

Libraries of synthetic stellar spectra – or are we building palaces upon sand?

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Abstract. The possibilities and problems of using calculated spectra from model atmospheres when analysing stellar populations in galaxies are reviewed. Various types of consistency tests for stellar models are discussed, as well as comparisons with observational data. It is argued that major improvements in the model spectra are possible and worthwhile.

Keywords. stars: atmospheres; galaxies: evolution, photometry

1. Introduction

When modelling the stellar populations of a galaxy on the basis of integrated spectra and colours different approaches may be taken. One may try to infer the properties of the stellar population directly from the observed spectrum, which in the ideal case will lead to the Hess diagram of the population, with additional information about the distribution of stars over different metallicities for each region in that diagram. Generally, however, it is necessary to add more constraints to this inversion process, which are obtained from constructing an evolutionary model of the stellar population, on the basis of evolutionary tracks for the individual stars. The basic free parameters of such a model will then be the star-formation rate as a function of time, the infall-rate of gas into the system, and the slope of the Initial Mass Function of the stars. More implicit but important parameters may describe the mixing efficiency of the ISM in the galaxy, and the yields of heavy elements from various types of stars.

Whether the most direct inversion of the spectrum to the Hess diagram is attempted, or a more or less elaborate chemical evolution model is made first, the calculation of the spectrum and spectral-energy distribution (SED) of the galaxy, to be compared with the observed one, requires knowledge of the spectra of the stars that the galaxy is supposed to consist of. Early population syntheses of galaxies (e.g. Spinrad & Taylor 1971) were usually based on observations of galactic template stars which were assumed to be representative of the populations in external galaxies. Although it was realized from the beginning that these stars may not fully match those of, e.g. the centres of galaxies like M31, there was no real alternative since the theoretical spectra calculated from model atmospheres were not of high enough accuracy to replace the observed template spectra.

The art of calculating theoretical stellar spectra was however gradually developed. Early pioneers were Nishimura (1958) who calculated TiO bands in M giants and Fay & Morgan (1967) who computed near-IR spectra of carbon stars. For less complicated spectra, continua and Balmer lines, considerable work was done by several people during the 1960's, for a summary see Cayrel (1969). Synthetic stellar colours, with statistical consideration of metal-line blocking, were calculated early by Baschek (1960) and later by Böhm-Vitense (1970) and Kurucz (1975). The great pioneer, in systematically developing the calculation of synthetic spectra to a high degree of realism for late-type stars was,

however, Roger A. Bell. After his first work on synthetic colour for F, G and K stars (e.g. Bell & Rodgers (1969), Bell (1970), Bell & Gottlieb (1971), Bell (1971)), he continued systematically improving the synthetic spectra and the model atmospheres (partly in collaboration with one of the present authors), and also provided theoretical calibrations of Lick indices for population synthesis (Tripicco & Bell 1995). Somewhat later, Bob Kurucz was the only colleague who matched the contribution of Bell in this field of research.

Being aware of the impressive advances made during the last four decades in this field of calculating theoretical stellar spectra one might hope that existing libraries of such spectra could be successfully applied in modelling galaxies. Sometimes, theoretical spectra are the only rescue, like for populations containing stars that are not present in the solar neighbourhood, such as massive metal-poor stars or stars with very high metallicities. In this review we shall explore whether such an expectation is well founded. A basic reason to scrutinize the adequacy of the theoretical spectra is, as was indicated above, the fact that the evolutionary models for the galaxies are loaded with so many free parameters, or even *ad-hoc* assumptions, that all measures must be taken to ascertain that further errors are not introduced in the analysis due to bad basic stellar data.

2. The physical failures of standard model atmospheres

A model stellar atmosphere is, as any theoretical model, built on a number of simplifying assumptions. For more than 3 decades these usually were: plane-parallel stratification in homogeneous layers (1D), hydrostatic equilibrium (HE), local thermodynamic equilibrium (LTE) and convective fluxes calculated from the local conditions according to the so-called mixing-length theory (MLT). More recently, model grids for extended stars with spherically symmetric stratification have been made, a minor but significant modification as will be illustrated below. The LTE assumption has also been relaxed, in particular for early-type stars, and in a few cases 3D models, with much more realistic convection, have been constructed. A second very significant ingredient in the models is a wealth of basic physics data, in particular transition probabilities and other data for the many millions of atomic and molecular spectral lines that contribute significantly to the spectrum of the star and to the energy transfer in its atmosphere.

The key question is now: How good are these models? How well do the model spectra reproduce those of stars with fundamental parameters (effective temperatures, radii, masses and chemical compositions) equal to those adopted for the models?

One way to explore this issue is to investigate the consequences of the inconsistency introduced by the basic assumptions. Another way is to compare the structures and spectra of models from various computer programs which may depart as regards numerical methods, the physical data used or even the basic assumptions made. A third way is to compare the model spectra with corresponding observed stellar spectra. In the present section we shall concentrate on the degree of physical consistency of the standard models and defer the other aspects to the following sections.

A major achievement in the modelling of stellar atmospheres has been made during the last decades in that 3D hydrodynamical and magneto-hydrodynamical models (relaxing both HE and MLT above) have been developed for solar-type stars (Nordlund 1982, Nordlund & Dravins 1990, Stein & Nordlund 2000, Asplund *et al.* 1999). Similar models for red giants have been constructed by Collet *et al.* (2006) and Kúćinskas, Ludwig & Hauschildt (2006). With a somewhat different approach, where the full star is represented in a computational spatial grid (“a star in a box”) Freytag (2003) has modeled supergiants. The mean structures of the models show considerable departures from standard 1D models. E.g., the cool metal-poor models of Asplund *et al.* (1999) and

in particular the very-metal-poor models of Collet *et al.* (2006) have considerably cooler surface layers than corresponding 1D models, which leads to severe effects on abundance determinations from the temperature-sensitive molecular lines. For the M giant models of Kúcinškas, Ludwig & Hauschildt, there are also considerable effects on the temperature structure, leading to typical differences of e.g. the V-K colour of 0.2 mag. Until now, however, no extensive grids of 3D models exist. In fact, although it has been shown that these models produce line profiles in much better agreement with observations, no full spectra have as yet been calculated for any of them. It may well take some years before such grids are available to the completeness needed for e.g. population synthesis.

Grids of line-blanketed model atmospheres of O- and B-type stars with the LTE assumption relaxed (i.e. in Statistical Equilibrium) were recently computed by Lanz & Hubeny (2003, 2006). Their B star spectra show somewhat larger Lyman and smaller Balmer continuum fluxes when compared to LTE models, which might be of some significance when models are used for reconstructing the star-formation history of young stellar populations. For B-type stars, the bolometric corrections presented by Lanz & Hubeny (2003) are systematically different by 0.1 mag from the LTE values by Castelli and Kurucz (2003). Model atmospheres for late type stars relaxing the assumption of LTE for various species have been explored by Short & Hauschildt (2003, 2005), Schweitzer, Hauschildt, and Baron (2000), Hauschildt *et al.* (1997) – but the results do not yet allow any conclusions as to their importance for galaxy spectra. The NLTE effects on models were either found to be negligible or difficult to judge due to the fact that other aspects of the models were incomplete (e.g. missing UV opacity).

Models for pulsating atmospheres of red giants, driven by a piston in the bottom of the models, have recently been produced by Höfner *et al.* (2005), see also Gautschy-Loidl *et al.* (2004). The models are fundamentally different from classical static models, in particular since the outer layers are far more extended by the pulsation shocks into an expanding atmosphere, forming a dust-driven wind. Also the spectrum energy distributions are severely affected, by this extension as well as by dust opacities which are quite uncertain. The latter authors show that these models have spectrum variations that agree at least qualitatively with the observed spectra of AGB stars. The models predict mass-loss rates that are, however, significantly dependent on the piston amplitude which at present cannot be calculated consistently. As an example of recent progress in this area, which also includes the calculation of extensive grids of models, see Wahlin, Höfner and Mattsson (2007, present volume). A major uncertainty in such attempts is our lack of a good theory for dust formation, in particular for oxygen-rich gases. This certainly limits our chances to properly model galaxy IR fluxes if AGB stars contribute significantly. We note in passing that Barmby *et al.* (2006) conclude that the 3.6 μm flux of M31, which represents old disk stars, is not dominated by AGB stars.

For very low-mass stars ($T_{\text{eff}} \leq 2800$ K), Chabrier *et al.* (2000) calculated model atmospheres, including the formation of dust grains. Colour-magnitude diagrams calculated from these models are significantly different from those neglecting dust formation, in particular for near-IR colours. This might affect population synthesis studies in the near-IR of galaxies, if low-mass stars are important contributors. If the latter can be the case is at the moment not clear. Simulations of simple stellar populations by Maraston (2005) show that even for old ages, the contribution of main-sequence stars to the total bolometric, V- and K-band luminosities approaches that of RGB stars.

For stars in different regions of the HR diagram, the effects of magnetic fields on atmospheric structures have been explored. Kochukhov, Kahn & Shulyak (2005) calculated models for A-type stars with enhanced line blanketing due to the intensification of spectral lines by a magnetic field. They found that magnetic models have lower fluxes

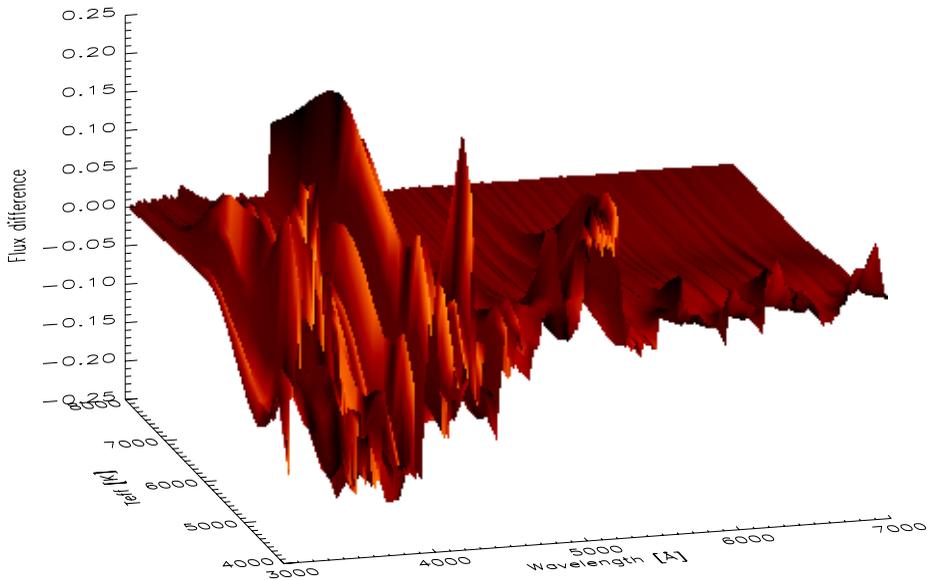


Figure 1. Relative flux difference between α -poor models ($[\alpha/\text{Fe}]=0.0$) and α -normal models ($[\alpha/\text{Fe}]=+0.4$) for $[\text{Fe}/\text{H}]=-1.0$ and $\log g = 4.5$. The spectra are binned in wavelength to $\approx 20\text{\AA}$ and the stepsize in T_{eff} is 250 K. The features in the “difference-landscape” are (from right to left) due to CaH/TiO (peaks at 6200–6500 \AA and 6700–7000 \AA , 4000 – 4500 K), MgH (peaks at 4950–5200 \AA and 4775 \AA , 4000 – 5000 K), Mg I at 5175 \AA (4000 – 6500 K), Ca I at 4226 \AA (4000 – 5000 K), Ca II, Ca I and Mg I at 3920–4000 \AA (from 5500 to 8000 K mainly Ca II), Mg I at 3830–3840 \AA (4000 – 5000 K). The difference in the continuum is due to the greater significance in the α -rich models of the H^- opacity as compared with Rayleigh scattering by H I, reflecting the increased abundance of the electron donors Mg, Si and Ca.

in the UV and higher in the visual spectral region. Thus, a magnetic star mimics a non-magnetic star with a temperature lower by maximally 500 K. With a percentage of magnetic and chemically peculiar stars of 5–10%, which is characteristic of the Milky Way (North 1993), effects of magnetic fields could be important for fluxes from galaxies dominated by B and A-type stars. Dorch (2004) has calculated MHD models of Betelgeuse, using a “star in a box” approach similar to that used by Freytag (2003). Dorch finds that “local dynamos” generate large-scale effects due to the large scales of convective patterns in this supergiant. He finds magnetic fields that are strong enough to effect the surface structures as well as the winds. The direct effects on the photospheric spectra and spectrum energy distributions remain to be explored.

Summing up, we see that the classical models are seriously questioned when the basic assumptions are scrutinized. I.e., their spectra may be systematically off as compared with corresponding stars, and this may have important effects on the interpretation of galaxy spectra. However, due to the very incomplete coverage of the HR diagram by these more advanced models, it is still not possible to replace the classical grids. In fact, the more realistic models are still so scant that more precise statements cannot yet be made on what errors are caused by using them.

Table 1. Recently published grids of synthetic spectra. The value-pairs in parentheses give lowest and highest value of a range of grid values. ^s: spherical models, ⁿ: non-LTE models. The MARCS models are available at <http://marcs.astro.uu.se/>.

Reference, <i>Code</i>	$T_{\text{eff}} [K]$	$\log g$ [cgs]	$[M/H]$	$[\alpha/Fe]$	$\lambda [\mu\text{m}]$
Coelho <i>et al.</i> (2005), <i>ATLAS9</i>	(3500, 7000)	(+0.0, +5.0)	(−2.5, +0.5)	+0.0, +0.4	(0.300, 1.80)
Rodríguez-Merino <i>et al.</i> (2005), <i>AT-</i> <i>LAS9</i>	(3000, 50000)	(+0.0, +5.0)	(−2.0, +0.5)		(0.085, 0.47)
Munari <i>et al.</i> (2005), <i>ATLAS9</i>	(3500, 47500)	(+0.0, +5.0)	(−2.5, +0.5)	+0.0, +0.4	(0.250, 1.05)
Brott & Hauschild (2005), <i>PHOENIX</i>	(2700, 5000)	(−0.5 ^s , +5.5)	(−3.5, +0.5)	(−0.2, +0.8)	(0.001, 50.0)
Martins <i>et al.</i> (2005), <i>TLUSTY, ATLAS, PHOENIX</i>	(3000, 55000 ⁿ)	(−0.5 ^s , +5.5)	(−1.0, +0.3)		(0.300, 0.70)
Gustafsson <i>et al.</i> (2003), <i>MARCS</i>	(4000, 8000)	(−1.0 ^s , +5.0)	(−5.0, +1.0)	(+0.0, +0.4)	(0.130, 20.0)

3. Some recent spectrum grids

Grids of synthetic flux spectra for stars within relatively wide parameter ranges have recently been published and are listed in Table 1. The spectra are based on model atmospheres from four different and independent codes, Kurucz’s ATLAS program (e.g. Castelli & Kurucz (2003)), the PHOENIX program of Hauschildt *et al.* (1996), TLUSTY (Lanz & Hubeny (2003) and references therein), and the MARCS program (Gustafsson *et al.* 2003). ATLAS models are in LTE and (predominantly) plane parallel, MARCS produces spherically symmetric LTE models while PHOENIX and TLUSTY may be used for calculating spherical or plane-parallel models in non-LTE, the first code mostly for late-type stars (although most of the published PHOENIX models are still based on the LTE assumption) and the latter code for hot stars. The spectra are calculated with input data fully consistent with those of the model atmospheres or in some cases (e.g. Coelho *et al.* 2005) with semiempirically modified line lists.

The grids of model spectra offer excellent possibilities to explore the variation of the spectrum properties with stellar fundamental parameters. An example is given in Fig.1 where ratios of spectra of models with different $[\alpha/Fe]$, i.e. logarithmic abundance ratios of the alpha elements (elements with even atomic numbers from O to Ti) relative to Fe, are shown as a function of wavelength and effective temperature.

Detailed comparisons of model spectra from different grids and calculated with different synthetic-spectrum programs have been made by Martins *et al.* (2005). In general, good agreement was found. When comparing spectra of MARCS models with those from the Coelho *et al.* (2005) grid a very satisfactory agreement is found for T_{eff} above 4000 K, while some clear discrepancies are seen for models for M-type stars, essentially reflecting differences in TiO line data. Even more severe discrepancies, however, are displayed in Fig. 2, reflecting the fact that the effects of sphericity for M-giants are not included in the Coelho *et al.* (2005) grid. Corresponding effects were corrected for empirically for plane-parallel Kurucz models by Lejeune, Cuisinier & Buser (1997), using broad-band colours. We have found, however, that such simple correction factors, assumed to be smoothly varying with wavelength, are not adequate for this purpose; the flux-ratio for spherical models vs plane-parallel ones changes rapidly with wavelength, e.g. across the various TiO bands, as may be seen from Fig. 2. Effects on sphericity on spectra were recently explored for F and K giants by Heiter & Eriksson (2006).

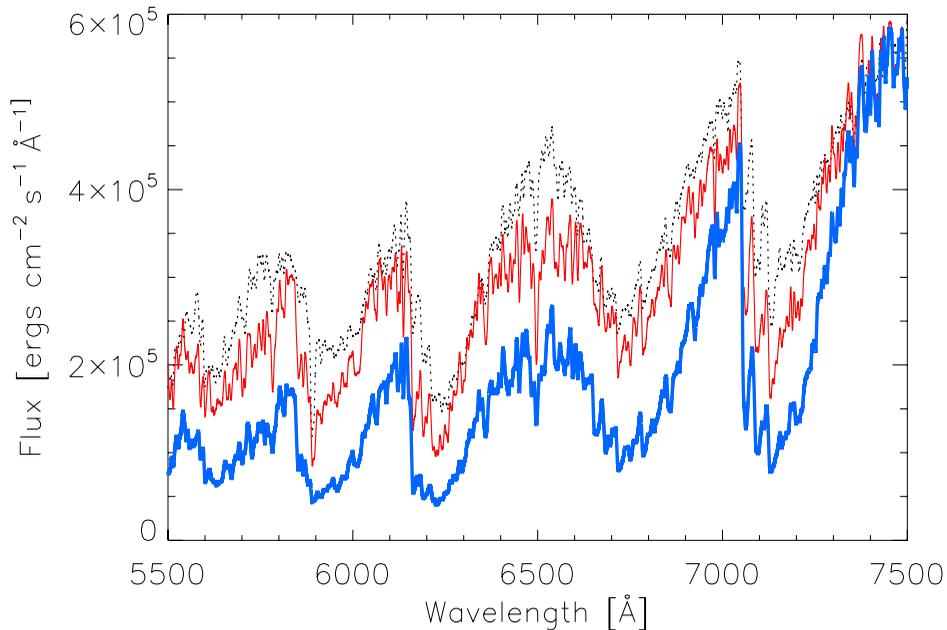


Figure 2. Comparison between calculated spectra from Coelho *et al.* (2005, dotted line) and the MARCS library (thin line: plane-parallel model, thick line: spherical model). (T_{eff} , $\log g$, $[M/H]$, ξ_t) = (3500 K, 0.0, 0.0, 5.0 km/s).

4. Do models match stars?

As a first test comparison of the standard models with stars we explore the agreement of a calculated solar flux spectrum with observations in Fig. 3. We find that the model matches the observations quite well – but there seems to be a tendency for an excess in the calculated flux in the interval 4400–4900 Å. The reason for this excess is still not known.

There are several libraries of absolutely calibrated stellar flux distributions or low-resolution spectra which may be compared with calculated spectra. Coelho *et al.* (2005) show several such comparisons with spectra in the STELIB library (Le Borgne *et al.* 2003) and demonstrate a generally good agreement. In Fig. 4 we show a comparison of MILES empirical spectra (Sánchez-Blázquez *et al.* 2006, Cenarro *et al.* 2007) with MARCS fluxes. We find again a good agreement, provided that the effective temperatures of the models are taken 100–200 K hotter than those ascribed to the stars in the MILES library. We note, as do Sánchez-Blázquez *et al.* (2006), that the MILES spectra tend to be bluer than corresponding STELIB spectra, as well as spectra in the ELODIE archive (Moultaka *et al.* 2004), although these two latter sets of data occasionally show considerable departures from each other. When comparing MARCS spectra with spectra from the HST-STIS low/medium resolution mode (helpfully provided by Michael Gregg) we find generally very good agreement. In these comparisons we have been anxious to limit them to stars with fundamental parameters well determined from independent data.

The overall good agreement in the near ultraviolet-visual-near IR wavelength region found for stars in the spectral interval B–K becomes somewhat less satisfactory for M stars and C stars, although examples of very good spectral fits, e.g. by MARCS models,

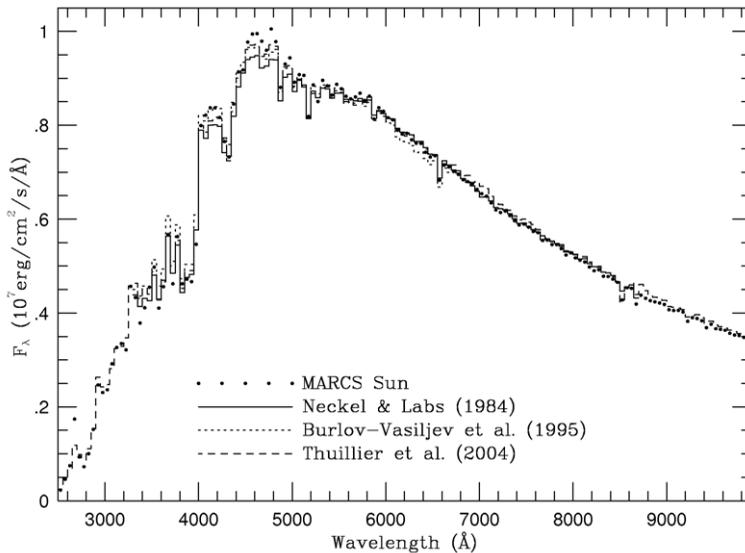


Figure 3. The MARCS solar model flux compared with absolute-calibrated observations. The Neckel & Labs (1984) and the Burlov-Vasiljev *et al.* (1995) data were obtained from the ground, while the Thuillier *et al.* (2004) data is a critical compilation of space-based observations with different instruments. The model fluxes generally agree well with observations, and there is no longer any indication of a so-called missing UV opacity. Note, however, the systematically higher model fluxes at the flux peak in the 4400–4900 Å region.

have also been presented for such stars (see, e.g. Garcia-Hernández *et al.* 2006). At longer wavelengths the predicted medium-resolution spectra of stars earlier than M0 are judged to be accurate to 3% in the middle IR and 5% in the far IR (Decin 2007).

For colours a generally satisfactory agreement between calculations and observations is obtained, see e.g. Munari *et al.* (2005), with some problems for the coolest stars. A detailed study of the situation for infrared colours beyond the K band remains to be made. Narrow-band indices are, however, not fully reproduced. E.g., for MARCS models Önehag *et al.* (2007) have been able to recover the effective-temperature scale of the Strömgren ($b - y$) and $H\beta$ indices very well, while the metallicity dependence of the m_1 index for F-type stars comes out wrong. This may be connected with a mismatch of the MARCS models with STIS spectra for subdwarfs, where we trace a flux deficiency of the models in the v band (cf. Fig. 5). We tentatively suggest that this may be due to the effects of convective temperature inhomogeneities in the stellar photospheres.

5. Should we build houses on sand? Recommendations

We have seen that the standard model atmospheres are not only physically inconsistent – attempts with more advanced modelling where the standard basic assumptions are partly relaxed indicate that the predicted fluxes from standard models may well be severely in error. When standard models from different grids are intercompared they tend to agree satisfactorily in most cases – the remaining differences are mainly due to differences in physical (atomic and molecular) input data. When testing the standard models relative to observed SEDs or spectra of stars with well-known fundamental parameters, a relatively good agreement is also often found. This may reduce our worries caused by the physical inconsistencies, but one should then note that a main use of the model

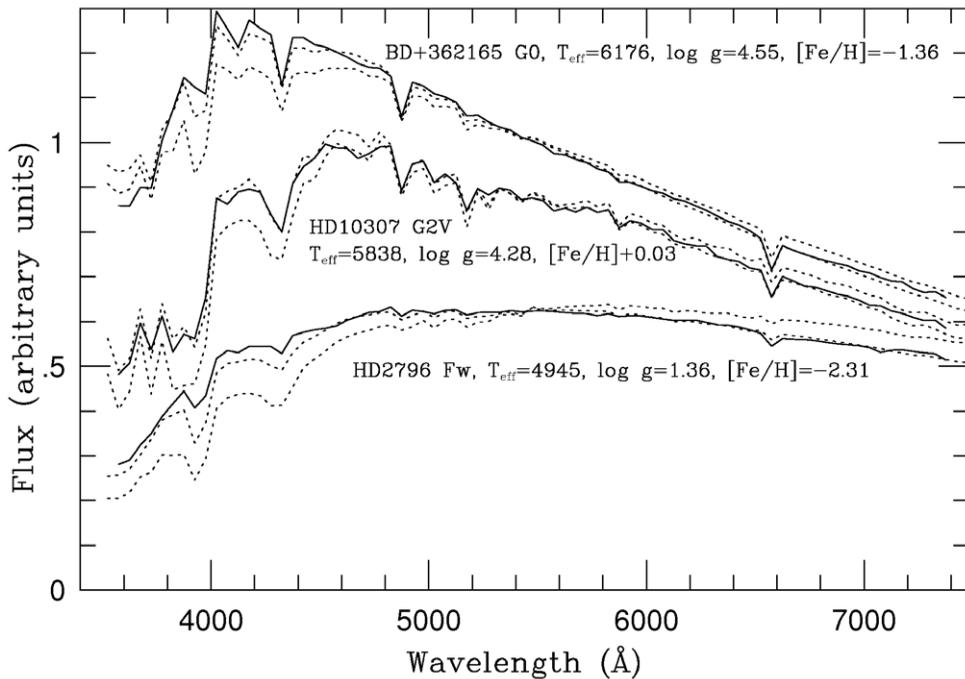


Figure 4. Comparison of observed MILES spectra (solid) to MARCS model fluxes (dotted). The fluxes have been binned to 50 Å wide bins, and are normalized in the 5000–6000 Å region. The stellar parameters according to MILES are shown in the figure. Model effective temperatures straddle the MILES values: 6000 and 6250 K for BD+362165, 5750 and 6000 K for HD10307, and 4750 and 5000 K for HD2796.

atmospheres is in extrapolating to stellar populations that are not represented in the solar neighbourhood, stars for which the model adequacy cannot be tested in any detail. Extrapolations to stars, such as very metal-rich ones, may therefore be quite dangerous. What may then be done to minimize the risks?

A first recommendation, which is comparatively cheap from an observational cosmologist's point of view is: *support those who work ambitiously on making the model atmospheres physically more self-consistent. One should not only calculate single models (that illustrate the phenomena in principle) but small grids of models and fluxes, so that the effects on e.g. integrated spectra can be tested.* Another important recommendation is: *develop criteria for the analysis of integrated spectra of stellar populations, that are sensitive to the parameters of this population but simultaneously minimally sensitive to the uncertainties in the model atmospheres.* One should calculate complementary grids of *artificially modified model atmospheres* with the surface temperature and the temperature gradient varied, and then select criteria that vary only a little with these perturbations. To succeed in this one must probably explore a broader spectral region, not the least out into the infrared. Another recommendation is: *when empirically correcting grids of theoretical spectra to force them to agree better with template stars, do this only after a detailed analysis of the situation.* The mis-match may be due to a complex interplay between several circumstances (observational calibration, fundamental parameter errors, physical inconsistencies in the models and errors in input physics data) and it may be quite inadequate to try to remedy it by, say, simple zero-point shifts.

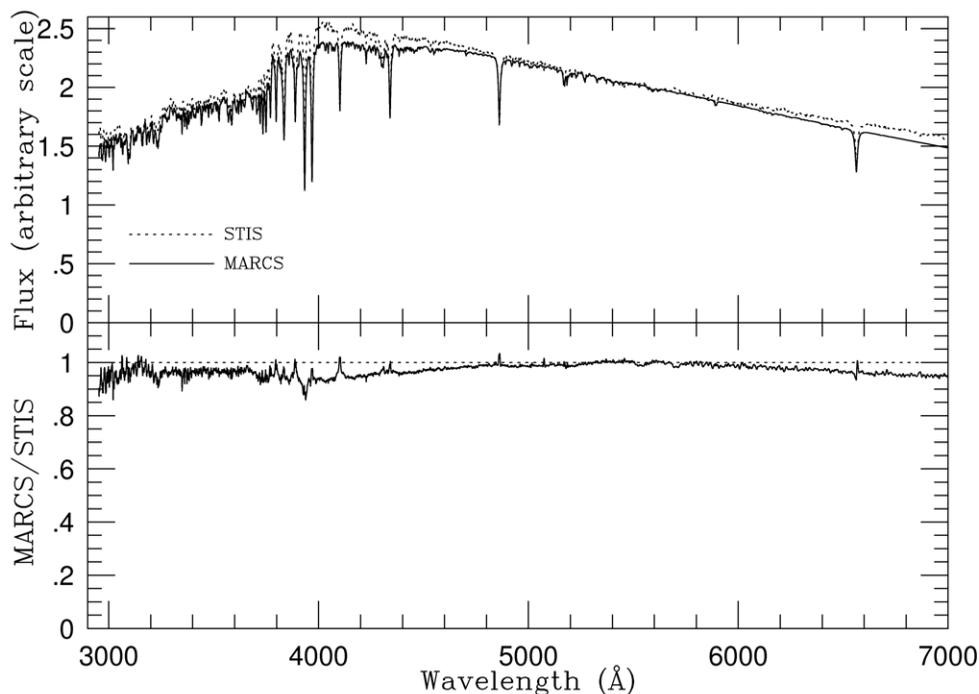


Figure 5. Comparison of the observed STIS flux of HD19445 with a spectrum of a MARCS model with $T_{\text{eff}} = 5191$ K, $\log g = 4.29$ (cgs), $[M/H] = -2.0$, $\xi_t = 1.0$ km/s (Önehag *et al.* 20007). The lower panel shows the ratio of model flux/observed flux.

Google has pointed us towards Kyle M Rollins, winner of the Arthur Wellington Prize from the American Society of Civil Engineers in 1996. He won the prize for his “dynamic compactation” of sand. In order to make it possible to build houses in a sandy field, one has used methods of watering the sand, or injecting it with salts. Professor Rollins instead tried to stabilize it by dropping a heavy weight of 30 tons from a height of 30 meters, repeatedly, and found that a satisfactory ground resulted. In the Brigham Young University Magazine from 1997 this story appears under the heading: “Wise professor seeks to build houses on sand.” Although we appreciate that this invention may be prize-worthy, we do not wish to project such a method into the problem of matching galaxy spectra with theoretical stellar spectra. The question is if brute force helps in this latter endeavour. Our firm belief is that this is not so. Instead we suggest that we should try to be clever.

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Discussion

THOMAS: How does the new metallicity of the Sun (factor 2 lower than previously measured) affect the calibration of model atmospheres?.

GUSTAFSSON: Except for features like CH, NH, OH, CO and CN bands the effects are very small on model spectra for solar-type stars. If, however, the new CNO abundances

by Asplund *et al.* are adopted for models of cooler stars like K, M and C stars (in the latter case with additional increase of C) the effects are considerable due to the significance of molecular-like blanketing. This includes direct effects – due to residual molecular absorption with the new abundances – but also indirect effects via the decreased cooling by CO of the surface layers or decreasing heating by TiO of the same layers, and decreased backwarming by several molecules. The resulting changed (often diminished) temperature gradients may then change the line-strengths (often weaken them). The effects are, however, probably not much greater than those of, e.g., neglecting the changes in C and N abundances by the first dredge-up.



The speaker (left) together with Rurik Wahlin and Bacham Reddy.