Report to ESF

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Report on the short research visit to Uppsala Observatory funded by the ESF within the GREAT activity

In the following, I report on the short research visit to Uppsala Observatory (Sweden), which took place between the 1-st and 5-th of September 2012.

I am a co-Investigator of the Gaia-ESO chemo-dynamical survey (GCDS), which is one of the important GREAT initiatives in connection with WGA3. One of my major tasks is to develop the methods for an *accurate* determination of element abundances and fundamental parameters of FGK stars. The aim of the visit to Uppsala was, in collaboration with local scientists involved in GCDS, to devise a new accurate scheme, which will be suitable for analysis of large data arrays of observed stellar spectra acquired within GCDS on the UVES/GIRAFFE instruments at Very Large Telescope (VLT, Chile). The Gaia-ESO survey has commenced in January 2012, and 8 observing blocks have been completed already, so that nearly 4000 high-quality spectra of stars in different populations of the Milky Way are now available to us.

Durting the visit, I held several meetings with scientists working at Uppsala, and specific work was done in collaboration with Nikolai Piskunov, Andreas Korn, and Thomas Nordlander (all Uppsala) on the algorithm development. We used the SME spectrum synthesis code originally designed by J. Valenti and N. Piskunov, which provides a solution to the problem by cross-matching an observed spectum of a star and a theoretical spectrum computed on the fly for different sets of input parameters.

So far, however, radiative transfer in SME has been treated under the simplifying assumption of local thermodynamic equilibrium (LTE), which significantly limited the accuracy of results. Our goal was therefore to develop SME towards being capable of solving more realistic, but also substantially more sophisticated, non-local thermodynamic equilibrium (non-LTE) radiative transfer problem. It has been demonstrated in numerous recent publications (Asplund 2005; Bergemann et al. 2012; Lind, Begremann, Asplund 2012) that only this approach leads to accurate fundamental stellar parametes free of systematic biases.

Despite a challenging task, a substantial progress has been made during the visit. This relates to several aspects of calculations with SME:

- First of all, we succeeded to impement the test grids of non-LTE (NLTE) departure coefficients for complete level systems of several elements, in particular Li, I Na I, and Fe I (see Fig. 1). The model atoms for these elements were taken from Lind et al. (2009), Lind et al. (2011), and Bergemann et al. (2012), and the full statistical equilibrium calculations were performed with the MULTI2.3 program as described in these references. Communication between the NLTE database and line transitions in the SME masterline lists proceeds via term designations, which must uniquely identify each atomic energy level. These levels must be present in both databases.

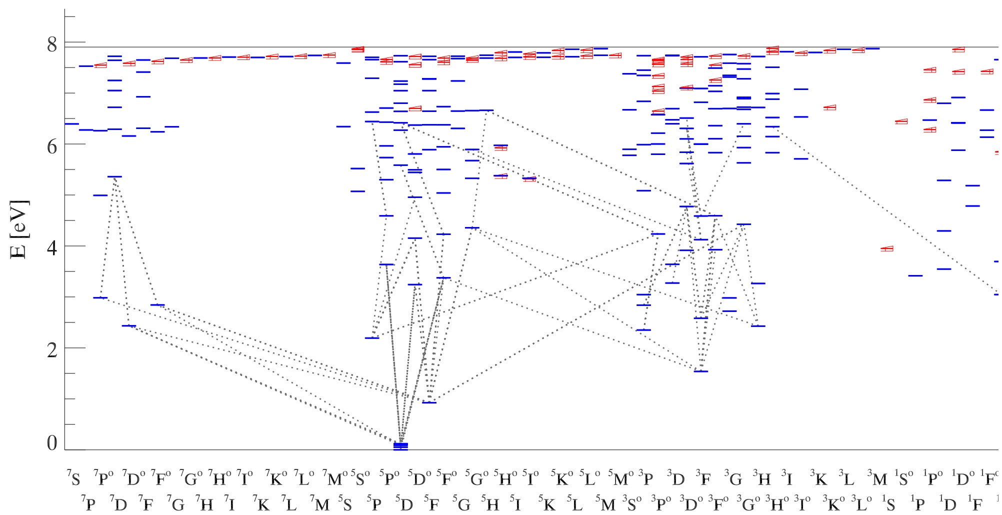

Fig. 1: The NLTE model atom of neutral iron, Fe I. The transitions, for which non-LTE radiative transfer is computed with SME, are shown by connecting lines.

The NLTE grids were computed on a very fine grid stellar parameters, corresponding to the MARCS model atmosphere grid, which is adopted within the Gaia-ESO survey. The departure coefficients were then used to correct the line opacity and source function in SME, thus recovering the full non-LTE line profile, identical to what is obtained by full statistical equilibirum calculations of an atom. The examples of the LTE and non-LTE Na I line profiles obtained in this way are shown in Fig. 2. It is clear that non-LTE provides a much better fit to the observed solar spectrum.

The major advantage of this approach using pre-computed grids of departure coefficients is that the calculation timescales can be kept quite small, so that 20 to 40 iterations with SME can be completed within 10 minutes of the CPU time. In particular, solving radiative transfer in multiple spectral lines of Fe and comparing with observed spectra provides *effective temperature, surface* *gravity, and metallicity* of star, and this set can be then used to determine individual elemental abundances, e.g., of Na and Li, which are of a key importance for the Gaia-ESO survey.

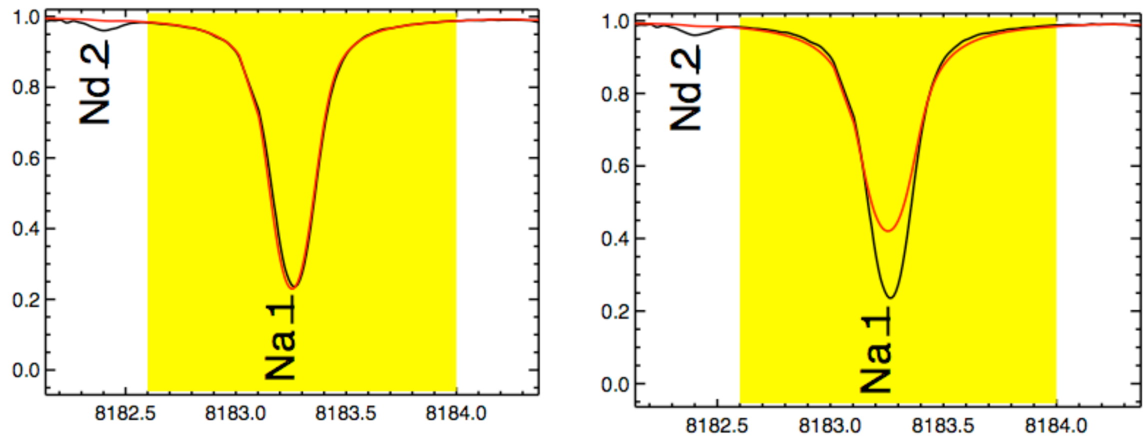

Fig. 2: Theoretical profiles of Na I spectral lines (red) in the solar spectrum computed with SME for the two radiative transfer modes: NLTE (left) and LTE (right). Black line shows the observed FTS solar spectrum.

- Several other modifications were made to the SME user interface, as well as optimization of the input and output processing IDL routines and efficient method to store the large NLTE grids.
- Finally, we made important modifications with respect to the interpolation scheme for the MARCS model atmospheres, and consequently, for the departure coefficients, which are specified on the node points of the MARCS grid only. While the standard mode of SME uses column mass as an independent depth variable, it is more reasonable and convenient to use optical depth at 500 nm, which is a standard optical depth in the MULTI2.3 non-LTE code. We have implemented a new numerical algorithm that efficiently interpolates in multiple dimensions in the model atmosphere and the departure coefficient grids on the tau(500) scale. An example of the interpolated and original model atmosphere for a model atmosphere corresponding to a metal-poor giant is shown in the Fig. 3.

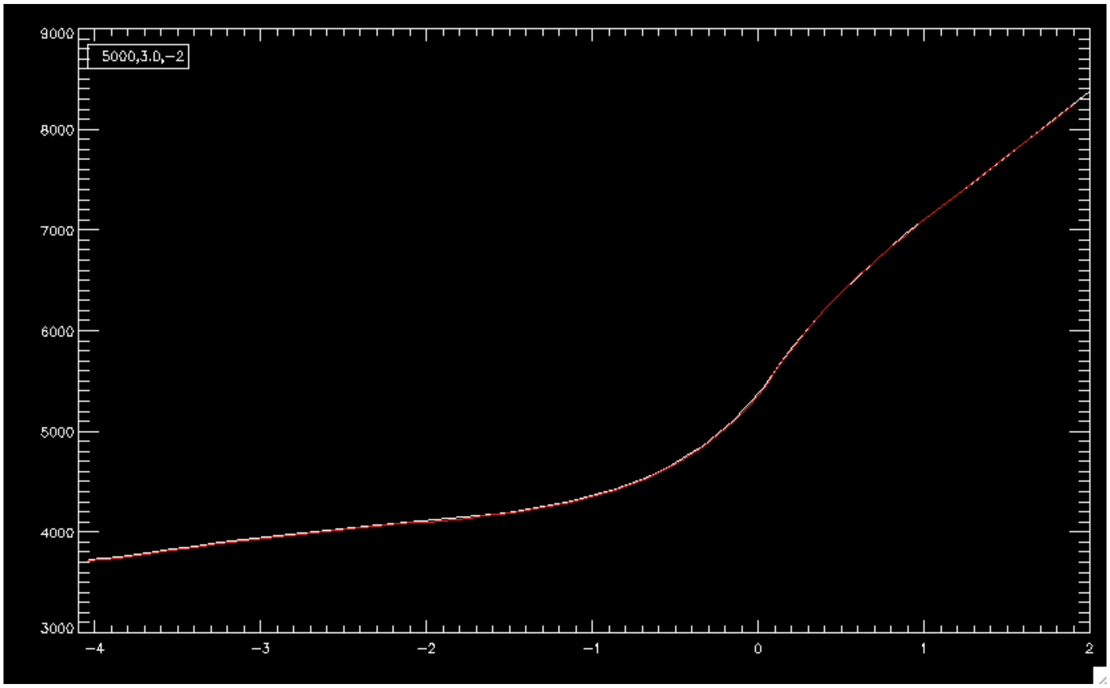

Fig. 3: The stratifications of temperature (y-axis) as a function of optical depth (log tau at 500 nm, x-axis) in the interpolated (white) and original (red) model atmospheres.

The outcome of the visit is the first version of SME capable of solving the NLTE radiative transfer problem. The software is now being tested, but first science runs with Gaia-ESO *reference calibration* stars will start shortly. Once the testing phase has been completed, we will begin with the analysis of all science targets observed within GCDS. It is expected that futher progress will be done in a collaborative effort by scientists from MPA (Garching), Uppsala and the Lund Observatory (Sweden), and my research visit to Uppsala demonstrated that exchance visits are very important for the efficiency of this collaboration.

The first scientific publication in connection with the work performed during the visit is expected by the mid of 2013, which is set by the regulations of the GCDS. The stellar parameters determined with SME must first pass the quality control performed by the GCDS work group 15, which is responsible for stellar parameter homogenization between all nodes involved in the Gaia-ESO survey.

I acknowledge that this research visit Uppsala was very successful for me in terms of scientific collaboration. With this, I would like to thank ESF for providing funding.

Sincerely yours,

Maria Bergemann