equil, vequil	Equilibrium ionization collisional plasma model from Borkowski.
etable	Table model for exponential of -1 times the input.
expabs	Low-energy exponential rolloff.
expdec	Exponential decay
expfac	Exponential factor.
ezdiskbb	Multiple blackbody disk model with zero-torque inner boundary.
gabs	Gaussian absorption line.

Model	Description
gauss, zgauss	Simple gaussian line profile.
gnei, vgnei	Generalized single ionization NEI plasma model.
grad	GR accretion disk around a black hole.
grbm	Gamma-ray burst model.
gsmooth	Gaussian smoothing with an energy dependent sigma.
highecut, zhighect	High energy cutoff.
hrefl	Simple reflection model good up to 15 keV.
kdblur	Convolve with the Laor model shape.
kdblur2	Convolve with the Laor2 model shape.
kerrbb	Multi-temperature blackbody model for thin accretion disk around a Kerr black hole.
kerrconv	Accretion disk line shape with BH spin as free parameter.
kerrd	Optically thick accretion disk around a Kerr black hole.
kerrdisk	Accretion disk line emission with BH spin as free parameter.
laor	Line from accretion disk around a black hole.
laor2	Line from accretion disk with broken power-law emissivity around a black hole.
lorentz	Lorentzian line profile.
lsmooth	Lorentzian smoothing with an energy dependent sigma.
meka, vmeka	Mewe-Gronenschild-Kaastra thermal plasma (1992).
mekal, vmekal	Mewe-Kaastra-Liedahl thermal plasma (1995).
mkcflow, vmcflow	Cooling flow model based on mekal.
mtable	Multiplicative table model.
nei, vnei	Simple nonequilibrium ionization plasma model.
notch	Notch line absorption.

Model	Description
npshock, vnpshock	Plane-parallel shock with ion and electron temperatures.
nsa	Neutron star with hydrogen atmosphere
nsagrav	Neutron star with hydrogen atmosphere for different g.
nsatmos	Neutron star H atmosphere with e- conduction and self-irradiation
nsmax	Neutron star magnetic atmosphere.
nteea	Pair plasma model.
nthcomp	Thermally comptonized continuum.
partcov	Convert absorption model into a partial covering absorption.
pcfabs, zpcfabs	Partial covering fraction absorption.
pegpwlw	Powerlaw with pegged normalization.
pexrav	Exponentially cut-off power-law reflected from neutral matter.
pexriv	Exponentially cut-off power-law reflected from ionized matter.
phabs, vphabs, zphabs, zvphabs	Photo-electric absorption
pileup	CCD pile-up model for Chandra
plabs	Absorption model with power-law dependence on energy.
plcabs	Cut-off powerlaw observed through dense, cold matter.
posm	Positronium continuum.
powerlaw, zpowerlw	Simple photon power law.
projct	3-D to 2-D projection mixing model.
pshock, vpshock	Constant temperature, plane-parallel shock plasma model.
pwab	Power-law distribution of neutral absorbers.
raymond, vraymond	Raymond-Smith thermal plasma.
rdblur	Convolve with the diskline model shape.

Model	Description
recorn	Change correction norm for a spectrum (replaces old recornrm command).
redden	IR/optical/UV extinction from Cardelli et al. (1989)
redge	Recombination edge.
reflect	reflection from neutral matter
refsch	E-folded power-law reflected from an ionized relativistic disk.
sedov, vsedov	Sedov model with electron and ion temperatures.
simpl	Comptonization of a seed spectrum.
smaug	Model for an optically-thin, spherically-symmetric thermal plasma.
smedge	Smoothed absorption edge.
spexpcut	Super-exponential cutoff absorption.
spline	Spline multiplicative factor.
srcut	Synchrotron radiation from cut-off electron distribution.
sresc	Synchrotron radiation from escape-limited electron distribution.
SSSice	Einstein Observatory SSS ice absorption.
step	Step function convolved with gaussian.
suzpsf	Suzaku PSF mixing model.
swind1	Absorption by partially ionized material with large velocity shear.
tbabs, ztbabs, tbgrain, tbvarabs	Absorption due to the ISM including molecules and grains.
uvred	UV reddening.
varabs, zvarabs	Photoelectric absorption with variable abundances.
wabs, zwabs	Photoelectric absorption (Morrison & McCammon).
wndabs, zwndabs	Photoelectric absorption with low energy window.
xion	The reflected spectrum from a photo-ionized accretion disk.

Model	Description
xmmpsf	XMM PSF model
zdust	Extinction by dust grains (Pei, 1992).
zredden	Redshifted IR/optical/UV extinction from Cardelli et al. (1989)
zsmdust	Extinction by dust grains in starburst galaxies.
zvfeabs	Redshifted absorption with variable iron abundance.
zxipcf	Partial covering absorption by partially ionized material.

6.2 Additive Model Components (Sources)

This and the following sections contain information on specific, installed XSPEC models. The parameters are given as `par1, par2,`, and `norm,` which is the normalization. Additive models represent sources of emission.

6.2.1 apec, vapec: APEC emission spectrum

An emission spectrum from collisionally-ionized diffuse gas calculated using the APEC code v1.3.1. More information can be found at

http://hea-www.harvard.edu/APEC

which should be consulted by anyone running this model. By default this model reads atomic physics continuum and line data from the files apec_v[version]_coco.fits and apec_v[version]_line.fits in the $HEADAS/../spectral/modelData directory. Different files can be specified by using the command xset APECROOT. There are three options. APECROOT can be set to a version number (eg 1.10, 1.2.0, 1.3.1). In this case the value of APECROOT will be used to replace 1.3.1 in the name of the standard files and the resulting files will be assumed to be in the modelData directory. Alternatively, a filename root (eg `apec_v1.2.0`) can be given. This root will be used as a prefix for the `_coco.fits` and `_line.fits` files. Finally, if neither of these work then the model will assume that the `APECROOT` value gives the complete directory path, e.g.

```
XSPEC12> xset APECROOT /foo/bar/apec_v1.2.0
```

will use the input files

`/foo/bar/apec_v1.2.0_coco.fits`

`/foo/bar/apec_v1.2.0_line.fits`.

Thermal broadening of lines can be included by using: `xset APECTHERMAL yes`. This runs significantly slower than the option without thermal broadening so you should only use this when necessary. Velocity broadening of lines can be included by using: `xset APECVELOCITY <velocity>`, where <velocity> is in km/s. This is added in Gaussian quadrature with any thermal broadening in use.

The **apec** model uses abundances set by the **abund** command. The **vapec** variant allows the user to set the abundance using additional parameters.

par1	plasma temperature, keV
par2	Metal abundances (He fixed at cosmic). The elements included are C, N, O, Ne, Mg, Al, Si, S, Ar, Ca, Fe, Ni. Relative abundances are set by the **abund** command.
par3	Redshift, z
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$,where D_A is the angular diameter distance to the source (cm), n_e and n_H are the electron and H densities (cm^{-3})

For the **vapec** variant the parameters are as follows.

par1	plasma temperature, keV
par2-par14	Abundances for He, C, N, O, Ne, Mg,Al, Si, S, Ar, Ca, Fe, Ni wrt Solar (defined by the abund command)
par15	redshift, z
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$,where D_A is the angular diameter distance to the source (cm), n_e and n_H are the electron and H densities (cm^{-3})

6.2.2 atable: tabulated additive model

An additive table model component. The filename to be used must be given immediately after atable in the **model** command. For example

model atable{mymod.mod}

uses `mymod.mod` as the input for the model. For specifications of the table model file, see the OGIP memo 92-009 on the FITS file format for table model files (available on the WWW or by anonymous ftp from **ftp://legacy.gsfc.nasa.gov/caldb/docs/memos** . Example additive table model files are `mekal.mod` and `raysmith.mod` in `$HEADAS/../spectral/modelData` and `testpo.mod` in `$HEADAS/../spectral/session`.

Any number of tabulated model components (additive, multiplicative or exponential) may be used simultaneously.

6.2.3 bapec, bvapec: velocity broadened APEC thermal plasma model

A velocity- and thermally-broadened emission spectrum from collisionally-ionized diffuse gas calculated using the APEC code v1.3.1. More information on APEC can be found at

http://hea-www.harvard.edu/APEC

which should be consulted by anyone running this model. By default this model reads atomic physics continuum and line data from apec_v[version]_coco.fits and apec_v[version]_line.fits in the $HEADAS/../spectral/modelData directory. Different files can be specified by using the command xset APECROOT. There are three options. APECROOT can be set to a version number (eg 1.10, 1.2.0, 1.3.1). In this case the value of APECROOT will be used to replace 1.3.1 in the name of the standard files and the resulting files will be assumed to be in the modelData directory. Alternatively, a filename root (eg `apec_v1.2.0`) can be given. This root will be used as a prefix for the `_coco.fits` and `_line.fits` files. Finally, if neither of these work then the model will assume that the `APECROOT` value gives the complete directory path, e.g.

```
XSPEC12> xset APECROOT /foo/bar/apec_v1.2.0
```

will use the input files

`/foo/bar/apec_v1.2.0_coco.fits`

`/foo/bar/apec_v1.2.0_line.fits`.

The **bapec** model uses abundances set by the **abund** command. The **bvapec** variant allows the user to set the abundance using additional parameters.

par1	plasma temperature, keV
par2	Metal abundances (He fixed at cosmic). The elements included are C, N, O, Ne, Mg, Al, Si, S, Ar, Ca, Fe, Ni. Relative abundances are set by the **abund** command.
par3	Redshift, z
par4	Gaussian sigma for velocity broadening (km/s)
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$,where D_A is the angular diameter distance to the source (cm), n_e and n_H are the electron and H densities (cm^{-3})

For the **bvapec** variant the parameters are as follows.

par1	plasma temperature, keV
par2-par14	Abundances for He, C, N, O, Ne, Mg,Al, Si, S, Ar, Ca, Fe, Ni wrt Solar (defined by the abund command)
par15	redshift, z
par16	Gaussian sigma for velocity broadening (km/s)
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$,where D_A is the angular diameter distance to the source (cm), n_e and n_H are the electron and H densities (cm^{-3})

6.2.4 bbody, zbbody: blackbody

A blackbody spectrum.

$$A(E) = \frac{K \times 8.0525 E^2 dE}{(kT)^4 \left[\exp\left(E / kT \right) - 1 \right]}$$

where

par1= kT temperature keV

norm= K L_{39} / D_{10}^2 , where L_{39} is the source luminosity in units of 10^{39} ergs^{-1}, D_{10} is the distance to the source in units of 10 kpc

The **zbbody** variant allows an additional (fixed) redshift parameter

$$A(E) = \frac{8.0525K\left[E(1+z)\right]^2 dE}{(1+z)kT^4\left(\exp\left[E(1+z)/kT\right]-1\right)}$$

where

par1= kT	temperature keV
z	Fixed redshift
norm= K	$\frac{L_{39}}{\left[D_{10}(1+z)\right]^2}$, where L_{39} is the source luminosity in units of 10^{39} ergs^{-1}, D_{10} is the distance to the source in units of 10 kpc

6.2.5 bbodyrad: blackbody spectrum, area normalized

A blackbody spectrum with normalization proportional to the surface area.

$$A(E) = \frac{K \times 1.0344 \times 10^{-3} E^2 dE}{\exp\left(E/kT\right)-1}$$

par1	temperature kT, keV
norm, K	R_{km}^2/D_{10}^2, where R_{km} is the source radius in km, and, D_{10} is the distance to the source in units of 10 kpc

6.2.6 bexrav: reflected e-folded broken power law, neutral medium

A broken power-law spectrum multiplied by exponential high-energy cutoff, $\exp\left(-E_c E\right)$, and reflected from neutral material. See Magdziarz & Zdziarski 1995, MNRAS, 273, 837 for details.

The output spectrum is the sum of an e-folded broken power law and the reflection component. The reflection component alone can be obtained for $\left|rel_{\rm refl}\right| < 0$. Then the actual reflection normalization is $|rel_{\rm refl}|$. Note that you need to change then the limits of $\left|rel_{\rm refl}\right|$ excluding zero (as then the direct component appears). If $E_c = 0$, there is no cutoff in the power law. The metal and iron abundance are variable with respect to those set by a command **abund**. The opacities are of Balucinska & McCammon (1992,

and 1994, private communication). As expected in AGNs, H and He are assumed to be fully ionized. Send questions or comments to **aaz@camk.edu.pl** .

par1	Γ_1, first power law photon index
par2	Ebreak, break energy (keV)
par3	Γ_2, second power law photon index
par4	Ec, the e-folding energy in keV (if $E_c = 0$ there is no cutoff)
par5	relrefl, reflection scaling factor (1 for isotropic source above disk)
par6	redshift, z
par7	abundance of elements heavier than He relative to the solar abundances
par8	iron abundance relative to the above
par9	cosine of inclination angle
norm	photon flux at 1 keV of the cutoff broken power-law only (no reflection) in the observed frame.}

6.2.7 bexriv: reflected e-folded broken power law, ionized medium

Broken power-law spectrum multiplied by exponential high-energy cutoff, $\exp(-E_c E)$, and reflected from ionized material. See Magdziarz & Zdziarski 1995, MNRAS, 273, 837 for details. Ionization and opacities of the reflecting medium is computed as in the procedure absori. The output spectrum is the sum of an e-folded broken power law and the reflection component. The reflection component alone can be obtained for $|rel_{\rm refl}| < 0$. Then the actual reflection normalization is $|rel_{\rm refl}| < 0$. Note that you need to change then the limits of $|rel_{\rm refl}| < 0$ excluding zero (as then the direct component appears). If $E_c = 0$, there is no cutoff in the power law. The metal and iron abundances are variable with respect to those set by a command abund. Send questions or comments to **aaz@camk.edu.pl** .

par1	Γ_1, first power law photon index
par2	$E_{\rm break}$, break energy (keV)
par3	Γ_2, second power law photon index

par4	E_c, the e-folding energy in keV (if $E_c = 0$ there is no cutoff)
par5	rel_{refl}, reflection scaling factor (1 for isotropic source above disk)
par6	redshift, z
par7	abundance of elements heavier than He relative to the solar abundances
par8	iron abundance relative to the above
par9	cosine of inclination angle
par10	disk temperature, K
par11	disk ionization parameter, $\xi = \frac{4\pi F_{ion}}{n}$, where F_{ion} is the 5eV–20 keV irradiating flux, n is the density of the reflector; see Done et al., 1992, ApJ, 395, 275}
norm	photon flux at 1 keV of the cutoff broken power-law only (no reflection) in the observed frame.}

6.2.8 bknpower: broken power law

A broken power law.

$$A(E) = \begin{cases} KE^{-\Gamma_1} & E \le E_{break} \\ KE_{break}^{\Gamma_2-\Gamma_1}(E/1\text{keV})^{-\Gamma_2} & E \ge E_{break} \end{cases}$$

where:

par1 $=\Gamma_1$	power law photon index for $E < E_{break}$
par2$=E_{break}$	break point for the energy in keV
par3$=\Gamma_2$	power law photon index for $E > E_{break}$
norm=K	photons keV^{-1}cm^{-2}s^{-1} at 1 keV}

6.2.9 bkn2pow: broken power law, 2 break energies

A three-segment broken power law (ie with two break energies).

$$A(E) = \begin{cases} KE^{-\Gamma_1} & E \le E_{\text{break},1} \\ KE_{\text{break},1}^{\Gamma_2-\Gamma_1}\left(E/1\text{keV}\right)^{-\Gamma_2} & E_{\text{break},1} \le E \le E_{\text{break},2} \\ KE_{\text{break},1}^{\Gamma_2-\Gamma_1}E_{\text{break},2}^{\Gamma_3-\Gamma_2}\left(E/1\text{keV}\right)^{-\Gamma_3} & E_{\text{break},2} \le E \end{cases}$$

where :

par1 = Γ_1 power law photon index for $E < E_{\text{break},1}$

par2 = $E_{\text{break},1}$ first break point for the energy, keV

par3 = Γ_2 power law photon index for $E_{\text{break},1} < E < E_{\text{break},2}$

par4 = $E_{\text{break},2}$ second break point for the energy, keV

par5 = Γ_3 power law photon index for $E > E_{\text{break},2}$

Norm = K photons $\text{keV}^{-1}\text{cm}^{-2}\text{s}^{-1}$ at 1 keV

6.2.10 bmc: Comptonization by relativistic matter

This is an analytic model describing Comptonization of soft photons by matter undergoing relativistic bulk-motion. The typical scenario involves thermal X-rays from the inner region of an accretion disk in a black-hole binary illuminating in-falling matter in close proximity to the black-hole event horizon. For a detailed description of the model, refer to Titarchuk, Mastichiadis & Kylafis 1997, ApJ, 487, 834; Titarchuk & Zannias, 1998, ApJ, 493, 863; Laurent & Titarchuk 1999, ApJ, 511, 289; Zannias, Borozdin, Revnivtsev., Trudolyubov, Shrader, & Titarchuk, 1999, ApJ, 517, 367; or Shrader & Titarchuk 1999, ApJ 521, L21. The model parameters are the characteristic black-body temperature of the soft photon source, a spectral (energy) index, and an illumination parameter characterizing the fractional illumination of the bulk-motion flow by the thermal photon source. It must be emphasized that this model is not an additive combination of power law and thermal sources, rather it represents a self-consistent convolution. The bulk-motion up-scattering and Compton recoil combine to produce the hard spectral tail, which combined with the thermal source results in the canonical high-soft-state spectrum of black hole accretion. The position of the sharp high energy cutoff (due to recoil) can be determined using the theta function $\theta\left(E_c - E\right)$. The model can also be used for the general Comptonization case when the energy range is limited from above by the plasma temperature (see compTT and compST).

par1 Temperature of thermal photon source in keV.

par2	Energy spectral index alpha.
par3	Log of the *A* parameter. Note that *f* in Borozdin *et al*. 1999 and Shrader & Titarchuk 1999 is $10^{\texttt{par3}}$
norm	A_N defined in Borozdin et al 1999 and Shrader & Titarchuk (1999)

6.2.11 bremss, vbremss, zbremss: thermal bremsstrahlung

A thermal bremsstrahlung spectrum based on the Kellogg, Baldwin & Koch (ApJ 199, 299) polynomial fits to the Karzas & Latter (ApJS 6, 167) numerical values. A routine from Kurucz (private communication) is used in at low temperature end. The He abundance is assumed to be 8.5 % of H by number.

Choice of fixed redshift is allowed by using **zbremss** variant

Choice of Hydrogen to Helium abundance ratio is allowed by using the **vbremss** variant.

The parameter settings are thus:

For **bremss**:

par1	plasma temperature in keV
norm	$\frac{3.02\times10^{-15}}{4\pi D^2}\int n_e n_I dV$, where D is the distance to the source (cm) and n_e, n_I are the electron and ion densities (cm^{-3})

For **zbremss**:

par1	plasma temperature in keV
par2 = z	redshift
norm	$\frac{3.02\times10^{-15}}{4\pi D^2}\int n_e n_I dV$, where D is the distance to the source (cm) and n_e, n_I are the electron and ion densities (cm^{-3})

For **vbremss**:

par1	plasma temperature in keV

par2 n(He)/n(H) (note that the Solar ratio is 0.085)

norm $\frac{3.02\times10^{-15}}{4\pi D^2}\int n_e n_I dV$, where D is the distance to the source (cm) and n_e, n_I are the electron and ion densities (cm^{-3})

6.2.12 c6mekl, c6vmekl, c6pmekl, c6pvmkl: differential emission measure using Chebyshev representations with multi-temperature mekal

c6mekl is a multi-temperature mekal model using sixth-order Chebyshev polynomial for the differential emission measure. The DEM is not constrained to be positive.. The switch parameter determines whether the mekal code will be run to calculate the model spectrum for each temperature or whether the model spectrum will be interpolated from a pre-calculated table. The former is slower but more accurate. The reference for this model is Singh *et al.* (1996, ApJ, 456, 766).

c6pmekl differs by using the exponential of the 6th order Chebyshev polynomial

c6mekl and **c6pmekl** use abundances relative to the Solar abundances set by the **abund** command

The variants **c6vmkl** and **c6pvmkl** with polynomial and exponential polynomial respectively allow the user to specify 14 elemental abundance.

For c6mekl and c6pmkl the parameters are:

par1-6 Chebyshev polynomial coefficients

par7 H density (cm^{-3})

par8 abundance wrt to Solar

par9 Redshift

par10
0 ⇒ calculate

1 ⇒ interpolate

2 ⇒ interpolate using APEC model

norm $\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm), n_e is the electron density (cm^{-3}), and n_H is the

hydrogen density (cm^{-3})

While for **c6vmkl** and **c6vpmkl** the parameters are:

par1-6 Chebyshev polynomial coefficients

par7 H density (cm^{-3})

par8-21 Abundances of He, C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca, Fe, Ni wrt Solar (defined by the **abund** command)

par22 Redshift

0 $\Rightarrow$ calculate

par23 1 $\Rightarrow$ interpolate

2  interpolate using APEC model

norm $\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm), n_e is the electron density (cm^{-3}), and n_H is the hydrogen density (cm^{-3})

6.2.13 cemekl, cevmkl: plasma emission, multi-temperature using mekal

A multi-temperature plasma emission model built from the mekal code. Emission measures follow a power-law in temperature (*i.e.* emission measure from temperature T is proportional to $(T/T_{max})^{\alpha}$. The switch parameter determines whether the mekal code will be run to calculate the model spectrum for each temperature or whether the model spectrum will be interpolated from a pre-calculated table. The former is slower but more accurate.

For the **cemekl** version, the abundance ratios are set by the **abund** command. The cevmkl variant allows the user to define the abundances.

The parameters for **cemekl** are:

par1=α index for power-law emissivity function

par2=T_{max} maximum temperature

par3 n_H (cm^{-3})

par4 abundance relative to solar

par5 redshift z

$0 \Rightarrow$ calculate

par6 $1 \Rightarrow$ interpolate

$2 \Rightarrow$ interpolate using APEC model

norm Normalization

For the **cevmkl** variant the parameters are:

par1 index for power-law emissivity function

par2 maximum temperature

par3 $n_{\rm H}$ ($\rm cm^{-3}$)

par4-17 abundance relative to solar Abundances for He, C, N, O, Ne, Na, Mg, Al, Si, S,Ar, Ca, Fe, Ni wrt Solar (defined by the **abund** command)

par18 redshift z

$0 \Rightarrow$ calculate

par19 $1 \Rightarrow$ interpolate

$2 \Rightarrow$ interpolate using APEC model

norm Normalization

6.2.14 cflow: cooling flow

A cooling flow model after Mushotzky & Szymkowiak (*Cooling Flows in Clusters and Galaxies*, ed. Fabian, 1988). An index of zero for the power-law emissivity function corresponds to emission measure weighted by the inverse of the bolometric luminosity at that temperature. The model assumes $H_0 = 50$ and $q_0 = 0$. The abundance ratios are set by the **abund** command.

par1 index for power-law emissivity function

par2	low temperature (keV)
par3	high temperature (keV)
par4	abundance relative Solar
par5	redshift, *z*
norm	Mass accretion rate (solar mass/yr)

6.2.15 compbb: Comptonization, black body

Comptonized blackbody model by Nishimura, Mitsuda and Itoh, 1986, PASJ, 38, 819. The electron temperature should normally be kept fixed since the Compton y parameter is the product of the electron temperature and optical depth.

par1	blackbody temperature (keV)
par2	electron temperature of the hot plasma (keV)
par3	optical depth of the plasma
norm	$\left(L_{39}/D_{10}\right)^2$, where L_{39} is the source luminosity in units of 10^{39} ergs^{-1} and D_{10} is the distance to the source in units of 10 kpc (the same definition used for the bbodyrad model)

6.2.16 compLS: Comptonization, Lamb & Sanford

A Comptonization spectrum after Lamb and Sanford, 1979, *M.N.R.A.S*, 288, 555. This model calculates the self-Comptonization of a bremsstrahlung emission from an optically thick spherical plasma cloud with a given optical depth and temperature. It was popular for Sco X-1.

par1	temperature in keV
par2	optical depth
norm	normalization

6.2.17 compPS: Comptonization, Poutanen & Svenson

Comptonization spectra computed for different geometries using exact numerical solution of the radiative transfer equation. The computational "iterative scattering method" is similar to the standard Lambda-iteration and is described in Poutanen J., Svensson R., 1996, ApJ, 470, 249 (PS96). The Compton scattering kernel is the exact one as derived by Jones F. C., 1968, Phys. Rev., 167, 1159 (see PS96 for references).

Comptonization spectra depend on the geometry (slab, sphere, hemisphere, cylinder), Thomson optical depth tau, parameters of the electron distribution, spectral distribution of soft seed photons, the way seed soft photons are injected to the electron cloud, and the inclination angle of the observer.

The resulting spectrum is reflected from the cool medium according to the computational method of Magdziarz & Zdziarski (1995) (see reflect, pexrav, pexriv models). rel_refl is the solid angle of the cold material visible from the Comptonizing source (in units 2 pi), other parameters determine the abundances and ionization state of reflecting material (Fe_ab_re, Me_ab, xi, Tdisk). The reflected spectrum is smeared out by rotation of the disk due to special and general relativistic effects using "diskline"-type kernel (with parameters Betor10, Rin, Rout).

Electron distribution function can be Maxwellian, power-law, cutoff Maxwellian, or hybrid (with low temperature Maxwellian plus a power-law tail).

Possible geometries include plane-parallel slab, cylinder (described by the height-to-radius ratio H/R), sphere, or hemisphere. By default the lower boundary of the "cloud" (not for spherical geometry) is fully absorbive (e.g. cold disk). However, by varying covering factor parameter cov_fac, it may be made transparent for radiation. In that case, photons from the "upper" cloud can also be upscattered in the "lower" cloud below the disk. This geometry is that for an accretion disk with cold cloudlets in the central plane (Zdziarski, Poutanen, et al. 1998, MNRAS, 301, 435). For cylinder and hemisphere geometries, an approximate solution is obtained by averaging specific intensities over horizontal layers (see PS96). For slab and sphere geometries, no approximation is made.

The seed photons can be injected to the electron cloud either isotropically and homogeneously through out the cloud, or at the bottom of the slab, cylinder, hemisphere or center of the sphere (or from the central plane of the slab if cov_frac ne 1). For the sphere, there exist a possibility (IGEOM=-5) for photon injection according to the eigenfunction of the diffusion equation sin (pi*tau'/tau)/(pi*tau'/tau), where tau' is the optical depth measured from the center (see Sunyaev & Titarchuk 1980).

Seed photons can be black body (bbodyrad) for Tbb>0 or multicolor disk (diskbb) for Tbb<0. The normalization of the model also follows those models: (1) Tbb>0, K = (RKM)**2 /(D10)**2, where D10 is the distance in units of 10 kpc and RKM is the source radius in km; (2) Tbb<0 K = (RKM)**2 /(D10)**2 cos(theta), where theta is the inclination angle.

Thomson optical depth of the cloud is not always good parameter to fit. Instead the Compton parameter y=4 * tau * Theta (where Theta= Te (keV) / 511) can be used. Parameter y is directly related to the spectral index and therefore is much more stable in fitting procedure. The fitting can be done taking 6th parameter negative, and optical depth then can be obtained via tau= y/(4* Te / 511).

The region of parameter space where the numerical method produces reasonable results is constrained as follows : 1) Electron temperature Te > 10 keV; 2) Thomson optical depth tau < 1.5 for slab geometry and tau < 3, for other geometries.

par1 = Te, electron temperature in keV

par2 = p, electron power-law index [N(gamma)=gamma^-p]

par3 = gmin, minimum Lorentz factor gamma

par4 = gmax, maximum Lorentz factor gamma

(a) if any of gmin or gmax < 1 then Maxwellian electron distribution with parameter Te

(b) if Te=0. then power-law electrons with parameters p, gmin, gmax

(c) if both gmin,gmax>=1 but gmax<gmin then cutoff Maxwellian with Te, p, gmin (cutoff Lorentz factor) as parameters

(d) if Te.ne.0, gmin, gmax >=1 then hybrid electron distribution with parameters Te, p, gmin, gmax

par5 = Tbb, temperature of soft photons

Tbb>0 blackbody

Tbb<0 multicolor disk with inner disk temperature Tbb

par6 = if > 0 : tau, vertical optical depth of the corona

if < 0 : y = 4*Theta*tau

limits: for the slab geometry - tau < 1

if say tau~2 increase MAXTAU to 50

for sphere - tau < 3

par7 = geom, 0 - approximate treatment of radiative transfer using escape probability for a sphere (very fast method); 1 - slab; 2 - cylinder; 3 - hemisphere; 4,5 - sphere

input photons at the bottom of the slab, cylinder, hemisphere or center of the sphere (or from the central plane of the slab if cov_fact not 1). if < 0 then geometry defined by |geom| and sources of incident photons are isotropic and homogeneous.

-5 - sphere with the source of photons distributed according to the eigenfunction of the diffusion equation

f(tau')=sim(pi*tau'/tau)/(pi*tau'/tau) where tau' varies between

0 and tau.

par8 = H/R for cylinder geometry only

par9 = cosIncl, cosine of inclination angle

(if < 0 then only black body)

par10 = cov_fac, covering factor of cold clouds

if geom =+/- 4,5 then cov_fac is dummy

par11 = R, amount of reflection Omega/(2*pi)

(if R < 0 then only reflection component)

par12 = FeAb, iron abundance in units of solar

par13 = MeAb, abundance of heavy elements in units of solar

par14 = xi, disk ionization parameter L/(nR^2)

par15 = temp, disk temperature for reflection in K

par16 = beta, reflection emissivity law (r^beta)

if beta=-10 then non-rotating disk

if beta=10 then 1.-sqrt(6./rg))/rg**3

par17 = Rin/Rg, inner radius of the disk (Schwarzschild units)

par18 = Rout/Rg, outer radius of the disk

par19 = redshift

6.2.18 compST: Comptonization, Sunyaev & Titarchuk

A Comptonization spectrum after Sunyaev and Titarchuk 1980, *A&A*, 86, 121. This model is the Comptonization of cool photons on hot electrons.

par1 temperature in keV

par2 optical depth

norm $\frac{Nf}{4\pi d^2}$, where N is the total number of photons from the source, d is the distance to the source, and f is the factor $\frac{z(z+3)y^z}{\Gamma(2z+4)\Gamma(z)}$. z is the spectral index, y is the injected photon energy in units of the temperature, and Γ is the incomplete gamma function.

6.2.19 compTT: Comptonization, Titarchuk

This is an analytic model describing Comptonization of soft photons in a hot plasma, developed by L. Titarchuk (see ApJ, 434, 313). This replaces the Sunyaev-Titarchuk Comptonization model in the sense that the theory is extended to include relativistic effects. Also, the approximations used in the model work well for both the optically thin and thick regimes. The Comptonized spectrum is determined completely by the plasma temperature and the so-called β parameter which is independent of geometry. The optical depth is then determined as a function of β for a given geometry. Thus `par5` switches between spherical and disk geometries so that β is not a direct input here. This parameter MUST be frozen. If `par5` ≥ 0, β is obtained from the optical depth using analytic approximation (e.g. Titarchuk 1994). If `par5` < 0 and $0.1 < \tau < 10$\$, β is obtained by interpolation from a set of accurately calculated pairs of β and τ from Sunyaev & Titarchuk 1985 (A&A 143, 374).

In this incarnation of the model, the soft photon input spectrum is a Wien law [$x^2 e^{-x}$ photons] because this lends itself to a particularly simple analytical form of the model. For present X-ray detectors this should be adequate. Note that in energy flux space the peak of the Wien law occurs at 3kT as opposed to 2.8kT for a blackbody. The plasma temperature may range from 2-500 keV, but the model is not valid for simultaneously low temperatures and low optical depth, or for high temperatures and high optical depth. The user is strongly urged to read the following references (esp. HT95 Fig 7) before and after using this model in order to fully understand and appreciate the physical assumptions made:

Titarchuk, L., 1994, ApJ, 434, 313; Hua, X-M., Titarchuk, L., 1995, ApJ, 449, 188;

Titarchuk, L., Lyubarskij, Y., 1995, ApJ, 450, 876.

par1	Redshift	
par2	Input soft photon (Wien) temperature (keV)	
par3	Plasma temperature (keV)	
par4	Plasma optical depth	
par5	Geometry switch. (sign denotes approximation technique, magnitude determines geometry)	
	≤ 1	disk
	>1	sphere
par5		
	≥ 0	use analytic approx for β vs τ
	< 0	β vs. τ from interpolation
norm	normalization	

6.2.20 cutoffpl: power law, high energy exponential cutoff

A power law with high energy exponential rolloff.

$$A(E) = KE^{-\alpha} \exp\left(-E/\beta\right)$$

par1 = α	power law photon index
par2 = β	e-folding energy of exponential rolloff (in keV)
norm = K	Photons $keV^{-1}cm^{-2}s^{-1}$ at 1 keV

6.2.21 disk: accretion disk, black body

The spectrum from an accretion disk, where the opacities are dominated by free-free absorption, i.e., the so-called blackbody disk model. Not correct for a disk around a neutron star.

par1	accretion rate in Eddington Luminosities
par2	central mass in solar mass units
par3	inner disk radius in gravitational (= 3 Schwarzschild radii)
norm	$2\cos i / d^2$ where i is the inclination of the disk and d is the distance in units of 10 kpc

6.2.22 diskbb: accretion disk, multi-black body components

The spectrum from an accretion disk consisting of multiple blackbody components. For example, see Mitsuda et al., PASJ, 36, 741, (1984), Makishima *et al.,* ApJ 308, 635, (1986).

par1	temperature at inner disk radius (keV)
norm	$\left(\left(R_{in}/km\right)/\left(D/10kpc\right)\right)^2 \cos\theta$, where $R_{\rm in}$ is "an apparent" inner disk radius, D the distance to the source, and θ the angle of the disk (θ = 0 is face-on). On the correction factor between the apparent inner disk radius and the realistic radius, see e.g., Kubota et al. 1998, PASJ, 50, 667.

6.2.23 Diskir: Irradiated inner and outer disk

The inner disk can be irradiated by the Compton tail. This can substantially change the inner disk temperature structure from that expected from an unilluminated disk in the limit where the ratio of luminosity in the tail to that in the disk, Lc/Ld>>1. This is generally the case in the low/hard state of accreting black holes, and neglecting this effect leads to an underestimate of the inner disk radius (Gierlinski, Done & Page 2008a MNRAS, 388, 753).

The irradiated inner disk and Compton tail can illuminate the rest of the disk, and a fraction f_out of the bolometric flux is thermalized to the local blackbody temperature at each radius. This reprocessed flux generally dominates the optical and UV bandpass of LMXBs (Gierlinski, Done & Page 2008b MNRAS, submitted).

par1 = kT_disk, innermost temperature of the UNILLUMINATED disk

par2 = Gamma, asymptotic power-law photon index

par3 = kT_e, electon temperature (high energy rollover)

par4 = Lc/Ld, ratio of luminosity in the Compton tail to that of the UNILLUMINATED disk

par5 = fin, fraction of luminosity in the Compton tail which is thermalized in the inner disk (generally fix at 0.1 as appropriate for an albedo of 0.3 and solid angle of 0.3)

par6 = rirr, radius of the Compton illuminated disk in terms of the inner disk radius

par7 = fout, fraction of bolometric flux which is thermalized in the outer disk

par8 = logrout, log10 of the outer disk radius in terms of the inner disk radius

K = normalization, as in diskbb

6.2.24 diskline: accretion disk line emission, relativistic

A line emission from a relativistic accretion disk. See Fabian et al., MNRAS 238, 729. Setting `par2` to 10 is the special case of the accretion disk emissivity law $\left(1-\sqrt{6/R}\right)\Big/R^3$.

par1 line energy

par2 power law dependence of emissivity. If this parameter is 10 or greater then the accretion disk emissivity law $\left(1-\sqrt{6/R}\right)\Big/R^3$ is used. Otherwise the emissivity scales as Rpar2

par3	inner radius (units of GM/c^2)
par4	outer radius (units of GM/c^2)
par5	inclination (degrees)
norm	photon cm-2 s-1 in the spectrum

6.2.25 diskm: accretion disk with gas pressure viscosity

A disk model with gas pressure viscosity. The spectrum from an accretion disk where the viscosity scales as the gas pressure. From Stella and Rosner 1984, ApJ, 277, 312.

par1	accretion rate in Eddington Luminosities
par2	central mass in solar mass units
par3	inner disk radius in gravitational (= 3 Schwarzschild radii)
par4	viscosity
norm	$2\cos i/d^2$ where i is the inclination of the disk and d is the distance in units of 10 kpc

6.2.26 disko: accretion disk, inner, radiation pressure viscosity

A modified blackbody disk model. The spectrum from the inner region of an accretion disk where the viscosity is dominated by radiation pressure.

par1	accretion rate in Eddington Luminosities
par2	central mass in solar mass units
par3	inner disk radius in gravitational (= 3 Schwarzschild radii)
par4	viscosity
norm	$2\cos i/d^2$ where *i* is the inclination of the disk and *d* is the distance in units of 10 kpc

6.2.27 diskpbb: accretion disk, power-law dependence for T(r)

A multiple blackbody disk model where local disk temperature T(r) is proportional to r^{-p}, where p is a free parameter. The standard disk model, diskbb, is recovered if p = 0.75. If radial advection is important then p < 0.75. See the discussion and examples in, e.g., Mineshige et al. 1994, ApJ, 426, 308, Hirano et al. 1995, ApJ, 446, 350, Watarai et al. 2000, PASJ, 52, 133, Kubota and Makishima 2004, ApJ, 601, 428, Kubota et al. 2005, ApJ, 631, 1062 .

par1	Tin: temperature at inner disk radius (keV)
par2	p: exponent of the radial dependence of the disk temperature
norm	$\left(\left(R_{in}/km \right) \Big/ \left(D/10kpc \right) \right)^2 \cos\theta$, where $R_{\rm in}$ is "an apparent" inner disk radius, D the distance to the source, and θ the angle of the disk (θ = 0 is face-on). On the correction factor between the apparent inner disk radius and the realistic radius, see e.g., Kubota et al. 1998, PASJ, 50, 667.

6.2.28 diskpn: accretion disk, black hole, black body

Blackbody spectrum of an accretion disk. This is an extension of the **diskbb** model, including corrections for temperature distribution near the black hole. The temperature distribution was calculated in Paczynski-Wiita pseudo-Newtonian potential. An accretion rate can be computed from the maximum temperature found. For details see Gierlinski et al., 1999, MNRAS, 309, 496. Please note that the inner disk radius (`par2`) can be a free parameter only close to `par2` = 6; otherwise `par2` is strongly correlated with K.

par1	maximum temperature in the disk (keV)
par2	inner disk radius in $R_g = GM/c^2$ units, $6 \le$ `par2` ≤ 1000
norm	$\frac{M^2 \cos i}{D^2 \beta^4}$ normalization, where M = central mass (solar masses), D distance to the source (kpc), i inclination of the disk, and β color/effective temperature ratio.

6.2.29 equil, vequil: collisional plasma, ionization equilibrium

Ionization equilibrium collisional plasma model. This is the equilibrium version of Kazik Borkowski's NEI models. Several versions are available. To switch between

them use the **xset** `neivers` command. **xset** `neivers 1.0` gives the version from xspec v11.1, **xset** `neivers 1.1` uses updated calculations of ionization fractions using dielectronic recombination rates from Mazzotta et al (1988), and **xset** `neivers 2.0` uses the same ionization fractions as 1.1 but uses APED to calculate the resulting spectrum. Note that versions 1.x have no emission from Ar. The default is version 1.1.

The **vequil** variant allows the user to set the abundances for the model.

For the **equil** model the parameters are:

par1	plasma temperature (keV)
par2	Metal abundances (He fixed at cosmic). The elements included are C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni. Abundances are defined by the abund command
par3	redshift
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm), n_e is the electron density (cm^{-3}), and n_H is the hydrogen density (cm^{-3})

For the **vequil** model, the parameters are:

par1	plasma temperature (keV)
par2-par13	Abundances for He, C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni wrt Solar (defined by the abund command)
par14	Redshift, z
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm), n_e is the electron density (cm^{-3}), and n_H is the hydrogen density (cm^{-3})

The references for this model are as follows:

Borkowski, Lyerly & Reynolds, 2001, ApJ, 548, 820

Hamilton, A.J.S., Sarazin, C. L. & Chevalier, R. A. , 1983,ApJS, 51,115

Borkowski, K.J., Sarazin, C.L. & Blondin, J.M. 1994, ApJ, 429, 710

Liedahl, D.A., Osterheld, A.L. Goldstein, W.H. 1995, ApJ, 438, L11

6.2.30 expdec: exponential decay

An exponential decay.

$$A(E) = \exp(-KE)$$

where:

par1 = K exponential factor

6.2.31 ezdiskbb: multiple blackbody disk model with zero-torque inner boundary

A multi-temperature blackbody model for a thin, steady-state, Newtonian accretion disk, assuming zero torque at the inner boundary for the disk at radius R_in. The temperature of the disk as a function of radius is assumed to be T(r) = T_* r^(-3/4) (1-r^(-1/2))^(1/4), where r = R/R_in and T_* = f(3 G M Mdot / 8 pi R_in^3 sigma)^(1/4). The maximum temperature in the disk is given by T_max = 0.488 T_*.

This model is an alternative to diskbb, which assumes a non-zero torque at the inner edge and a temperature profile T(r) = T_* r^(-3/4), and it should be used to fit spectra of disks when the zero-torque inner boundary condition is appropriate. For details see Zimmerman et al. (2004) astro-ph/0408209.

par1 = maximum temperature in the disk (keV)

par2 = (1/f^4) (R_in/D)^2 cos i, where R_in is the inner radius of the disk in km, D is the distance to the source in units of 10 kpc, i is the inclination, and f is the color to effective temperature ratio.

6.2.32 gauss, zgauss: gaussian line profile

A simple gaussian line profile. If the width is ≤ 0, then itis treated as a delta function. The **zgauss** variant computes a redshifted gaussian.

$$A(E) = K \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-{(E - E_l)^2}\Big/{2\sigma^2} \right)$$

where:

par1 = E_l line energy in keV

par2 = σ line width in keV

Norm = K total photons $cm^{-2} s^{-1}$ in the line

For **zgauss** the corresponding formula is:

$$A(E) = \frac{K}{\sqrt{2\pi}\sigma^2(1+z)} \exp\left(\frac{1}{2}\left[{(E(1+z) - E_{\mathrm{L}})}\Big/{\sigma} \right]^2 \right)$$

and parameter settings are:

par1 = E_{L} line energy in keV

par2 = σ line width in keV

par3 = z redshift

norm = K total photons $cm^{-2} s^{-1}$ in the line

6.2.33 gnei, vgnei: collisional plasma, non-equilibrium, temperature evolution

Non-equilibrium ionization collisional plasma model. This is a generalization of the **nei** model where the temperature is allowed to have been different in the past *i.e.* the ionization timescale averaged temperature is not necessarily equal to the current temperature. For example, in a standard Sedov model with equal electron and ion temperatures, the ionization timescale averaged temperature is always higher than the current temperature for each fluid element. The references for this model can be found under the description of the equil model. Several versions are available. To switch between them use the **xset** `neivers` command. **xset** `neivers 1.0` gives the version from xspec v11.1, **xset** `neivers 1.1` uses updated calculations of ionization fractions using dielectronic recombination rates from Mazzotta et al (1988), and **xset** `neivers 2.0` uses the same ionization fractions as 1.1 but uses APED to calculate the resulting spectrum. Note that versions 1.x have no emission from Ar. The default is version 1.1.

The **vgnei** variant allows the user to set the abundances of the model.

For the **gnei** model the parameters are:

par1	plasma temperature (keV)
par2	Metal abundances (He fixed at cosmic). The elements included are C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni. Abundances are defined by the abund command
par3	Ionization timescale in units of s cm^{-3}.
par4	Ionization timescale averaged plasma temperature (keV)
par5	(fixed) redshift
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm), n_e and n_H (cm^{-3}) are the electron and hydrogen densities respectively.

For **vgnei** the parameters are:

par1	plasma temperature (keV)
par2-par13	(Fixed) Abundances for He, C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni wrt Solar (defined by the abund command)
par14	Ionization timescale in units of s cm^{-3}.
par15	Ionization timescale averaged plasma temperature (keV)
par16	(fixed) redshift
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm), and n_e , n_H (cm^{-3}) are the electron and hydrogen densities respectively.

6.2.34 grad: accretion disk, Schwarzschild black hole

General Relativistic Accretion Disk model around a Schwarzschild black hole. Inner radius is fixed to be 3 Schwarzschild radii, thus the energy conversion efficiency is 0.057. See Hanawa, T., 1989, ApJ, 341, 948 and Ebisawa, K. Mitsuda, K. and Hanawa, T. 1991, ApJ, 367, 213. Several bugs were found in the old GRAD model which was included in xspec 11.0.1ae and before. Due to these bugs, it turned out that the mass obtained by fitting the old GRAD model to the observation was 1.4 times over-estimated. These bugs were fixed, and a new parameter (par6) was added to make the distinction between the old and new codes clear.

par1 distance (kpc)

par2 disk inclination angle (deg; 0 for face-on)

par3 mass of the central object (solar units)

par4 mass accretion rate 10^{18} gs^{-1}

par5 spectral hardening factor, T_{col}/T_{eff}. Should be greater than 1.0, and considered to be 1.5–1.9 for accretion disks around a stellar-mass black hole. See, *e.g.,* Shimura and Takahara, 1995, ApJ, 445, 780

par6 A flag to switch on/off the relativistic effects (never allowed to be free). If positive, relativistic calculation; if negative or zero, Newtonian calculation (the inner radius is still fixed at 3 Schwarzschild radii, and the efficiency is 1/12).

norm Should be fixed to 1.

6.2.35 grbm: gamma-ray burst continuum

A model for gamma-ray burst continuum spectra developed by D. Band, et. al., 1993 (ApJ 413, 281).

$$A(E) = \begin{cases} K\left(E/100.\right)^{\alpha_1} \exp(-E/E_c) & E < (\alpha_1 - \alpha_2)E_c \\ K\left[(\alpha_1 - \alpha_2)E_c/100.\right]^{(\alpha_1-\alpha_2)} \left(E/100.\right)^{\alpha_2} \exp\left[-(\alpha_1 - \alpha_2)\right] & E > (\alpha_1 - \alpha_2)E_c \end{cases}$$

where E is in units of 100 keV.

par1 $= \alpha_1$ first power law index

par2 $= \alpha_2$ second power law index

par3 $= E_c$ characteristic energy in keV

norm $= K$ normalization constant

6.2.36 kerrbb: multi-temperature blackbody model for thin accretion disk around a Kerr black hole

A multi-temperature blackbody model for a thin, steady state, general relativistic accretion disk around a Kerr black hole. The effect of self-irradiation of the disk is considered, and the torque at the inner boundary of the disk is allowed to be non-zero. This model is intended as an extension to grad, which assumes that the black hole is non-rotating. For details see Li et al., ApJSuppl, 157, 335, 2005.

par1 = eta, ratio of the disk power produced by a torque at the disk inner boundary to the disk power arising from accretion. It must be >= 0 and <=1. When eta = 0, the solution corresponds to that of a standard Keplerian disk with zero torque at the inner boundary.

par2 = specific angular momentum of the black hole in units of the black hole mass M (geometrized units G=c=1). Should be >= -1 and < 1.

par3 = disk's inclination angle (the angle between the axis of the disk and the line of sight). It is expressed in degrees. i=0 is for a "face-on" accretion disk. i should be <= 85 degree.

par4 = the mass of the black hole in units of the solar mass.

par5 = the "effective" mass accretion rate of the disk in units of 10^18 g/sec. When eta = 0 (zero torque at the inner boundary), this is just the mass accretion rate of the disk. When eta is nonzero, the effective mass accretion rate = (1+eta) times the true mass accretion rate of the disk. The total disk luminosity is then "epsilon" times "the effective mass accretion rate" times "c^2", where epsilon is the radiation efficiency of a standard accretion disk around the Kerr black hole

par6 = the distance from the observer to the black hole in units of kpc.

par7 = spectral hardening factor, T_col/T_eff. It should be greater than 1.0, and considered to be 1.5-1.9 for accretion disks around a stellar-mass black hole. See, e.g., Shimura and Takahara 1995, ApJ, 445, 780

par8 = a flag to switch on/off the effect of self-irradiation (never allowed to be free). Self-irradiation is included when > 0. Self-irradiation is not included when <= 0.

par9 = a flag to switch on/off the effect of limb-darkening (never allowed to be free). The disk emission is assumed to be limb-darkened when > 0. The disk emission is assumed to be isotropic when lflag is <= 0.

K = normalization. Should be set to 1 if the inclination, mass and distance are frozen.

6.2.37 kerrd: optically thick accretion disk around a Kerr black hole

Optically thick extreme-Kerr disk model based on the same tranfer-function used in the "laor" Kerr disk-line model. Local emission is simply assumed to be the diluted blackbody. See Laor 1991, ApJ, 376, L90 for explanation of the transfer function. See Ebisawa et al. 2003, ApJ, 597, 780 for

examples of using this model.

par1 = distance (kpc)

par2 = spectral hardening factor, Tcol/Teff. Should be
greater than 1.0, and considered to be 1.5-1.9
for accretion disks around a stellar-mass black hole.
See, e.g., Shimura and Takahara, 1995, ApJ, 445, 780

par3 = mass of the central object (solar unit)

par4 = mass accretion rate (1e18 g/s)

par5 = disk inclination angle (deg; 0 for face-on)

par6 = inner radius (units of GM/c**2). 1.235 is the
last stable orbit.

par7 = outer radius (units of GM/c**2)

K = normalization factor. should be fixed to 1.

6.2.38 kerrdisk: accretion disk line emission with BH spin as free parameter

Model for an accretion disk broad emission line with the black hole spin allowed to be a free parameter. A detailed description can be found in Brenneman & Reynolds (2006ApJ...652.1028B).

This model is quite slow so is best used after models such as laor or diskline have been employed to get an estimate of the best-fit parameters.

par1 = rest frame line energy (keV)

par2 = emissivity index for the inner disk

par3 = emissivity index for the outer disk

par4 = break radius separating the inner and outer portions of the disk (gravitational radii)

par5 = dimensionless black hole spin

par6 = disk inclination angle to the line of sight (degrees)

par7 = inner radius of the disk in units of the radius of marginal stability

par8 = outer radius of the disk in units of the radius of marginal stability

par9 = redshift z

K = flux in line (photons/cm^2/s)

6.2.39 laor: accretion disk, black hole emission line

An emission line from an accreti on disk around a black hole. Ari Laor's calculation including GR effects (ApJ 376, 90).

par1	Line energy in keV
par2=α	power law dependence of emissivity (scales as $R^{-\alpha}$)
par3	inner radius (units of GM/c^2)
par4	outer radius (units of GM/c^2)
par5	inclination (degrees)
norm	photons cm^{-2}s^{-1} in the line

6.2.40 laor2: accretion disk with broken-power law emissivity profile, black hole emission line

An emission line from an accreti on disk with a broken power-law emissivity profile around a black hole. Uses Ari Laor's calculation including GR effects (ApJ 376, 90). Modified from laor model by Andy Fabian.

par1	Line energy in keV
par2	Index: power law dependence of emissivity (scales as $R^{-\mathrm{Index}}$)
par3	inner radius (units of GM/c^2)
par4	outer radius (units of GM/c^2)
par5	inclination (degrees)
par6	radius at which emissivity power-law index changes
par7	Emissivity power-law index for radii > par6
norm	photons $cm^{-2}s^{-1}$ in the line

6.2.41 lorentz: lorentz line profile

A Lorentzian line profile.

$$A(E) = K \frac{\sigma/2\pi}{\left[(E - E_L)^2 + (\sigma/2)^2\right]}$$

where:

par1 $= E_L$	line energy in keV
par2 $= \sigma$	FWHM line width in keV
norm $= K$	photons cm^{-2} s^{-1} in the line

6.2.42 meka, vmeka: emission, hot diffuse gas (Mewe-Gronenschild)

An emission spectrum from hot diffuse gas based on the model calculations of Mewe and Gronenschild (as amended by Kaastra). The model includes line emissions from several

elements. Abundances are the number of nuclei per Hydrogen nucleus relative to the Solar abundances set by the **abund** command.

The **vmeka** variant allows the user to set the abundances for the model.

Parameters for the **meka** model are:

par1	plasma temperature in keV
par2	H density (cm^{-3})
par3	Metal abundances (He fixed at cosmic). The elements included are C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca, Fe, Ni.
par4	redshift, z
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm), , and n_e , n_H (cm^{-3}) are the electron and hydrogen densities respectively.

Parameters for the **vmeka** model are:

par1	plasma temperature in keV
par2	H density (cm^{-3})
par3-par14	Abundances for He, C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni wrt Solar (given by the Anders & Grevesse mixture)
par15	redshift, z
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm), and n_e , n_H (cm^{-3}) are the electron and hydrogen densities respectively.

The references for the MEKA model are as follows :

Mewe, R., Gronenschild, E.H.B.M., and van den Oord, G.H.J. 1985 A &AS, 62, 197

Mewe, R., Lemen, J.R., and van den Oord, G.H.J. 1986, A &AS, 65, 511

Kaastra, J.S. 1992, An X-Ray Spectral Code for Optically Thin Plasmas (Internal SRON-Leiden Report, updated version 2.0)

Similar credit may also be given for the adopted ionization balance:

Arnaud, M., and Rothenflug, M. 1985, A & AS, 60, 425

Arnaud, M., and Raymond, J. 1992, ApJ, 398, 394

6.2.43 mekal, vmekal: emission, hot diffuse gas (Mewe-Kaastra-Liedahl)

An emission spectrum from hot diffuse gas based on the model calculations of Mewe and Kaastra with Fe L calculations by Liedahl. The model includes line emissions from several elements. The switch parameter determines whether the mekal code will be run to calculate the model spectrum for each temperature or whether the model spectrum will be interpolated from a pre-calculated table. The former is slower but more accurate. Relative abundances are set by the **abund** command for the **mekal** model. The **vmekal** variant allows the user to set the individual abundances for the model.

par1	plasma temperature in keV
par2	H density (cm^{-3})
par3	Metal abundance (He fixed at cosmic). The elements included are C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca, Fe, Ni.
par4	(fixed) redshift
	0 $\Rightarrow$ calculate
Par5	1 $\Rightarrow$ interpolate
	2 $\Rightarrow$ interpolate using APEC model
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm), and n_e, n_H (cm^{-3}) are the electron and hydrogen densities respectively.

Parameters for the **vmekal** variant are:

par1	plasma temperature in keV
par2	H density (cm^{-3})
par3-par16	Abundances for He, C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca, Fe, Ni wrt Solar (given by the Anders & Grevesse mixture)
par17	(fixed) redshift
	0 $\Rightarrow$ calculate
par18	1 $\Rightarrow$ interpolate
	2 $\Rightarrow$ interpolate using APEC model
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm), and n_e, n_H (cm^{-3}) are the electron and hydrogen densities respectively.

The references for the MEKAL model are as follows :

Mewe, R., Gronenschild, E.H.B.M., and van den Oord, G.H.J. 1985,A&AS, 62, 197

Mewe, R., Lemen, J.R., and van den Oord, G.H.J. 1986, A&AS}, 65, 511

Kaastra, J.S. 1992, An X-Ray Spectral Code for Optically Thin Plasmas (Internal SRON-Leiden Report, updated version 2.0)

Liedahl, D.A., Osterheld, A.L., and Goldstein, W.H. 1995, ApJL, 438, 115

Similar acknowledgement may also be given for the adopted ionization balance:

Arnaud, M., and Rothenflug, M. 1985, A&AS, 60, 425

Arnaud, M., and Raymond, J. 1992, ApJ, 398, 394

6.2.44 mkcflow, vmcflow: cooling flow, mekal

A cooling flow model after Mushotzky & Szymkowiak (*Cooling Flows in Clusters and Galaxies* ed. A. C. Fabian, 1988). This one uses the mekal (or vmekal) model for the individual temperature components and differs from cflow in setting the emissivity function to be the inverse of the bolometric luminosity. The model assumes H_0 = 50 and q_0 = 0. Abundance ratios are set by the **abund** command. The switch parameter determines whether the mekal code will be run to calculate the model spectrum for each

temperature or whether the model spectrum will be interpolated from a pre-calculated table. The former is slower but more accurate.

For the mkcflow model the parameters are:

par1	low temperature (keV)
par2	high temperature (keV)
par3	abundance relative to Solar
par4	(fixed) redshift
	0 $\Rightarrow$ calculate
par5	1 $\Rightarrow$ interpolate
	2 $\Rightarrow$ interpolate using APEC model
norm	Mass accretion rate (solar mass/yr)

While for the vmcflow variant the parameters are:

par1	low temperature (keV)
par2	high temperature (keV)
par3-par16	Abundances for He, C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca, Fe, Ni wrt Solar (given by the Anders & Grevesse mixture)
par17	Redshift
	0 $\Rightarrow$ calculate
par18	1 $\Rightarrow$ interpolate
	2 $\Rightarrow$ interpolate using APEC model
norm	Mass accretion rate (solar mass/yr)

6.2.45 nei, vnei: collisional plasma, non-equilibrium, constant temperature

Non-equilibrium ionization collisional plasma model. This assumes a constant temperature and single ionization parameter. It provides a characterization of the spectrum but is not a physical model. The references for this model can be found under the description of the equil model. The references for this model can be found under the description of the equil model. Several versions are available. To switch between them use the **xset** `neivers` command. **xset** `neivers 1.0` gives the version from xspec v11.1, **xset** `neivers 1.1` uses updated calculations of ionization fractions using dielectronic recombination rates from Mazzotta et al (1988), and **xset** `neivers 2.0` uses the same ionization fractions as 1.1 but uses APED to calculate the resulting spectrum. Note that versions 1.x have no emission from Ar. The default is version 1.1.

The **vnei** variant allows the user to set the abundance vector.

For the nei version the parameters are

par1	plasma temperature (keV)
par2	Metal abundances (He fixed at cosmic). The elements included are C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni. Relative abundances are defined by the abund command.
par3	Ionization timescale in units of s cm^{-3}.
par4	redshift z
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm), and n_e, n_H (cm^{-3}) are the electron and hydrogen densities respectively.

For the **vnei** variant the parameters are:

par1	plasma temperature (keV)
par2	H density in cm^{-3}

par3-par14 Abundances for He, C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni wrt Solar (defined by the abund command)

par15 Ionization timescale in units of s cm^{-3}.

par16 redshift z

norm $\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm) , and n_e , n_H (cm^{-3}) are the electron and hydrogen densities respectively.

6.2.46 npshock, vnpshock: shocked plasma, plane parallel, separate ion, electron temperatures.

Plane-parallel shock plasma model with separate ion and electron temperatures. This model is slow. `par1` provides a measure of the average energy per particle (ions+electrons) and is constant throughout the postshock flow in plane shock models (Borkowski et al., 2001, ApJ, 548, 820). `par2` should always be less than `par1`. If `par2` exceeds `par1` then their interpretations are switched (ie the larger of `par1` and `par2` is always the mean temperature). Additional references can be found under the help for the equil model. Several versions are available. To switch between them use the **xset** `neivers` command. **xset** `neivers 1.0` gives the version from xspec v11.1, **xset** `neivers 1.1` uses updated calculations of ionization fractions using dielectronic recombination rates from Mazzotta et al (1988), and **xset** `neivers 2.0` uses the same ionization fractions as 1.1 but uses APED to calculate the resulting spectrum. Note that versions 1.x have no emission from Ar. The default is version 1.1.

The npshock version uses relative abundances from the Anders & Grevesse (1993) mix, while the vpnshock version allows the user to set the abundances.

Parameters for **npshock** are:

par1 Mean shock temperature (keV)

par2 electron temperature immediately behind the shock front (keV)

par3 Metal abundances (He fixed at cosmic). The elements included are C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni. Abundances are given by the Anders & Grevesse mixture.

par4	Lower limit on ionization timescale in units of s cm^{-3}.
par5	Upper limit on ionization timescale in units of s cm^{-3}.
par6	redshift z
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm) , and n_e , n_H (cm^{-3}) are the electron and hydrogen densities respectively.

For **vnpshock** the parameters are:

par1	Mean shock temperature (keV)
par2	electron temperature immediately behind the shock front (keV)
par3	H density in cm^{-3}
par4-par15	Abundances for He, C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni wrt Solar (given by the Anders & Grevesse mixture)
par16	Lower limit on ionization timescale in units of s cm^{-3}.
par17	Upper limit on ionization timescale in units of s cm^{-3}.
par18	redshift z
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm) , and n_e , n_H (cm^{-3}) are the electron and hydrogen densities respectively.

6.2.47 nsa: neutron star atmosphere

This model provides the spectra in the X-ray range (0.05-10 keV) emitted from a hydrogen atmosphere of a neutron star. There are three options : nonmagnetized (B < 10^8

- 10^9 G) with a uniform surface (effective) temperature in the range of $\log T_{eff}(K) = 5.0 - 7.0$; a field B = 10^{12} G with a uniform surface (effective) temperature in the range of $\log T_{eff}(K) = 5.5 - 6.8$; a field B = 10^{13} G with a uniform surface (effective) temperature in the range of $\log T_{eff}(K) = 5.5 - 6.8$. The atmosphere is in radiative and hydrostatic equilibrium; sources of heat are well below the atmosphere. The Comptonization effects (significant at $T_{eff} > 3 \times 10^6 K$) are taken into account. The model spectra are provided as seen by a distant observer, with allowance for the GR effects. The user is advised to keep M_{ns} and R_{ns} fixed and fit the temperature and the normalization. MagField must be fixed at one of 0, 10^{12}, or 10^{13}.
The values of the effective temperature and radius as measured by a distant observer (``values at infinity'') are :

$$T_{eff}^{\infty} = T_{eff} g_r$$

$$R_{ns}^{\infty} = R_{ns} / g_r$$

where

$$g_r = \left(1 - 2.952 M_{ns} / R_{ns}\right)^{1/2}$$

is the gravitational redshift parameter.

Please send your comments/questions to Slava Zavlin (VYACHESLAV.ZAVLIN@msfc.nasa.gov) and/or George Pavlov (pavlov@astro.psu.edu). If you publish results obtained using these models, please reference Zavlin, V.E., Pavlov, G.G., & Shibanov, Yu.A. 1996, A&A, 315, 141 for nonmagnetic models, and Pavlov, G.G., Shibanov, Yu.A., Zavlin, V.E., & Meyer, R.D. 1995, in “The Lives of the Neutron Stars,” ed. M.A. Alpar, U. Kiziloglu, & J. van Paradijs (NATO ASI Ser. C, 450; Dordrecht: Kluwer), p. 71 for magnetic models.

par1	$\log T_{eff}$, (unredshifted) effective temperature
par2	M_{ns}, neutron star gravitational mass (in units of solar mass)
par3	R_{ns}, neutron star radius (in km)
par4	neutron star magnetic field strength (0, 1e12, or 1e13 G)
K	$1/D^2$, where D is the distance of the object in pc.

6.2.48 nsagrav: NS H atmosphere model for different g

This model provides the spectra emitted from a nonmagnetic hydrogen atmosphere of a neutron star with surface gravitational acceleration g ranging from 1e13 to 1e15 cm/s^2, allowed by equations of state for the neutron star matter (the **nsa** model gives the spectra calculated for g=2.43e14 cm/s^2). The uniform surface (effective) temperature is in the range of Log T_{eff}(K) = 5.5 - 6.5. The atmosphere is in radiative and hydrostatic equilibrium; sources of heat are well below the atmosphere. The radiative force and electron heat conduction are included in the models, but they are of no importance in the specified ranges of T_{eff} and g. The model spectra are provided as seen by a distant observer, with allowance for the GR effects.

The neutron star mass M and radius R determine the redshift parameter,

$$g_r=[1-2.952*M/R]^{0.5},$$

and the gravitational acceleration at the surface,

$$g=1.33e16*M/R^2/g_r \text{ cm/s}^2,$$

where M is in units of solar mass, and R is in km. The allowed domain in the M-R plane corresponds to $g_r^2 > 1/3$ and 1e13 < g < 1e15 cm/s^2. (This domain is restricted by the solid curves in the figure). If chosen M and R values correspond to g_r or/and g values outside the allowed domain, then the code sets the latter to be the closest limiting values (e.g., if one chooses M=2, R=8, then the code will use $g_r=3^{-1/2}=0.578$ instead of $g_r=0.512$ corresponding to the M and R chosen), which would lead to unphysical results.

The values of the effective temperature and radius as measured by a distant observer ("values at infinity") are:

$$T^{\infty} = g_r T_{eff}, R^{\infty} = R / g_r$$

The nsagrav model may be useful for putting constraints on M and R from spectral fits to thermal emission detected from neutron stars, provided the quality of the observational data are good enough to warrant a detailed analysis. The parameters M and R can be fixed at specific values or allowed to vary within a reasonable range (see the note above). For example, one can run spectral fits on a M-R grid (using the **steppar** command) within the allowed parameter domain (see above).

Please send your comments/questions (if any) to Slava Zavlin (vyacheslav.zavlin@msfc.nasa.gov) and/or George Pavlov (pavlov@astro.psu.edu). If you publish results obtained using this model please reference Zavlin et al. (1996, A&A 315, 141).

par1	Log T_{eff} : (unredshifted) effective temperature
par2	M_{ns} : neutron star gravitational mass (in units of Solar mass)

par3	R_{ns} : "true" neutron star radius (km)
K	$1/D^2$ where D is the distance to the object in pc

6.2.49 nsatmos: NS Hydrogen Atmosphere model with electron conduction and self-irradiation

This model interpolates from a grid of NS atmosphere calculations provided by George Rybicki and Ramesh Narayan to output a NS atmosphere spectrum. The model grids cover a wide range of surface gravity and effective temperature, and incorporate thermal electron conduction and self-irradiation by photons from the compact object. This code assumes negligible (less than 10^9 G) magnetic fields and a pure hydrogen atmosphere. A detailed description of the model is given in Heinke et al. (2006), ApJ in press, astro-ph/0506563 (see also McClintock et al. 2004, ApJ, 615, 402).

par1	Log T_{eff} : (unredshifted) effective temperature
par2	M_{ns} : neutron star gravitational mass (in units of Solar mass)
par3	R_{ns} : "true" neutron star radius (km)
par4	dist : distance to the neutron star (in kpc)
K	fraction of the neutron star surface emitting

6.2.50 nsmax: Neutron Star Magnetic Atmosphere

This model interpolates from a grid of neutron star (NS) atmosphere spectra to produce a final spectrum that depends on the parameters listed below. The atmosphere spectra are obtained using the latest equation of state and opacity results for a partially ionized, strongly magnetized hydrogen or mid-Z element plasma. The models are constructed by solving the coupled radiative transfer equations for the two photon polarization modes in a magnetized medium, and the atmosphere is in radiative and hydrostatic equilibrium. The atmosphere models mainly depend on the surface effective temperature T_{eff} and magnetic field strength B and inclination Θ_B; there is also a dependence on the surface gravity $g=(1+z_g)GM/R^2$, where $1+z_g=(1-2GM/R)^{-1/2}$ is the gravitational redshift and M and R are the NS mass and radius, respectively.

Two sets of models are given: one set with a single surface B and T_{eff} and a set which is constructed with B and T_{eff} varying across the surface according to the magnetic dipole model (for the latter, θ_m is the angle between the direction to the observer and the magnetic axis). The effective temperatures span the range log T_{eff}=5.5-6.8 for hydrogen and log $T_{eff.}$=5.8-6.9 for mid-Z elements(note: for the latter, change temperature range in nsmax_lmodel.dat) The models with single (B,T_{eff}) cover the energy range 0.05-10 keV, while the models with (B,T_{eff})-distributions cover the range 0.09-5 keV.

par1 = logTeff, surface (unredshifted) effective temperature

par2 = $1+z_g$, gravitational redshift

par3 = switch indicating model to use (see nsmax.dat or **model list**)

A = $(R_{em}/d)^2$, normalization, where R_{em} is the size (in km) of the emission region and d is the distance (kpc) to the object Note: A is added automatically by XSPEC.

Please send your comments/questions to Wynn Ho (**wynnho@slac.stanford.edu**). If you publish results obtained using NSMAX, please reference **Ho, W.C.G., Potekhin, A.Y., & Chabrier, G. (2008, ApJS, 178, 102)** and also **Mori, K. & Ho, W.C.G. (2007, MNRAS, 377, 905)** if using the mid-Z models.

6.2.51 nteea: non-thermal pair plasma

A nonthermal pair plasma model based on that of Lightman & Zdziarski (1987, ApJ 319, 643) from Magdziarz and Zdziarski. It includes angle-dependent reflection from Magdziarz & Zdziarski (1995, MNRAS 273, 837). The abundances are set up by the command **abund**. Send questions or comments to **aaz@camk.edu.pl**

par1	nonthermal electron compactness
par2	blackbody compactness
par3	scaling factor for reflection (1 for isotropic source above disk)
par4	blackbody temperature in eV
par5	the maximum Lorentz factor
par6	thermal compactness (0 for pure nonthermal plasma)
par7	Thomson optical depth of ionization electrons (*e.g.,* 0)
par8	electron injection index (0 for monoenergetic injection)
par9	minimum Lorentz factor of the power law injection (not used for monoenergetic injection)
par10	minimum Lorentz factor for nonthermal reprocessing $1 < \texttt{par10} \leq \texttt{par9}$
par11	radius in cm (for Coulomb/bremsstrahlung only)
par12	pair escape rate in c (0-1, see Zdziarski 1985, ApJ, 289, 514)

par13	cosine of inclination angle
par14	iron abundance relative to that defined by **abund**
par15	redshift *z*
norm	photon flux of the direct component (w/o reflection) at 1~keV in the observer's frame.

6.2.52 Nthcomp: Thermally comptonized continuum

Nthcomp is a *much* better description of the continuum shape from thermal comptonisation than an exponentially cutoff power law, but is not that much more complicated in terms of parameters. The high energy cutoff is sharper than an exponential, and is parameterized by the electron temperature (kT_e). VERY roughly, an exponential rollover energy E_c=2-3kT_e but the shape is very different, so it impacts on the reflected fraction as well. Another major effect (especially for X-ray binaries) is that it incorporates the low energy rollover. The hot electrons Compton UPscatter seed photons so there are few photons in the scattered spectrum at energies below the typical seed photon energies, making it significantly different to a power law below this energy. Typically the physical picture is that these seed photons are (quasi)blackbody (eg neutron star boundary layer) or disk blackbody in shape. Either of these shapes can be selected (input type), both being parameterized by a seed photon temperature (kT_bb). Between the low and high energy rollovers the shape of the spectrum is set by the combination of electron scattering optical depth and electron temperature. It is not necessarily a power law, but can be parameterized by an asymptotic power law index (Gamma). Details of this are given in Zycki, Done & Smith (1999), including a self-consistent reflection component which is NOT released here as it was written using non-FITS standard files so has significant issues with portability.

This is the thermally comptonized continuum model of Zdziarski, Johnson & Magdziarz 1996, MNRAS, 283, 193, as extended by Zycki, Done & Smith 1999, MNRAS 309, 561. Please reference these papers if you use it.

par1 = Gamma, asymptotic power-law photon index.

par2 = kT_e, electron temperature (high energy rollover)

par3 = kT_bb, seed photon temperature (low energy rollover)

par4 = inp_type, 0 or 1 for blackbody or disk-blackbody seed photons, respectively

par5 = redshift

K = normalization, unity at 1 keV for a norm of 1.

6.2.53 pegpwrlw: power law, pegged normalization

A power law with pegged normalization.

$$A(E) = KE^{-\alpha}$$

where :

par1 $= \alpha$	photon index of power law (dimensionless)
par2	lower peg energy range
par3	upper peg energy range
norm	flux (in units of 10^{-12} erg cm^{-2}s^{-1} over the energy `par2`–`par3`). If `par2` = `par3`, it is the flux in μJy at `par2`

6.2.54 pexrav: reflected powerlaw, neutral medium

Exponentially cut off power law spectrum reflected from neutral material (Magdziarz & Zdziarski 1995, MNRAS, 273, 837). The output spectrum is the sum of the cut-off power law and the reflection component. The reflection component alone can be obtained for $rel_{\rm refl} < 0$. Then the actual reflection normalization is $|rel_{\rm refl}|$. Note that you need to change then the limits of $rel_{\rm refl}$ excluding zero (as then the direct component appears). If $E_{\rm c} = 0$ there is no cutoff in the power law. The metal and iron abundance are variable with respect to those defined by the command **abund**. The opacities are from Balucinska & McCammon (ApJ 400, 699 and 1994, private communication). H and He are assumed to be fully ionized. Send questions or comments to **aaz@camk.edu.pl** .

par1	Γ, first power law photon index, $N_E \propto E^{-\Gamma}$
par2	$E_{\rm c}$, cutoff energy (keV) (if $E_{\rm c} = 0$ there is no cutoff)
par3	$rel_{\rm refl}$, reflection scaling factor (0, no reflected component < $rel_{\rm refl}$ < 1 for isotropic source above disk)
par4	redshift, z
par5	abundance of elements heavier than He relative to the solar abundances
par6	iron abundance relative to that defined by **abund**
par7	cosine of inclination angle

norm	photon flux at 1 keV (photons $keV^{-1}cm^{-2}\ s^{-1}$) of the cutoff broken power-law only (no reflection) in the observed frame.

6.2.55 pexriv: reflected powerlaw, ionized medium

Exponentially cut off power law spectrum reflected from ionized material (Magdziarz & Zdziarski MNRAS, 273, 837; 1995). Ionization and opacities of the reflecting medium is computed as in the procedure absori. The output spectrum is the sum of the cutoff power law and the reflection component. The reflection component alone can be obtained for $rel_{\rm refl} < 0$. Then the actual reflection normalization is $|rel_{\rm refl}|$. Note that you need to change then the limits of $rel_{\rm refl}$ excluding zero (as then the direct component appears). If $E_{\rm c} = 0$ there is no cutoff in the power law. The metal and iron abundances are variable with respect to those defined by the command **abund**. Send questions or comments to **aaz@camk.edu.pl** .

par1	Γ, first power law photon index, $N_E \propto E^{-\Gamma}$
par2	$E_{\rm c}$, cutoff energy (keV) (if $E_{\rm c} = 0$ there is no cutoff)
par3	$rel_{\rm refl}$, reflection scaling factor (0, no reflected component < $rel_{\rm refl}$ < 1 for isotropic source above disk)
par4	redshift, z
par5	abundance of elements heavier than He relative to the solar abundances
par6	iron abundance relative to that defined by **abund**
par7	cosine of inclination angle
par8	disk temperature in K
par9	disk ionization parameter, $\xi = 4\pi \frac{F_{ion}}{n}$, where $F_{\rm ion}$ is the 5eV – 20keV irradiating flux, n is the density of the reflector; see Done et al., 1992, ApJ, 395, 275.
norm	photon flux at 1 keV (photons $keV^{-1}cm^{-2}\ s^{-1}$) of the cutoff broken power-law only (no reflection) in the observed frame.

6.2.56 plcabs: powerlaw observed through dense, cold matter

This model describes X-ray transmission of an isotropic source of photons located at the center of a uniform, spherical distribution of matter, correctly taking into account Compton scattering. The model can be used for radial column densities up to 5×10^{24} cm^{-2}. The valid energy range for which data can be modeled is between 10 and 18.5 keV, depending on the column density. Details of the physics of the model, the approximations used and further details on the regimes of validity can be found in Yaqoob (1997; ApJ, 479, 184). In this particular incarnation, the initial spectrum is a power law modified by a high-energy exponential cut-off above a certain threshold energy.

Also, to improve the speed, a FAST option is available in which a full integration over the input spectrum is replaced by a simple mean energy shift for each bin. This option is obtained by setting parameter 9 to a value of 1 or greater and cannot be made variable. Further, for single-scattering albedos less than ACRIT (*i.e.* `par8`) energy shifts are neglected altogether. The recommended value is ACRIT=0.1 which corresponds to about 4 keV for cosmic abundances and is more than adequate for ASCA data.

Note that for column densities in the range 10^{23} – 10^{24} cm^{-2}, the maximum number of scatterings which need be considered for convergence of the spectrum of better than 1% is between 1 and 5. For column densities as high as 5×10^{24} cm^{-2}, the maximum number of scatterings which need be considered for the same level of convergence is 12. This parameter cannot be made variable.

par1	Column density in units 10^{22} cm^{-2}
par2	Maximum number of scatterings to consider.
par3	Iron abundance.
par4	Iron K edge energy.
par5	Power-law photon index.
par6	High-energy cut-off threshold energy.
par7	High-energy cut-off e-folding energy.
par8	Critical albedo for switching to elastic scattering.
par9	If `par9` > 1, function uses mean energy shift, not integration.
par10	Source redshift, *z*
norm	Normalization factor

6.2.57 posm: positronium continuum

Positronium continuum (Brown & Leventhal 1987 ApJ 319, 637)

$$K\left[\frac{2}{(\pi^2 - 9)E_C}\right] *$$

$$A(E) = \left[\frac{E(E_C - E)}{(2E_C - E)^2} + \frac{2E_C(E_C - E)}{E^2}\log\left(\frac{E_C - E}{E_C}\right) - \frac{2E_C(E_C - E)^2}{(2E_C - E)^3}\log\left(\frac{E_C - E}{E_C}\right) + \frac{2E_C - E}{E}\right]$$

for E < Ec = 511 keV, where:

norm = K normalization.

6.2.58 powerlaw, zpowerlw: power law photon spectrum

powerlaw is a simple photon power law. The **zpowerlw** variant computes a redshifted spectrum.

$$A(E) = KE^{-\alpha}$$

par1 = α photon index of power law (dimensionless)

norm= K photons $keV^{-1}cm^{-2}s^{-1}$ at 1 keV

For **zpowerlw** the formula and corresponding parameters are:

$$A(E) = K\left[E(1+z)^{-\alpha}\right]/(1+z)$$

where :

par1= α photon index of power law (dimensionless)

par2= z Redshift

norm= K photons $keV^{-1}cm^{-2}s^{-1}$ at 1 keV

6.2.59 pshock, vpshock: plane-parallel shocked plasma, constant temperature

Constant temperature, plane-parallel shock plasma model. The references for this model can be found under the description of the equil model. Several versions are available. To switch between them use the **xset** `neivers` command. **xset** `neivers 1.0` gives the version from xspec v11.1, **xset** `neivers 1.1` uses updated calculations of ionization fractions using dielectronic recombination rates from Mazzotta et al (1988), and **xset** `neivers 2.0` uses the same ionization fractions as 1.1 but uses APED to calculate the resulting spectrum. Note that versions 1.x have no emission from Ar. The default is version 1.1. **]**

The pshock version has abundances given by the Anders & Grevesse (1993) mixture, while the vpshock variant allows the user to set the abundance vector.

Parameters for the **pshock** version are:

par1	plasma temperature (keV)
par2	Metal abundances (He fixed at cosmic). The elements included are C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni in ratios set by the abund command.
par3	Lower limit on ionization timescale in units of s cm^{-3}.
par4	Upper limit on ionization timescale in units of s cm^{-3}.
par5	redshift z
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm), and n_e, n_H (cm^{-3}) are the electron and hydrogen densities respectively.

Parameters for **vpshock** are:

par1	plasma temperature (keV)
par2	H density in cm^{-3}
par3-par14	Abundances for He, C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni wrt the solar as defined by the abund command.

par15 Lower limit on ionization timescale in units of s cm^{-3}.

par16 Upper limit on ionization timescale in units of s cm^{-3}.

par17 redshift z

norm $\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm) , and n_e , n_H (cm^{-3}) are the electron and hydrogen densities respectively.

6.2.60 raymond, vraymond: emission, hot diffuse gas, Raymond-Smith

An emission spectrum from hot, diffuse gas based on the model calculations of Raymond and Smith (ApJS 35, 419 and additions) including line emissions from several elements. This model interpolates on a grid of spectra for different temperatures. The grid is logarithmically spaced with 80 temperatures ranging from 0.008 to 80 keV.

The **vraymond** variant allows independent parameters to set the abundances. Abundances are the number of nuclei per Hydrogen nucleus relative to the Solar abundances as set by the **abund** command.

For **raymond** the parameters are:

par1 plasma temperature (keV)

par2 Metal abundances (He fixed at cosmic). The elements included are C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni. Abundances are given by the Anders & Grevesse mixture.

par3 redshift z

norm $\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm), and n_e , n_H (cm^{-3}) are the electron and hydrogen densities respectively.

For **vraymond** the parameters are:

par1 plasma temperature (keV)

par2-par13 Abundances for He, C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni wrt Solar (defined by the **abund** command)

par14 redshift z

norm $\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_{\rm e} n_{\rm H} dV$ where D_A is the angular diameter distance to the source (cm), and $n_{\rm e}$, $n_{\rm H}$ (cm^{-3}) are the electron and hydrogen densities respectively.

6.2.61 redge: emission, recombination edge

Recombination edge emission.

$$A(E) = \begin{cases} 0 & E < E_{\rm c} \\ K(1/T_p)\exp\left[-\frac{(E-E_c)}{T_P}\right] & E \geq E_{\rm c} \end{cases}$$

where:

par1= $E_{\rm c}$ Threshold energy

par2= $T_{\rm p}$ Plasma temperature (keV)

norm= K Photons cm^{-2}s^{-1} in the line

6.2.62 refsch: reflected power law from ionized accretion disk

Exponentially cut-off power-law spectrum reflected from an ionized relativistic accretion disk. In this model, spectrum of **pexriv** is convolved with a relativistic disk line profile `diskline`. See Magdziarz & Zdziarski 1995 MNRAS, 273, 837 for details of Compton reflection. See Fabian et al. 1989, MNRAS, 238, 729 for details of the disk line profile.

par1 Γ, power law photon index, $N_E \propto E^{-\Gamma}$

par2	E_c, cutoff energy (keV) (if $E_c = 0$ there is no cutoff)
par3	rel_{refl}, reflection scaling factor (0, no direct component < rel_{refl} < 1 for isotropic source above disk)
par4	redshift, z
par5	abundance of elements heavier than He relative to the solar abundances
par6	iron abundance relative to that defined by **abund**
par7	inclination angle (degrees)
par8	disk temperature in K
par9	disk ionization parameter, $\xi = 4\pi \frac{F_{ion}}{n}$, where F_{ion} is the 5eV – 20keV irradiating flux, n is the density of the reflector; see Done et al., 1992, ApJ, 395, 275.
par10 = ε	power law dependence of emissivity. the emissivity $\propto R^{\varepsilon}$
par11	inner radius (units of GM/c^2)
par12	outer radius (units of GM/c^2)
par13	internal model accuracy - points of spectrum per energy decade
norm	photon flux at 1 keV (photons $keV^{-1}cm^{-2}s^{-1}$) of the cutoff broken power-law only (no reflection) in the observed frame.

6.2.63 sedov, vsedov: sedov model, separate ion/electron temperature

Sedov model with separate ion and electron temperatures. This model is slow. `par1` provides a measure of the average energy per particle (ions+electrons) and is constant throughout the postshock flow in plane shock models (Borkowski et al., 2001, ApJ, 548, 820). `par2` should always be less than `par1`. If `par2` exceeds `par1` then their interpretations are switched (ie the larger of `par1` and `par2` is always the mean temperature). Additional references can be found under the help for the equil model. Several versions are available. To switch between them use the **xset** `neivers` command. **xset** `neivers 1.0` gives the version from xspec v11.1, **xset** `neivers 1.1` uses updated calculations of ionization fractions using dielectronic recombination rates from Mazzotta et al (1988), and **xset** `neivers 2.0` uses the same ionization fractions as

1.1 but uses APED to calculate the resulting spectrum. Note that versions 1.x have no emission from Ar. The default is version 1.1.

The **sedov** model has relative abundances determined by the solar Anders and Grevesse mixture, while the **vsedov** variant allows the user to set the abundances.

Parameters for **sedov** are:

par1	mean shock temperature (keV)
par2	electron temperature immediately behind the shock front (keV)
par3	Metal abundances (He fixed at cosmic). The elements included are C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni. Relative abundances are defined by the abund command
par4	ionization age (s cm^{-3}) of the remnant (= electron density immediately behind the shock front multiplied by the age of the remnant)
par5	redshift z
norm	$\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm) , and n_e, n_H (cm^{-3}) are the electron and hydrogen densities respectively.

For **vsedov** the parameters are:

par1	mean shock temperature (keV)
par2	electron temperature immediately behind the shock front (keV)
par3	H density in cm^{-3}
par4-par15	Abundances for He, C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni wrt Solar (defined by the abund command)

par4 ionization age (s cm^{-3}) of the remnant (= electron density immediately behind the shock front multiplied by the age of the remnant)

par5 redshift z

norm $\frac{10^{-14}}{4\pi\left[D_A(1+z)\right]^2}\int n_e n_H dV$ where D_A is the angular diameter distance to the source (cm) , and n_e , n_H (cm^{-3}) are the electron and hydrogen densities respectively.

6.2.64 smaug: optically-thin, spherically-symmetric thermal plasma.

This model performs an analytical deprojection of an extended, optically-thin and spherically-symmetric source. A thorough description of the model is given in Pizzolato et al. (ApJ 592, 62, 2003). In this model the 3D distributions of hydrogen, metals and temperature throughout the source are given specific functional forms dependent on a number of parameters, whose values are determined by the fitting procedure. The user has to extract the spectra in annular sectors, concentric about the emission peak. The inner boundary (in arcmin), the outer by the fitting procedure. The user has to extract the spectra in annular sectors, concentric about the emission peak. The inner boundary (in arcmin), the outer boundary (also in arcmin), and the width (in degrees) of each annular sector are specified (respectively) by the three additional keywords XFLT0001, XFLT0002, and XFLT0003, to be added to the spectrum extension in each input file (e.g. with the ftool FKEYPAR). Some parameters of smaug define the redshift and other options (see below). The other, 'relevant' ones define the 3D distributions of hydrogen density, temperature and metal abundance, determined by a simultaneous fit of the spectra. The cosmological parameters can be set using the cosmo command.

par1 central temperature [keV]

par2 max difference of temperature [keV]

par3 exponent of the inner temperature

par4 radius of the inner temperature [Mpc]

par5 exponent of the middle temperature

par6	radius of the middle temperature [Mpc]
par7	exponent of the outer temperature
par8	radius of the outer temperature [Mpc]
par9	central hydrogen density [cm**-3]
par10	fraction of nH.cc relative to the 1st beta component
par11	exponent of the first beta component
par12	radius of the 1st beta component [Mpc]
par13	exponent of the 2nd beta component
par14	radius of the 2nd beta component [Mpc]
par15	central metallicity [solar units]
par16	exponent of the metal distribution
par17	radius of the metal distribution [Mpc]
par18	redshift of the source
par19	number of mesh-points of the dem summation grid
par20	cutoff radius for the calculation [Mpc]
par21	mode of spectral evaluation: 0 = calculate, 1 = interpolate, 2 = APEC interpolate
par22	type of plasma emission code, 1 = Raymond-Smith, 2 = Mekal, 3 = Meka, 4 = APEC
K	model normalisation (nH.cc squared [cm**-6])

Note that if the interactive chattiness level in XSPEC is set to a value > 10, smaug also prints on screen the following quantities:

H_0	Hubble constant [km/s/Mpc]

q_0	deceleration parameter
L_0	cosmological constant
DA	source angular distance [Mpc]
DSET	dataset no. to which the quantities listed below are
IN	inner rim of the projected annular sector [Mpc]
OUT	outer rim of the projected annular sector [Mpc]
WID	width of the projected annular sector [deg]
EVOL	emitting volume within the integration radius cutoff [Mpc^3]
EINT	emission integral within the integration radius cutoff [Mpc^3 cm^-6]. If nH.cc is frozen to 1, the actual EI is obtaned by multiplying this figure by the square root of the model normalisation

6.2.65 srcut: synchrotron spectrum, cutoff power law

`srcut` describes the synchrotron spectrum from an exponentially cut off power-law distribution of electrons in a homogeneous magnetic field. This spectrum is itself a power-law, rolling off more slowly than exponential in photon energies. Though more realistic than a power-law, it is highly oversimplified, but does give the maximally curved physically plausible spectrum and can be used to set limits on maximum accelerated-electron energies even in remnants whose X-rays are thermal. See Reynolds, S.P. & Keohane, J.W. 1999, ApJ, 525, 368 and Reynolds, S.P., 1998 ApJ 493, 357. Note that the radio spectral index and flux can be obtained from Green's Catalogue at **http://www.mrao.cam.ac.uk/surveys/snrs** for galactic SNRs.

par1	alpha: radio spectral index
par2	break Hz: approximately the frequency at which the flux has dropped by a factor of 10 from a straight power law.
norm	1 GHz flux (Jy)

6.2.66 sresc: synchrotron spectrum, cut off by particle escape

The synchrotron spectrum from an electron distribution limited by particle escape above some energy. The electrons are shock-accelerated in a Sedov blast wave encountering a constant-density medium containing a uniform magnetic field. The model includes variations in electron acceleration efficiency with shock obliquity, and post-shock radiative and adiabatic losses, as described in Reynolds, S.P., ApJ 493, 357 1998. This is a highly specific, detailed model for a fairly narrow set of conditions. See also Reynolds, S.P., ApJL 459, L13 1996. Note that the radio spectral index and flux can be obtained from Green's Catalogue at **http://www.mrao.cam.ac.uk/surveys/snrs** for galactic SNRs.

par1	alpha: radio spectral index (flux proportional to frequency $f^{-\alpha}$)
par2	break Hz: approximately the frequency at which the flux has dropped by a factor of 6 below a straight power law extrapolation from radio frequencies. This frequency is 5.3 times the peak frequency radiated by electrons with energy E_{m3} in a magnetic field of $4B_1$, in the notation of Reynolds (1998), Eq. (19).
norm	1 GHz flux (Jy)

6.2.67 step: step function convolved with gaussian

A step function convolved with a gaussian.

$$A(E) = \frac{K}{2}\left[1 - \mathrm{erf}\left(\frac{E - E_S}{\sqrt{2}\sigma}\right)\right]$$

par1= E_s	start energy (keV)
par2= σ	gaussian sigma (keV)
norm= K	step amplitude

6.3 Multiplicative Model Components

6.3.1 absori: ionized absorber

An ionized absorber based on that of Done et al. (1992, ApJ 395, 275) and developed by Magdziarz & Zdziarski. See also Zdziarski et al. (1995, ApJ 438, L63).

Photoionization rates are from Reilman & Manson (1979, ApJS 40, 815), who employ the Hartree-Slater approximation (accurate to about 5%), and recombination rates are from Shull & Steenburg (1982, ApJS 48, 95). The cross sections are extrapolated with E^{-3} above 5 keV. The abundances are set up by the command abund. Send questions or comments to **aaz@camk.edu.pl**

par1	power-law photon index.
par2	Hydrogen column in units of 1022cm–2
par3	Absorber temperature in K.
par4	Absorber ionization state (L/nR2), see Done et al. (1992)
par5 = z	redshift.
par6	Iron abundance relative to that defined by the command abund

6.3.2 acisabs: Chandra ACIS q.e. decay

This model accounts for the decay in the ACIS quantum efficiency most likely caused by molecular contamination of the ACIS filters. The user needs to supply the number of days between Chandra launch and observation. The `acisabs` parameters related to the composition of the hydrocarbon and the rate of decay should be frozen and not modified. The present version of `acisabs` is to be used for the analysis of bare ACIS I and ACIS S data. For the present version of `acisabs` one must use the standard qe file vN0003 instead of the optional vN0004 file.

Because of the present large uncertainty in the ACIS gain at energies below 350eV we recommend that events in the 0—350eV range be ignored in the spectral analysis until the gain issue is resolved.

acisabs calculates the mass absorption coefficients of the contaminant from atomic scattering factor files provided at

http://henke.lbl.gov/optical_constants/asf.html .

par1	Days between Chandra launch and ACIS observation
par2	Slope of linear quantum efficiency decay
par3	Offset of linear quantum efficiency decay
par4	Number of carbon atoms in hydrocarbon
par5	Number of hydrogen atoms in hydrocarbon

par6 Number of oxygen atoms in hydrocarbon

par7 Number of nitrogen atoms in hydrocarbon

6.3.3 cabs: Compton scattering, optically thin, non-relativistic.

Non-relativistic, optically-thin Compton scattering.

$$M(E) = \exp\left(-n_{\mathrm{H}}\sigma_{\mathrm{T}}(E)\right)$$

where

$\sigma_{\mathrm{T}}(E)$ is the Thomson cross-section.

par1= n_{H} hydrogen column (in units of 10^{22} atoms cm^{-2})

6.3.4 constant: energy-independent factor

An energy-independent multiplicative factor.

`par1`= factor

6.3.5 cyclabs: absorption line, cyclotron

A cyclotron absorption line as used in pulsar spectra. See Mihara *et al.*, Nature, 1990 or Makishima *et al.* PASJ, 1990.

$$M(E) = \exp\left[-D_{\mathrm{f}}\frac{\left(W_{\mathrm{f}}E/E_{\mathrm{cycl}}\right)^2}{(E-E_{\mathrm{cycl}})^2+W_{\mathrm{f}}^2} + D_{2\mathrm{h}}\frac{\left(W_{2h}E/2E_{\mathrm{cycl}}\right)^2}{(E-2E_{\mathrm{cycl}})^2+W_{2\mathrm{h}}^2}\right]$$

par1= D_{f} depth of the fundamental

par2= E_{cycl} cyclotron energy

par3= W_{f} width of the fundamental

par4= $D_{2\mathrm{h}}$ depth 2nd harmonic

par5= $W_{2\mathrm{h}}$ width of the 2nd harmonic

6.3.6 dust: dust scattering

A modification of a spectrum due to scattering off dust on the line-of-sight. The model assumes that the scattered flux goes into a uniform disk whose size has a 1/E dependence and whose total flux has a $1/E^2$ dependence.

par1 scattering fraction at 1 keV

par2 size of halo at 1 keV in units of the detector beamsize

6.3.7 edge, zedge: absorption edge

The edge model is absorption edge, given by.

$$M(E) = \begin{cases} 1 & E \le E_c \\ \exp\left[-D\left(E/E_c\right)^{-3}\right] & E \ge E_c \end{cases}$$

where:

par1= E_c threshold energy

par2 = D absorption depth at the threshold

The zedge model given by

$$M(E) = \begin{cases} 1 & E < E_c \\ \exp\left(-D\left[E(1+z)/E_c\right]^3\right) & E > E_c \end{cases}$$

allows a redshift z where:

par1 = E_c threshold energy

par2= D absorption depth at threshold

par3= z redshift

6.3.8 etable: exponential tabular model

An exponential table model. The filename to be used should be given immediately after etable in the model command. For example:

```
XSPEC12>model etable{mymod.mod}
```

uses mymod.mod as the input for the model. XSPEC will multiply the contents of the model by –1 then take the exponential *i.e.* this model is for calculating absorption functions. For specifications of the table model file, see the OGIP memo 92-009 on the FITS file format for table model files (available on the WWW or by anonymous ftp from **ftp://legacy.gsfc.nasa.gov/caldb/docs/memos**.).

6.3.9 expabs: exponential roll-off at low E

A low-energy exponential rolloff.

$$M(E) = \exp(-E_c / E)$$

where:

par1= E_c e-folding energy for the absorption

6.3.10 expfac: exponential modification

An exponential modification of a spectrum.

$$M(E) = \begin{cases} 1 + A\exp(-fE) & E > E_c \\ 1 & E < E_c \end{cases}$$

where:

par1= A amplitude of effect

par2= f exponential factor

par3= E_c start energy of modification

6.3.11 gabs: gaussian absorption line

$$M(E) = \exp\left(-\left(par3 \Big/ \sqrt{2\pi}\, par2\right)\exp\left(-.5\left(\left(E - par1\right)/ par2\right)^2\right)\right)$$

where :

par1 = line energy in keV

par2 = line width (sigma) in keV

par3 = optical depth

6.3.12 highecut, zhighect: high-energy cutoff

A high energy cutoff.

$$M(E) = \begin{cases} \exp\left[(E_c - E)/E_f\right] & E \geq E_c \\ 1.0 & E \leq E_c \end{cases}$$

where

par1= E_c cutoff energy in keV

par2= E_f e-folding energy in keV

The redshifted version **zhighect** has.

$$M(E) = \begin{cases} \exp\left[\left(E_c - E\left[1+z\right]\right)/E_s\right] & E \geq E_c \\ 1.0 & E \leq E_c \end{cases}$$

where :

par1= E_c cutoff energy in keV

par2= E_f e-folding energy in keV

par3 = z redshift

6.3.13 hrefl: reflection model

A simple multiplicative reflection model due to Tahir Yaqoob. This model gives the reflected X-ray spectrum from a cold, optically thick, circular slab with inner and outer radii (R_i & R_o, respectively) illuminated by a point source a height H above the center of the slab. The main difference between this model and other reflection models is that analytic approximations are used for the Chandrasekar H functions (and their integrals) and ELASTIC SCATTERING is assumed (see Basko 1978, ApJ, 223, 268). The elastic-scattering approximation means that the model is ONLY VALID UP TO ≈ 15 keV in the

source frame. Future enhancements will include fudge factors that will allow extension up to 100 keV. The fact that no integration is involved at any point makes the routine very fast and particularly suitable for generating error contours, especially when fitting a large number of data channels. The model is multiplicative, and so can be used with ANY incident continuum.

Parameters are as follows:

par1	minimum angle (degrees) between source photons incident on the slab and the slab normal $\left[=\tan^{-1}\left(R_i/H\right)\right]$
par2	maximum angle (degrees) between source photons incident on the slab and the slab normal $\left[=\tan^{-1}\left(R_o/H\right)\right]$
par3	Angle (degrees) between the observer's line of sight and the slab normal.
par4	Iron abundance relative to Solar
par5	Iron K-edge energy
par6	Fraction of the direct flux seen by the observer
par7	Normalization of the reflected continuum
par8	redshift

Suppose the incident photon spectrum is N(E) photons $cm^{-2}s^{-1}keV^{-1}$ and that the incident continuum is steady in time, and suppose further that the reflected continuum from the slab is R(E). When you multiply the incident spectrum with `hrefl`, what you actually get is the following:

$$M(E) = \texttt{par6}\cdot N(E) + \texttt{par7}\cdot R(E)$$

Thus, the actual physical situation described above corresponds to

`par6`=1.0
`par7` =1.0.

You may decide to float par6 and/or par7. In that case, you must decide what the best-fitting values of these parameters mean physically for your case. It may imply time-lags between the direct and reflected components, different source and/or disk geometries to those assumed, or something else.

6.3.14 mtable: multiplicative tabular model

A multiplicative table model. The filename to be used should be given immediately after `mtable` in the **model** command. For example:

```
XSPEC12>model mtable{mymod.mod}
```

uses `mymod.mod` as the input for the model. For specifications of the table model file, see the OGIP memo 92-009 on the FITS file format for table model files (available on the WWW or by anonymous ftp from **ftp://legacy.gsfc.nasa.gov/caldb/docs/memos** . A sample multiplicative table model file is `testpcfabs.mod` in `$HEADAS/../spectral/session.`

6.3.15 notch: absorption line, notch

A notch line absorption. This is model is equivalent to a very saturated absorption line.

$$M(E) = \begin{cases} (1-f) & \text{for } E_L - W/2 < E < E_L + W/2 \\ 1 & \text{elsewhere} \end{cases}$$

where

par1= E_L line energy (keV)

par2= W line width (keV)

par3= f covering fraction

6.3.16 pcfabs, zpcfabs: partial covering fraction absorption

A partial covering fraction absorption. The relative abundances are set by the **abund** command.

$$M(E) = f\exp\left[-n_H\sigma(E)\right] + (1-f)$$

where σ(E) is the photo-electric cross-section (NOT including Thomson scattering) (see `phabs`) and:

par1= n_H equivalent hydrogen column (in units of 10^{22} atoms cm^{-2})

par2= f covering fraction $0 < \texttt{par2} < 1$ (dimensionless)

The redshifted variant zpcfabs is given by:

$$M(E) = n_H\exp\left[-f\sigma\left(E\left[1+z\right]\right)\right] + 1 - f$$

where σ(E) is the photo-electric cross-section (NOT including Thomson scattering) (see `phabs`). Relative abundances are as for **pcfabs**. Parameters are:

par1= n_H equivalent hydrogen column (in units of 10^{22} atoms cm^{-2})

par2= f dimensionless covering fraction $(0 < f \leq 1)$

par3= z redshift

6.3.17 phabs, vphabs, zphabs, zvphabs: photoelectric absorption

A photoelectric absorption using cross-sections set by the **xsect** command. The relative abundances are set by the **abund** command.

$$M(E) = \exp\left[-n_H \sigma(E)\right]$$

where σ(E) is the photo-electric cross-section (NOT including Thomson scattering). Note that the default He cross-section changed in v11. The old version can be recovered using the command

xsect `obcm`

par1= n_H equivalent hydrogen column (in units of 10^{22} atoms cm^{-2})

The redshifted variant, **zphabs**, uses the formula

$$M(E) = \exp\left[-n_H \sigma\left(E\left[1+z\right]\right)\right]$$

and has parameters

par1= n_H equivalent hydrogen column (in units of 10^{22} atoms cm^{-2})

par2= z Redshift

The variants **vphabs**, **zvphabs** allow the user to set fixed abundance parameters with respect to the solar composition, as defined by the **abund** command. For **vphabs** (rest-frame) the parameters are

par1= n_H equivalent hydrogen column (in units of 10^{22} atoms cm^{-2})

par2–par18 abundances for He, C, N, O, Ne, Na, Mg, Al, Si, S, Cl, Ar, Ca, Cr, Fe, Co, Ni wrt to Solar

While the corresponding redshifted variant **zvphabs** has parameters

par1= n_H equivalent hydrogen column (in units of 10^{22} atoms cm^{-2})

par2-par18 abundances for He, C, N, O, Ne, Na, Mg, Al, Si, S, Cl, Ar, Ca, Cr, Fe, Co, Ni wrt to Solar (defined by the abund command)

par19= z redshift

6.3.18 plabs: power law absorption

Absorption as a power-law in energy. Useful for things like dust.

$M(E) = KE^{-\alpha}$

par1= α index

par2= K coefficient

6.3.19 pwab: power-law distribution of neutral absorbers

An extension of partial covering fraction absorption into a power-law distribution of covering fraction as a function of column density, built from the wabs code. See Done & Magdziarz 1998 (MNRAS 298, 737) for details.

par1 = minimum equivalent hydrogen column (in units of 10**22 atoms/cm**2)

par2 = maximum equivalent hydrogen column (in units of 10**22 atoms/cm**2)

par3 = power law index for covering fraction.

6.3.20 redden: interstellar extinction

IR/optical/UV extinction from Cardelli et al. (1989, ApJ, 345, 245). The transmission is set to unity shortward of the Lyman limit. This is incorrect physically but does allow the model to be used in combination with an X-ray photoelectric absorption model such as phabs.

`par1` E(B-V)

6.3.21 smedge: smeared edge

A smeared edge (Ebisawa PhD thesis, implemented by Frank Marshall).

$$M(E) = \begin{cases} 1 & E < E_c \\ \exp\left[-f(E/E_c)^{\alpha}\right]\left[1-\exp\left(\{E_c - E\}/W\right)\right] & E \geq E_c \end{cases}$$

where:

par1= E_c the threshold energy (keV)

par2= f the maximum absorption factor at threshold

par3= α index for photo-electric cross-section (normally –2.67)

par4= W smearing width (keV)

6.3.22 spexpcut: super-exponential cutoff absorption

A high-energy super-exponential roll-off.

$$M(E) = \exp\left(-\left(E/E_C\right)^{\alpha}\right)$$

useful for fitting gamma-ray spectra of pulsars (see eg Nel & de Jager 1995), where:

par1= E_c e-folding energy for the absorption

par2 = α exponent index

Caveat : the absorption for an energy bin is calculated as the arithmetic mean of the function value at the start and end energies of the bin. If the energy bins are large this can be inaccurate and the energies command should be used to define a finer energy grid on which to calculate the model.

6.3.23 spline: spline modification

A cubic spline modification.

par1 start x-value

par2 start y-value

par3 end y-value

par4 start *dy/dx*

par5 end *dy/dx*

par6 end x-value

6.3.24 SSS ice: Einstein SSS ice absorption

The Einstein Observatory SSS ice absorption.

`par1` ice thickness parameter

6.3.25 swind1: absorption by partially ionized material with large velocity shear

A model to fit the soft excess in AGN by partially ionized absorbing material with large velocity shear. It approximates this by using XSTAR kn5 photoionization absorption model grids (calculated assuming a microturbulent velocity of 100km/s), and then convolving this with Gaussian smearing. This is the model used by Gierlinski & Done 2006, Sobolewska & Done 2006 and Done et al 2006. It is an update (uses a newer version of XSTAR) of the original model of Gierlinski & Done 2004.

par1 = column density (10^{22} cm^{-2})

par2 = log(xi) where $xi=L/nr^2$

par3 = sigma : Gaussian sigma for velocity smearing (v/c)

par4 = redshift

6.3.26 tbabs, ztbabs, tbgrain, tbvarabs: ISM grain absorption

The Tuebingen-Boulder ISM absorption model. This model calculates the cross section for X-ray absorption by the ISM as the sum of the cross sections for X-ray absorption due to the gas-phase ISM, the grain-phase ISM, and the molecules in the ISM. In the grain-phase ISM, the effect of shielding by the grains is accounted for, but is extremely small. In the molecular contribution to the ISM cross section, only molecular hydrogen is considered. In the gas-phase ISM, the cross section is the sum of the photoionization cross sections of the different elements, weighted by abundance and taking into account depletion onto grains.

In addition to the updates to the photoionization cross sections, the gas-phase cross section differs from previous values as a result of updates to the ISM abundances. These updated abundances are available through the **abund** `wilm` command. Details of updates to the photoionization cross sections as well as to abundances can be found in Wilms, Allen and McCray (2000, ApJ 542, 914).

tbabs allows the user to vary just the molecular hydrogen column.

par1 equivalent hydrogen column (in units of 10^{22} atoms/cm^{-2})

ztbabs is similar, but allows the user to set a fixed redshift parameter

par1 equivalent hydrogen column (in units of 10^{22} atoms/cm^{-2})
z redshift

tbgrain allows the user to vary the molecular hydrogen column and the grain distribution parameters.

par1 equivalent hydrogen column (in units of 10^{22} atoms cm^{-2})
par2 molecular hydrogen column (in units of 10^{22} atoms cm^{-2})
par3 grain density (in gm/cm^{-3})
par4 grain minimum size (in μm)
par5 grain maximum size (in μm)
par6 power-law index of grain sizes

tbvarabs additionally allows the user to vary the elemental abundances and the redshift

par1	equivalent hydrogen column (in units of 10^{22} atoms cm^{-2})
par2 -par18	abundance (relative to Solar) of He, C, N, O, Ne, Na, Mg, Al, Si, S, Cl, Ar, Ca, Cr, Fe, Co, Ni
par19	molecular hydrogen column (in units of 10^{22} atoms cm^{-2})
par20	grain density (in gm/cm^{-3})
par21	grain minimum size (in μm)
par22	grain maximum size (in μm)
par23	power-law index of grain sizes
par24 - par41	grain depletion fractions of He, C, N, O, Ne, Na, Mg, Al, Si, S, Cl, Ar, Ca, Cr, Fe, Co, Ni}
par42	redshift

6.3.27 uvred: interstellar extinction, Seaton Law

A UV reddening using Seaton's law (M.N.R.A.S. 187, 75p). Valid from 1000–3704Å. The transmission is set to unity shortward of the Lyman limit. This is incorrect physically but does allow the model to be used in combination with an X-ray photoelectric absorption model such as `phabs`.

`par1`	E(B-V)

6.3.28 varabs, zvarabs: photoelectric absorption

A photoelectric absorption with variable abundances using cross-sections set by the **xsect** command. The column for each element is in units of the column in a solar abundance column of an equivalent hydrogen column density of $10^{22}cm^{-2}$. The Solar abundance table used is set by the **abund** command. These models differ from the models vphabs, zvphabs only by the units in which the abundances are expressed (vphabs, zvphabs define these relative to the solar abundance, not in terms of column density).

par1- par18	equivalent columns for H, He, C, N, O, Ne, Na, Mg, Al, Si, S, Cl, Ar, Ca, Cr, Fe, Co, Ni

The zvarabs variant allows the user to specify a (fixed) redshift, i.e. the parameters are:

par1–par18	equivalent columns for H, He, C, N, O, Ne, Na, Mg, Al, Si, S, Cl, Ar, Ca, Cr, Fe, Ni, Co
par19	redshift

6.3.29 wabs, zwabs: photoelectric absorption, Wisconsin cross-sections

A photo-electric absorption using Wisconsin (Morrison and McCammon; ApJ 270, 119) cross-sections.

$$M(E) = \exp\left[-n_H \sigma(E)\right]$$

where σ(E) is the photo-electric cross-section (NOT including Thomson scattering). Note that this model uses the Anders & Ebihara relative abundances (1982, Geochimica et Cosmochimica Acta 46, 2363) regardless of the **abund** command.

par1= n_H	equivalent hydrogen column (in units of 10^{22} atoms cm^{-2})

The **zwabs** variant allows the user to specify a (fixed) redshift parameter, and uses the corresponding formula

$$M(E) = \exp\left[-n_H \sigma\left(E\left[1+z\right]\right)\right]$$

par1= nH	equivalent hydrogen column (in units of 1022 atoms cm–2)
par2= z	redshift

6.3.30 wndabs, zwndabs: photo-electric absorption, warm absorber

Photo-electric absorption from approximation to a warm absorber using Balucinska,-Church, and McCammon (ApJ 400, 699) cross-sections. Relative abundances are set by the **abund** command.

$$M(E) = \begin{cases} 1 & E > E_W \\ \exp\left[-n_H \sigma(E)\right] & E \le E_W \end{cases}$$

where σ(E) is the photo-electric cross-section (NOT including Thomson scattering) and

par1= n_H equivalent hydrogen column (in units of 10^{22} atoms cm^{-2})

par2= E_W window energy (keV)

The **zwndabs** variant allows the user to specify a (fixed) redshift and uses the corresponding formula:

$$M(E) = \begin{cases} \exp\left[-n_H \sigma\left(E\left[1+z\right]\right)\right] & E \le E_W \\ 1 & E > E_W \end{cases}$$

with parameters:

par1= nH equivalent hydrogen column (in units of 1022 atoms cm–2)

par2= EW window energy (keV)

par3= z redshift

6.3.31 xion: reflected spectrum of photo-ionized accretion disk/ring

This model describes the reflected spectra of a photo-ionized accretion disk or a ring if one so chooses. The approach is similar to the one used for tables with stellar spectra. Namely, a large number of models are computed for a range of values of the spectral index, the incident X-ray flux, disk gravity, the thermal disk flux and iron abundance. Each model's output is an un-smeared reflected spectrum for 5 different inclination angles ranging from nearly pole-on to nearly face on, stored in a look-up table. The default geometry is that of a lamppost, with free parameters of the model being the height of the X-ray source above the disk, h_X, the dimensionless accretion rate through the disk, $\dot{m}$, the luminosity of the X-ray source, L_X, the inner and outer disk radii, and the spectral index. This defines the gravity parameter, the ratio of X-ray to thermal fluxes, etc., for each radius, which allows the use of a look-up table to approximate the reflected spectrum. This procedure is repeated for about 30 different radii. The total disk spectrum is then obtained by integrating over the disk surface, including relativistic smearing of the spectrum for a non-rotating black hole (e.g., Fabian 1989).

In addition, the geometry of a central sphere (with power-law optically thin emissivity inside it) plus an outer cold disk, and the geometry of magnetic flares are available (`par13` = 2 and 3, respectively). One can also turn off relativistic smearing to see what the local disk spectrum looks like (`par12` = 2 in this case; otherwise leave it at 4). In addition, `par11` = 1 produces reflected plus direct spectrum/direct; `par11` =2 produces (incident + reflected)/incident [note that normalization of incident and direct are different because of solid angles covered by the disk; 2 should be used for magnetic flare model]; and `par11` =3 produces reflected/incident. Abundance is controlled by `par9` and

varies between 1 and 4 at the present. A much more complete description of the model will be presented in Nayakshin et al. 2001 (currently available at **http://adsabs.harvard.edu/cgi-bin/nph-bib_query?bibcode=2001ApJ...546..406N&db_key=AST&data_type=HTML&format=&high=4230b2429423803**)

par1	height of the source above the disk (in Schwarzschild radii)
par2	ratio of the X-ray source luminosity to that of the disk
par3	accretion rate (in Eddington units)
par4	$\cos i$ the inclination angle (1 = face-on)
par5	inner radius of the disk (in Schwarzschild radii)
par6	outer radius of the disk (in Schwarzschild radii)
par7	photon index of the source
par8	redshift z
par9	Fe abundance relative to Solar (which is defined as 3.16×10^{-5} by number relative to H)
par10	Exponential high energy cut-off energy for the source
	$1\Rightarrow$ (reflected+direct)/direct
par11	$2\Rightarrow$ (reflected+incident)/incident
	$3\Rightarrow$ reflected/incident
par12	$2\Rightarrow$ no relativistic smearing
	$4\Rightarrow$ relativistic smearing
par13	$1\Rightarrow$ lamppost
	$2\Rightarrow$ central hot sphere with outer cold disk
	$3\Rightarrow$ magnetic flares above a cold disk

Note that setting par13 to 2 gives a central hot sphere with luminosity law $dL/dR = 4\pi R^2 R^{-10y}$. The inner radius of the sphere is 3 Schwarzschild radii and the outer radius is equal to par1. Only the case with par5 $\geq$ par1 has been tested so far.

6.3.32 zdust: extinction by dust grains

Extinction by dust grains from Pei (1992, ApJ 395, 130), suitable for IR, optical and UV energy bands, including the full energy ranges of the Swift UVOT and XMM-Newton OM detectors. Three models are included which characterize the extinction curves of (1) the Milky Way, (2) the LMC and (3) the SMC. The models can be modified by redshift and can therefore be applied to extragalactic sources. The transmission is set to unity shortward of 912 Angstroms in the rest frame of the dust. This is incorrect physically but does allow the model to be used in combination with an X-ray photoelectric absorption model such as phabs. Parameter 1 (method) describes which extinction curve (MW, LMC or SMC) will be constructed and should never be allowed to float during a fit. The extinction at V, A(V) = E(B-V) x Rv. Rv should typically remain frozen for a fit. Standard values for Rv are MW = 3.08, LMC = 3.16 and SMC = 2.93 (from table 2 of Pei 1992), although these may not be applicable to more distant dusty sources.

par1	method: 1 = Milky Way, 2 = LMC, 3 = SMC
par2	E(B-V): color excess
par3	Rv: ratio of total to selective extinction
par4	z: redshift

6.3.33 zredden: redshifted version of redden

IR/optical/UV extinction from Cardelli et al. (1989, ApJ, 345, 245). The transmission is set to unity shortward of 900 Angstroms. This is incorrect physically but does allow the model to be used in combination with an X-ray photoelectric absorption model such as phabs.

par1 = E(B-V)

par2 = redshift

6.3.34 zsmdust: extinction by dust grains in starburst galaxies

Extinction by dust grains suited to starburst galaxies and the hosts of gamma ray bursts. The model can be applied over the IR, optical and UV energy bands, including the full

energy ranges of the Swift UVOT and XMM-Newton OM detectors. The transmission is set to unity shortward of 912 Angstroms in the rest frame of the dust. This is incorrect physically but does allow the model to be used in combination with an X-ray photoelectric absorption model such as phabs. The extinction curve contains no spectral features and is characterized by a powerlaw slope over spectral wavelength. This model has been justified by e.g. Savaglio & Fall (2004, ApJ, 614, 293) because the apparent low metallicities within GRB hosts result in no significant spectral features within the extinction curve, unlike those found in local galaxies. The extinction at V, A(V) = E(B-V) x Rv. Standard values for Rv are Milky Way = 3.08, LMC = 3.16 and SMC = 2.93 (from table 2 of Pei 1992, ApJ, 395, 130), although these may not be applicable to more distant dusty sources.

par1	E(B-V): color excess
par2	ExtIndex: spectral index of the extinction curve
par3	Rv: ratio of total to selective extinction
par4	z: redshift

6.3.35 zvfeabs: photoelectric absorption with free Fe edge energy

Redshifted photoelectric absorption with all abundances tied to Solar except for iron. The Fe K edge energy is a free parameter.

par1	equivalent hydrogen column (in units of 10^{22} atoms cm^{-2})
par2	abundance relative to Solar
par3	iron abundance relative to Solar
par4	Fe K edge energy
par5	redshift *z*

6.3.36 zxipcf: partial covering absorption by partially ionized material

This model uses a grid of XSTAR photionized absorption models (calculated assuming a microturbulent velocity of 200km/s) for the absorption, then assumes that this

only covers some fraction f of the source, while the remaining (1-f) of the spectrum is seen directly. This is the model used by Reeves et al (2008) 'On why the iron K-shell absorption in AGN is not the signature of the local warm-hot intergalactic medium', and may also be more generally applicable to the spectral complexity seen in Narrow Line Seyfert 1 AGN (Miller et al 2007, A&A, 463, 13).

par1 = column density (10^{22} cm^{-2})

par2 = log(xi) where $xi=L/nr^2$

par3 = covering fraction

par4 = redshift

6.4 Convolution Model Components

Convolution components apply a convolution operator to an input model flux calculated from a source (additive) model, as modified by other components (multiplicative factors or other convolution operators). They differ from multiplicative components, which only apply a bin-wise multiplicative factor, by allowing transformations of the flux across energy bins.

6.4.1 cflux: calculate flux

A convolution model to calculate the flux of other model components. For example :

suppose the model is :

phabs*(pow + gauss)

then

cflux*phabs*(pow + gauss)

with the normalizaton of the power-law model fixed gives the flux and error on the entire model.

phabs*cflux*(pow + gauss)

again with the normalization of the power-law fixed gives the unabsorbed flux and error. Finally,

phabs*(pow + cflux*gauss)

with the normalizaton of the gaussian fixed gives the flux and error on the gaussian component. It is important to ensure that the energy range over which the model is calculated (which is determined by the response matrix in use) covers the energy range for which the flux is calculated.

Parameters are :

par1= Emin Minimum energy over which flux is calculated.

par2= Emax Maximum energy over which flux is calculated.

par3=lg10Flux log (base 10) flux in erg/cm^2/s

6.4.2 gsmooth: gaussian smoothing

Gaussian smoothing with a variable width $\Sigma(E)$, which varies as the `par2` power of the energy. The width at 6 keV is set with `par1`

$$dC(E) = \frac{1}{\sqrt{2\pi\Sigma(E)^2}} \exp\left[-\frac{1}{2}\left(\frac{E-X}{\Sigma(E)}\right)^2\right] A(X)dX$$

$$\Sigma(E) = \sigma\left(E/6\right)^{\alpha}$$

where :

par1= σ gaussian sigma at 6 keV

par2= α power of energy for sigma variation

6.4.3 kdblur: convolve with the laor model shape

A convolution model to smooth a spectrum by relativistic effects from an accretion disk around a rotating black hole.. Uses Ari Laor's calculation including GR effects (ApJ 376, 90). Modified from laor model by Andy Fabian and Roderick Johnstone.

par1 Index: power law dependence of emissivity (scales as $R^{-\mathtt{Index}}$)

par2 inner radius (units of GM/c^2)

par3 outer radius (units of GM/c^2)

par4 inclination (degrees)

6.4.4 kdblur2: convolve with the laor2 model shape

A convolution model to smooth a spectrum by relativistic effects from an accretion disk around a rotating black hole. The accretion disk has a broken-power law emissivity profile. Uses Ari Laor's calculation including GR effects (ApJ 376, 90). Modified from laor2 model by Andy Fabian and Roderick Johnstone.

par1	Index: power law dependence of emissivity (scales as $R^{-\mathtt{Index}}$)
par2	inner radius (units of GM/c^2)
par3	outer radius (units of GM/c^2)
par4	inclination (degrees)
par5	radius at which emissivity power-law index changes
par6	Emissivity power-law index for radii > par6

6.4.5 kerrconv: accretion disk line shape with BH spin as free parameter

Convolves the current spectrum with the line shape from the kerrdisk model. A detailed description can be found in Brenneman & Reynolds (2006ApJ...652.1028B). This model is quite slow so is best used after models such as laor or diskline have been employed to get an estimate of the best-fit parameters.

par1 = rest frame line energy (keV)
par2 = emissivity index for the inner disk
par3 = emissivity index for the outer disk
par4 = break radius separating the inner and outer portions of the disk (gravitational radii)
par5 = dimensionless black hole spin
par6 = disk inclination angle to the line of sight (degrees)
par7 = inner radius of the disk in units of the radius of marginal stability
par8 = outer radius of the disk in units of the radius of marginal stability

6.4.6 lsmooth: lorentzian smoothing

Lorentzian smoothing with a variable width, which varies as the `par2` power of the energy. The width at 6 keV is set with `par1`.

$$dC(E) = \frac{\Sigma(E)}{2\pi\left[(E-X)^2 + (\Sigma(E)/2)^2\right]} A(X)dX$$

$$\Sigma(E) = \sigma\left(E/6\right)^{\alpha}$$

where:

par1= σ lorentzian sigma at 6 keV

par2= α power of energy for sigma variation

6.4.7 partcov: partial covering

A convolution model to convert some absorption model into a partial covering absorption. If the absorption model is M(E) then this is converted to (1-CvrFract) + Cvrfact * M(E). Note that when specifying the model it is important to put parentheses in the right place. Let this model be P(E) which we want to apply to an absorption model M(E) then use the result to multiply an additive model A(E). The combined model should be specified as (P*M)*A, not P*M*A or P*(M*A).

The parameters are :

par1=CvrFract Covering fraction (0 < par1 < 1).

6.4.8 rdblur: convolve with the diskline model shape

A convolution model to smooth a spectrum by relativistic effects from an accretion disk around a non-rotating black hole.. Modified from diskline model (Fabian et al., MNRAS 238, 729) by Andy Fabian and Roderick Johnstone.

par1 Index: power law dependence of emissivity (scales as $R^{-\mathrm{Index}}$) . If this parameter is 10 or greater then the accretion disk emissivity law $\left(1-\sqrt{6/R}\right)\Big/R^3$ is used.

par2 inner radius (units of GM/c^2)

par3 outer radius (units of GM/c^2)

par4 inclination (degrees)

6.4.9 reflect: reflection from neutral material

Convolution model for reflection from neutral material according to the method of Magdziarz & Zdziarski (1995, MNRAS, 273, 837). This is a generalization of the pexrav and bexrav models. When using this model it is essential to extend the energy range over which the model is calculated because photons at higher energies are Compton downscattered into the target energy range. The energy range can be extended using the extend command. The upper limit on the

energies should be set above that for which the input spectrum has significant flux. See the help on pexrav or bexrav for further information and admonitions.

par1	reflection scaling factor (1 for isotropic source above disk)
par2 = *z*	redshift
par3	abundance of elements heavier than He relative to the solar abundances
par4	iron abundance relative to the above
par5	cos *i*, the inclination angle

6.4.10 simpl: comptonization of a seed spectrum

An empirical convolution model of Comptonization in which a fraction of the photons in an input seed spectrum is scattered into a power-law component. The model is described in Steiner et al. (2008, in prep), with details related to the XSPEC implementation given in the appendix. It is designed for soft plasmas which are not Compton thick, and Gamma>1. When using this model, it may be necessary to extend the energy grid over which the model is calculated. This can be accomplished using the energies command.

par1	Gamma, the photon power law index.
par2	the scattered fraction (between 0 and 1).
par3	a flag to switch between up-scattering only (>0) and both up- and down-scattering (<=0).

6.5 Pile-Up Model Components

6.5.1 pileup: CCD pile-up model for Chandra

CCD pile-up model used for brightish point sources observed by Chandra. This is an implementation of the fast pile-up algorithm proposed by John Davis (see **http://space.mit.edu/~davis/papers/pileup2001.pdf**). The frame time and maximum number of photons to pile up should be fixed. The grade morphing is expressed through a single parameter, alpha, which should be left as a free parameter. This model should be considered in beta test. Note that to calculate fluxes etc. for the model you must remove the pileup component. The pile-up model is similar to the operation of the convolution models, differing only in the treatment of the detector efficiency during the convolution.

par1	frame time (in seconds)
par2	maximum number of photons to pile up
par3	grade correction for single photon detection
par4	grade morphing parameter (good grade fraction is assumed proportional to $\texttt{par4}^{p-1}$ where p is the number of piled photons)
par5	PSF fraction. Only this fraction will be treated for pile-up
par6	Number of regions. The counts to be piled-up will be distributed among `par6` regions, which will be piled-up independently.

6.6 Mixing Model Components

Mixing models perform transformations on the available spectra. The spectra must be assigned to more than one data group in order have any effect. Each data group is a "region" of the observation, and the "mixing transformation" allows the model flux from one such "region" to influence another region. Thus, these models, unlike all the others, can be two-dimensional in effect. It follows they that differ from all the other models in that the data must be read before the model can be defined. In most cases also, the input data must contain additional information in order to use the model. This additional information can be in the form of the OGIP standard XFLT keys, which allow a set (currently up to 10) of scalar real values, or in some cases additional files to be read containing spatial information.

XSPEC12 will return error messages if the data are not loaded, not compatible with the model (i.e. do not contain the required additional information), loaded inconsistently with the use of the model (the division of data into regions is incorrect, or data within a given region fail consistency checks). It will also return error messages if the data are subsequently changed to a set that violates these consistency checks, and additionally remove the model definition.

6.6.1 ascac: ASCA surface brightness model

Mixing model for ASCA data. Written for cluster data so uses beta or two power-law surface brightness models. Includes a calculation of the telescope effective area so no arf should be applied to input files. Note that this model is very slow if any of the parameters are free.

The model is used by reading spectra in as separate datagroups. Each input file requires the XFLT0001 keyword set to a different number (eg if concentric annuli are in use then number outwards). The normalizations for each datagroup should be linked since the ascac model takes care of the relative normalizations based on the surface

brightness model used. A maximum of five different spatial regions is allowed. The absolute normalization is not reliable so this model should not be used to derive fluxes.

par1	Alpha
par2	Beta
par3	Core (arcmin)
par4	0 ⇒ beta model, 1 ⇒ 2-power-law

6.6.2 projct: project 3-D ellipsoidal shells onto 2-D elliptical annuli

This model performs a 3-D to 2-D projection of prolate ellipsoidal shells onto elliptical annuli. The annuli can have varying ellipticities and position angles but must have the same center. The user should extract spectra in a series of annuli. Each spectrum needs three additional keywords (XFLT0001, XFLT0002, XFLT0003) in the spectrum extension. These keywords contain the semi-major axis, semi-minor axis, and position angle (in degrees) for the outer boundary of the annulus. It is assumed that the inner boundary is specified by the outer boundary of the next annulus in. The lengths can be in any consistent units although for numerical accuracy they should have reasonable values. Optional pairs of extra keywords (eg XFLT0004/5, XFLT0006/7, etc.) can be used to specify start and end angles for a partial annulus. These angles should be given relative to the same zero as the position angle.

The user reads in the spectra as separate datagroups and sets model parameters for each datagroup. The model for datagroup J will be the model in the shell whose outer boundary is a prolate ellipsoid of semi-major and semi-minor axes given by the semi-major and semi-minor axes in the XFLT keywords for dataset J. The projct model sums up the appropriate fractions of each ellipsoid model to make the projected spectrum.

For example, suppose we extract spectrum from three elliptical regions defined by (1,0.5,0), (2,1,0), (3,1.5,0). That is the first region is in an ellipse of semi-major axis 1 and semi-minor axis 0.5. The second region is an elliptical annulus whose inner boundary has semi-major axis 1 and semi-minor axes 0.5 and whose outer boundary has semi-major axis 2 and semi-minor axis 1. The third region is defined similarly. The model fit has a temperature of 2 keV for the first datagroup, 3 keV for the second, and 4 keV for the third. The actual model fit to the first dataset has contributions from all three temperatures, the second only from the 3 and 4 keV components, and the third only from the 4 keV component. The weighting is the fraction of the ellipsoidal volume intersected by the elliptical annular cross-section. Thus the normalizations correspond to the emission measure in each ellipsoidal shell.

If multiple observations are to be analyzed, data sets from different observations corresponding to the same annulus should be part of the same data group. For example, given the following 4 data files:

Data sets for obs 1: obs1_an1, obs1_an2

Data sets for obs 2: obs2_an1, obs2_an2

The proper data loading command is:

```
XSPEC12>data 1:1 obs1_an1 1:2 obs2_an1 2:3 obs1_an2 2:4 obs2_an2
```

The `projct` model has 3 (fixed) parameters, which can be used to define the inner ellipse of the region being analyzed. For instance, in the example above we could have only read in spectra for the outer two regions but then set the projct parameters to (1.0,0.5,0.0). This would have allowed us to determine the temperatures and emission measures of the outer two annuli without having to worry about fitting a model to the central region.

par1	semi-major axis of inner boundary ellipse
par2	semi-minor axis of inner boundary ellipse
par3	position angle of inner boundary ellipse

6.6.3 recorn: change correction norm for a spectrum

This model is a replacement for and improvement on the old xspec command recornrm. If a correction file is in use for a spectrum then its normalization can be fitted for using this model. The first parameter, which is not variable, is the spectrum number and the second the correction file normalization. The starting value of the second parameter should be set to the current value of the correction file norm (this can be independently set using the cornorm command).

par1	specnum: spectrum number
par2	cornorm: correction file normalization

6.6.4 suzpsf: suzaku surface brightness model

Mixing model for Suzaku data. Mixes the spectra between datagroups based on the PSF overlap between selected regions. A surface brightness model is required to calculate the mixing and this can be supplied in several ways. If SUZPSF-IMAGE has been set to some image file (using **xset**) then this image will be used for the surface brightness distribution. If SUZPSF-IMAGE has not been set then either a beta or two

power-law model is used. In this case the model parameters determine the shape of the surface brightness distribution. If SUZPSF-RA and SUZPSF-DEC are set they are used as the center of the distribution. They should be specified either in decimal degrees or as hh:mm:ss.s and dd:mm:ss.s. If SUZPSF-RA and SUZPSF-DEC are not set then the centroid of the wmap will be used as the center of the surface brightness distribution.

The PSF used is an empirical model of a sum of two exponentials and a Gaussian with coefficients determined from an observation of MCG-6-30-15 performed early in the mission.

The model works by calculating the mixing factors. It will recalculate these factors if any of the SUZPSF-* or any of the model parameters are changed. Calculating the mixing factors is very slow so should be avoided as much as possible. To speed things up, it is possible to save the mixing factor array to a FITS file and re-use it during a later calculation. To save a mixing factor calculation, prior to loading the mixing model (using the **model** command), use **xset** to set the variable SUZPSF-MIXFACT-OFILEn to the name of the output FITS file, and where n is an integer corresponding to the observation number:

```
XSPEC12> xset SUZPSF-MIXFACT-OFILE1 fact_obs1.fits
```

Conversely, a saved factor array can be read in by setting SUZPSF-MIXFACT-IFILEn:

```
XSPEC12> xset SUZPSF-MIXFACT-IFILE1 fact_obs1.fits
```

Multiple observations can be fit simultaneously. In this case the observations should be read in each datagroup in the same order, e.g.

```
XSPEC12> data 1:1 obs1reg1 1:2 obs2reg1 1:3 obs3reg1 2:4 obs1reg2 2:5 obs2reg2
```

par1	Alpha (not used if Switch=0
par2	Beta
par3	Core (arcmin)
par4	Switch (0 = beta model, 1 = 2-power-law)

6.6.5 xmmpsf: xmm surface brightness model

Mixing model for XMM data. Mixes the spectra between datagroups based on the PSF overlap between selected regions. A surface brightness model is required to calculate the mixing and this can be supplied in several ways. If XMMPSF-IMAGE has been set to some image file (using **xset**) then this image will be used for the surface brightness distribution. If XMMPSF-IMAGE has not been set then either a beta or two power-law model is used. In this case the model parameters determine the shape of the surface brightness distribution. If XMMPSF-RA and XMMPSF-DEC are set they are used as the center of the distribution. They should be specified either in decimal degrees or as hh:mm:ss.s and dd:mm:ss.s. If XMMPSF-RA and XMMPSF-DEC are not set then the centroid of the wmap will be used as the center of the surface brightness distribution.

The model works by calculating the mixing factors. It will recalculate these factors if any of the XMMPSF-* or any of the model parameters are changed. Calculating the mixing factors is very slow so should be avoided as much as possible. To speed things up, it is possible to save the mixing factor array to a FITS file and re-use it during a later calculation. To save a mixing factor calculation, prior to loading the mixing model (using the **model** command), use **xset** to set the variable XMMPSF-MIXFACT-OFILEn to the name of the output FITS file, and where n is an integer corresponding to the observation number:

```
XSPEC12> xset XMMPSF-MIXFACT-OFILE1 fact_obs1.fits
```

Conversely, a saved factor array can be read in by setting XMMPSF-MIXFACT-IFILEn:

```
XSPEC12> xset XMMPSF-MIXFACT-IFILE1 fact_obs1.fits
```

Multiple observations can be fit simultaneously. In this case the observations should be read in each datagroup in the same order, e.g.

```
XSPEC12> data 1:1 obs1reg1 1:2 obs2reg1 1:3 obs3reg1 2:4 obs1reg2 2:5 obs2reg2
```

par1 Alpha (not used if Switch=0

par2 Beta

par3 Core (arcmin)

par4 Switch (0 = beta model, 1 = 2-power-law)

Appendices

Appendix A The User Interface

A-1 Introduction

All communication with the user in XSPEC is performed through the tcl user interface. When XSPEC starts, a tcl interpreter is initialized, and the XSPEC commands are added to it so that the tcl interpreter understands them. The XSPEC commands, which are C++ functions, define the syntax through a new built-in library of utility functions. The parser used in earlier versions of XSPEC has been discontinued: however the syntax understood by XSPEC12 is much the same as before.

XSPEC and tcl/tk

Because tcl is a full scripting language, users can write complex scripts with loops, branching, etc., which utilize XSPEC commands. Here we describe how to use those features of tcl necessary to give the user similar functionality to that available in previous versions of XSPEC, and to give information on the details of our tcl implementation that may be useful to experienced tcl users. For a description of tcl, see, for example, *Practical Programming in Tcl and Tk*, B. Welch, (1997, Prentice Hall).

Tk, tcl's companion graphical user interface (GUI) toolkit, is also loaded by XSPEC on startup. It is planned that future versions of XSPEC will provide an optional GUI side-by-side with the command line interface (CLI). Although XSPEC does not currently use tk, its presence allows users to write XSPEC scripts with graphical interfaces using Tk commands.

A-2 A note on command processing

To emulate the performance of the former XSPEC parser, the command functions are programmed to react similarly to some of its features.

The # sign is used for comments in tcl, but may appear only at the beginning of a command. tcl and XSPEC both ignore carriage returns on a new line, but XSPEC also ignores the skip character `'/'`. The character sequence `'/*'` entered during a command exits that command, sets any responses to the default response, and returns the user to the prompt. The `'\'` character is used in tcl for continuing a command onto the next line.

Additionally, note that in tcl, commands and their arguments are delimited by white space. They are terminated by a newline or semicolon, *unless* there is an open set of parentheses `'{ }'` constituting a loop or test structure. In other words, in tcl the following starts a loop:

```
while { condition } {
….
}
```

but

```
while { condition }
{

}
```

is incorrect, since in the latter case the `while` command terminates at the end of the first line.

A-3 Command Recall/Editing

The XSPEC/tcl interface also uses gnu readline for command input, which allows command line editing and interactive command recall. On most systems, the left and right arrow keys and the backspace/delete key can be used to navigate and edit the command line. The up and down arrow keys can be used to step thru the command history list. Gnu readline is highly customizable, and many more editing/recall functions are available. Readline documentation can be generated in either postscript or html format from the files in the xanadu/readline/doc directory distributed with the source.

The default implementation of tcl also supports a C-shell like command recall mechanism. The `history` command gives a numbered list of the most recently entered commands. Any command in the list can be re-executed by entering `!n`, where `n` is the number of the command in the history list. The previous command can be re-executed by entering `!!`. The most recent command that begins with a string can be re-executed by entering `!prefix`, where `prefix` is the string the command begins with.

Note that command recall is implemented using the tcl `unknown` procedure, part of which is a script file loaded by tcl at run time. See the section on the `unknown` command for more details on how it is implemented in XSPEC.

A-4 Logging

The `log` command can be used to open a log file to which all input and and output to tcl will be written. Reading these log files can potentially be confusing when logging tcl flow control commands such as `while` or `for`. This is because tcl treats the body of these commands as an argument of the command. Thus when the command is echoed to the log file, the entire body of the command is echoed with it.

In order to make this situation less confusing, before commands are echoed to the command file, all newline characters are replaced by semicolons, and the resulting command line is trucated to 80 characters. Then any commands executed with in the body of a flow control command are echoed as they are executed.

Consider the following sequence of tcl commands within XSPEC:

```
XSPEC12> log
Logging to file: xspec.log
XSPEC12> set i 1 ; set product 1
1
XSPEC12> while {$i <= 5} {
XSPEC12> set product [expr $product * $i]
XSPEC12> incr i
XSPEC12> }
XSPEC12> set product
```

```
 120
 XSPEC12>
```

This would produce the following output in the file `xspec.log`:

```
Logging to file: xspec.log
 XSPEC12> set i 1
 set product 1
 1
 XSPEC12> while {$i <= 5} {;set product [expr $product * $i];incr i;}
   expr $product * $i
  set product [expr $product * $i]
  incr i
   expr $product * $i
  set product [expr $product * $i]
  incr i
   expr $product * $i
  set product [expr $product * $i]
  incr i
   expr $product * $i
  set product [expr $product * $i]
  incr i
   expr $product * $i
  set product [expr $product * $i]
  incr i
 XSPEC12> set product
 120
 XSPEC12>
```

A-5 Command Completion

tcl attempts to match the name of any entered command as an abbreviation of a valid command (either a tcl or XSPEC command). If the entered command matches more than one valid command, tcl then lists the possible choices, but does not execute the command. For XSPEC commands, aliases have been constructed matching the command to its minimum abbreviation, as listed when typing `?' at the XSPEC prompt (see under Aliases).

For example, the minimum abbreviation for the `plot' command is `pl'. Thus, typing `pl' will execute the plot command, even though this would otherwise be ambiguous with the tk command `place'. Command completion is also implemented using the tcl `unknown` procedure, part of which is a script file loaded by tcl at run time, and may be different or not exist on your system. See the section in this help file on the `unknown` command for more details on how it is implemented in XSPEC.

N.B. tcl explicitly switches off command completion for scripts. Because of the way scripts are implemented in XSPEC, however, command abbreviations nevertheless do work in scripts entered with the **@** command, but not when entered from the command line or using the source command. See below for more details about tcl scripting.

A-6 Unknown Procedure

tcl provides a facility whereby if it cannot match an entered command to its list of known commands, it calls the `unknown` procedure, with the unmatched command (along with its arguments) as its argument. The version of `init.tcl` distributed with tcl contains a version of the unknown procedure. When tcl initializes, it looks in several standard places for a script file named `init.tcl`, which it executes if found. The `unknown` procedure is where tcl does command completion and automatic shell command execution.

At start up time, XSPEC loads its own `unknown` procedure, , which it uses to intercept script processing requests of the form

```
XSPEC12>@<script>
```

and renames the previously defined `unknown` procedure to `tclunknown`. If XSPEC is not doing any special processing, it simply passes any unmatched commands on to `tclunknown`, which then processes them as usual. XSPEC has its own special version of the `unknown` procedure

These factors need to be taken into consideration for programmers writing tcl scripts for use within XSPEC. For example, if after initialization, users wishing to load a different version of the standard tcl `unknown` procedure should name that procedure `tclunknown`, rather than `unknown`.

A-7 Aliases

Command name aliases can be constructed using the tcl `interp` command:

```
interp alias {} <command_alias> {} <xspec_command>
```

where `<xspec_command>` is the name of the command you wish to make an alias for, and `<command_alias>` is the name of the alias you wish to set for the command. The `{}` are *required* syntax.

To delete the alias `<command_alias>`, simply nullify it with:

```
interp alias {} <command_alias> {}
```

A-8 Initialization Script

When running interactively, the user has the option of providing an initialization script, which will be executed after XSPEC completes its startup procedure, ie. just before it begins prompting for commands. The file should be named `xspec.rc` and located in the directory $HOME/.xspec. **If one runs XSPEC in batch mode, by specifying a script on the command line, this initialization script is not executed.**

When multiple users are accessing a single system-wide XSPEC build, the installer can also provide additional initialization that will apply to all users. See the section “XSPEC Overview and Helpful Hints: Customizing XSPEC” for more details.

A-9 XSPEC Command Result

After being executed, many tcl commands return a result string, which is echoed to the terminal when the command is entered on the command line. When writing complex tcl scripts, this result can be stored and/or used as a test in loops, etc. When XSPEC commands are executed, they write information to the terminal by writing directly to the appropriate output channel. However, when running interactively, the tcl result string is also written to the terminal after the command is executed. The tclout command (see command description) creates tcl variables from xspec's calculations.

A-10 Script Files

XSPEC/tcl script files can be executed in three different ways, as follows:

xspec - <script>	executing script on initialization
XSPEC12>@ <script>	executing script from within the program
XSPEC12>source tclscript	use tcl's source command from within the program.

Each of these usages does something slightly different. In the first form, XSPEC will execute a file called `<script>`. One may execute a series of script files at startup with the following command syntax:

unix> xspec - file1 file2 file3 ...

Note that the space following the - is required.

The second form is `@<name>`, where `<name>` is the name of the script file to be executed. Here the default extension of `.xcm` is assumed. Scripts containing valid tcl or XSPEC commands will be executed using this form, and (unless the script ends in **quit** or **exit**) will return to the interactive prompt after completion.

The final form, using tcl's source command, is intended for the special case where the script contains the implementation of a new command written in tcl/tk. See the section on **writing custom commands** for more details. In current tcl versions it compiles the script into bytecode representation for more efficient execution, and adds any procedures defined in the script to the set of commands understood by the interpreter. **It will *not* work for general scripts containing XSPEC/tcl commands, for example those produced by XSPEC's save command. These should rather be executed using the @ form.**

Note that only in the second case `@` is there a default filename suffix (i.e. .xcm) for both the other methods of script execution the filename must be given in full.

tcl internally switches off the mechanism that expands command abbreviations when scripts are executed. If this were not done, the user could specify command abbreviations that change the behavior of the tcl command set (e.g. `set` for the **setplot** command would redefine tcl's command for setting variables). This behavior can be overridden with the statement

set tcl_interactive 1

near the beginning of the script, but it is not recommended to do so. Instead, we strongly recommend spelling out command names in full within XSPEC scripts.

A-11 Command Echoing

By default, when XSPEC is executing a script file, it echoes each command to the terminal before it is executed. This can be controlled using the tcl variable `xs_echo_script`, whose default value is 1. If this variable is set to 0, the commands from the script file will not be echoed to the terminal.

A-12 Summary

In summary, we suggest the following convention:

- Running an xspec script from the unix command prompt is intended to be used for background processing or overnight batch jobs. Using the unix `at` command, one can arrange to receive the log file by e-mail.
- The `@` usage is intended for processing previously run xspec command sequences, such as are produced by the **save** command.
- The `source` usage, as well as executing the commands in the script, performs the equivalent of pre-compiling the script for later invocation. Its most appropriate use is in preparing new custom XSPEC command procedures. Once the script is working correctly, it can be placed in the user script directory and become part of the user's standard command set. For examples, see the scripts addline.tcl and modid.tcl in the directory

  `$SPECTRAL/scripts`

  that implement the commands **addline** and **modid**. These also show how to make commands self-documenting.

A-13 Unix Shell Commands

Shell commands can be executed within XSPEC using the `exec` command (see the help entry on the `exec` command). When running interactively, if tcl cannot find a command that matches that entered on the command line, it will search for a shell command that matches the entered command. If it finds a match, it automatically executes the shell command via `exec`. Note that this feature is implemented using the tcl `unknown` procedure, part of which is a script file loaded by tcl at run time, and may be different or not exist on your system. See the section in this help file on the `unknown` command for more details on how it is implemented in XSPEC.

Note that the tcl `exec` command executes the given command directly, without first passing it on to the shell. Thus no globbing (ie. expansion of wildcards such `*.pha`) is performed. If you wish to pass you command through a shell for wildcard expansion, etc, use the `syscall` command.

If you want to start a subshell from within XSPEC, simple type the command for starting that shell, ie. type

```
XSPEC12>csh
```

in order to start a C-shell. Note that typing

XSPEC12>exec csh

will not work properly.

Giving the

XSPEC12>syscall

command with no arguments will start a subshell using your current shell (csh, tcsh, bash, sh, etc).

A-14 Writing Custom XSPEC commands

XSPEC commands can be written by users as tcl procedures, which have similarities with fortran subroutines. Within XSPEC, tcl procedures can take arguments and execute XSPEC and tcl commands. The syntax for specifying arguments to a tcl procedure is as follows:

```
proc my_proc {arg1 arg2}{
...

data 1:1 ${arg1}_s0_20
data 2:2 ${arg2}_s1_20
...
}
```

Here, arg1, arg2 are values supplied by the user (here, part of a filename) from the command line, and substituted wherever `${arg1}`, `${arg2}` appear within the script. One may also give an argument a default value, so that the command so created may be invoked even without needing to specify the argument:

```
proc my_proc {arg1    {arg2 file2} }  {
...
}
```

Note that the parentheses enclosing both `${arg2}` and `file2` in this expression distinguish this from the case where 3 arguments are required for `my_proc`. Once this file is created, it needs to be `source`'d once, which compiles the script into an internal bytecode representation (this is similar to the way Java operates). Alternatively, one may place it in the user script directory and create an index in that directory, after which case it will be found automatically and compiled the first time it is invoked.

The user script directory is given by the line

```
USER_SCRIPT_DIRECTORY:
```

in the Xspec.init file that is copied into $HOME/.xspec when the user starts xspec12 for the first time (the supplied default value for this directory is the $HOME/.xspec directory itself). After the script is placed there, perform the following command

```
%xspec12
XSPEC12>cd <USER_SCRIPT_DIRECTORY>
```

```
XSPEC12>auto_mkindex .
XSPEC12>exit
```

This will instruct XSPEC to build an index of scripts to be loaded on xspec startup.

On the next invocation of XSPEC, the script will be sourced on startup and will appear in the list of commands XSPEC understands.

The `my_proc` procedure is then defined such that one may type:

XSPEC12>my_proc eso103 eso104

and the data statement in the above example will be executed as if the following had been entered:

```
data 1:1 eso103_s0_20
data 2:2 eso104_s1_20
```

The tcl `info` command can be used to show which procedures have been defined:

```
XSPEC12>info commands <procedure name>
```

This will return <procedure name> if that procedure has been compiled (source'd) already or is a built-in command, or nothing if it has not (yet) been invoked or defined.

A-15 Scripting commands that prompt the user

The commands **model**, **editmod**, **addmod**, **newpar**, and **fakeit** may prompt the user for more information when used interactively. In order to write scripts that use these commands, one must know how to force XSPEC to enter the information that would be prompted for. The technique is exemplified as follows. Suppose we defined a procedure `xmodel` that makes a model with certain predefined parameter values:

```
set p1  {1.5 0.001 0 0 1.E05 1.E06}
set p2  {1 0.001 0 0 1.E05 1.E06}
 proc xmodel {modelString param1 param2 args} {


  model $modelString & $param1 & param2 & /*


 }
```

Here the "`&`" character is taken by XSPEC as a carriage return, delimiting the model string and parameter arguments into separate input lines.

The procedure `xmodel` may be compiled with the command

```
XSPEC12> source xmodel.tcl
```

This creates xmodel as a command with two arguments which sets subsequent parameters to their default values. It can be invoked e.g. by

```
XSPEC12>xmodel {wa(po + peg)} $p1 $p2
```

Note that the model string, which contains spaces, needs to be entered in `{}` or double quotes. Note also that tcl understands a single string argument, `args`, as in

```
proc  tclscript { args } {
…
}
```

to mean a variable number of arguments to a procedure (it is supplied as a tcl list, which can be split within the procedure into separate strings for digestion by xspec if present).

A-16 Script Example

In the directory `$HEADAS/../spectral/session` is a script file called `tclex.xcm`. This script gives an example of how one might use the power of tcl's scripting language in an XSPEC session. This script should be executed with

```
XSPEC12> @tclex

# This script gives an example of how one might use the power of tcl's
# scripting language in an XSPEC session.  In this example, XSPEC loops
# thru 3 data files (file1, file2 and file3) and fits them each to the
# same model `wabs(po+ga)'.  After the fit the value of parameter 4
(the
# line energy for the gaussian) for each data set is saved to a file.

# Keep going until fit converges.
query yes

# Open the file to put the results in.
set fileid [open fit_result.dat w]

for {set i 1} {$i < 4} {incr i} {

# Set up the model.
  model wabs(po+ga) & /*

# Get the file.
  data file$i

# Fit it to the model.
  fit

# Get the values specified for parameter 4.
  tclout param 4
  set par4 [string trim $xspec_tclout]

# Turn it into a Tcl list.
  regsub -all { +} $par4 { } cpar4
  set lpar4 [split $cpar4]

# Print out the result to the file.  Parameter value is
# the 0th element of the list `lpar4'.
  puts $fileid "$i [lindex $lpar4 0]"

}
```

```
# Close the file.
close $fileid
```

The user is encouraged to read the voluminous on-line documentation and literature available about tcl in order to benefit fully its flexible command processing, graphical interfacing, and scripting capabilities. See **http://www.tcl.tk** for much more information and extensive bibliography.

Appendix B Fitting with few counts/bin

B-1 Theory

No background

Cash (1979) showed that the χ^2 minimization criterion is a very bad one if any of the observed data bins had few counts. A better criterion is to use a likelihood function:

$$C = 2\sum_{i=1}^{N} y(x_i) - y_i \ln y(x_i) + \ln y_i !$$

where y_i are the observed data and $y(x_i)$ the values of the function. Minimizing C for some model gives the best-fit parameters. Furthermore, this statistic can be used in the same, familiar way as the χ^2 statistic to find confidence intervals. One finds the parameter values that give

$$C = C_{min} + N$$

where N is the same number that gives the required confidence for the number of interesting parameters as for the χ^2 case.

Castor (priv. comm.) has pointed out that a better function to use is :

$$C = 2\sum_{i=1}^{N} y(x_i) - y_i + y_i \left(\ln y_i - \ln y(x_i)\right)$$

This differs from the first function by a quantity that depends only upon the data. In the limit of a large number of counts this second function does provide a goodness-of-fit criterion similar to that of χ^2 and it is now used in XSPEC. It is important to note that the C-statistic assumes that the error on the counts is pure Poisson, and thus it cannot deal with data that already has been background subtracted, or has systematic errors.

With background

Arnaud (2003, ApJ submitted) has extended the method of Cash to include the case when a background spectrum is also in use. Note that this requires the source and background spectra to both be available, it does not work on a background-subtracted spectrum.

Suppose we have an observation which produces S_i events in the $i = \{1, N\}$ spectral bins in an exposure time of t_s. This observation includes events from the source of interest along with background events. Further suppose that we perform a background observation which generates B_i events in an exposure time t_b. If the source count rate in bin *i* is y_i then the new fit statistic is

$$W = 2\sum_{i=1}^{N} \{t_s y_i + (t_s + t_b) f_i - S_i \log(t_s y_i + t_s f_i) - B_i \log(t_b f_i) - S_i(1 - \log S_i) - B_i(1 - \log B_i)\}$$

where

$$f_i = \frac{S_i + B_i - (t_s + t_b) y_i \mp d_i}{2(t_s + t_b)}$$

and

$$d_i = \sqrt{\left[(t_s + t_b) y_i - S_i - B_i\right]^2 + 4(t_s + t_b) B_i y_i}\ .$$

The sign of d_i in f_i is chosen so that $f_i > 0$.

In the limit of large numbers of counts/bin a second-order Taylor expansion shows that W tends to

$$\sum_{i=1}^{N} \left(\frac{[S_i - t_s y_i - t_s f_i]^2}{t_s y_i + t_s f_i} + \frac{[B_i - t_b f_i]^2}{t_b f_i} \right)$$

which is distributed as χ^2 with $N - M$ degrees of freedom, where the model y_i has M parameters (including the normalization).

B-2 Practice

No background

XSPEC's default minimization algorithm is a variant of Marquardt's method (the Levenberg-Marquadt algorithm) described in §11.5 of *Data Reduction and Error Analysis for the Physical Sciences* by Bevington (2002). (The reader is advised that this description is designed to be read in conjunction with Bevington.) This method is appropriate for fitting models that are twice differentiable. We illustrate the implementation of this W statistic using this method. The algorithm works by finding a matrix α_{jk} and a vector β_k such that the equation :

$$\beta_k = \sum_j \delta a_j \alpha_{jk}$$

gives sensible values of the change in parameters, δa_j, for the fitting function.

Bevington §11.4 gives the derivation of α and β and shows that β is parallel to the gradient of χ^2.

Now the C-statistic has a gradient with respect to the parameters of the fitting function of :

$$-\frac{1}{2}\frac{\partial C}{\partial a_k} = \sum_i \left(\frac{y_i}{y} - 1 \right) \frac{\partial y}{\partial a_k} = \beta_k$$

So, following Bevington, expand $y(x_i)$ about y_0 :

$$y(x_i) = y_0(x_i) + \sum_j \frac{\partial y_0(x_i)}{\partial a_j} \delta a_j\ .$$

substitute into C and minimize with respect to the changes in the parameters :

$$\frac{\partial C}{\partial \delta a_k} = 2\sum_i \left[\frac{\partial y_0(x_i)}{\partial a_k} - y_i \left(y_0(x_i) + \sum_j \frac{\partial y_0(x_i)}{\partial a_j} \delta a_j \right)^{-1} \frac{\partial y_0(x_i)}{\partial a_k} \right]$$

setting this to zero we obtain, to first order in the parameter changes,

$$\sum_i \left(\frac{y_i}{y_0(x_i)} - 1 \right) \frac{\partial y_0(x_i)}{\partial a_k} = \sum_j \left(\sum_i \frac{y_i}{y_0^2(x_i)} \frac{\partial y_0(x_i)}{\partial a_j} \frac{\partial y_0(x_i)}{\partial a_k} \delta a_j \right)$$

or :

$$\beta_k = \sum_j \delta a_j \alpha_{jk}$$

where:

$$\alpha_{jk} = \sum_i \frac{y_i}{y_0^2(x_i)} \frac{\partial y_0(x_i)}{\partial a_j} \frac{\partial y_0(x_i)}{\partial a_k}$$

These α and β then are substituted for those used in the χ^2 case and the algorithm works as required. Note that α_{jk} is $-\partial^2 C / \partial a_k \partial a_j$ to first order in partial derivatives in y, evaluated at y_0.

There is one further difference in XSPEC between the χ^2 and likelihood methods, which is caused by the fact that XSPEC uses an analytic formula for setting the model normalization. In the χ^2 case, this means multiplying the current model by:

$$\sum_i \frac{y_i y(x_i)}{\sigma_i^2} \Big/ \sum_i \frac{y(x_i)^2}{\sigma_i^2}$$

where σ_i is the error on y_i. In the likelihood case the corresponding factor is:

$$\sum_i y_i \Big/ \sum_i y(x_i)$$

With background

An analogous argument to the above can be followed through for the *W* statistic. We need the partial derivatives of *W* which are evaluated as follows.

$$\frac{\partial W}{\partial a_j} = 2\sum_i \left\{ t_s + g_i(t_s + t_b) - \frac{S_i(1+g_i)}{y_i + f_i} - \frac{B_i g_i}{f_i} \right\} \frac{\partial y_i}{\partial a_j}$$

$$\frac{\partial^2 W}{\partial a_j \partial a_k} = 2\sum_i \left\{ (t_s + t_b)h_i - \frac{S_i h_i}{y_i + f_i} - \frac{S_i(1+g_i)^2}{(y_i + f_i)^2} - \frac{B_i h_i}{f_i} - \frac{B_i g_i^2}{f_i^2} \right\} \frac{\partial y_i}{\partial a_j} \frac{\partial y_i}{\partial a_k}$$

where

$$g_i \frac{\partial y_i}{\partial a_j} = \frac{\partial f_i}{\partial a_j} = \frac{1}{2d_i}\left((t_s + t_b)y_i - S_i + B_i - d_i\right)\frac{\partial y_i}{\partial a_j}$$

and

$$h_i \frac{\partial y_i}{\partial a_j} = \frac{\partial g_i}{\partial a_j} = \frac{2(t_s + t_b)S_i B_i}{d_i^3}\frac{\partial y_i}{\partial a_j}$$

Note that in this case there is no analytic formula that can be used to set the model normalization.

References

Arnaud, K. A. 2003, Astrophysical Journal, submitted

Bevington, P. 2002 Data Reduction and Error Analysis for the Physical Sciences Third Edition (McGraw Hill:Columbus)

Cash, W. 1979 Parameter estimation in astronomy through application of the likelihood ratio Astrophysical Journal 228, 939

Appendix C Adding models to XSPEC

XSPEC includes a large collection of standard models that can be fit to data. However, sometimes these are not enough and a new model might be required. In order of increasing complexity the ways to do this are: use the mdefine command; create a table model; load a model function created by someone else; create and load your own model function. The mdefine command can be used for a model which can be described using a simple formula and is documented under the commands section of the manual so we do not discuss it further. This appendix describes the other three methods then finishes with a note about the more complex issue of mixing models.

C-1 Table models

A very simple way of fitting with user-defined models is available for a particular class of models. These are models that can be defined by a grid of spectra, with the elements of the grid covering the range of values of the parameters of the model. For instance, for a one-parameter model, a set of model spectra can be tabulated for different values of the parameter (P1, P2, P3, etc.) The correct model spectrum for a value P is calculated by interpolation on the grid. The generalization to more parameters works in the obvious way. The table is specified in the model command by the special strings atable, mtable, or etable with the filename following in brackets – see the entries in the models section of the manual. Any number of table model components can be used simultaneously.

Table model components can be much slower than most standard models if there are significant numbers of parameters. The memory requirements increase as 2^n where n is the number of parameters in the model. A table model with more than 3 or 4 fitting parameters is not recommended. Additionally, the interpolation is linear, which implies that the second derivatives used by the default Levenberg-Marquadt algorithm may not be accurate. If the fit does not work well it may be worth trying the migrad (minuit library) algorithm which makes no assumptions about the second derivative.

As with standard models, the spectra should be in terms of flux-per-bin and not flux-per-keV. Any set of energy bins can be used, and XSPEC will interpolate the model spectra onto the appropriate energy bins for the detectors in use. It is therefore a good idea to choose energy bins such that the spectrum is well-sampled over the range of interest. The file structure for these models is a FITS format described at :

http://heasarc.gsfc.nasa.gov/docs/heasarc/ofwg/docs/general/ogip_92_009/ogip_92_009.html

or:

ftp://legacy.gsfc.nasa.gov/fits_info/fits_formats/docs/general/ogip_92_009

C-2 Loading a new model function

New model functions either downloaded from the XSPEC additional models webpage at :

http://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/newmodels.html

or acquired privately are added using the two commands **initpackage**, which prepares and compiles a library module containing them, and the **lmod** command which actually loads them into the program. These commands are described in the XSPEC commands section of the manual, to which the user is referred. Any number of different user model packages may be added to XSPEC from the user prompt, and the user has control over the directory from which models are loaded. On Cygwin, local model libraries must be built and linked to XSPEC statically prior to runtime, and therefore cannot be loaded with **lmod**. Cygwin users should consult the **static_initpackage** section of the **initpackage** command documentation.

Note that the **lmod** command requires write-access to the particular directory specified. This is because **lmod** uses the Tcl 'make package' and 'package require' mechanisms for automatic library loads and these require Tcl write an index file (pkgIndex.tcl) to the directory. Consequently we recommend using the Tcl **load** command instead of **lmod** if the library is being used by a number of users on a local network. Note that such a library can be loaded automatically by placin the command in the global_customize.tcl script (see the section "Customizing XSPEC").

C-3 Writing a new model function

A model function is a subroutine that calculates the model spectrum given an input array of energy bins and an array of parameter values. The input array of energy bins gives the boundaries of the energy bins and hence has one more entry than the output flux arrays. The energy bins are assumed to be contiguous and will be determined by the response matrix in use. The subroutine should thus make no assumptions about the energy range and bin sizes. The output flux array for an **additive** model should be in terms of photons $cm^2 s^{-1}$ (not photons $cm^2 s^{-1}$ keV^{-1}) i.e. it is the model spectrum integrated over the energy bin. The output array for a **multiplicative** model is the multiplicative factor for that bin. Convolution models are operators on the output from additive or multiplicative models. Model subroutines can be written in fortran, either in single or double precision, in C++ using either C++-style arguments or C style arguments, and in C.

The "model.dat" entry

In addition to the subroutine, XSPEC requires a text file describing the model and its parameters. The standard models are specified in the model.dat file so we usually refer to this text file by that name. A sample model.dat entry has the following form:

```
modelentry        5  0.          1.e20           modelfunc    add  0 0
lowT    keV     0.1   0.0808  0.0808 79.9      79.9       0.001
highT   keV     4.    0.0808  0.0808 79.9      79.9       0.001
Abundanc " "    1.    0.      0.      5.        5.        0.01
*redshift " "   0.0
$switch    1
```

The first line for each model gives the model name, the number of parameters, the low and high energies for which the model is valid, the name of the subroutine to be called and the type of model (add, mul, mix, or con, or acn). The final argument two arguments are flags: the

first should be set to 1 if model variances are calculated by modelfunc and the second should be set to 1 if model should be forced to perform a calculation for each spectrum. This final flag is necessary because if multiple spectra have the same energy bins, the default behavior is to perform the model calculation for just one spectrum and copy the results for each of the others. However if a model depends on information about the spectrum in addition to its energy ranges, it must be forced to perform a calculation for each spectrum.

The remaining lines in the text file specify each parameter in the model. For regular model parameters the first two fields are the parameter name followed by an optional units label. If there is no units label then there must be a quoted blank (" ") placeholder. The remaining 6 numerical entries are the default parameter value, hard min, soft min, soft max, hard max, and fit delta, which are described in the **newpar** command section.

There are three special types of parameter which can be used. If the name of the parameter is prefixed with a "*" the parameter is a "scale" parameter and cannot be made variable or linked to an other kind of parameter other than another scale parameter. Since the parameter value can never vary only the initial value need be given. If the name of the parameter is prefixed with a "$" the parameter is a "switch" parameter which is not used directly as part of the calculation, but switches the model component function's mode of operation (i.e. calculate or interpolate). Switch parameters only have 2 fields: the parameter name and an integer value. If a P is added at the end of the line for a parameter then the parameter is defined to be periodic. During a fit, a periodic parameter will not be pegged if it tries to exceed its hard limits. Instead it will be assigned a value within its limits: f(max + delta) = f(min + delta), f(min-delta) = f(max-delta). The soft min and max settings are irrelevant for period parameters and will be ignored.

The model subroutine function

The following table lists the function arguments required for the different language options. The second column is the way the function name should be included in the model.dat entry.

Call Type	Specification	Arguments and Type	Meaning
Single precision fortran	modelfunc	real*4 ear(0:ne)	Energy array
		integer ne	Size of flux array
		real*4 param(*)	Parameter values. (Dimension must be specified inside the function)
		integer ifl	The spectrum number being calculated
		real*4 photar(ne)	Output flux array

		real*4 photer(ne)	Output flux error array (optional)
Double precision fortran	F_modelfunc	real*8 ear(0:ne)	As above
		integer ne	"
		real*8 param()	"
		integer ifl	"
		real*8 photar(ne)	"
		real*8 photer(ne)	"
C/C++, C-style	c_modelfunc	const Real* energy	Energy array (size Nflux+1)
		int Nflux	Size of flux array
		const Real* parameter	Parameter values
		int spectrum	Spectrum number of model component being calculated
		Real* flux	Output flux array
		Real* fluxError	Output flux error array (optional)
		const char* init	Initialization string (see below)
C++, C++ style	C_modelfunc	const RealArray& energy	Energy array
		const RealArray& parameter	Parameter values
		int spectrum	Spectrum number of model component being calculated
		RealArray& flux	Output flux array
		RealArray& fluxError	Output flux error array (optional)

		const string& init	Initialization string (see below)

For example, a model component in double precision fortran is specified by:

```
modelentry        5  0.         1.e20           F_modelfunc    add  0
```

XSPEC then picks out the right function definition, and calls the function modelfunc which expects double precision arguments. The C-style call can clearly be compiled and implemented by either a C or a C++ compiler: however we recommend using the C++ call if the model is written in C++ as it will reduce overhead in copying C arrays in and out the XSPEC internal data structures. To prevent unresolved symbol linkage errors, we also recommend prefacing C++ local model function definitions with the **extern "C"** directive.

Example C/C++ function definitions:

```
/* C -style */
extern "C" void modelfunc(const Real* energy, int Nflux, const Real* parameter, int spectrum,
Real* flux, Real* fluxError, const char* init)
{
    /* Model code:  Do not allocate memory for flux and fluxError arrays.  XSPEC's
    C-function wrapper will allocate arrays prior to calling the function (and will free them
    afterwards). */
}
    // C++
extern "C" void modelfunc(const RealArray& energy, const RealArray& parameter, int
spectrum, RealArray& flux, RealArray& fluxError, const string& init)
{
    // Model code:  Should resize flux RealArray to energy.size() - 1.  Do the same for
    // fluxError array if calculating errors, otherwise leave it at size 0.
}
```

Note on type definitions for (C and C++): XSPEC provides a typedef for **`Real`**, in the xsTypes.h header file. The distributed code has

```
typedef Real double;
```

i.e. all calculations are performed in double precision. This is used for C models and C++ models with C-style arguments.

The type **`RealArray`** is a dynamic (resizeable) array of **`Real.`** XSPEC uses the std::valarray template class to implement **`RealArray`**. The internal details of XSPEC require that the **`RealArray`** typedef supports vectorized assignments and mathematical operations, and indirect addressing (see C++ documentation for details). However, we do not recommend using

specific features of the std::valarray class, such as array slicing, in case the typedef is changed in future.

The input energies are set by the response matrices of the detectors in use. IFL is an integer which specifies to which response (and therefore which spectrum) these energies correspond. It exists to allow multi-dimensional models where the function might also depend on eg pulse-phase in a variable source. The output flux array should not be assumed to have any particular values on input. It is assumed to contain previously calculated values only by convolution/pileup models, which have the nature of operators. The output flux error array allows the function to return model variances.

The C and C++ call types allow one extra argument, which is a character string that can be appended to the top line of the model component description. This string is read on initialization and available to the model during execution. An example of its use might be the name of a file with specific data used in the model calculation: this allows different models to be implemented the same way except for different input data by specifying different names and input strings.

C-4 Writing new mixing models

Mixing models are fundamentally different from the other kinds of models since they apply a transformation to a set of modeled fluxes (as enumerated by the spectra in the fit), rather than modify the flux designed to fit a single spectrum. The need to store temporary results, as well as the requirements of the model calculation, lead to many workspace arrays: further, the transformations applied are often fixed during a fit, or can be split to avoid redundant calculations into parts that are fixed and parts that change during iteration in order. XSPEC's internal organization (data structures) can be mapped straightforwardly to the requirements of these models so to implement them efficiently and handle memory allocation, we recommend that mixing models be written in C++ or C. At present only a C++ implementation is available. Users considering adding new mixing model types should contact the developers of XSPEC at **xspec12@athena.gsfc.nasa.gov**

Appendix D Overview of PLT

As in previous versions, the initial release of XSPEC12 uses the PLT library, which is in turn based on PGPLOT[5], to implement its plotting capabilities.

Future versions will be able to offer other plotting library options.

Extensive documentation for the PLT graphics routine is available in the ***The QDP/PLT Users's Guide*** and from PLT's interactive help. This appendix is intended to provide information to assist in using PLT from within the XSPEC program.

Within XSPEC, it is possible to set your graphics device using the CPD command. Any PGPLOT device supported by your local version of PGPLOT is accepted. The CPD command can also be used to display a list of all PGPLOT devices. If you fail to enter a device name, you will be prompted for a PGPLOT device every time you generate a new plot.

From XSPEC, there are two ways to call the PLT routine. Both have the same syntax which is described in the corresponding manual section.

- The **plot** `<plot mode>` command will produce a graph and control will return immediately to XSPEC.
- The **iplot** `<plot mode>` command will put XSPEC into interactive plot mode. The `PLT>` prompt will appear after the XSPEC plot command has finished producing the same graph. At this point, you can enter PLT commands to inspect interesting parts of the graph, add labels, or make a hardcopy file for later printing.

D-1 Getting started with PLT

In the following description of PLT commands, the full command is descried. Capital letters denote the shortest abbreviation of the command that will be recognized. Here is a brief guide to some of the PLT commands that can be entered when **iplot** is invoked.

HElp will provide you with descriptions of the PLT commands.

Plot redraws the display using all of the commands that change the graph entered since the last plot.

Rescale `[<X,Y>]`

followed by two numbers, will set the minimum and maximum of the plotted x-range to the numbers specified. Without further arguments, **Rescale** X or Y will reset the minimum and maximum values to their default values. **Rescale** also updates the screen immediately. Other

---

[5] PGPLOT is the name of a Graphics Subroutine Library written by T. J. Pearson

at the California Institute of Technology

commands allow you to make several changes to the the graph without having to wait for the screen to be updated after every change.

LAbel `<Top,X,Y> [<string>]`

add labels to various locations on the graph. For example, typing

LA Top EXOSAT was great

Will cause the message "EXOSAT was great" to appear at the top of the graph the next time the display is redrawn. Without the string argument the current label for Top, X, or Y is set to the empty string.

Hardcopy [?, PGPLOT plot device]

Create a file that can later be printed. Since it redraws the graph and sends it to a file, it does not reproduce what currently is visible on the graphics display, but rather what you would see if you re-issued the **Plot** command. With the optional "?" argument, **Hardcopy** returns the current hardcopy plotting device. This can be overridden with **Hardcopy** `[PGPLOT device name].`

EXit return control to XSPEC. Any changes you have made to the plot will be lost.

D-2 PLT Command summary

CLear	Immediately clear the graphics device
COlor	Change the default colour index
CONtour	Produce a contour plot
CPD	Change the plotting device
CQuit	Clear the graphics device and return control to XSPEC
CSize	Change the default character size
Error	Control whether errors are displayed and used in fitting
EXit	Exit PLT and return control to XSPEC
Fit	Fit the PLT model to the data
FNy	Evaluate the model at the specified location
FOnt	Change the default text font

Freeze	Freeze a parameter value
GAp	Change the default gap size between the data and the edge
Grid	Control the location of the major and minor tic marks
Hardcopy	Make a file that can later be printed
HElp	Obtain help on any PLT command
Imodel	Numerically integrate the model over specified range
LAbel	Add or remove labels from the plot
LIne	Control whether a line is used to connect data points
LOg	Control whether data is plotted using a $\log_{10}$ scale
LStyle	Change the default style of the line connecting the data points
LWidth	Change the default line width
MArker	Control whether the data points are plotted with markers
MOdel	Define a PLT model
Newpar	Change a parameter value associated with the model
PLot	Immediately re-plot the data
PRompt	Change the `PLT>` prompt
Rescale	Reset the minimum and maximum plot range
SCr	Change the color representation of the specified color index
SHow	Display the values of PLT internal variables
SKip	Control how PLT divides data into vectors
STatistics	Compute various statistical properties of the data
THaw	Allow a parameter value to vary during a fit
Time	Control whether the time stamp is plotted
Uncertainty	Compute the uncertainty in a parameter value
VErsion	Display date of the most recent modification to PLT

Viewport	Control the size of the viewport plotting area
WData	Write a QDP data file to disk
WEnviron	Write both QDP data and header files to disk
WHead	Write a QDP header file to disk
WModel	Write a model file to disk
Xaxis	Define the method used to calculate the x-variable
Yaxis	Define the y-axis scale for a contour plot
$	Execute operating system commands
@filename	Read commands from a PLT command (.PCO) file

Appendix E Associated programs

Introduction

The **HEAsoft** package provides a number of programs and subroutine libraries to manipulate the FITS files used by XSPEC. A description of most tasks can be obtained by typing help taskname or to get a complete list fhelp ftools.

HEAsoft reading tasks

FTLIST Prints the contents of a FITS file to the screen or to a file.

DMPRMF Prints the contents of a FITS RMF file to the screen or to a file.This tool prints the RMF file in a more legible fashion than FTLIST.

HEAsoft manipulation tasks

FPARKEY Changes the value of a keyword in a FITS extension header.

GRPPHA Defines (or redefines) and/or displays the grouping and quality flags, the important keywords, and the fractional systematic errors.

RBNPHA Compresses a FITS PHA file to a user-defined number of channels. The output is a new file containing the revised PHA extension plus a direct copy of any other extensions in the original file.

MATHPHA Performs arithmetical operations on PHA files.

CMPPHA Convert a type II pha file to a type I pha file.

RBNMF Bins a FITS RMF file (the detector response matrix) in channel or energy space.

CMPRMF Compress an RMF by removing all response below a threshold value.

ADDARF Adds together ARFs.

ADDRMF Adds together RMFs.

MARFRMF Multiplies an RMF file by an ARF file.

GENRSP A generic spectral response generator.

HEAsoft subroutines

The directory `ftools/callib/src/gen` in the HEAsoft distribution contains a number of subroutines for reading and writing the extensions in FITS format spectral and response files. More information on their use can be obtained from the xspec website at:

http://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/fits/fitsfiles.html

RDPHA2 Read a spectrum extension

WTPHA3 Write a spectrum extension

RDRMF5 Read the matrix extension

WTRMF5 Write the matrix extension

RDEBD4 Read the channel boundaries extension

WTEBD4 Write the channel boundaries extension

RDARF1 Read the effective area extension

WTARF1 Write the effective area extension

Appendix F Using The XSPEC Models Library In Other Programs

For those who wish to incorporate the standard XSPEC model functions library into their own programs, XSPEC provides a set of functions and wrappers that can be called from external C, C++ or Fortran programs.

F-1 Calling Model Functions From C And Fortran

An increasing number of XSPEC model functions are written in C++, and have the C++-style function interface described in Appendix C. XSPEC provides function wrappers for each of these to make them callable from Fortran or C programs. The wrappers are stored in the files funcWrappers.h and funcWrappers.cxx in the XSFunctions directory.

For each C++ model function there are 2 wrappers: one for passing single precision arrays and one for double precision, with the interfaces as shown in Appendix C for single precision Fortran-style and C-style respectively. The single precision wrapper function name will be the original C++ function name appended with a "f_ " prefix, while the double precision wrapper will have a "C_ prefix".

For example, XSPEC's model.dat entry for the power law model lists the function name C_powerLaw. This shows that the actual function name is "powerLaw" and the "C_" indicates it has a C++ interface inside XSPEC. funcWrappers.cxx defines the following 2 wrappers:

```
void f_powerLaw(const float* energy, int nFlux, const float* params, int
                spectrumNumber, float* flux, float* fluxError)
```

```
void C_powerLaw(const double* energy, int nFlux, const double* params, int
                  spectrumNumber, double* flux, double* fluxError, const char*
                  initStr)
```

The second function is intended to be called from C programs, while Fortran programs may call either (funcWrappers.cxx also includes CERN <cfortran.h> definitions to make these accessible to Fortran).

F-2 Interface Routines

XSPEC also provides a set of functions for accessing some of the model functions' internal data. The C++ functions are listed in the file FunctionUtility.h in the XSUtil/FunctionUtils directory. For C and Fortran access, equivalent wrapper functions are listed in the same directory in xsFortran.h. The wrapper functions have C-style function declarations, and are also made available to Fortran calling routines via the CERN <cfortan.h> interface.

The currently provided C/Fortran wrapper functions are (see xsFortran.h for the function signatures):

FNINIT	Initializes data directory locations needed by the models. See below for a fuller description.
FGABND	Get an element abundance.
FGCHAT	Get current chatter level setting for model functions' output verbosity.
FPCHAT	Set the chatter level. Default is 10, higher chatter levels produce more output.
FGDATD	Get the model .dat files path.
FPDATD	Set the model .dat files path.
FGMODF	Get the model ion data path.
FGMSTR	Get a model string value (see XSPEC xset command).
FPMSTR	Set a model string value.
FPSLFL	Load values of a "file" solar abundance table (see abund command).
FGSOLR	Get the solar abundance table setting.
FPSOLR	Set the solar abundance table.
FGXSCT	Get the cross section table setting.
FPXSCT	Set the cross section table.

csmgh0	Get the cosmology H0 setting (see the cosmo command).
csmph0	Set H0.
csmgl0	Get Λ0.
csmpl0	Set Λ0.
csmgq0	Get q0.
csmpq0	Put q0.
fzsq	Computes the luminosity distance, (c/H0)*fzsq. The function is valid for small values of q0*z for the case of no cosmological constant and uses the approximation of Pen (1999 ApJS 120, 49) for the case of a cosmological constant and a flat Universe. The function is not valid for non-zero cosmological constant if the Universe is not flat.
xs_getVersion (or xgvers)	Retrieve XSPEC's version string.

F-3 Initializing the Models Library

The external program should always call the FNINIT routine prior to any other call into the models library. This initializes the locations of the various data files needed by the models, and also sets the abundance and cross-section tables. Unless the user has overridden the model ion data directory location with the XSPEC_MDATA_DIR environment variable, the initial settings are:

Model ion data location	$HEADAS/../spectral/modelData
Abundance and cross-section .dat files location	$HEADAS/../spectral/manager
Solar abundance table	angr
Photoelectric cross-section table	bcmc

F-4 Building with the Models Library

The XSFunctions library depends on three lower-level XSPEC libraries, XS, XSUtil, and XSModel, and also the CCfits and cfitsio libraries distributed with HEASOFT. A Makefile for a small Fortran program linking with the models library therefore may look like this on Linux:

```
myprog : myprog.o
        g77 -g myprog.o -o myprog \
                -L/path/to/headas/installed/location/lib \
                -lXSFunctions -lXSModel -lXSUtil -lXS -lCCfits_2.1 -lcfitsio_3.11
myprog.o: myprog.f
        g77 -g -c myprog.f
```

Appendix G Adding a Custom Chain Proposal Algorithm

When running a Monte Carlo Markov Chain with the **chain** command, XSPEC provides several built-in proposal options from which to draw trial parameter values for the next step in the chain. A **built-in** proposal is selected prior to the chain run with the command:

chain proposal <distribution> <source>

where <distribution> is the statistical distribution used to randomize the parameter values (e.g. `gaussian`, `cauchy)`, and <source> refers to the source of the applied covariance information (see the **chain** command for details).

It is also possible for the user to create an arbitrary new proposal scheme and add it to the options available under the chain proposal command. This is done in a way similar to the adding of local models described in Appendix C, though in this case the code can only be written in C++. Essentially three steps are involved, each described in greater detail below:

- Create a small text file named randomize.dat.
- Write a class which inherits from XSPEC's abstract base class RandomizerBase.
- Run XSPEC's **initpackage** and **lmod** commands to build and load the shared library containing the new proposal class(es).

G-1 The randomize.dat Initialization File

This file must be placed in the same directory as the user's proposal code files, and plays a role similar to the local models' .dat initialization files, though it has a much simpler structure. It also MUST be named randomize.dat, for this name is the only clue **initpackage** has to distinguish between creating a chain proposal or local models library.

All that needs to be entered into this file is a line of the form:

<class name> [<opt string arg1> <opt string arg2> … <opt string argN>]

for each proposal class that will go in the library. <class name> must be a case-sensitive match to the actual C++ class name, and is the only required entry on the line. The class should also be stored in code files <class name>.h and <class name>.cxx.

Any additional arguments on the line will be placed in a single C++ string (including any separating whitespace), and passed to the class constructor. This is to allow the option of setting initialization parameters at the class construction stage. Therefore if optional arguments are included, the class must have a constructor which takes a single string argument. Otherwise, the constructor should contain no arguments.

For example, a randomize.dat file declaring two classes might contain:

```
MyProposal1
MyProposal2    1.4773     on      false
```

In the code files, the constructor declarations corresponding to this would then be:

MyProposal1.h

```
class MyProposal1 : public RandomizerBase
{
   public:
   // …
   MyProposal1();
   // …
};
```

MyProposal2.h

```
class MyProposal2 : public RandomizerBase
{
   public:
   // …
   MyProposal2(const string& initArgs);
   // …
};
```

G-2 Writing a Chain Proposal Class

All user proposal classes must inherit from XSPEC's abstract class RandomizerBase, whose interface is defined in the file:

headas-<version>/Xspec/src/XSFit/Randomizer/RandomizerBase.h.

The proposal class must declare a constructor as described in the previous section, and which explicitly calls the RandomizerBase constructor, passing it a lower-case name string. This name will become the proposal identifier when making a selection using the `chain proposal` option during an XSPEC session. For example:

MyProposal1.cxx

```
MyProposal1::MyProposal1()
   : RandomizerBase("myprop1")
{
}
```

In XSPEC:

```
XSPEC12> chain proposal myprop1 [<optional initializing args>]
```

The RandomizerBase class contains 5 private virtual functions: doRandomize, doInitializeLoad, doInitializeRun, doAcceptedRejected, and getCovariance:

doRandomize is the only pure virtual function and therefore is the only one which **must** be overridden in the inheriting class. Its signature is:

virtual void doRandomize(RealArray& parameterValues, const Fit* fit)

where RealArray is a typedef for std::valarray<double> and is defined in src/main/xsTypes.h. This function is called by XSPEC for each chain iteration, and XSPEC passes in the current variable

model parameter values. The overridden doRandomize function performs the necessary parameter modifications and sends them back in the same array.

The function's second argument is a const pointer to XSPEC's global Fit class object. For those willing to further explore XSPEC's internals, this pointer provides access to various fit and chain information (such as covariance matrices), which may be necessary for the user's proposal scheme.

doInitializeLoad and doInitializeRun may be optionally overridden to perform initialization tasks at different stages during runtime. The default versions of these functions in RandomizerBase do nothing. doInitializeLoad is called by XSPEC immediately after the proposal is selected with the `chain proposal` command. Therefore one may find it useful to have this function process any additional arguments which may be entered on the command line:

```
chain proposal myprop [<optional initializing args>]
```

XSPEC automatically bundles `[<optional initializing args>]` into a single string and places it in the m_initString data member of RandomizerBase, to which the inheriting class has access. doInitializeRun is called once at the start of a chain run, and is useful for any tasks which must be performed one time immediately after the `chain run` command is entered.

doAcceptedRejected is called after each iteration in the chain. Its first argument is an array filled with the most recently attempted model parameter values, and its second argument is a boolean true or false indicating whether the attempt was accepted or rejected. The base class function does nothing with this, but an inherited class may want to use this information in an overriden function.

In its simplest form, a proposal class may be declared and defined as in the following example. This doesn't actually do anything since the doRandomize function is empty and the parameterValues array is left unchanged.

MyProposal.h

```
#ifndef MYPROPOSAL_H
#define MYPROPOSAL_H

#include <xsTypes.h>
#include <XSFit/Randomizer/RandomizerBase.h>

class Fit; // only a forward declaration is required for Fit

class MyProposal : public RandomizerBase
{
   public:
      MyProposal();
      virtual ~MyProposal();
   private:
      virtual void doRandomize(RealArray& parameterValues, const Fit* fit);
};

#endif
```

MyProposal.cxx

```
#include "MyProposal.h"
#include <XSFit/Fit/Fit.h>

MyProposal::MyProposal()
   : RandomizerBase("myprop")
{
}

MyProposal::~MyProposal()
{
}

void MyProposal::doRandomize(RealArray& parameterValues, const Fit* fit)
{
   // This is where the proposal algorithm should modify the variable
   // model parameters in the parameterValues array.
}
```

G-3 Building and Loading the Proposal Class Library

Once the randomizer.dat file and the class(es) have been written, the library can be built and loaded during an XSPEC session using the same **initpackage** and **lmod** sequence that is used for local model libraries. To create a Makefile and build the library:

```
XSPEC12> initpackage <name> randomizer.dat <directory>
```

To load the new proposal(s) into XSPEC:

```
XSPEC12> lmod <name> <directory>
```

where `<name>` is the name you choose for the package collection of proposal classes. It will also become the library file name. The only differences from the local models case are that here the initializer file MUST be named randomizer.dat, and that the directory path to the proposal classes (either relative or absolute) must be provided on the command line. If this is left off XSPEC will default to looking in the directory set by LOCAL_MODEL_DIRECTORY, and these classes should NOT be stored in the same directory as local models. If the building and loading has successfully completed, you should see the proposal name (the same name string that was passed to the RandomizerBase constructor) appear in the chain proposal list displayed by typing `chain proposal` with no other arguments.

Appendix H Changes between v11 and v12

In 1998 we decided to re-engineer XSPEC using modern computer science methods so it could continue fulfilling its role as a mission-independent X-ray spectral fitting program.

The program's internal design, layout, and data structures have largely been rewritten in ANSI C++ using **object oriented design techniques**, generic programming techniques, and **design patterns**. The thoroughgoing reanalysis has also allowed a number of improvements in overall design and, at robustness, as well as maintainability, *without changing the familiar syntax*. With a few exceptions here and there, the new program syntax is fully backward-compatible with that of v11: most of the exceptions support new features that are enhancements

(and can be ignored if not relevant to the user's problems). Some features of v11 previously declared to be deprecated have been removed.

At the same time, the core of the XSPEC calculation scheme has been retained, in particular the models library, written almost exclusively in fortran77.

Model implementation has been rewritten to support allow models written not only in single precision fortran, but double precision fortran, C, and C++. Further, XSPEC can now be used as a development environment for local models by allowing recompilation from the command prompt.

In v12, spectra can be fit with more than one distinct model simultaneously, provided separate model components can be assigned distinct response functions. This is particularly useful for spectra from coded aperture masks.

A new internal dynamic expression implementation allows more complex (multiply-nested) models, and also allows parameter links to be polynomial functions of one or more parameters.

Great care has been taken to optimize the program for memory usage and execution speed. A revision of the numerical derivative algorithm has reduced the number of convolution operations required during fitting. On the other hand, v12 performs its calculations in double precision (apart from the models library), and this with the more complex model expression evaluations reduces execution speed. Taken together, v12 should outperform v11 when the number of channels is large and the model to be fitted is relatively simple and should be comparable in other circumstances.

The default fitting algorithm (Levenberg-Marquadt) has been retained intact. New fitting algorithms and objective functions (statistics) may be added to the program at runtime. The CERN Minuit/migrad algorithm has been better integrated into the code and its documentation is now directly accessible during XSPEC sessions.

Type II (multi-spectrum) OGIP files are now fully supported. Multiple ranges can be selected in the data command, and support is present for Type II background and arf files. Observation simulations (the **fakeit** command) now operate on Type II inputs.

The online documentation scheme is now implemented using pdf or html files, replacing the older VMS-style help system. The help scheme can be configured to use external applications such as Adobe Acrobat or the xpdf readers as well as web browsers. Users can document their own local models and tcl-scripted procedures in pdf and html files and add them to the help system.

Plotting within v12 is backward compatible with a few small extensions. Although it is currently implemented using PLT, explicit dependence on the plot library has been removed. This will allow alternative plotting libraries to be used in future. The PLT plotting package is described briefly in Appendix D and in more detail in the "QDP/PLT User's Guide" (Tennant, 1989).

v12 communicates with the user through the familiar command line interface. The input/output streams, however, can in future be easily redirected to communicate with the user through a graphical user interface (GUI).

Finally, the design implements a new error handling system can return the program safely to the user prompt when an error occurs and leave the program in a state from which the user can continue working. Also, for the first time there is now an **undo** command.

Integral Spectrometer/Coded Mask Instrument Support

The **INTEGRAL** Spectrometer (**SPI**) is a coded-mask telescope, with a 19-element Germanium detector array. There are several complications regarding the spectral de-convolution of coded-aperture data. For XSPEC the most obvious problem is the source confusion issue; as there may be multiple sources in the FoV leading to different degrees of shadowing on different detectors. Thus, a separate instrumental response must be applied to a spectral model for each possible source, for each detector. If there are multiple sources in the FoV, then additional spectral models can be applied to an additional set of response matrices, enumerated as before over detector and dither pointing. This capability —to model more than one source at a time in a given minimization procedure—did not exist in XSPEC prior to v12. The other unique aspect of the INTEGRAL analysis is that the background is modeled along with the source(s) in a single de-convolution.

XSPEC analysis of INTEGRAL/SPI data is very different from other instruments is the manner in which the response matrices are handled. Since there are a large number of responses involved in the de-convolution problem, memory use becomes a concern. To load the required response matrices (as XSPEC normally does), would require $\sim(N_{ch})^2 \times N_p \times N_d$ floating-point memory locations per source. This could become quite large for high-spectral resolution and/or long observation scenarios. To address this problem, a methodology has been developed to reconstruct the required 2-D response matrices from a basis set, consisting of a small number (3) of 2-D objects (template RMFs), and a larger number of 1-D objects (component ARFs). The full matrices can then be reconstructed "on the fly" at the minimization step of the calculation, and discarded after each use. This, in principle, occurs all very transparently to the user.

A fuller description of Integral data analysis appears in section **2** of this manual and a walkthrough example is given in **4.6**.

Current Exclusions

The v11 commands and features not provided in v12 are:

Feature	Rationale for exclusion
recornorm	With version 12.5.0, this has been replaced and improved upon by the recorn mixing model.
thleqw	Rarely used command not yet implemented.
extend	Beginning with version 12.3.0, this has been replaced by the more flexible **energies** command.
background models	This has been replaced by v12's multiple source modeling techniques

Additionally, we have withdrawn seldom-used fitting methods anneal and genetic. Future development will add new techniques.

Appendix I Older Release Notes

v12.5.0 Nov. 2008

- Two of the remaining unimplemented v11 commands have now been added.

  mdefine allows dynamic definition of models that can be expressed algebraicly.

  recornrm has been replaced by the **recorn** model. This allows the correction norm to be treated as a fit parameter, a better solution than the v11 recornrm command.

- The complete HTML help files are included in a tar file. These can be made available on a local machine if remote access is now available and selected in the Xspec.init file.
- Convolution components can now operate on multiplicative components. For example, in the model = (CM)A, the convolution component acts on only the multiplicative component. Previously this would have been treated the same as C(MA). The **partcov** partial covering model takes advantage of this new capability.
- There is a new simple way of estimating fluxes (and their errors) from parts of the model. Apply the **cflux** convolution model to the component(s) for which the flux is required.
- The following models have been added as standard
  - **diskir** : irradiated disk
  - **kerrdisk** : broad iron line from a disk around a Kerr BH
  - **nsmax** : NS magnetic atmosphere
  - **nthcomp** : thermally Comptonized continuum
  - **spexpcut** : super-exponential cut-off
  - **swind1** : partially ionized absorbing material with velocity shear
  - **zxipcf** : partial covering of partially ionized absorbing material
  - **cflux** : calculate the flux from model component(s)
  - **kerrconv** : broadening due to rotation around a Kerr BH
  - **partcov** : partial covering modifier for absorption models
  - **simpl** : Comptonization of a seed spectrum

- **recorn** : Vary the correction file normalization

- The **lrt.tcl** and **simftest.tcl** scripts perform the likelihood ratio and F-tests, respectively.
- The **writefits.tcl** script writes filenames and current fit parameters and errors to a single row of a FITS file. This script can be used as a template for saving other information.
- A response of "/*" to a "y/n" prompt will jump out of the current operation and return to the XSPEC command prompt. This is particularly useful for escaping nested fits during an **error** command run.
- The units have been changed for **setplot** wave plots. model and ufspec have a y-axis in photons/cm^2/s/Hz, emodel and eufspec in Jy (10^-23 erg/cm^2/s/Hz), eemodel and eeufspec in erg/cm^2/s.
- **Fakeit** can now work with multiple-extension response files. It also works correctly when multiple models are in use (this was release in patch v12.4.0r).
- The active|inactive|options can be applied to the default (unnamed) model (released in patch v12.4.0v).
- Support for GLAST GBM extensions to the standard file formats including multiple response matrix extensions in the same file (released in patch 12.4.0am).
- There are additional diagnostics available at high chatter levels from MCMC **chain** runs. User's custom proposal classes have access to information about acceptances and rejections.
- Initial support for multicore processors using the OpenMP parallel processing compiler option. Multiplication of the model and response is performed in parallel across the multiple spectra in a datagroup.
- All bug fixes to v12.4.0 released as patches a - ar are included in v12.5.0. In addition the following problems have been corrected.
  - When a runtime error is encountered during the calculation of a parameter's error bounds (using the **error** command), the value is now filled in with 0.0 rather than retaining its previous value.
  - **Steppar** will now correctly step in reverse direction if the range values were entered in high-to-low order.
  - Model expression parsing has been improved for nested expressions.
  - Log file output has been fixed so '#' comments are placed correctly.
  - The chi-square calculation includes the **corfile** contribution even if there is no background file associated with the spectrum.

  - There are minor plotting fixes to the confidence line in 1-D steppar/margin plots, the rescaling of the Y=0 green line in lower-panel plots, and the Y-axis label in plot delchi.
  - **Tclout** peakrsid no longer fails for a spectrum whose model was not assigned to source 1.
- The XSFunctions library now also depends on XSModel, requiring the addition of a -lXSModel flag to the Makefile of external programs linking with the XSPEC model functions library. (See **Appendix F**)
- The modelIonData model data files directory has been renamed to modelData.
- Portions of some model functions have been translated from Fortran to C++ to reduce use of the udmget memory allocation function. Future versions will remove all references to udmget.