High Resolution X-ray Spectroscopy: Issues for Creating an Atomic Database for a Collisional Plasma Spectral Emission Code

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ABSTRACT

We are developing a set of tools which will calculate the line and continuum emission from a hot, collisionally ionized plasma. This project is a successor to the Raymond & Smith plasma code, but unlike that code we separate the problem into two distinct parts:

- *APEC*: the Astrophysical Plasma Emission Code. This is a C program which calculates the emissivity of a collisionally ionized plasma as a function of temperature and ionization state.
- *APED*: the Astrophysical Plasma Emission Database. The database consists of a set of FITS format files containing wavelengths, oscillator strengths, fits to the collisional excitation rate coefficients, and other data necessary for calculating emissivity.

1. Introduction

Our goals for the new code are that:

- Together, *APEC* and *APED* will be able to calculate both continuum spectra and an emission line list from a collisionally ionized plasma.
- *APEC* will be able to estimate the errors on both the wavelengths and emission intensities due to uncertainties in the atomic physics listed in *APED*.
- *APED* will be easy to update as new atomic data becomes available, with only minor modifications to *APEC* (for example, to include a new fitting function).
- *APEC* will be usable either independently or be callable as a library routine from a plasma model, such as a magnetohydrodynamic code.

We present here a report of our progress to date.

2. Why create a new plasma code?

Some publicly-available collisionally excited plasma emission models already exist: SPEX/MEKAL (Mewe, Kaastra, & Liedahl 1993), Chianti (Dere *et al.* 1997), and the Raymond & Smith (1977) code. Why is a new code needed? Some advantages of *APEC* and *APED*:

- **Cross-checking** – Since each plasma emission code requires choosing from a large overlapping but incomplete set of atomic data, having independent models allows critical comparison and evaluation of errors in the code and database.
- **Distribution** – When complete, the entire *APEC* and *APED* will be distributed. As *APEC* is written in ANSI C, and *APED* uses FITS files, both are easily portable. The first line list and emission spectra will be available before AXAF launch.
- **Modification** – *APEC* will be able to use any set of atomic data in the FITS format. For example, the *APEC* could use a version of *APED* where many fine structure levels were bundled together, reducing the number of lines calculated but improving the speed of the code.
- **Error analysis** – *APED* will include error estimates for every parameter, value, or fit. See **error analysis** on this poster.
- **Uniformity** – *APEC* and *APED* attempt to treat each physical process in a general fashion, to avoid ad hoc solutions. For example, the recombination of an electron in the continuum into an excited level of an ion is considered as part of the level population calculation for the recombined ion.

3. *APEC*

APEC emphasizes simplicity and logical flow, at some sacrifice in speed and size. It is written in ANSI-standard C. The primary numerical routines–those for matrix inversion–are from standard public domain math packages LAPACK and BLAS.

APEC calculates the plasma emission by:

1. Reading the user command file
2. Reading *APED* to get the necessary atomic data
3. Calculating the ionization balance (if desired; otherwise a tabular ionization balance can also be input)

4. Calculating the level population and emission lines for each ion from the excitation and de-excitation rates along with radiative transitions and population by radiative or dielectronic recombination.

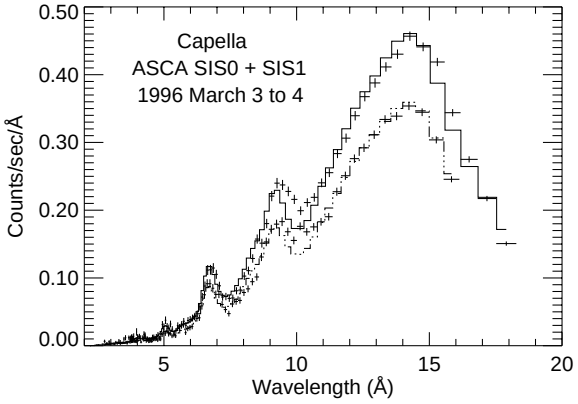
5. Calculating continuum radiation processes such as bremsstrahlung, two-photon emission, and radiative recombination.

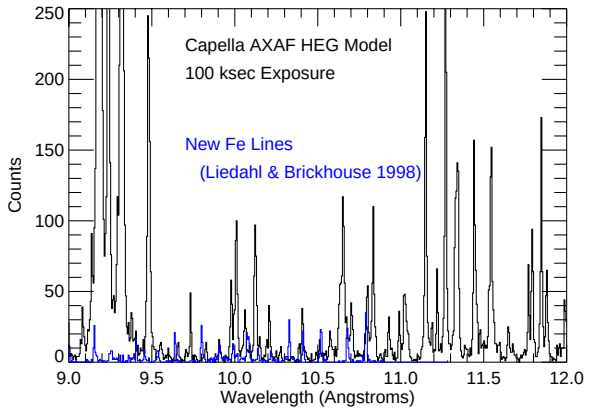
6. Outputting the emission line and spectral data in a FITS file

We are working with both the developers of XSPEC and the AXAF Science Center data analysis software so that our output FITS file will be directly readable by their analysis packages.

4. Emission Line Project (ELP)

The upper figure shows the flux deficit near 10 Å in the ASCA spectrum of Capella (Brickhouse *et al.* 1998). The spectrum of Capella (simulated, lower) will allow us to assess the completeness of plasma spectral emission models. The ELP is a collaborative effort to produce X-ray spectral line catalogs of 3 bright stellar coronal sources – Procyon, Capella, and HR 1099. These targets cover the range of elements and ionization states available to the LETG and HETG spectrometers, thus providing benchmarks for *APEC* and *APED*.





Simultaneous observations with EUVE will allow the extension of the benchmarks to longer wavelengths, and cross-calibration of XMM and AXAF will further improve our understanding of the X-ray spectrum.

5. *APED*

APED currently consists of five different types of FITS files.

- **Emission Line** – Wavelengths, Einstein A coefficients
- **Electron Collision** – Fits or tables for $\Upsilon(T)$, the thermally-averaged excitation rate.
- **Proton Collision** – Same for proton excitation, if significant.
- **Energy Levels** – Including the energy and degeneracy for each level
- **Ionization/Recombination** – collisional ionization and recombination rates, as well as photoionization cross section for each shell.

Depending on what calculations are desired, each ion may have data in any or all of these file types. These files can be examined and even modified using the HEASARC FITS viewer *fv* or the ASC browser, and we plan to develop other visualization tools.

This ease of access will, for example, allow users to update wavelengths or oscillator strengths, or to test the sensitivity of a particular line ratio to the underlying atomic physics.

6. Example

Although not completed, *APEC* and *APED* are already generating output. Currently, the data in *APED* has come from:

- Fe XVII - Fe XXIV : D. Liedahl at LLNL, using HULLAC code
- Hydrogenic and Helium-like ions : Sampson, Goett, & Clark 1983
- All other ions: The Chianti project, Dere et al. (1997)

As an example, we show below a comparison of the emission calculated by the Raymond & Smith (1993 update) code and *APEC*. These spectra are from a 10^6 K plasma in collisional ionization equilibrium.

7. Error Analysis

Perhaps the most vital new feature of *APEC* and *APED* is the ability to do internal error analysis, beyond benchmarking against other plasma codes or the available laboratory results. *APEC* and *APED* will provide three methods for evaluating the model errors resulting from the error in the underlying atomic physics:

1. **Comparison of data** – *APED* already contains data for some ions from more than one source. Although we will choose a standard "best" set for the emission tables, simply running *APEC* with various datasets provides a direct comparison.

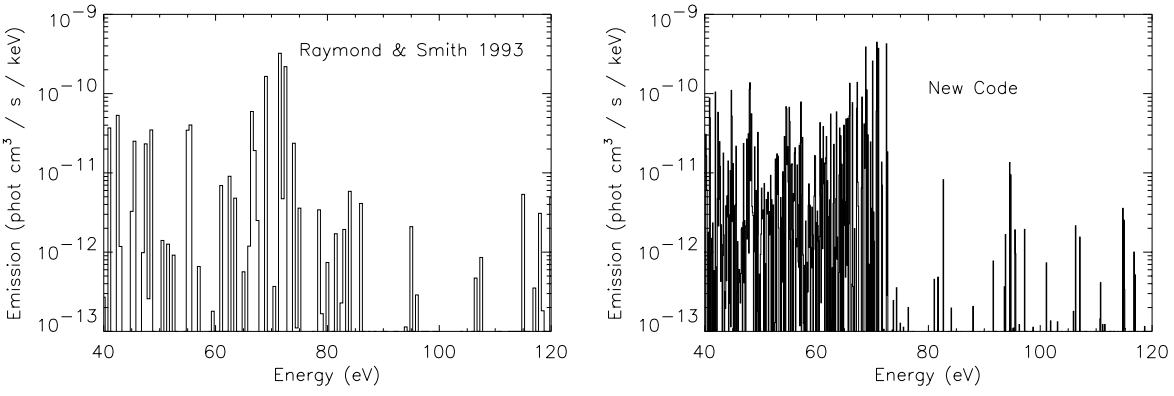
2. **Sensitivity testing** – *APED* contains numerical error estimates. A user can then explore with *APEC* the consequences of using the best rate $\pm 1\sigma$ for a particular ion or line parameter.

3. **Monte Carlo modeling** – When calculating the atomic rates, *APEC* is capable of varying the rate within the given errors. Since theoretical atomic physics calculations tend to have systematic errors, each rate will be given a single offset and then calculated for a range of temperatures. When completed, we will have the best possible estimate of the error on the emissivity and selected line ratios.

8. The missing line problem

While the accuracy of the atomic data used for high resolution spectral diagnostics is of obvious importance, accounting for the entire spectral content is also of great importance. While the atomic database will contain estimates of the accuracy of particular data, the overall quality of modeling also requires an estimate of what has been left out. With X-ray grating spectroscopy, the assessment of lines that are missing in the plasma emission code is needed to interpret line ratio diagnostics. For moderate resolution spectroscopy incompleteness in bands comparable to a resolution element can seriously degrade the global fits. Systematic errors can also derive from missing atomic processes in the line formation.

Published collisional excitation rate data generally exist only for levels with low principal quantum numbers ($n \lesssim 6$). While individual lines of higher n are weak, lines become increasingly close together as one approaches the ionization limit. Thus the net contribution of such lines to the flux at moderate resolution can be significant. This figure (Liedahl, private communication) shows energy bands where one might expect high n lines to contribute.



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