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IrOnIc: How to Consider Hundreds of Millions of Iron-Group Lines in NLTE Model-Atmosphere Calculations

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The iron-group elements have a very high number of atomic levels and an overwhelming number of spectral lines. No NLTE model-atmosphere code can cope with these levels and lines in a classical way. In order to decrease the number of levels and lines to a manageable number, a statistical approach was developed over the last decade.

The Iron Opacity and Interface (*IrOnIc*) code calculates sampled cross-sections and model-atom files as input for model-atmosphere calculations. *IrOnIc* is presently transferred into a parallelized version, using MPI as well as GPU (CUDA) techniques. It will be made accessible to the public as a service of the German Astrophysical Virtual Observatory (*GAVO*).

Stellar Model Atmospheres

The consideration of metal-line blanketing is essential for the reliability of stellar model atmospheres. State-of-the-art codes like the Tübingen NLTE Model-Atmosphere Package (*TMAP*, http://astro.uni-tuebingen.de/~TMAP, Werner et al. 2003) can consider opacities of all elements from hydrogen to nickel (Rauch 2003). The iron-group elements (here Ca - Ni) have hundreds of thousands of atomic levels and hundreds of millions of respective line transitions due to their partly filled 3d and 4s atomic sub-shells. Classical model atoms (Rauch & Deetjen 2003) go far beyond the scope of *TMAP*. With a statistical approach, it is possible to consider 200 million iron-group lines.

Statistical Treatment of Iron-Group Atomic Data

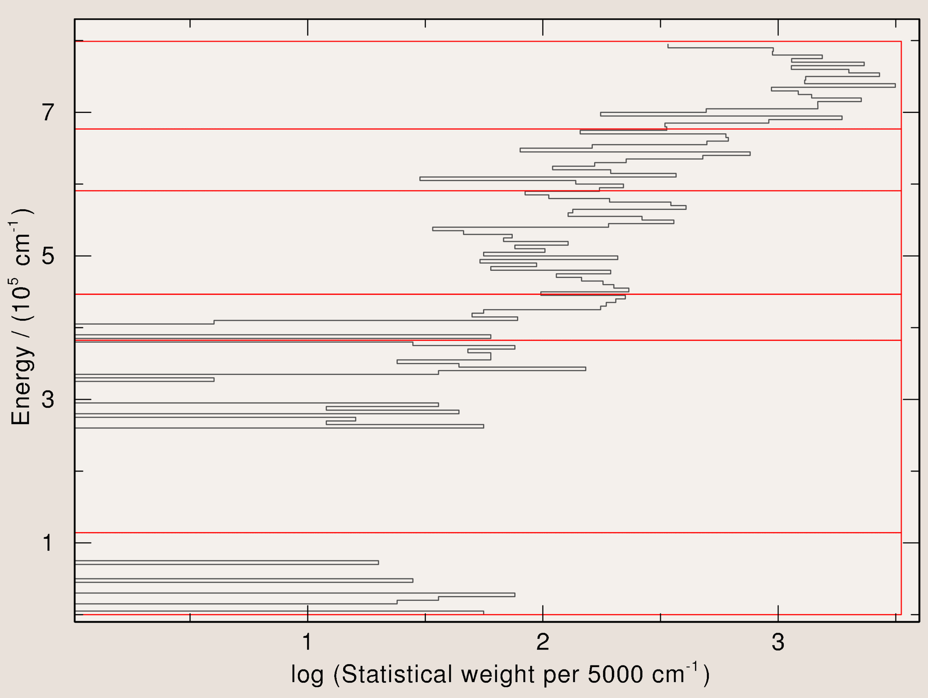

Fig. 1: Example of a band structure for Fe VI. The ionization energy is 799000 cm^{-1}.

IrOnIc (Rauch & Deetjen 2003) combines the large number of atomic levels of an ion to a few so-called super-levels (Fig. 1). All levels within one band are in LTE relation while the super-levels are treated in NLTE.

The super-levels are combined by respective super-lines (Fig. 2) that are, on the other hand, calculated from the huge number of lines that combined the original levels.

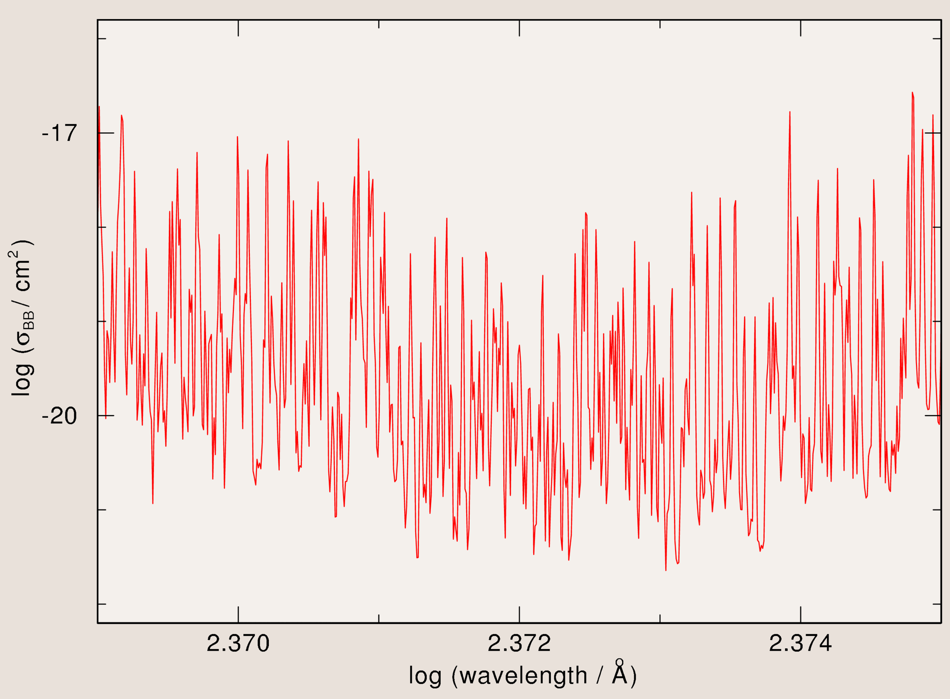

Fig. 2: Detail of a cross-section for Fe VI between the bands 2 and 6 (Fig. 1).

IrOnIc uses an opacity-sampling method to create the cross-section data of transitions between and within super-levels. Every line is thus represented with its real strength at its correct wavelength. Source of the atomic data are Kurucz' line lists (Kurucz 2009) and the Opacity Project (Seaton et al. 1994).

The Current Project

Depending on the size of the frequency grid, *IrOnIc* calculations to prepare atomic data files for *TMAP* presently need a couple of days. The bottleneck of these calculations are the millions of theoretical line profiles (approximated by Voigt profiles). To accelerate the computational process, MPI parallelization (for the ions of a species) as well as GPU support (for the Voigt profiles) is introduced.

As the calculation of the Voigt profiles consumes nearly 90% of the total computation time, different Voigt algorithms were tested. Without parallelization, the variations come to about a factor ten, with accelerators a speed-up with a factor of about 40 is feasible. Implementing this into the code will make it about a factor of 20 faster.

Within the framework of a *GAVO* (http://g-vo.org) project, a new, easy-to-use WWW interface will be created to control *IrOnIc*. Once all data are generated, the user gets an email notification with an appropriate wget command to retrieve the data.

The new *IrOnIc* will use a fixed, fine frequency-point discretization to sample the opacity data. Then, the model-atmosphere code interpolates all data internally to the actually used frequency grid. This makes the use of the data more flexible and avoids a complete *IrOnIc* recalculation in case that this frequency grid is changed.

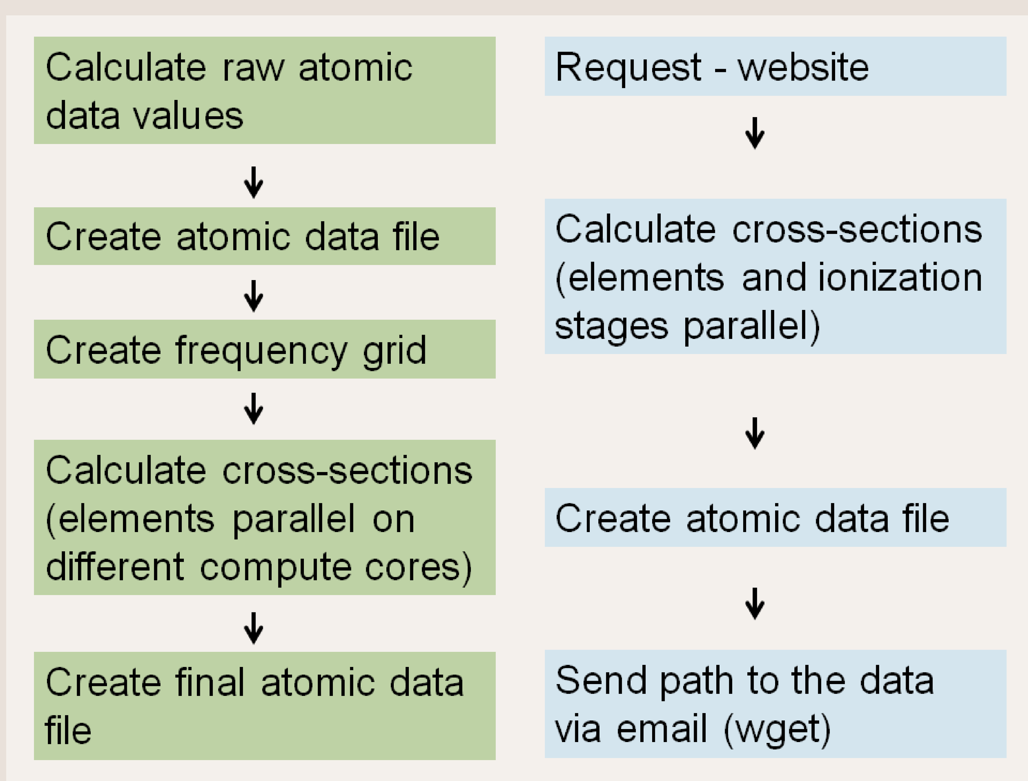

Fig. 3: Scheme of the old (left) and new (right) *IrOnIc* versions.

The aim of our project is to reduce the "waiting time", i.e. the time before new model-atmosphere calculations can start, to a reasonable value of a few hours. In addition, we provide easy access via a new WWW interface to the *IrOnIc* calculations. Thus, all other model-atmosphere codes can benefit.

References
Kurucz, R. 2009, AIPC, 1171, 43
Rauch, T. 2003, A&A, 403, 709
Rauch,T. & Deetjen, J. L. 2003, in: Hubeny, Mihalas, & Werner (eds.), ASP-CS, 288, 103
Seaton, M. J., Yan, Y., Mihalas, D., & Pradhan, A. K. 1994, MNRAS, 266, 805
Werner, K., Deetjen, J. L., Dreizler, S., et al. 2003, in: Hubeny, Mihalas, & Werner (eds.), ASP-CS, 288, 31

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