AtomDB 3.0 Documentation

Adam R. Foster

March 25, 2015
Revision 1.0

Contents

1 Introduction

This document describes the release of AtomDB version 3.0 for non-equilibrium ionization. This is not an academic paper, it is a user guide with a brief outline of the physics involved. A real publication will be produced describing the atomic data and using the data in an analysis at a later data.

Consider this an FAQ/work in progress. More will be added. Apologies for the very rough nature of the document.

2 AtomDB

AtomDB is a project to collect atomic data relevant to emission from hot, collisionally ionized astrophysical plasmas, with $10^4 \leq T_e \leq 10^9$K. From this, line emissivities are generated for an optically thin plasma, assuming collisional excitation dominates the excitation. The previous release of AtomDB, v2.0.2, includes data for most astrophysically relevant ions from hydrogen to nickel. The AtomDB model is implemented in XSPEC as the `apec` model (along with many variations, which include `vapec`, `bvapec` etc etc.). The `apec` model assumes that the plasma is in collisional ionization equilibrium

AtomDB 2.0.2 did not include any information for inner shell ionization or excitation processes. This meant the database was missing all fluorescence lines (e.g. the $n = 2 \rightarrow 1$ transition of Fe I to Fe XXIV in the 6.4–6.6keV). A non-equilibrium model was made by Borkowski, adding in the fluorescence lines. This is implemented in XSPEC as the `nei` model. Revised data sets have been produced for this model, with the latest being the `APEC_nei_v11_line.fits` files available at `ftp://legacy.gsfc.nasa.gov/software/lheasoft/release/xspec-nei-apec-data.tar.gz`

The AtomDB database was massively updated in 2012 with the release of AtomDB v2.0.2. However the nei data was frozen at the 2001 data set, and was not simple to update. It was also incomplete for many ions, including no ions below Fe XIV and no $n = 3 \rightarrow 1$ inner shell transition data.

This release of AtomDB represents a major update to both AtomDB and the APEC code, which converts the atomic data into collisional plasma emissivities. Very little existing data has been changed - this release is not focusing on improving existing data. Instead, there has been a large increase in the types of data, including inner shell excitation, inner shell ionization and auto-ionization. In addition, the XSTAR photo-ionization database has been incorporated into AtomDB. This is not related to non-equilibrium issues, but does affect the continuum calculations.

3 Calculating Emission

The emission from a line in a given plasma, $I_{j\rightarrow k}$ photons cm^{-3} s^{-1}, is given by

$$I_{j\rightarrow k} = N_j A_{j\rightarrow k} \tag{1}$$

where N_j is the number of ions of element Z, ion $z1$, in state j cm^{-3}, and $A_{j\rightarrow k}$ is the Einstein A coefficient of spontaneous emission (in s^{-1}). N_j can be calculated as follows:

$$N_j = \frac{N_j}{N_{z1}} \frac{N_{z1}}{N_Z} \frac{N_Z}{N_H} \frac{N_H}{N_e} N_e \tag{2}$$

Where N_j/N_{z1} is the fraction of the ion's population in level j, N_{z1}/N_Z is the ion fraction, N_Z/N_H is the elemental abundance (by default in AtomDB, from Andres and Grevesse 1989), and N_H/N_e is the hydrogen to electron density ratio.

In equilibrium version of AtomDB, the emissivity $\epsilon_{j\rightarrow k}$ for each line is tabulated by calculating each of these quantities separately: the level population for each ion is calculated, then multiplied by the equilibrium ion abundance, then the elemental abundance, and finally the electron to hydrogen ratio, which is 1.2 for a plasma with 90%H, 10%He and trace amounts of every other element. The final result of this is tabulated in the AtomDB line files (e.g. `apec_v2.0.2_line.fits`) if the emissivity is greater than the cutoff value of 10^{-20}ph cm^3 s^{-1}. If it is less than this, it is added to a pseudo-continuum of weak lines. The observed flux is then obtained by multiplying the emissivity by the emission measure and dividing by area of a sphere of radius D:

$$\Gamma_{j\rightarrow k} \left(\text{ph cm}^{-2}\text{ s}^{-1}\right) = \epsilon_{j\rightarrow k} \frac{1}{4\pi D^2} \int n_e n_H dV \tag{3}$$

where D is the distance to the object, and $\int n_e n_H dV$ is the emission measure.

Similar calculations are made when calculating continuum emission, with the exception that instead of individual line fluxes, fluxes are tabulated as flux per unit energy (or wavelength), as suits a continuum calculation.

3.1 Level populations

The APEC code, which converts the atomic data in AtomDB into emissivities used to calculate the spectra above, is a collisional-radiative model. In this model, the level populations are assumed to respond immediately to any change in the electron temperature. The ion populations may change much more slowly. The result is a decoupling of the ionization balance calculation and the related line emission.

The collisional-radiative matrix is created by considering all the populating processes for each level: collisional excitation and de-excitation, spontaneous emission, recombination (dielectronic and radiative) into the level, and ionization into and out of the level. Combining this matrix with the conservation of particles (i.e. all level populations sum to 1), we can solve for the level populations. The populations are then multiplied by the Einstein A coefficient to give an emissivity for each line per ion of element Z.

3.2 Ion population

The ionization balance is solved by taking the total ionization and recombination rates (currently from [2] in AtomDB), and solving the tri-diagonal matrix formed by the ionization and recombination rates for $dN_z/dt = 0$. For a non-equilibrium plasma, the ion population is solved using the method of [4]. The line emissivities from Section 3.1 are multiplied by this ion population.

As most of these values can be

4 NEI population calculation: AtomDB 3.0

In AtomDB 3.0 we have overhauled the APEC code to provide astrophysically relevant calculations for NEI plasma. This has also required a slew of new atomic data. Here we identify the changes made.

NEI plasma can be either ionizing (also known as underionized) or recombining (overionized). In an ionizing plasma, ions are exposed to electrons of a much higher energy than they would in an equilibrium plasma. Typical X-ray features include the K-shell line of iron at 6.4-6.7 keV. Modeling this requires the addition of data for inner shell ionization and inner-shell excitation, complete with the radiative stabilization and auto-ionization rates for each doubly excited level.

Recombining plasmas produce significantly enhance radiative recombination continua (RRCs) and dielectronic satellite lines. Data for both of these processes was already available in AtomDB 2.0.

4.1 Atomic Data Changes in Version 3.0

In AtomDB 3.0 there have been very few updates to the existing atomic data - that is corrections to or improvements on existing values. Instead, there has been a significant expansion of the database to include the data required to model the NEI plasma, with most data being generated by extensive runs of the Flexible Atomic Code (FAC).

Improvements have included:

1. Calculation of level-resolved inner shell ionization rates, from the ground to the n$\leq$4 shell for all ions.
2. Calculation of level-resolved inner shell excitation rates, from the ground to the n$\leq$4 shell for all ions.
3. Calculation of auto-ionization and Einstein A values for transitions from all doubly excited levels to all lower levels.

4.2 Spectral Calculation (APEC) Changes in Version 3.0

The APEC code has been rewritten in python, making extensive use of the linear algebra routines in the `numpy` and `scipy` packages. These in turn call the BLAS and LAPACK libraries, which were used by the C version of APEC. Results have been checked and found to be consistent for equilibrium plasmas between the two versions of the codes. The following changes have then been made to the physics of the calculation:

1. The code now calculates the level population explicitly for each ion, including population of excited states of adjacent ions *e.g.* excitation and auto-ionization into an excited level of the next ion.
2. Cascades within the adjacent ion population are propagated assuming zero density, i.e. only radiative cascade to the ground or further auto-ionization.
3. For ions with less than 12000 levels (those with 20 electrons or less), the level populations are calculated directly by making one collisional-radiative matrix including the auto-ionizing levels. For those with more than 12000 levels, a projection matrix is formed connecting the auto-ionizing levels to the bound levels. This is then used to solve the bound level populations, then the auto-ionizing level populations are obtained based on these fixed low level populations. After renormalization (so the population totals 1), the calculation proceeds as before. This is done to preserve memory.
4. Extrappolation has been built into the code for collisional excitation rates. Many AtomDB holdings only cover a small subset of the full temperature range ($10^4 - 10^9$K), as these were the temperatures at which these ions exist in equilibrium plasma. We have implemented the approach of [3] to obtain excitation rates at higher and lower temperatures than tabulated. Where such extrappolations have been used, we make note in the headers of the HDU in the fits files.

In addition, the output of the code for non-equilibrium data is significantly changed. Instead of:

$$\epsilon_{\rm APEC} = A_{j\rightarrow k}\frac{N_j}{N_{z1}}\frac{N_{z1}}{N_Z}\frac{N_Z}{N_H} \tag{4}$$

we have:

$$\epsilon_{\rm APECNEI} = A_{j\rightarrow k}\frac{N_j}{N_{z1}}\frac{N_Z}{N_H} \tag{5}$$

i.e. the epsilons are tabulated, ready to be multiplied by the ionization balance. In addition, due to the fact that a line can be created from an adjacent ion by ionization or recombination into an excited state, we add two columns into the output line emissivity files: the `ion_drv` and `elem_drv`, which are the original ion and element respectively. So the resonance transition of O VII (`elem`=8, `ion`=7), $1s2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0$, can be driven by ionization from O^{5+} (ion_drv=6), excitation within O^{6+} (ion_drv=7), or recombination from O^{7+} (ion_drv=8). Currently in all cases elem_drv is the same as the element.

Similarly, this leads to a new way of labeling some lines. Typically, DR satellite lines are labeled by the ion whose lines they are similar too. So DR lines of O VI are really transitions in O V driven by recombination from O VI. Recombination continuua, and weak lines, are stored by the driving ion as well.

Due to this increase in data which has to be preserved, the non-equilibrium emissivity files are quote large (around 700Mb). The equilibrium versions, which are identical in format to previous versions of AtomDB, are still fairly small (around 30Mb).

5 Using the new data

To use the new data in your favorite modeling code, there are several things to be aware of. First is what the new data is. Second is how to load it into XSPEC, and third is how to use new or existing models with it. We will cover XSPEC in detail here: there are other modeling packages (Sherpa, ISIS) which can access the new data, and run the XSPEC models relevant to APEC. As they all run XSPEC to use these models, the same description applies, although with some differences in calling syntax.

WARNING: There is a bug in XSPEC which affects using the AtomDB 3.0 data. It is fixed in version 12.8.2.i. If your version of XSPEC is older than this, or if you are using Sherpa, you will need to use the workaround which will be described below.

5.1 3.0 data in XSPEC

For the equilibrium data, you can simply download the relevant files and set the APECROOT variable to point to them. XSPEC automatically add the _line.fits and _coco.fits to the filename, so you should write:

```
xspec> xset APECROOT /path/to/atomdb_3.0/apec_v3.0.1
```

This will then load the new data for the equilibrium models (e.g. `apec, bvapec`.

An NEI plasma calculation underlies many of the models in XSPEC: `nei`, `pshock`, `sedov`. It consists of 2 parts: first, the ionization balance calculation, then secondly, the emission per ion calculation. The results of these are multiplied together to give a spectrum.

The data set for the ionization balance calculation is set by the `NEIVERS` parameter. Version 1.1 is the default, version 2.0 is the data of [1], and version 3.0 is the latest AtomDB 3.0.1 data. The files for this are not related to anything downloaded from the AtomDB website: the necessary eigenvector files were provided to XSPEC and have been included since version 12.8.2 was released. To set the NEIVERS parameter:

```
xspec> xset NEIVERS 3.0
```

The spectral calculation requires the `NEIAPECROOT` variable to point to the new nei apec files.

```
xspec> xset NEIAPECROOT /path/to/atomdb_3.0/apec_v3.0.1_nei
```

Again, XSPEC automatically adds the relevant suffixes, _line.fits and _comp.fits.

Note that the version 3.0 data includes all elements up to Nickel in it. However, prior versions of the NEI codes only included the 14 most commone elements. Therefore if you load up an `nei` model with the new data, you will find no chromium emission even if you thing you should.

A new model, called `rnei`, or revised NEI, has been created which solves 2 problems at once. First, it includes all the trace elements. Their abundances are set to 1.0 by default. The `vrnei` and `vvrnei` models allow you alter the abundances of various elements individually. In addition, the `rnei` allows you to set an initial temperature, T_{init}. This initial temperature is the ionizatoin balance which the plasma started from, before evolving for time constant τ (cm^{-3} s) at the new temperature T. If T_{init} is set to its minimum, 10^4K, then you have the same as the existing `nei` model. By setting it to a higher temperature than T you can simulate a recombining plasma.

6 Bugs

6.1 XSPEC 12.8.2 before i patch, Sherpa, ISIS(?)

In XSPEC version 12.8.2, there is a parameter misalignment in the vrnei, vnpshock and vsedov models. This causes faulty results. This was fixed in 12.8.2.i.

If you are using an older version of XSPEC, or Sherpa (which has XSPEC 12.8.2.e), you can work around this by using the vvrnei, vvnpshock and vvsedov models. It will create a lot more parameters, but you can freeze them and get the same effect at the single v models.

References

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[2] P. Bryans, E. Landi, and D. W. Savin. A NEW APPROACH TO ANALYZING SOLAR CORONAL SPECTRA AND UPDATED COLLISIONAL IONIZATION EQUILIBRIUM CALCULATIONS. II. UPDATED IONIZATION RATE COEFFICIENTS. *The Astrophysical Journal*, 691(2):1540–1559, February 2009.

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