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

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Abstract. 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 in a classical way. A statistical approach was developed over the last decade to decrease the number of levels and lines to a manageable amount. The Iron Opacity and Interface (IrOnIc) calculates sampled cross-sections and model-atom files as input for model-atmosphere computations. IrOnIc is presently transferred into a parallelized code to reduce the calculation time to a reasonable value. It will be accessible by the public as a service of the German Astrophysical Virtual Observatory.

1. Stellar Model-Atmospheres and Statistical Treatment of Iron-Group Lines

Stellar model-atmosphere codes generally solve the radiation-transfer equation together with constraint equations like e.g. hydrostatic and radiative equilibrium. Each of these determines a distinct quantity. E.g. the effective temperature $T_{\text{eff}}$ is obtained by solving the radiative equilibrium. For NLTE codes, the Saha-Boltzmann equation is replaced by the rate equations which leads to a set of coupled, highly non-linear equations.

A stellar model-atmosphere calculation needs to consider metal-line blanketing to create reliable models. Iron-group elements (here Ca-Ni) are very important because they 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, the levels of iron-group elements are located in very narrow energy range and, thus, they can be seen as a quasi-continuum.

With classical model atoms (Rauch & Deetjen 2003) for the iron-group elements, the numerical capability even of state-of-the-art NLTE codes like the Tübingen NLTE Model-Atmosphere Package (TMAP), Werner et al. 2003 is exceeded by far. TMAP has been developed since the 1980s and is well established (e.g. Rauch et al. 2007; Wassermann et al. 2010). It is suitable for hot, compact objects with $20\,000\,K < T_{\text{eff}} < 200\,000\,K$, and surface gravities $4 \leq \log g \leq 9$. It can consider opacities from hydrogen to nickel (Rauch 2003). For the iron-group elements, a statistical treatment enables a consideration of an unlimited number of line transitions.

In order to reduce the quantity of levels and lines for the stellar atmosphere code without loosing opacity, IrOnIc has been developed since the late 1990s. The basic

\[\text{http://astro.uni-tuebingen.de/~TMAP}\]
idea of this code was presented by Anderson (1985, 1989) and adopted for TMAP by Dreizler & Werner (1992, 1993). It combines all atomic levels of an ion into a few so-called superlevels. E.g. 24112 levels of Fe vi are combined into six superlevels (Fig. 1). All levels within one superlevel are in LTE relation and contribute to its energy and statistical weight. The superlevels are treated by TMAP in NLTE. Transitions between these superlevels as well as transitions within the bands are allowed. They are calculated with an opacity-sampling technique. In this way, every transition is represented with its correct strength and position (Fig. 2). Source of the atomic data are e.g. Kurucz’ line lists (Kurucz 2009) and the Opacity Project (Seaton et al. 1994).

2. The IrOnIc Project

Presently, the calculation of cross-sections with IrOnIc needs about one to three days. As the user cannot start the model-atmosphere calculation until the IrOnIc run is performed, a new, faster version of this code, using MPI as well as GPU techniques, is
developed. This happens within the framework of a German Astrophysical Virtual Observatory (GAVO) project.

To speed-up the code, three main approaches will be implemented:

1. With the old IrOnIc version, the user has to perform three runs to get the atomic data file and cross-sections (Fig. 3). The new version will be controlled via a web interface. The user only has to enter the requested parameters and gets an email notification with a wget command to retrieve cross-sections, atomic data, and frequency file.

2. The new IrOnIc version will use a fixed, fine frequency grid. The cross-sections are later interpolated by the model-atmosphere code to the frequency grid of the actual calculation. This avoids a complete IrOnIc recalculation in case that the frequency grid is changed when e.g. new atoms are taken into account.

3. The code itself will be transferred into a parallel code. The elements as well as their ions will run in parallel with MPI parallelization. The bottleneck of the calculations are the millions of theoretical line profiles (approximated by Voigt profiles). Their calculation presently consumes nearly 90% of the total calculation time. We tested different Voigt function algorithms and got variations up to a factor of ten. Performing these calculations on a GPU gives a speed-up of a factor $\approx 40$ for the line-profile calculation.

In summary, a new, faster version of the IrOnIc code to calculate sampled cross-sections and model atoms for iron-group elements is written. As this happens within a GAVO project, the service will be available to the community. Speed-up will be

\footnote{http://g-vo.org/}
achieved through parallelization and restructuring. The new version is estimated to be a factor of about 20 faster. This reduces the waiting time until the stellar model-atmosphere calculation can start to a value of a few hours instead of days. In addition, a web interface (Fig. 4) is created to ensure easy control and accessibility, and to provide the data in VO-compliant format. In this way, any model-atmosphere codes can benefit.

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Figure 4. The new IrOnIc web interface (presently a test version only).