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Cool star model atmospheres for Gaia : ATLAS, MARCS, and PHOENIX

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Abstract. I present the widely used model atmosphere codes ATLAS, MARCS, and PHOENIX, and I compare their output model structures and spectra for cool stars of FGKM-types. While model atmosphere stratifications agree closely with each other in the 1-D approximation, this is not the case for spectra. Differences between model spectra from different codes are largest in the blue-UV, but smaller differences appear in all regions, especially in the molecular features of cooler model spectra. I recommend the groups to try to solve these discrepancies together. In the meantime, users must be careful when using these spectra in regimes where they differ.

I discuss here only comparisons of spectra at solar metallicity, and this should be extended to other metallicities. Detailed comparisons with carefully calibrated spectrophotometric data, and high resolution spectra for stars with well known parameters are also of prime importance. It appears that we still need better line positions for molecules. Finally we should remember that 1-D models are only a step towards a better representation of reality, and we should keep developing, and carefully test 3-D, NLTE models.

1. Introduction

Lots of information we have on stars comes from our comparison of observed spectra with spectra we compute. Synthetic spectra are calculated using a variety of physical data (e.g., atomic and molecular line data, partition functions, dissociation energies), and a physical description of the environment in which spectral lines and continuum occur, the stellar atmosphere. Models of stellar atmospheres are thus a key ingredient in our quest of information on stars. Real star atmospheres display a wealth of dynamical phenomena, such as convection and mass-loss, are structured by magnetic field, with frequent departures from equilibrium in the population of atomic levels. Some recent attempts to include this complexity in stellar atmosphere modeling have widened our capacity to interpret observations, at a considerable computing cost (see, e.g. [1], and Collet in this Volume). On the other hand, it is possible to achieve a quite satisfactory description of stellar atmospheres and spectra, at a much lower cost, by imposing a few, although quite restrictive approximations: local thermodynamic equilibrium (LTE, actually not strictly, as scattering in the continuum is properly treated in 1-D, an issue only recently tackled in 3-D models [2],[3]), hydrostatic equilibrium, 1-D geometry (plane-parallel, PP, or spherically symmetric, Sph), and an energy balance that includes convection treated with the mixing length approximation (MLT). It is surprising how well these approximations work, as long as one is not concerned with extreme cases, or one is not looking at the few percent accuracy level. I will

discuss only such classical modeling, and the main three codes available to compute cool star atmospheres. One should, however, keep in mind the limitations of these models discussed at length in numerous papers, and in this Volume by Collet, Przybilla, and Groh.

2. Model atmosphere codes

2.1. *ATLAS*

The ATLAS code was developed by R. Kurucz in the 1970s [4], and later updated by him and colleagues, see e.g. [5], [6]. The currently used versions are ATLAS9, using Opacity distribution functions (ODF), and ATLAS12, using OS, with 30 000 points. A major contribution of R. Kurucz was to compute, and provide to the community with an extensive database of atomic and molecular line data (see kurucz.harvard.edu, for data, and codes, including the synthetic spectrum code SYNTHE). They are in wide use in the community, and the atomic data is included in the VALD database [7]. A comparison of ODF and OS models of FGK stars shows very little differences, for the same chemical composition and line data. It was shown, however, by [8] that ODF is a poor approximation when different sources of opacity uncorrelated in wavelength occur at different atmospheric depths. This is the case in, e.g., cool carbon stars, with CO and CN at depth, and HCN and C₂H₂ in the surface layers. Opacity sampling offers a better description of the radiation field, provided a sufficiently large number of wavelength points are used (of the order of 10⁵, [9]). Comparisons of ATLAS9 and ATLAS12 models were made by U. Heiter (camd08.ast.cam.ac.uk/Greatwiki/WGB4StellarAtmospheres/Workshop2010), who also gives useful information on the code and its history, as well as a number of links to grids of models (wwwuser.oat.ts.astro.it/castelli/, and www.univie.ac.at/nemo/cgi-bin/dive.cgi). There is a spherical version of ATLAS by J. Lester and H. Neilson [10], on www.astro.utoronto.ca/lester/Programs. A workshop was dedicated to ATLAS12, and the various tools and data associated with it in 2005 (see sait.oat.ts.astro.it/MSAIS/8/index.html)

2.2. *MARCS2008*

The MARCS model atmosphere code has been in use since the mid-1970s [11]. A detailed history of its development may be found in [9], and in [12]. The models are computed in PP or Sph 1-D geometry, LTE, hydrostatic equilibrium, with a detailed account of opacity through opacity sampling (OS) with more than 10⁵ wavelength points. A major update of the input physical data, esp. of opacities, resulted in the publication of a new grid [12], available online (www.marcs.astro.uu.se). The inclusion of a huge number of molecular lines allows the computation of cool stars, including M, S, and C-types. The temperature range is limited downwards to M dwarfs, due to the lack of dust opacities, and to the use of the electron pressure as a primary variable. The hot end is early F or late A-type stars, due to limits in the number of ions that are included. The details of the implementation of the code and of the input data are discussed in [12]. Sphericity effects were discussed by [13], [14], and [12]. There is a synthetic spectrum code, turbospectrum [15], available upon request to B. Plez, that includes the same physical data, and routines than the MARCS code.

2.3. *PHOENIX*

The PHOENIX code was born in the 1990s see, e.g. [16], and references therein. It is much more general than MARCS and ATLAS, as it can handle relativistic dynamical media, and massive NLTE, in 1-D. Models published through the years cover supernovae to brown dwarfs and planetary atmospheres. A 3-D version has been developed recently [17].

2.4. Limitations of the models

We may improve opacities, input data, as it has been extensively done in the past decade, but there are limitations intrinsic to the methods : sampling of the opacities, LTE, 1-D. The relaxation of the LTE hypotheses is outside the scope of this paper, but discussions can be found elsewhere in this volume. Opacity sampling is now routinely done with a number of wavelengths in excess of 10^5 , which is a big advantage of simple classical models over more sophisticated 3-D, or NLTE models. A 1-D model can be computed within minutes on a laptop, whereas it is a major computational effort to increase the number of frequency bins in 3-D hydrodynamical models. The impact of a coarse sampling of opacities on the thermal structure, and the emergent sampled spectral energy distributions (SED) was discussed by [9]. The conclusion is that 10^5 sampling points between 100 and 20 000 nm are sufficient to compute cool star (FGKM) model atmospheres with errors on the thermal stratification not exceeding a few degrees Kelvin in any layer. One exception is the optically thin layers of metal-poor stars due to the fact that only a few lines dominate their thermal equilibrium. However, other effects (hydrodynamical, and NLTE) are likely to have a stronger impact on the temperature of these layers. Sampled SEDs are more a problem, as many lines affect the emergent flux, without effects on the thermal structure. A sampling density sufficient for an accurate thermal structure may not allow the computation of a sampled SED to better than 10% in some spectral regions. Detailed spectra can, and should of course be computed afterwards with much larger spectral resolution ($> 10^6$ points), based on the thermal stratification calculated with much less points.

3. Comparison of model structures

Before looking at emergent spectra, it is important to verify if the three codes, using different numerical methods and schemes, as well as different input physical data, produce similar model stratifications. [12] show comparisons between MARCS, ATLAS, and PHOENIX thermal structures for solar and metal-poor composition, for dwarfs, giants, and supergiants models of effective temperatures, T_{eff} between 3000 K and 7000 K. Large differences are not found, except with previous generation PHOENIX models (NextGen).

4. Comparison of spectra

4.1. The SED

A comparison of ATLAS and previous generation PHOENIX (NextGen) models was made by [18], by fitting the SEDs of a sample of target stars. Here, I wish to compare models between each other. They should of course also be compared to observations. This was done for MARCS models, in a preliminary way, by [19]. One simple way to look at the differences in the overall shape of spectra is color-color, and color- T_{eff} diagrams. I therefore computed Johnson-Cousins UBVR_IJHK photometry for a number of MARCS and PHOENIX (kindly provided by P. Hauschildt) model spectra using the filters of [20]. For ATLAS models the photometry computed with the same filters is available on wwwuser.oat.ts.astro.it/castelli/. This was done for solar metallicity models only. Figure 1 shows the T_{eff} - V-K relation for giants and dwarfs. Small differences may be seen around 3500 K and below (note that there are no ATLAS models cooler than 3500 K). With its large leverage on the SED of cool stars, the V-K index is a very powerful tool for temperature determination, quite insensitive to gravity (except for M-type stars), and metallicity, and thus not so sensitive to modeling details. It is, however, affected by reddening. Figure 2 shows that there seems to be a problem in the near-IR flux (too blue) of the dwarf ATLAS models for $T_{\text{eff}} \leq 4000$ K. The T_{eff} - B-V relation of Figure 3 is more affected by metallicity and gravity. The calculations of the three codes agree well above 4000 K for both giants and dwarfs, which indicates that opacities are accounted for in very similar ways in the blue-green part of the spectrum. This is not so surprising as they all use the VALD or Kurucz atomic line data, which is part of VALD. Below 4000 K large differences show up. The

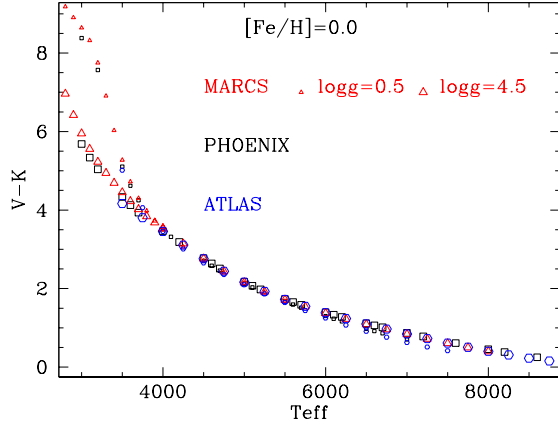


Figure 1. T_{eff} - $V-K$ relation for dwarf (large symbols) and giant (small symbols) star models ($\log g=4.5$ and 0.5 cgs respectively). Blue circles are ATLAS models, red triangles are MARCS models, and black squares are PHOENIX models.

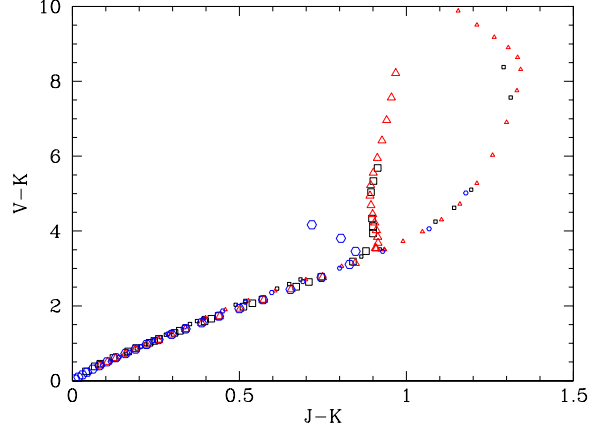


Figure 2. $J-K$ - $V-K$ relation. Symbols as in Figure 1.

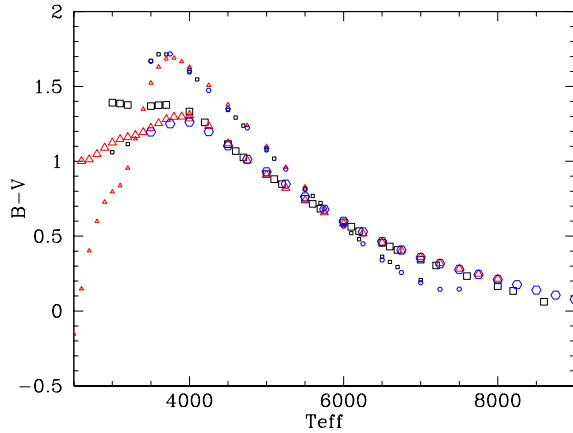


Figure 3. T_{eff} - $B-V$ relation. Symbols as in Figure 1.

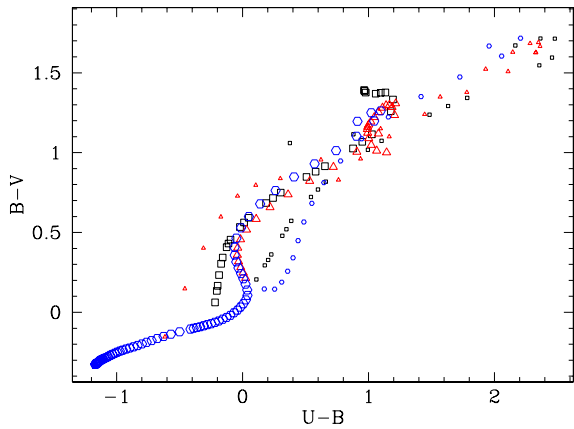


Figure 4. $U-B$ - $B-V$ relation. Symbols as in Figure 1.

$U-B$ - $B-V$ plot of Figure 4 displays differences of up to half a magnitude. It appears that the blue-violet part of the spectrum is the most problematic, and these differences should be investigated in detail, in order to pinpoint their origin, and find a cure.

4.2. the RVS domain

The next comparison we can make of direct interest to Gaia is high-resolution spectra in the RVS domain. To that end I computed high-resolution ($R = \lambda/\Delta\lambda = 500\,000$) spectra for a number of MARCS models using the Turbospectrum code. The input atomic line data comes from VALD, and the molecular lines from the MARCS database. I collected PHOENIX spectra (courtesy of P. Hauschildt) for similar models, that use a partly different set of line data. All spectra

were degraded to the resolution of the RVS by convolution with a Gaussian profile of 26 km s^{-1} . This comparison thus gives an estimate of remaining discrepancies due to both differences in the model structures, and in the line data used to compute the spectra in different groups. Figure 5

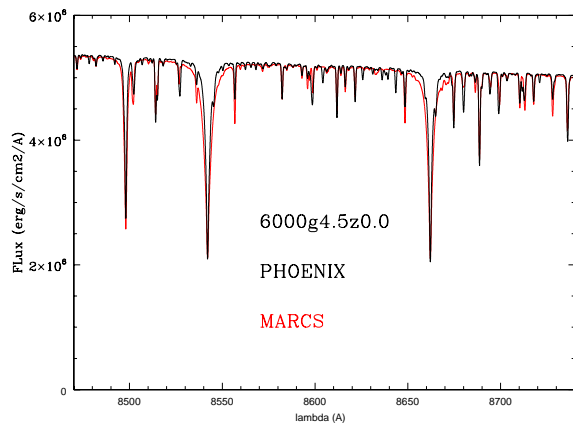


Figure 5. Synthetic spectra in the Gaia/RVS range for stellar parameters typical of a solar composition G dwarf. The black solid line is for a PHOENIX model, and the red solid line for a MARCS calculation. Spectra were degraded to the resolution of the Gaia/RVS.

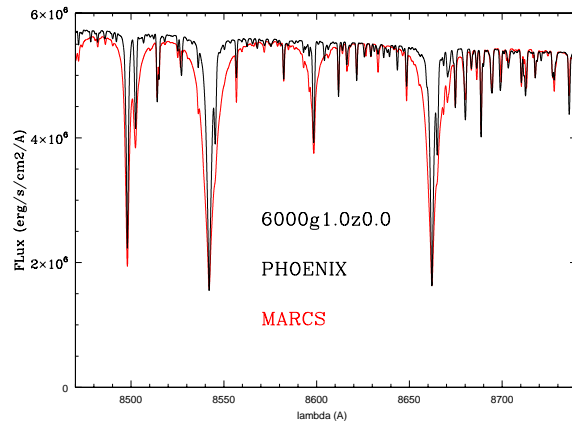


Figure 6. Synthetic spectra in the Gaia/RVS range for stellar parameters typical of a solar composition G supergiant. Symbols as in Figure 5.

to Figure 10 show comparisons at this resolution. Note that to really understand where the differences stem from, it is necessary to carry out an analysis at much higher resolution, as most features seen at the RVS resolution are blends of lines, both atomic and molecular, especially at lower T_{eff} . My purpose here is only to estimate at which level two independent calculations (codes, and physical and line data) differ. This gives us an idea of the magnitude of errors we may expect from the current models. Figure 5 and Figure 6 display model spectra representative of a dwarf, and a supergiant star slightly hotter than the Sun. The most prominent difference between MARCS and PHOENIX spectra is that the latter have markedly narrower Ca II lines. In MARCS/Turbospectrum collisional line broadening is treated according to the recipes of [21], [22]. This is obviously not the case in PHOENIX, but this implementation is under way. There are a number of other differences in the details of fainter features. An interesting fact is that MARCS predicts broader Ca II lines in the lower gravity model, with lower pressure. Naively one would expect the opposite. This is a well-known effect of contrast between line and continuum opacity. In the supergiant model, the electron pressure is 30 times lower than in the dwarf, leading to a 30 times lower H^- opacity, and thus to stronger lines. In both cases Ca is almost fully ionized. Figure 7 and Figure 8 show a similar comparison for a dwarf and a supergiant model of K-type. In the supergiant model, molecular lines begin to show up, and they become much more prominent in M-type stars, like in the M dwarf model of Figure 9. The enlarged plot of the same spectra in Figure 10 demonstrates that there is work to be done on molecular line lists (TiO here), at least on the line positions. This demands careful comparisons with observed spectra of standard stars. It is also obvious from Figure 7 that the situation is much worse for FeH (with band head at 8690 \AA), with a large uncertainty in the line strengths.

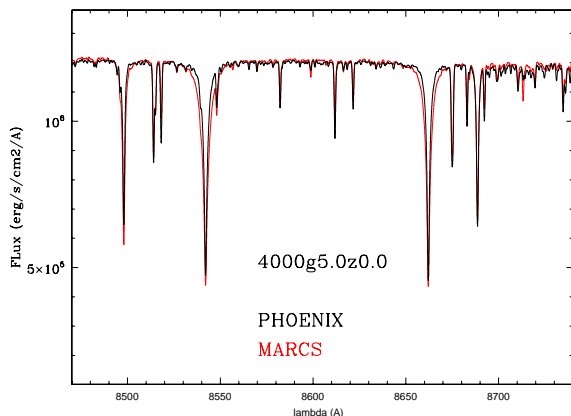


Figure 7. Synthetic spectra in the Gaia/RVS range for stellar parameters typical of a solar composition K dwarf. Symbols as in Figure 5.

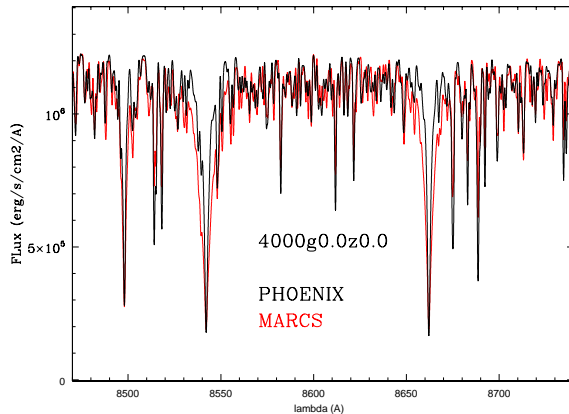


Figure 8. Synthetic spectra in the Gaia/RVS range for stellar parameters typical of a solar composition K supergiant. Symbols as in Figure 5.

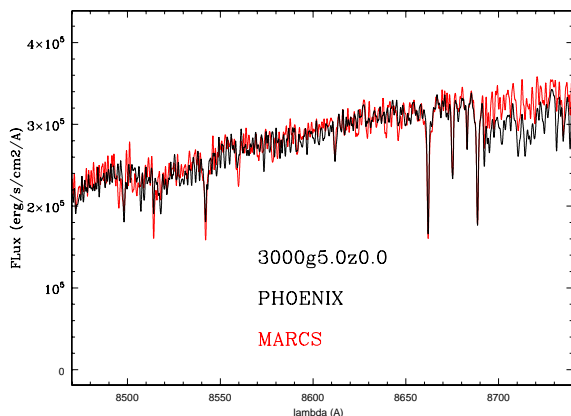


Figure 9. Synthetic spectra in the Gaia/RVS range for stellar parameters typical of a solar composition M dwarf. Symbols as in Figure 5.

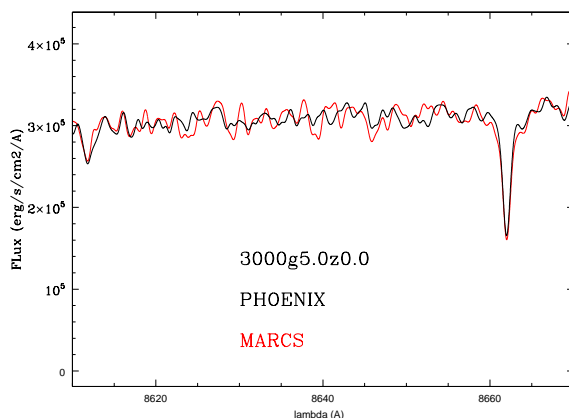


Figure 10. Zoom in on the 8610-8670 Å window of the spectra of Figure 9. Symbols as in Figure 5.

5. Conclusions and recommendations

The non-exhaustive comparisons presented above show that there are still significant differences between ATLAS, MARCS, and PHOENIX model spectra, although model structures are quite similar. Judging from color comparisons, most large differences are in the UV, and their origin should be investigated. ATLAS model spectra deviate in the near-IR, below 4000 K. PHOENIX model spectra deviate in B–V below 4000 K. In the RVS domain, from the comparison of MARCS and PHOENIX model spectra, it appears that a number of faint features do not match each other. In PHOENIX calculations, collisional broadening is too approximate, and should be improved following the recipe of [21], [22]. This is under way. M dwarf model spectra reveal important differences in the details of TiO bands, and in the strength of FeH. The MARCS and PHOENIX groups should compare in detail their line lists, and settle this problem. I discuss

here only comparisons of spectra at solar metallicity, and this should be extended to other metallicities. While model atmosphere stratifications agree closely with each other in the 1-D approximation, this is not the case for spectra. Detailed comparisons with carefully calibrated spectrophotometric data, and high resolution spectra for stars with well-known parameters are of prime importance to test the models. Large efforts are indeed being devoted within the Work Package "Provide calibration training data" of CU8 to this end. It appears that we still need better line positions for molecules. Close collaboration with physicists is very productive, and must be encouraged. Progress is being made for, e.g., CN, C₂, CH, C₂H₂. Finally we should remember that 1-D models are only a step towards a better representation of reality, and we should keep developing, and carefully test 3-D, NLTE models.

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