Stellar atmospheres and synthetic spectra for GAIA

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Abstract. In this paper we discuss our new model atmosphere grids for objects relevant to the GAIA mission. The grids are computed using version 13 of our general-purpose model atmosphere code PHOENIX and included the most recent updated to the micro-physics and line opacities added to the code. We will make the synthetic spectra of the new grid available to support the preparation of the GAIA mission. By the time results from GAIA become available, we expect that advances in modeling stellar atmospheres will result in vastly improved models, but the current grids will be perfectly adequate for the preparation of the mission and initial data analyses.

1. Introduction

Stellar atmosphere modeling has experienced a renaissance in the past decade with the advent of better algorithms and faster computers. This has allowed research groups to remove or relax many of the standard assumptions that were made in the 70s through 80s and that had become accepted wisdom over the years. Not surprisingly the new calculations show that many of these assumptions are actually quite bad and can lead to spurious results or incorrect interpretations of observed spectra. The intricate connection between geometry (plane parallel or spherical), line blanketing (atomic and/or molecular) and non-LTE effects (using small to extremely large model atoms and molecules) began
Figure 1.  The effects of line blanketing on the emitted spectrum of M dwarfs is illustrated in the top panel, the bottom panel demonstrates the effects of metallicity changes on the emitted spectra. From Allard et al. (1997).
to emerge slowly as crucial ingredients for physically correct and meaningful interpretations and analyses of stellar spectra. Unfortunately, easy and simple solutions do not really work for stellar atmospheres (although everybody likes the easy way out and some of them are useful for teaching purposes) and have actually hindered progress and reduced the reliability of results.

Our group has developed the very general non-LTE (NLTE) stellar atmosphere computer code PHOENIX (Hauschildt 1992, 1993, Hauschildt et al. 1995, Allard & Hauschildt 1995, Hauschildt et al. 1996, Baron et al. 1996a, Hauschildt et al. 1997, Baron & Hauschildt 1998, Hauschildt & Baron 1999, Allard et al. 2001) which can handle extremely large model atoms as well as line blanketing by hundreds of millions of atomic and molecular lines. This code is designed to be both portable and flexible: it is used to compute model atmospheres and synthetic spectra for, e.g., novae, supernovae, M, L, and T dwarfs, irradiated atmospheres of extrasolar giant planets, O to M giants, white dwarfs and accretion disks in active galactic nuclei (AGN). The radiative transfer in PHOENIX is solved in spherical geometry and includes the effects of special relativity (including advection and aberration) in the modeling.

The PHOENIX code allows us to include a large number of NLTE and LTE background spectral lines and solves the radiative transfer equation for each of them without using simple approximations like the Sobolev approximation. Therefore, the profiles of spectral lines must be resolved in the co-moving (Lagrangian) frame. This requires many wavelength points (we typically use 150,000 to 300,000 points). Since the CPU time scales linearly with the number of wavelength points, the CPU time requirements of such calculations are large. In addition, (NLTE) radiative rates for both line and continuum transitions must be calculated and stored at every spatial grid point for each transition, which requires large amounts of storage and can cause significant performance degradation if the corresponding routines are not optimally coded.

An important problem in stellar atmosphere calculations is to find a consistent solution of the very diverse equations that describe the various physical processes. We have developed a scheme of nested iterations that enables us to separate many of the variables (e.g., separating the temperature correction procedure from the calculation of the NLTE occupation numbers). This allows us to compute far more detailed stellar atmosphere models than was previously possible (see references for details).

In order to take advantage of the enormous computing power and vast aggregate memory sizes of modern parallel supercomputers, both potentially allowing much faster model construction as well as more sophisticated models, we have developed a parallel version of PHOENIX which is now the default production version for all our model grids.

2. Methods and models

For our model calculations, we use our multi-purpose stellar atmosphere code PHOENIX (version 13). Details of the numerical methods are given in the above references, so we do not repeat the description here.

One of the most important recent improvements of cool stellar atmosphere models is that new molecular line data have become available and that they have
improved the fits to observed spectra significantly. Our combined molecular line list includes about 700 million molecular lines. The lines are selected for every model from the master line list at the beginning of each model iteration to account for changes in the model structure (see below). Both atomic and molecular lines are treated with a direct opacity sampling method (dOS). We do not use pre-computed opacity sampling tables, but instead dynamically select the relevant LTE background lines from master line lists at the beginning of each iteration for every model and sum the contribution of every line within a search window to compute the total line opacity at arbitrary wavelength points. The latter feature is crucial in NLTE calculations in which the wavelength grid is both irregular and variable from iteration to iteration due to changes in the physical conditions. This approach also allows detailed and depth dependent line profiles to be used during the iterations. This is important in situations where line blanketing and broadening are crucial for the model structure calculations and for the computation of the synthetic spectra. It is highlighted in Figure 1 which shows the dramatic effects of line blanketing on M dwarf spectra and the correspondingly large effects of metallicity on the emergent spectrum (and model structure).

Although the direct line treatment seems at first glance computationally prohibitive, it leads to more accurate models. This is due to the fact that the line forming regions in cool stars and planets span a huge range in pressure and temperature so that the line wings form in very different layers than the line cores. Therefore, the physics of line formation is best modeled by an approach that treats the variation of the line profile and the level excitation as accurately as possible. To make this method computationally more efficient, we employ modern numerical techniques, e.g., vectorized and parallelized block algorithms with high data locality Hauschildt et al. 1997, and we use high-end workstations or parallel supercomputers for the model calculations. With these techniques, a complete model calculation (about 20 iterations) takes less than 20 minutes on 24 CPUs of an IBM pSeries 690 parallel supercomputer.

In the calculations presented in this contribution, we have included a constant statistical velocity field, \( \xi = 2 \text{ km s}^{-1} \), which is treated like a microturbulence. The choice of lines is dictated by whether they are stronger than a threshold \( \Gamma \equiv \chi_l / \kappa_c = 10^{-4} \), where \( \chi_l \) is the extinction coefficient of the line at the line center and \( \kappa_c \) is the local b-f absorption coefficient (see Hauschildt et al. 1999 for details of the line selection process). This typically leads to about \( 10 - 250 \times 10^9 \) lines which are selected from the master line lists. The profiles of these lines are assumed to be depth-dependent Voigt or Doppler profiles (for very weak lines). Details of the computation of the damping constants and the line profiles are given in Schweitzer et al. (1996). We have verified in test calculations that the details of the line profiles and the threshold \( \Gamma \) do not have a significant effect on either the model structure or the synthetic spectra. In addition, we include about 2000 photo-ionization cross sections for atoms and ions (Mathisen 1984, Verner & Yakovlev 1995).

The equation of state (EOS) is an enlarged and enhanced version of the EOS used in Allard & Hauschildt (1995). We include about 1000 species (atoms, ions and molecules) in the EOS. The EOS calculations themselves follow the method discussed in Allard & Hauschildt (1995). For effective temperatures,
Figure 2. Detailed comparison of the solar spectrum from the Kitt Peak Atlas to a simple LTE PHOENIX model with $T_{\text{eff}} = 5770\, \text{K}$, log $g = 4.4$ and solar abundances. No attempts of fine tuning were made.

$T_{\text{eff}} < 2500\, \text{K}$, the formation of dust particles has to be considered in the EOS. In our models we allow for the formation (and dissolution) of a variety of grain species. For details of the EOS and the opacity treatment see Allard et al. (2001).

The NLTE treatment of large model atoms or molecules such as H$_2$O and TiO which have several million transitions is a formidable problem which requires an efficient method for the numerical solution of the multi-level NLTE radiative transfer problem. Classical techniques, such as the complete linearization or the Equivalent Two Level Atom method, are computationally prohibitive for large model atoms and molecules. Currently, the operator splitting or approximate $\lambda$-operator iteration (ALI) method (e.g. Cannon 1973, Rybicki 1972, Rybicki 1984, Scharmer 1984) seems to be the most effective way of treating complex NLTE radiative transfer and rate equation problems. Variants of the ALI method have been developed to handle complex model atoms, e.g., Anderson’s multi-group scheme (Anderson 1987, 1989) or extensions of the opacity distribution function method (Hubeny & Lanz 1995). However, these methods have problems if line overlaps are complex or if the line opacity changes rapidly with optical depth, a situation which occurs in cool stellar atmospheres. The ALI rate operator formalism, on the other hand, has been used successfully to treat very large model atoms such as Fe directly and efficiently (Hauschildt &
Baron 1995, Hauschildt et al. 1996, Baron et al. 1996b). It allows us to currently treat a large number of species and atomic levels in direct NLTE. NLTE models are absolutely necessary for effective temperatures larger than about 10 000 K as the structure of the atmosphere starts to depend significantly on a proper treatment of NLTE effects. Using LTE models will cause misleading results and should be avoided. In general, models with low gravities will require a full NLTE treatment (with spherical geometry) for lower $T_{\text{eff}}$ than high gravity models.

3. Some results

In the following paragraphs we will give a few representative results that highlight the type of results that can be obtained today.

With our current model code we can fit the spectra of such fundamental standards like the Sun (Figure 2) and Vega (Figure 3) quite well. For cool giants the models can reproduce high-resolution spectra (e.g., Figure 4) and fit simultaneously the interferometrically observed size as function of wavelength. This demonstrates that current models can reproduce the detailed radiation field of giants very well, which strongly supports of the model approaches that were taken since the early 1990's.

For cooler objects, e.g., M, L & T dwarfs, progress in modeling has been substantial over the last few years. This is shown in Figure 5 where we compare
Figure 4. Comparison of the spectrum of $\gamma$ Sge to a PHOENIX model with $T_{\text{eff}} = 3900$ K, $\log g = 0.55$, $M = 1.0 M_\odot$, and solar abundances (top) and the measured wavelength dependent size distribution (bottom). From Aufdenberg & Hauschildt (2002).

models for an L3.5 dwarf with model spectra that were computed under the assumptions (a) dust forms and remains at the depth that it formed (Dusty), (b) dust forms and immediately and completely rains out below the photosphere of the object (Cond) to (c) the physically better model in which the amount
Figure 5. The spectrum of an L3.5 dwarf compared to Dusty, Cond and preliminary dust Settling calculations.

of dust in a given layer is calculated by balancing depletion by gravitational settling with mixing by convection and other global motions in the atmosphere (Settling; Allard et al, in preparation).

4. The GAIA grid

The current state of the art in model atmosphere and synthetic spectra calculations will be able to reliably aid the development of the filter and resolution system and also help the design of analysis packages for the GAIA mission. With modern algorithms and fast parallel computers it is possible to construct a fairly
detailed grid of synthetic spectra for this purpose. While it is clear that this grid will be obsolete by the time GAIA will be launched, however, the basic features of the models will stay the same even in 10-15 years (after all, current models reproduce observed spectra quite well!). We have thus started to compute such a PHOENIX grid that will cover the parameter range of interest to the GAIA community. We will make the grid of synthetic spectra publicly available as models are completed. The grid will use simplifying assumptions, e.g., LTE, for the effective temperature range of $T_{\text{eff}} = 2500$ K to $10000$ K, but will feature the latest set of line lists and be calculated in spherical symmetry for a fixed mass of $1M_\odot$.

We use a setup of the microphysics that gives the currently best fits to observed spectra of M, L, and T dwarfs for the low $T_{\text{eff}}$ regime and that also updates the microphysics used in the NextGen (Hauschildt et al. 1999a, 1999b) model grid. The water lines are taken from the AMES calculations Partridge & Schwenke (1997), this list gives the best overall fit to the water bands over a wide temperature range. TiO lines are taken from Schwenke (1998) for similar reasons. The overall setup is similar to the one described in more detail in Allard et al. (2001).

5. Conclusions

In this paper we have discussed a few new results of stellar atmosphere modeling that have helped to resolve some outstanding problems understanding and interpreting observed stellar spectra. During the last decade, progress was made by breakthroughs in both methodology and computer technology, which has led to substantially improved models and synthetic spectra. This is in good part due to the pioneering work of R. Kurucz who has provided superb atomic line lists that are crucial to obtain reasonable fits. Although there is still a lot of work to be done, advances over the last decade or so have enabled us to deliver far better models than ever before. In many cases, even our current ‘best effort’ models cannot reproduce observed spectra satisfactorily, this is in particular the case for L and T dwarfs. However, this is due to physical effects that we ‘know’ but we cannot currently describe well enough (e.g., incomplete line lists for key molecules or dust and cloud formation processes). Another area that requires much more work is our detailed understanding of winds from both hot and cool stars. There is currently a lot of effort being put into the solution of these key problems, although it is clear that once they are solved, others will pop up in unexpected places.

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