Mem. S.A.It. Suppl. Vol. 8, 165

Memorie della
Supplementi

Stellar models and opacity.

The LLMODELS approach

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Abstract. Computation of the opacities of the millions of spectral lines contributing to the absorbtion is one of the main tasks in modelling stellar atmospheres. Several statistical techniques have been developed in the past to represent line absorbtion. They do well for stars meeting the method's assumptions close enough. We implemented a general method, the line by line (LL) method, in the widely used ATLAS9. It avoids problems resulting from statistical techniques and allows us to calculate complex models resembling individual abundance patterns and stratification of element abundances and turbulent velocity. Still the implemented numerical routines make it feasible to calculate models on modern PC's in a time comparable to the time required by classical routines.

Key words. Radiative Transfer – Stars: atmospheres – Stars: chemically peculiar

1. Introduction

Modelling stellar atmospheres is an important tool for investigating stellar structure and evolution and deriving their fundamental parameters. Investigations like abundance analysis, pulsation mode identification, synthesis of galaxy spectra, various methods to determine stellar fundamental parameters and many more rely on accurate models of the atmospheric structure, because we cannot directly probe a star's interior.

One of the main challenges for stellar atmosphere modelling are the millions of spectral lines which have to be taken into account in radiative transfer. Straight forward opacity calculation, line by line, seems not to be economical in terms of computing time, so several statistical methods have been developed to represent the line absorbtion. Best known are the Opacity Distribution Function method (ODF) (see Strom & Kurucz 1966) and the Opacity Sampling method (OS) (see Peytremann 1974). Due to their statistical nature these methods have various shortcommings (Carbon 1974; Castelli & Kurucz 1994).

As our observation techniques and instruments gained in quality new questions emerged, stellar atmospheres with individual abundances (peculiar stars, horizontal branch stars, etc.). In particular in the case of chemically peculiar stars (CP) it may be necessary to take into account stratification of elements, since spectra of several of these stars indicate

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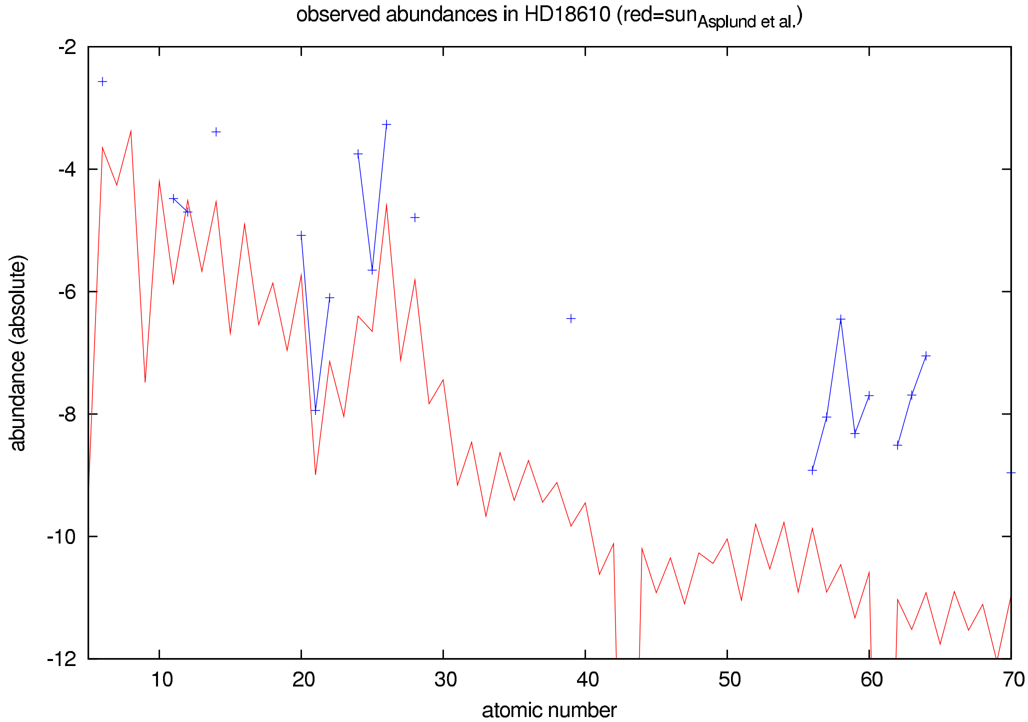

Fig. 1. Observed element abundances (blue) of HD18610 (Stütz et al. 2003) compared to the sun (red) (Asplund et al. 2004).

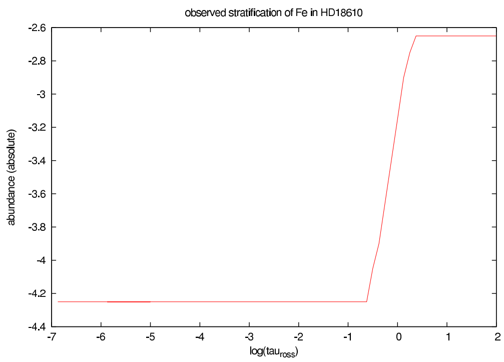

Fig. 2. Observed stratification profile of Fe for HD18610 (Stütz et al. 2003).

a vertical abundance distribution. Additionally we are now able to tackle the phenomena of turbulent velocities (ξ_t(z)) and strong global magnetic fields from the theoretical point of view. To give an example, fig.1 and fig.2 show the CP2 star HD 18610. Its element pattern deviates strongly from solar scaled case and iron changes its abundance by a factor of 40 through the atmosphere.

2. The Line by Line technique

In order to describe the frequency and the depth dependence of atomic line absorbtion coefficients as accurate as possible we went back to the roots (calculate opacities line by line), trying to do it fast. The LLMODELS stellar atmosphere code (Shuliak et al. 2004) is based on the main program blocks of Atlas9 (Strom & Kurucz 1966; Kurucz 1994) and STARSP (Tsymbal 1996) concerning the line opacity calculations. What we call the line by line method (LL) is to compute the line absorbtion on a very fine wavelength grid (typically 0.1 Å), including also opacities caused by other lines on both sides of the given grid point. The spectrum is reproduced in detail in this procedure.

2.1. Line opacities

Computing time is driven by the large number of lines which have to be considered and the small wavelength steps in the spectral regions which are to be integrated. The number of spectral lines can be reduced by only taking into account the 'important' atomic lines. Typically we preselect lines with absorbtion of at least 1/100 the continuum opacitiy in the line center.

When the line opacity is derived at a certain grid point, also all nearby possibly contributing lines have to be considered. Kurucz' ATLAS12 (Kurucz 1993) which applies the OS method for example uses 200 grid points with a step size of about 1 Å to compute the absorbtion of a single line. This covers a spectral interval comparable to a Balmer line of an A–type star. Obviously such a procedure would slow down a LL calculation immensely. Fortunately the wings of most atomic lines cover only a few Å and we do not need to calculate their profiles far beyond a reasonably choosen limit. Thus we can separate the lines in many narrow lines and a few broad lines (hydrogen lines, CaII H and K, etc.). Experimentally it was found that a spectral interval of ±2.5 Å is accurate enough the most atomic lines (i.e. the narrow lines). The wide lines are treated differently. Hydrogen line opacities are derived within an interval of ±50 Å and a step size of 1 Å. For other wide lines we use the same fine wavelength grid as for the narrow lines but a larger spectral interval of ±30 Å.

2.2. Hydrostatic equation

Other major changes to the ATLAS9 program blocks affect the hydrostatic equation, convection modelling and convergence criteria. In ATLAS9 as well as in ATLAS12 the hydrostatic equation is solved using precalculated tables of $\kappa_{\rm ross}$ for choosen T, $P_{\rm gas}$ and ξ_t and for fixed abundances. But these are unhandy for models with pronounced abundance patterns or even stratification. Computing $\kappa_{\rm ross}$ on the fly on the other hand is time consuming, because it requires an integration over a frequency interval (for details see Shuliak et al. 2004). Instead we use the monochromatic optical depth τ_{5000} and determine the absorbtion at 5000 Å. After $T_{\rm new}$ and $P_{\rm new}$ are derived, they are interpolated back on the standart $\tau_{\rm ross}$ grid to prevent the model from fluctuating along the atmospheric depths and we continue working in terms of $\tau_{\rm ross}$.

2.3. Other physics and performance

Additional to the mixing length theory (MLT) we implemented the local full spectrum turbulence convection model of Canuto & Mazzitelli (1991). This was done in the same manner as for ATLAS9 by Heiter et al. (2002). The CM convection model proves its advantage mainly in the regime of weaker convection. Furthermore it eliminates the necessity of tuning a mixing length.

Converging a model, we demand constancy of the total flux and conservation of radiative equilibrium. The first criterion is not very sensitive to temperature variations in the optically thin layers. This is why we introduced the second one, which becomes more relevant in this regions of the atmosphere.

Table 1. LLMODELS statistics

Physics	
Basic routines	ATLAS9+ numerics
Line opacities	LL (STARSP), ODF
Hydrogen lines	Griem, VCS
Convection	CM, MLT
Performance	1.8GHz Athlon
ODF model	10 – 20 sec
LL model	70 – 90 min
ODF+LL model	30 – 60 min

Summarizing we will present some statistics for the LLMODELS model atmosphere code in table 1. The references for the treatment of hydrogen lines are Griem (1960) and Vidal et al. (1973) (VCS). Of course a good starting model reduces the number of iterations and thus increases the performance. For that

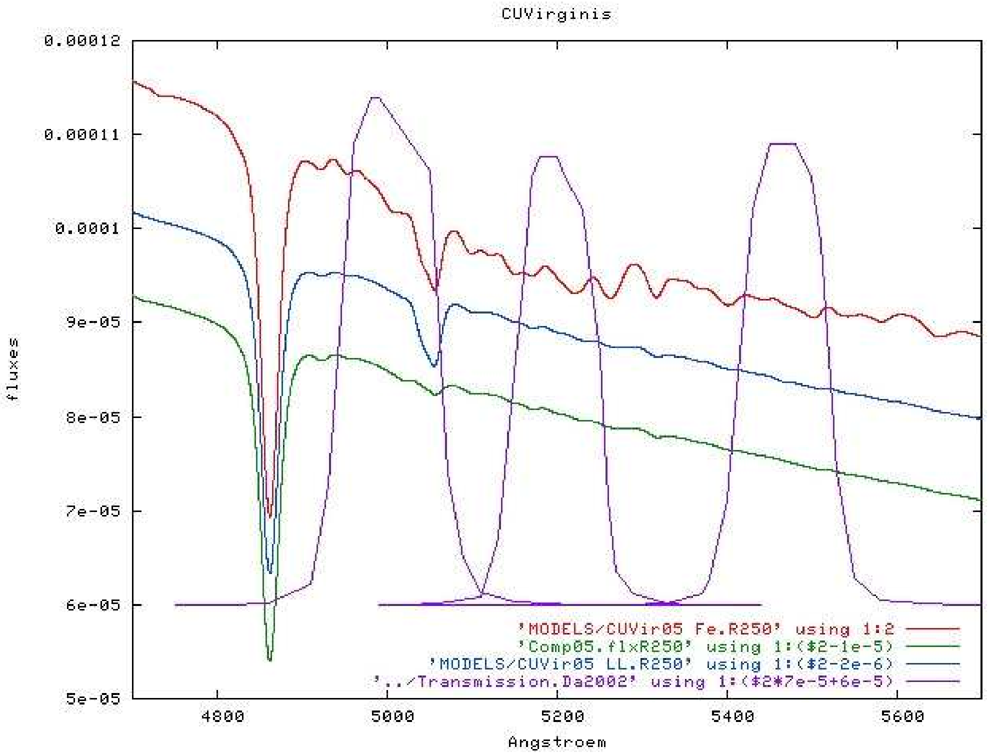

Fig. 3. CU Virginis, red - stratified model, blue - individual abundance pattern green - solar scaled model. Scaled transmission curves of g_1, g_2, and y (from left to right).

reason we reimplemented the ODF method in our code to do the first iterations.

3. Example of a CP2 star

To illustrate the consequences of stratification in modelling, spectrum synthesis and synthetic photometry we show a recent result in an investigation on the connection of the photometric Δa index (Maitzen 1976) to the atmospheric structure of A–type stars (Kupka et al. 2005). Amongst other features, a flux depression around 5200 Å is typical for CP2 stars (magnetic chemical peculiar stars). This feature can be detected photometrically.

In figure 3 the 3 filters of the Δa photometric system are plotted over 3 theoretical spectra corresponding to models with the fundamental atmospheric parameters of CU Virginis. The spectra differ only in abundance pattern (bottom = solar scaled to the metalicity of CU Virginis, upper two = analyzed abundance pattern of CU Virginis) and stratification of Fe and Si (top spectrum). It clearly can be seen that the Δa indices

$$\Delta a = a_0 - a_{star} \tag{1}$$

$$a = g_2 - \frac{g_1 + y}{2} \tag{2}$$

of these models will differ. Comparing our final model, resembling the individual abundance pattern and stratification profile of this star, to independent photometric observations we find that our synthetic Δa index of 29^{mmag} (mmag = millimagnitudes) compares very well to the observed Δa index of 30^{mmag} (observations and synthesis are for the rotation phase 0.5). The individual abundance pattern alone, although supporting the feature, cannot explain the observed depth of the depression at

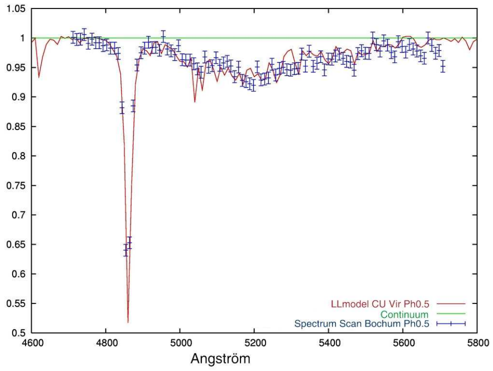

Fig. 4. Synthetic fluxes for CU Virginis (line) compared to observations with the Bochum RSS on La Silla (bars indicating error of observations).

5000 Å. Figure 4 shows a comparison of the resultant theoretical spectrum to spectrum scans obtained with the Bochum Rapid Spectrum Scanner on La Silla.

4. Conclusions

The LL method implemented in the LLMODELS atmosphere code naturally allows to account for pronounced individual abundance patterns of stellar atmospheres and stratification effects of element abundances and velocities. The routines have been developed to investigate this phenomena in peculiar A–type stars, but calculations can be done fast enough to use line by line models also in other fields of astronomy (e.g., synthesis of galaxy spectra, horizontal branch stars, IR method for determining fundamental parameters, etc.).
Note that the treatment of stratification is strictly phenomenological. Stratification profiles are not determined but put into the models as observables.

Acknowledgements. We want to thank Denis Shuliak the main developer of LLMODELS for heavy programming and Vadim Tsymbal for his ideas and the source of STARSP. This research was funded by the Austrian *Fonds zur Förderung der wissenschaftlichen Forschung* (P–14984).

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