MIT Center for Space Research **AXAF Science Center**

CSR

ISIS: Interactive Spectral Interpretation System
Overview of Functionality

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1 Science Goals

To make full use of the high resolution X-ray spectra from AXAF HETGS and LETGS and from other upcoming missions including XMM, Astro-E and Constellation-X, spectroscopic analysis techniques similar to those used in high resolution optical spectroscopy must be introduced in the X-ray community. ISIS (Interactive Spectral Interpretation System) will support these analysis techniques by facilitating spectroscopy database searches and by performing standard spectroscopic measurements adapted for the X-ray band. The database search tools in ISIS will help X-ray astronomers take full advantage of the detailed X-ray spectroscopy database of Smith, Brickhouse, Liedahl & Raymond (1998) (see Appendix) and will also provide access to older spectral models such as Raymond-Smith, MEKA and MEKAL. The ISIS spectroscopic measurement tools will provide both a complement and an important alternative to the forward-folding analysis approach currently used in X-ray astronomy. Fundamentally, ISIS supports a shift from “model-driven” analysis to “data-driven” analysis.

The forward-folding approach now common in X-ray astronomy is necessarily “model-driven” because the algorithm requires a global spectral model to be folded through the instrumental response for comparison with the data. In contrast, standard optical spectroscopic analysis techniques are “data-driven” in the sense that one measures the characteristics of spectral features (e.g. emission line intensities) *independent* of a theoretical model of the spectrum. Interpretation of these measurements necessarily requires a theoretical model, but the measurements themselves represent model-independent observables that can be used to test future alternative theoretical models of astrophysical sources.

2 Status

ISIS is currently in prototype stage under interative development and in evolution. The current version is v0.2.

3 Features

The principal new feature of ISIS that distinguishes it from other spectral analysis systems such as ASCFit and XSPEC is that it provides tools to aid in understanding the detailed physics of spectrum formation down to the level of the formation of individual emission lines and line complexes. ISIS gives users access to an extensive database of atomic data and plasma emission models, allowing them to display energy level diagrams, to filter line lists and to gain access to individual emission components contributing to theoretical models of plasma X-ray emission.

Another important feature of ISIS is its high-level scripting language. This feature is particularly important because, given the evolving nature of high-resolution X-ray spectral analysis, users need the ability to implement and refine newly invented analysis techniques. With its powerful scripting language, ISIS will be extensible either through use of command scripts (including branching and looping structures) or through user-defined commands which access external functions coded in C (via dynamic linking). Through this mechanism, users will be able to add functionality to the system and supply alternate algorithms for supplied commands. Furthermore, the core routines of ISIS will also be made available as an ANSI-C subroutine library with a documented interface so that users can access the spectroscopy database using the ISIS subroutines directly in their own programs.

The initial release of ISIS will be command line or script driven (with command history mechanism and command line editing), and the plot window will support mouse cursor interaction (e.g. as an alternate method for specifying wavelength regions of interest). ISIS will also support logging of all interactive commands.

The primary input data for ISIS are 1) high resolution X-ray spectra (either a count histogram or flux-corrected spectrum) 2) the spectroscopy database, and 3) mission calibration data (rmf, arf, detector gap locations, etc.). Detailed descriptions of these files may be found in the Interface Control Documents for Level 2 Data Products (Version 1.2), the Spectroscopy Database (Version 0.7), Analysis Reference Data (Version 1.1) respectively. These documents are available from

`http://hea-www.harvard.edu/asclocal/sds/development/ICD/index.html`.

ISIS output files may contain database-selected inputs (e.g. lists of selected emission lines, edges or other atomic data, line intensities and line ratios as a function of temperature and density, model spectra or spectral components) as well as line and continuum fit parameters with confidence limits. A key component will be a file which contains a list of observed spectral features or regions of interest along with analysis results for each feature (feature identification information, fit parameters, etc.). While the detailed format of the output files is TBD, the output formats will build on existing file formats to the extent possible, making it easier for other programs to read ISIS output for further processing. For example, to write out a model spectrum using a particular wavelength grid, ISIS will probably use a FITS file format which is similar to a standard PHA file. The format most useful for each of the various output files is likely to evolve during ISIS development. In particular, it is desirable that the ASC DataModel be capable of working with all ISIS FITS input and output files. As development proceeds, output file formats will be frozen and clearly documented in ICDs.

3.1 Database Queries

The initial ISIS release will be developed to make use of the X-ray spectroscopy database of Smith, Brickhouse, Liedahl & Raymond (1998) (see Appendix), although ISIS will be designed to allow working with alternate spectroscopy databases. Spectral models will be assembled using line and continuum emissivities, abundances and ionization fractions retrieved from the database. The atomic structure parameters and atomic transition rates on which the emissivities are based will also be available. Access to the outputs of older spectral models such as Raymond-Smith, MEKA and MEKAL will also be provided, although with much less functionality, because the detailed input atomic data for those models are not available in a convenient format.

- Lines
  - Retrieve line lists based on a wide range of search criteria (e.g. filter on element, ion, upper level, lower level, wavelength, wavelength uncertainty, ionization potential of parent ion, temperature of peak abundance of parent ion, density sensitivity, predicted intensity range for given input model, potential absorption optical depth based on Einstein A value and user-specified column, etc.).
  - Generate, change, and refer to a user-defined subset of the line list (useful for e.g. correcting wavelengths of a subset of lines of interest).
  - Plot line intensities and line ratios vs. temperature, density or other line ratios.
  - Overlay color-coded line identification labels on plot of observed data or computed theoretical model.
  - Save retrieved line data to a conveniently formatted file (the detailed format is TBD).
- Continua
  - Read in continuum components from individual elements and ions.
  - Display continuum components along with total continuum for a given input model
  - Save continuum and components to conveniently formatted file (the detailed format is TBD).
- Edges
  - Retrieve list of edges in a given wavelength range, for given input model. Select useful subset (e.g. just the strong edges using user-supplied criterion).
  - View high-resolution data on edge structure where available.
  - Over-plot predicted edge positions on spectral data.
- Atomic Structure
  - Display plots of energy level structure of individual ions and display the strongest transitions between energy levels.
  - Given a particular line identification, display the relevant energy level structure and show related lines.
  - Report source and accuracy of input atomic data where that information is available.
- Spectral Models
  - Read in a set of single-component collisional equilibrium models with user-defined abundances, temperatures, densities and construct multi-component models with user-defined normalizations. Modify models by applying user-supplied redshifts or line broadening.
  - Over-plot model and data.

- Save model (along with all components) to a conveniently formatted file (the detailed format is TBD).
- Apply user-defined ionization balance.
- View ionization fractions as function of temperature and density.
- Allow substitution of an alternate emissivity database (computed using the same atomic data set) or of both the atomic data set and a matching emissivity database.
- Ability to test robustness of line emissivity predictions. This will probably involve extracting a subset of relevant atomic data from the database, altering selected parameters (rates) and re-computing line emissivities to see the effect of the change. (This approach may only be practical for line complexes whose behavior can be modeled with a relatively small number of energy levels.)

3.2 Measurement Features

Early ISIS development will deal almost exclusively with database access functionality, although we may also include some simple spectral measurement capability. Eventually, it will be necessary to have much more powerful measurement features within the same system that provides access to the spectroscopy database. In a future ISIS release, these functions could be provided by linking to ASCFit (and/or XSPEC).

Ultimately, ISIS will handle multiple data sets simultaneously (e.g. to analyze multiple HEG and MEG plus and minus orders simultaneously as separate spectra). In model fitting (e.g. fitting one or more line profiles plus continuum), the user will be able to freeze individual or multiple fit parameters at known values and to specify limited allowed ranges for otherwise free fit parameters. It will also be possible to fold a theoretical model through the instrumental response for comparison with the raw count histograms. Fitting of differential emission measure models is unlikely to be supported in the initial release although may be included in a later version. Measurement results will be logged to a conveniently formatted file (the detailed format is TBD). Both screen and postscript plots will be supported. Screen plots will allow multiple plot windows with zoom and overplotting of data and models.

- Lines
  - Compute total counts or total flux between two bins or between two wavelengths.
  - Fit line profile (instrumental, thermal, convolution, user-defined) plus continuum (polynomial, power-law, bremsstrahlung, user-defined) and compute goodness of fit with confidence limits. Allow user-defined continuum, either by eye or from external model.
  - Account for instrumental features by referring to relevant calibration data (locations and effects of edges, chip gaps, etc.).
  - Fit multiple line profiles plus continuum to small spectral regions which appear to have blended lines.
  - Supply Gaussian, Lorentzian, Voigt profiles, plus instrumental, convolution operator and user-defined profile.
  - Display position of higher-order features (useful for LETG).
- Continua
  - Fit polynomial, power-law, brems, thermal, multi-temperature, user-defined.

  - Include ISM absorption using the most detailed available atomic data.

- Edges
  - Fit piecewise functional model or user-defined model.

4 Possible Future Improvements

These are features which may be desirable, but may fall outside the scope of the ISIS development effort, may require significant algorithm development and testing, or which should reasonably occur at a later date.

- Fitting differential emission measure models.
- LETG order-separation via bootstrapping from high energy/low order to low energy/high order. Existing algorithms need to be tested against realistic data, beginning with the Emission Line Project data. Until algorithms are tested and shown to be effective, this should be a low priority for ISIS development.
- Capability to fit 2-D detector image/grating spectral data. Algorithms should be tested and proven before integration into ISIS.
- Ability to use pipeline functions (*specdetect, specmeasure, specidentify*) in an interactive mode. This should occur naturally once ISIS is integrated into the ASCDS. [*specdetect* automatically finds emission lines in grating spectra, *specmeasure* fits line profiles, *specidentify* generates candidate line identifications.]

5 Appendix: Content of the Spectroscopy Database

This is a brief summary of the content of the spectroscopy database of Smith, Brickhouse, Liedahl, & Raymond 1998; formatting details may be found in the Spectroscopy Database ICD (Version 0.7). The database will contain, among others, the following tables:

- elemental abundances
- ionization balance models as a function of temperature and density
- continuum emissivity tables
- For each ion:
  - energy levels
  - emission line wavelengths, transition probabilities
  - line intensities as a function of density and temperature
  - collisional excitation rate coefficients
  - ionization and recombination rates with errors

All data will be stored in FITS files with the atomic data kept separate from the emissivities and other quantities dependent on the physical state of the plasma. It is intended that the format be as generic as possible so that all or part of the database can be easily replaced, perhaps to substitute an alternate ionization balance calculation, or an alternate table of line intensities.

6 References

Smith, R., Brickhouse, N., Liedahl, D., & Raymond, J., 1998, "High Resolution X-Ray Spectroscopy: Issues for Creating an Atomic Database for a Collisional Plasma Spectral Emission Code", in "Science with XMM: The First XMM Workshop", in press.