Astronomical Data Analysis Software and Systems IX
ASP Conference Series, Vol. 216, 2000
N. Manset, C. Veillet, and D. Crabtree, eds.

ISIS: An Interactive Spectral Interpretation System for High Resolution X-Ray Spectroscopy

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Abstract. The Interactive Spectral Interpretation System (ISIS) is designed to facilitate the interpretation and analysis of high resolution X-ray spectra like those obtained using the grating spectrographs on Chandra and XMM and the microcalorimeter on Astro-E. It is being developed as an interactive tool for studying the physics of X-ray spectrum formation, supporting measurement and identification of spectral features, and interaction with a database of atomic structure parameters and plasma emission models. The current version uses the atomic data and collisional ionization equilibrium models in the Astrophysical Plasma Emission Database (APED) of Brickhouse et.al., and also provides access to earlier plasma emission models including Raymond-Smith and MEKAL. Although the current version focuses on collisional ionization equilibrium plasmas, the system is designed to allow use of other databases to provide better support for studies of non-equilibrium and photoionized plasmas. To maximize portability between Unix operating systems, ISIS is being written entirely in ANSI C using free-software components (CFITSIO, PGPLOT and S-Lang).

1. Introduction

To make full use of the high resolution X-ray spectra from Chandra HETGS and LETGS and from other 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 supports 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 help users take full advantage of the detailed X-ray spectroscopy database of Smith, Brickhouse, Liedahl & Raymond (1998) and also provide access to older spectral models such as Raymond-Smith (1977), MEKA and MEKAL (see Mewe, Kaastra & Liedahl 1996 and references therein). The ISIS spectroscopic measurement tools 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.

ISIS supports data-driven analysis by combining support for basic data analysis functions (e.g. computing total counts detected in a line or performing chi-squared fits of line-profiles) with access to a comprehensive spectroscopy database. This database access can be used to facilitate line identification and to support application of line-based spectral diagnostics such as density sensitive line-ratios. It can also be used to investigate the sensitivity of spectral models to various assumptions and input parameters including elemental abundances and ionization balance.

2. Features and Availability

The principal new feature of ISIS that distinguishes it from other spectral analysis systems such as 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 provides quick access to an extensive database of atomic data and plasma emission models making it much easier to extract and manipulate detailed plasma parameters including ionization fractions, line emissivities and continuum emissivities broken down by ion and physical process. Input atomic data values are also available, including energy levels and radiative transition probabilities.

The initial ISIS release has been developed to make use of the X-ray spectroscopy database of Smith, Brickhouse, Liedahl & Raymond (1998), although the design should allow future upgrades to support working with alternate spectroscopy databases. Multicomponent spectral models can be assembled using line and continuum emissivities, abundances and ionization fractions retrieved from the database (see Figure 1). Selected atomic structure parameters and atomic transition rates on which the emissivities are based will also be available. ISIS supports direct access to the outputs of older spectral models such as Raymond-Smith, MEKA and MEKAL, although with much less functionality, because the detailed input atomic data for those models are not available in a convenient format.

Another important feature of ISIS is its high-level command language, S-Lang. This flexible C-like interpreted language provides a wide range of control structures and, because it was designed to be embedded in C programs, provides an easy-to-use mechanism for linking with user-defined software. S-Lang also supports array-based mathematical operations (similar to IDL), providing strong support for operations common to a broad range of analysis tasks. These features are important because, given the evolving nature of high-resolution X-ray spectral analysis, users need the ability to rapidly implement and refine new analysis techniques. ISIS is programmable and extensible either through user-defined command scripts (which may include branching and looping structures) or through the addition of user-defined commands which may access external

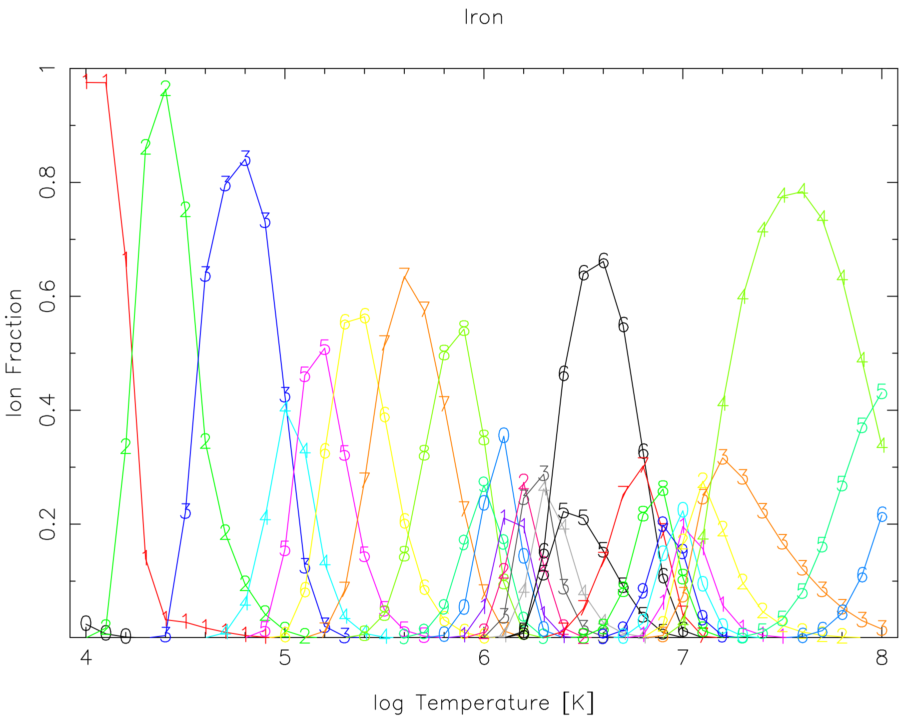

Figure 1. This figure, generated by ISIS, shows the abundance of iron ions as a function temperature in collisional ionization equilibrium (Arnaud & Raymond 1992). Each curve is labeled with the least significant digit of the ion charge; e.g. Fe I is labeled with a "0" and both Fe II and Fe XII are labeled with a "1".

subroutine libraries (via dynamic linking). In this way, users can easily add specialized functionality to the system or supply alternate algorithms for existing functions. In addition, the core routines of ISIS will be available as an ANSI-C subroutine library with a documented interface so that users can use the ISIS subroutines directly in their own programs.

The current version of ISIS can read spectral data in either FITS or ASCII format. The ASCII data format is extremely simple and should make it easy to import data from other formats, the FITS format is the type II pha file format used for Chandra transmission grating observations (see Figure 2). Fitting tools are included to provide support for chi-square fitting of multiple line profiles; several common line profile functions are included and multiple user-defined fit functions may be added as well.

As an example of linking to other software, the current version of ISIS includes dynamically linked modules which provide direct access to selected XSPEC and PGPLOT subroutines. By packaging this functionality in dynamically linked modules, we increase the available functionality while minimizing the amount of software required to install and use ISIS (users not interested in

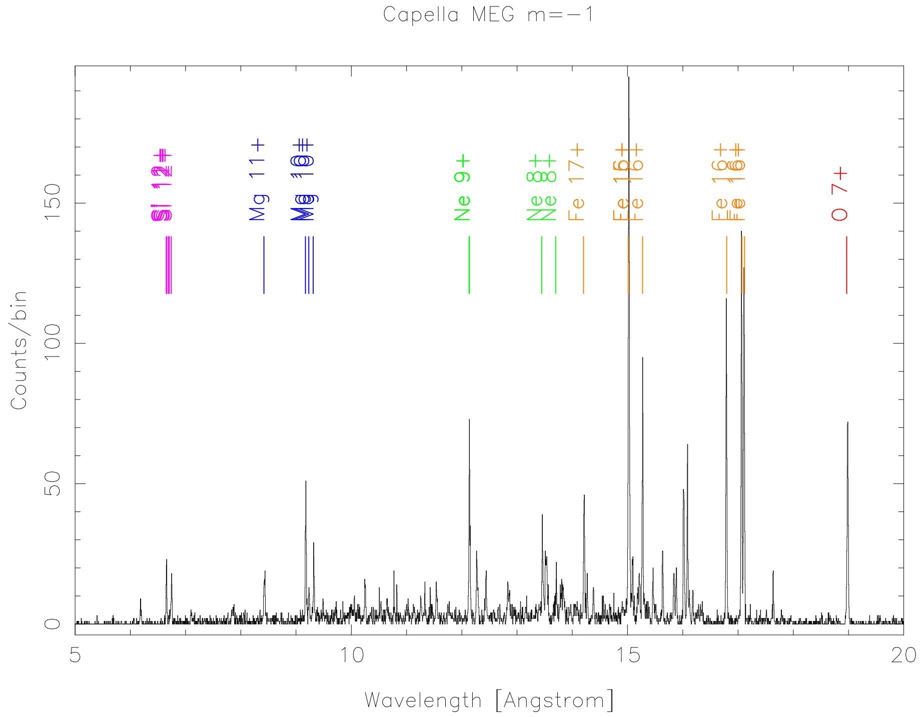

Figure 2. Spectrum of Capella from a 15 ksec observation by the Chandra X-ray Observatory High Energy Grating Transmission Spectrograph (HETGS) on Aug 28, 1999 during the orbital activation and checkout phase.

using the XSPEC module are not required to install XSPEC before using ISIS). Updated information on ISIS is available from the ISIS web page[1].

Acknowledgments. We would like to thank David Davis and Dan Dewey for testing several versions of ISIS and for suggesting numerous improvements. We would also like to thank John Davis for his assistance with the overall design, for contributions of source code and for numerous helpful conversations and suggestions.

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[1] `http://space.mit.edu/ASC/ISIS`