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PINTofALE: Analysis of UV–X-Ray High-Resolution Emission Spectra

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Abstract. We have developed an IDL-based[1] software for *interactive analysis* of astrophysical spectra, with particular emphasis on the high resolution X-ray spectra obtained by *Chandra* and *XMM-Newton*, as well as UV, FUV and EUV spectra from *HST*, *FUSE* and *EUVE*. This package for interactive analysis of line emission (PINTofALE) is based on a modular set of tools that interact with an atomic database and with observational data. The tools are designed to allow easy identification of spectral features, measure line fluxes, and carry out detailed modeling. The basic philosophy of the package is to provide access to the innards of atomic line databases, and to have flexible tools to interactively compare with the observed data. It is motivated by the large amount of bookkeeping, computation and iterative interaction that is required between the researcher and observational and theoretical data in order to derive astrophysical results. The tools link together the processes of spectral "browsing", feature identification, measurement, and computation and derivation of results. Unlike standard modeling and fitting engines currently in use, PINTofALE opens up the "black box" of atomic data required for UV/X-ray analyses and allows the user full control over the data that are used in any given analysis. PINTofALE is publically available at `http://hea-www.harvard.edu/PINTofALE/` .

1. Rationale

Imaging spectrometers such as those of *Beppo*SAX, ASCA, *Chandra*/ACIS, etc. provide modest resolving power of up to $\sim$ 10 at soft X-ray wavelengths — sufficient to resolve broad, blended line complexes from underlying continuum emission but well below that required to investigate individual spectral lines. However, the diffraction gratings of *Chandra* and *XMM-Newton* improve upon this by an order of magnitude, with resolving powers of between several hundred and about 2000. Moreover, these instruments are *broad-band*, simultaneously covering large wavelength ranges that, even in the case of the Sun, have only before been studied in much smaller bandpasses. For the first time, the multitude of soft X-ray plasma diagnostics available through the detailed analysis of individual spectral lines are accessible for the study of hot astrophysical plasmas.

[1]Interactive Data Language, from Research Systems, Inc.

Low resolution spectra are usually analysed by means of modeling and fitting "engines" such as XSPEC (Arnaud 1996), SPEX (Kaastra et al. 1996), or CIAO/Sherpa (Freeman et al. 2001). These powerful tools enable spectral models to be compared with observed spectra and best-fit model parameters to be derived based on minimization of a test statistic such as χ^2 or the maximization of a likelihood (van Dyk et al. 2001). They come complete with "internal" emission models, such as the optically thin radiative loss models of Raymond & Smith (1977) and Kaastra et al. (1996). However, while other models can be input for the computations ("table models"), these tools are not conducive or flexible for the analysis of individual emission lines. Global model fitting of high resolution X-ray spectra is also fraught with problems ranging from the simple fact that current radiative loss models are signficantly incomplete in terms of the line emission included compared to that in actual spectra (e.g. Beiersdorfer et al. 1999), to the fact that the wavelengths of most spectral lines in the soft X-ray range are simply not known to sufficient accuracy.

To carry out such line-by-line analyses, a general list of steps might be as follows: (1) Start with a cursory knowledge of the features one expects to see in the observed spectra — a line list, or a model prediction of lines or other features and their intensities; (2) Identify selected features in the spectra; (3) Measure the strengths of individual lines and features; (4) Input measured data into computations that, though the appropriate atomic data and description of processes giving rise to observed flux, provide meaningful astrophysical information; and (5) Possibly re-enter derived information back into simulations or predictions that enable better measured quantities to be derived. An example might be a continuum level against which emission line fluxes need to be measured: measurements of strong line fluxes are unaffected by a relatively weak continuum and can be used to predict it; weak line fluxes might depend on the assumed continuum level.

To carry out such an analysis one might have a source or list of spectral lines, or a program to compute models; a plotting device to compare predictions and observations; a package to measure spectral features such as line fluxes; and an atomic database and programs that perform calculations based on measured quantities. The problem is that in these individual programs, relevant information and data are not in any homogeneous form and the individual programs and tools do not in general talk to each other. Even different sources of atomic data describing the same transition can have any number of different formats or units. The researcher is then faced with a general problem of bookkeeping for all the operations, steps and relevant data, and with the problem of transferring information from one task to the next — e.g. what were the first guess wavelengths for features in the blend to be de-blended by the line fitting and measuring tool? Or which atomic data is now used for a particular measured quantity to derive a result? The central theme in PINTofALE is that, from the first identification of observed features with features in the atomic databases or line lists, this association is passed through the whole process transparently to the user.

2. Structure

There are 3 basic components to PINTofALE: (1) routines to handle externally compiled atomic databases; (2) quick access database of lines and continua compiled from the external databases; and (3) tools to carry out various analysis tasks.

2.1. Atomic Databases

None of the existing compilations of atomic line transitions in the EUV and X-ray region such as `CHIANTI` (Dere et al. 1996), `SPEX` (Kaastra et al. 1996), and `RS` (Raymond & Smith 1977) are complete. Indeed they all differ in their selection of lines, the wavelength regions of interest, the types of transitions included, etc. Efforts to make a comprehensive list of line transitions in the X-ray regime are underway, notably in the creation of the `APED` (Brickhouse et al. 1999, Smith et al. 1999). Clearly, each database is geared towards specific goals, and it is often necessary to pick and choose line transitions from these databases.

We therefore re-cast these databases into a uniform format that allows us to pick the appropriate line transitions from any of the supported databases, and to add new atomic data as desired. The data stored are line emissivities as functions of temperature for a variety of densities and pressures, thus considerably reducing computations times during further analyses. We also separate out ion populations from the direct atomic contribution function, and are thus able to consider different versions of ion balance calculations (e.g. Arnaud & Rothenflug 1986, Arnaud & Raymond 1992, Mazzotta et al. 1998), as well as allow for flux calculations in the absence of ionization equilibrium.

The uniform database consists of the following tables, one set for each compilation, and supports filtering in wavelength space. We note in passing that we also treat continua similarly: *Wavelengths* of the transitions in the original database; *Temperatures* at which the emissivities are computed and stored ($4 \leq \log_{10}(\mathrm{T[K]}) \leq 8$); *Atomic numbers* of the elements giving rise to the line transition; *Ionic state* corresponding to the transition and the *ionic state* that determines the intensity (e.g., recombination line intensities are governed by the fraction of ions in the higher ionization stage); *Emissivity matrix*, for all the temperatures for each wavelength, computed for a particular density or pressure; e^- *configuration* and *level designations* corresponding to the transition, where available; and *Source* of the emissivity data.

2.2. Analysis Routines

The analysis tools are written entirely in IDL. They take advantage of the multi-platform support, as well as the native graphics capabilities provided by IDL. The routines are highly modular, and while not object-oriented, are designed to be flexible and fault-tolerant. In most cases I/O is in regular scalar and vector variables, but in some special cases (see below) all the necessary data are stored in well-defined structure variables.

The spectral browser is used to explore the spectrum and in parallel examine the linelist, database or predicted model. Regions of the spectrum can be zoomed in to by mouse control and a feature or line can be selected. A GUI is spawned by this selection process that lists the lines in the database or model that might be relevant for the observed feature. These lines can be based on model predictions and can have expected fluxes listed that include the instrument response, such that observed and predicted features can be compared on an equal basis. Any number of these lines can be tagged as an "identification" of the observed feature—from a single line in the case of the observed line being apparently unblended, to a slew of lines in the case of a complex blend. The product of this spectral browser is an "ID data structure" that forms the heart of our analysis procedure — a virtual scribbling pad that lists the interesting lines and features picked out in the spectrum and the corresponding links of these features to their respective relevant atomic data.

Line-identification is controlled by a line measuring and fitting engine GUI that reads the contents of the ID structure and sets up everything for measurement of line fluxes, including the option of using a model or "by eye" estimate of the continuum. All the information required to construct first guess parameters is provided automatically in the ID structure such as the locations of lines, the different components of blends and their expected relative positions and strengths, etc. This saves considerable time and effort compared to the option of typing in all the set-up parameters for line deblending and fitting manually. More components and lines can be added interactively if required. Results from Levenberg-Marquardt minimization (other convergence algorithms such as Markov-Chain Monte Carlo will be implemented in future versions) of three-parameter models such as Gaussians, Beta-profiles, etc. are written onto the ID structure.

The ID structure at this point contains the list of features in the observed spectrum for analysis, the measured strengths of these features, and the appropriate atomic data and links required for computations to derive results. Routines developed for this purpose operate on the ID structure; examples might be a scheme for determining the source *Emission Measure Distribution* that can be folded back into the predicted source model (this iteration is important when, e.g., attempting to assess the presence of hidden blends); another might be a tool for plotting line identifications.

The lynch-pin of the system is the manner in which line identifications are stored. Storing them in an unambiguous fashion is non-trivial because of problems such as the presence of line blends, multiple grating orders, instrument wavelength miscalibrations, etc. In order to facilitate bookkeeping, all the relevant variables are carried together in a single structure. A feature in the spectrum is characterized by a wavelength, and has one set of identifications associated with it. Each ID consists of: One or more *wavelengths* corresponding to the identifications, *atomic numbers* of the atoms giving rise to the corresponding transitions; corresponding *ionic states*; the share of the observed *flux* in each of the components or the predicted flux if the former is unavailable; the *error* on the fluxes; the *line contribution function* for each line including the adopted ion balance; the *temperatures* at which the above are defined; and a *description* of the transition, and any *comments* noted by the user.

Such a structure can easily account for the complex analysis requirements routinely encountered in spectral analysis. For example, a feature may have multiple identifications, of any element or ionic state, and the number of such identifications may be altered as needed. Identifications are stored by direct association and not by nearness to the wavelength of the observed feature, so that IDs from higher grating orders are correctly handled (the matched wavelengths are vastly different from the 1^{st}-order wavelength scale). For the same reason, wavelength shifts in the observed spectrum, which may arise either due to errors in wavelength calibration or due to doppler shifting of the source, also do not pose any problems.

Standardizing the output of the line identification process allows us to transparently handle the following steps such as flux measurement, derivation of the emission measure, deducing the plasma density, etc.

3. Availability

PINTofALE v1.0 was released publically on 3 Feb 2001. It is available for download from `http://hea-www.harvard.edu/PINTofALE` . An updated release, including improved color plot support, line lists from `APED`, and support for DEM reconstruction, is planned for December 2001.

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References

Arnaud, K.A., 1996, Astronomical Data Analysis Software and Systems V, Eds. G.Jacoby and J.Barnes, p17, ASP Conf.Ser., v.101

Arnaud, M., & Raymond, J.C. 1992, ApJ 398, 39

Arnaud, M., & Rothenflug, R. 1986, A&AS 60, 425

Beiersdorfer, P., Lepson, J.K., Brown, G.V., Utter, S.B., Kahn, S.M., Liedahl, D.A., & Mauche, C.W. 1999, ApJ, 519, 185

Brickhouse, N.S., Smith, R.K., & Houck, J.C. 1999a, in AAS-HEAD, 31, 33.11

Dere, K.P., Landi, E., Mason, H.E., Monsignori-Fossi, B.C., & Young, P.R., 1997, A&AS, 125, 145

Freeman, P.E., Doe, S., Siemiginowska, A. 2001, to appear in Proc. SPIE Conf. 4477, astro-ph/0108426

Kaastra, J.S., Mewe, R., Liedahl, D.A., Singh, K.P., White, N.E., & Drake, S.A. 1996, A&A 314, 547

Mazzotta, P., Mazzitelli, G., Colafrancesco, S., & Vittorio, N. 1998, A&ASS, 133, 403

Raymond, J.C., & Smith, B.W., 1977, ApJS, 35, 419

Smith, R.K., Brickhouse, N.S., Raymond, J.C., & Liedahl, D.A. 1999, in AAS-HEAD, 31, 33.07

van Dyk, D., Connors, A., Kashyap, V.L., & Siemiginowska, A. 2001, ApJ, 548, 224