New ATLAS9 model atmosphere grids

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ABSTRACT

We present several new sets of grids of model stellar atmospheres computed with modified versions of the ATLAS9 code. The individual sets differ essentially in the physics used for the treatment of the convective energy transport and in the number of layers used to describe the vertical structure of the atmospheres. These grids of model atmospheres provide a basis for the characterization of the COROT seismology targets, in particular the precise and reliable determination of their effective temperatures, surface gravities and abundances.

1. Introduction

In the recent years, the following problems with published grids of model atmospheres (e. g., Kurucz 1993) crystallized:

- The convection zone (CZ) is treated using the mixing length theory (MLT) with a large value for the mixing length to pressure scale height ratio ($\alpha = 1.25$). It has been shown by Schmidt (1999) that synthetic colors (in the Geneva system) calculated using model atmospheres with a smaller value of α are in better agreement with the observed colors of standard stars. Furthermore, van 't Veer-Menneret & Mégessier (1996) found that in order to reproduce the Balmer line profiles of the Sun they had to reduce the value of α down to 0.5.
- Convective overshooting is included in the model atmosphere calculations available on CD-ROM in a way which leads to discontinuities in synthetic color indices (Castelli 1996). Furthermore Castelli et al. (1997) showed that effective temperatures derived from color indices computed without overshooting were, on average, closer to T_{eff} determined from the infrared flux method for A to K-type stars. The corresponding model grids are now available on the website of R. Kurucz (http://kurucz.harvard.edu). These results were confirmed by Smalley & Kupka (1997), who showed in addition that models using turbulent convection theory (CM, see below) give Strömgren color indices that are in best overall agreement with observations.
- The spacing in T_{eff} and $\log g$ between grid points is rather large.
- Only one choice for the resolution of the model structure ($\Delta \log \tau_{\text{ross}}$) is available.
- No information on the convergence of the individual models is provided.

	Min	Max	Step	
$T_{\rm eff}$[K]	4000	10000	200	
$\log g$	2.0	5.0	0.2	
[M/H]	-2.0, -1.5, -1.0, -0.5, -0.3, -0.2, -0.1, 0.0, +0.1, +0.2, +0.3, +0.5, +1.0			
$v_{\rm micro}$	0, 1, 2, 4 $\rm km\,s^{-1}$			
Convection	MLT	CGM	CGM	CM
Number of layers	72	72	288	288

Table 1: Atmospheric and computational parameters of the model atmosphere grid.

Therefore we started the computation of new grids of model atmospheres, corresponding fluxes and colors, using three versions of the ATLAS9 code: First, the original version from CD-ROM 13 of Kurucz (1993), but without overshooting and using α = 0.5 (MLT). The other two versions were provided by F. Kupka, who modified the code to include turbulent convection models from Canuto & Mazzitelli (1991, CM), and from Canuto, Goldman & Mazzitelli (1996, CGM), with the fine-tuning parameter set to 0.09.

2. Model grid computations

The parameters for which computations are planned are listed in Tab. 2. Convection has been turned off for models with $T_{\rm eff}\geq$8600 K, because the convective flux can be neglected for higher temperatures. The uppermost layer is located at log $\tau_{\rm ross} = -6.875$ and the difference of consecutive layers in log $\tau_{\rm ross}$ is 0.125 and 0.03125 for models with 72 and 288 layers, respectively. Up to now, computations of the grids with $v_{\rm micro}$ = 2 $\rm km\,s^{-1}$ have been completed and will be available on CD-ROM on request from the author, including model structure and convergence information as described below.

The grid computations were performed with the Perl package SMGT (Stellar Model Grid Tool), written by W. Schmidt (1999). This program handles the following tasks for each grid node defined by grid parameters given by the user: it creates an input deck for ATLAS9, runs the ATLAS9 program until convergence criteria are satisfied for each individual model, and directly evaluates the output to summarize information on convergence and model structure. The information provided by SMGT for each model comprises the flux and flux derivative root mean square (RMS) and maximum values, the numbers of the layers between which errors greater than the rms occur, the maximum of convective to total flux, the numbers of the top and bottom convection zone layers, and the optical depth where the temperature equals $T_{\rm eff}$.

The program can be run in either of two modes depending on the temperature structure used for initialization: In *static* mode, an existing model file or a grey atmosphere is used. In *dynamic* mode, an existing model file or a weighted average of all existing models within one grid step of each parameter is

	RMS	Maximum	
primary			
ΔF_l	$\leq 1\%$	$\leq 5\%$	
$\Delta F_l'$	$\leq 2\%$	$\leq 10\%$	or $\leq 10\%$ $(N/10 \leq l \leq N)$
ΔT_l			$\leq$ 1K $(0 \leq l \leq N/10)$
secondary			
$\Delta F_l, \Delta F_l'$	$\leq 10\%$	$\leq 100\%$	

Table 2: Convergence criteria used for the grid computations. N is the number of layers of a model.

used. The weights are calculated in the following way:

$$\prod_k \exp\left(-\frac{|p_k^i - p_k^m|}{\Delta p_k}\right),$$

where the product is calculated over all atmospheric parameters p_k, i denotes the initialization model, m the model to be computed, and Δp_k the range of parameter p_k in the whole grid.

The state of convergence of a particular model is evaluated by calculating the root mean square (RMS) and the maximum of the flux errors (ΔF_l), the flux derivative errors ($\Delta F_l'$) and the temperature correction (ΔT_l) in all layers l. A model is considered as fully converged if these values satisfy certain criteria, which are given in Tab. 2 (labelled "primary"). Models for which these criteria cannot be achieved after a reasonable number of iterations are also stored, if they satisfy the criteria labelled "secondary" in Tab. 2, but the corresponding file names are marked accordingly.

In order to achieve the convergence criteria without wasting time when no further improvements can be expected from further iterations, the required number of iterations is calculated and checked dynamically, after an initial sequence of 12 iterations. From a sequence of n iterations the ATLAS9 output is processed every n/4 iteration and the speed of convergence is characterized by calculating the ratios between the rms errors of two subsequent iterations. "Damping exponents" are computed for the flux and flux derivative errors from these ratios. From the damping exponents in turn, the total number of iterations is calculated, involving the ratio of the current RMS errors to that given by the primary criterion. The larger of the values resulting from ΔF_l or $\Delta F_l'$ is taken. The computations are terminated if the errors increase (after a few further trials) or if the predicted total number of iterations exceeds a certain limit. (480 for the current computations).

3. Conclusion

We presented model atmosphere grids which have been computed automatically for four combinations of convection models and depth resolutions, 13 metallicity values, large ranges and small spacings for $T_{\rm eff}$ and $\log g$. Convergence as described above could be achieved in almost all cases. This is illustrated in Fig. 1,

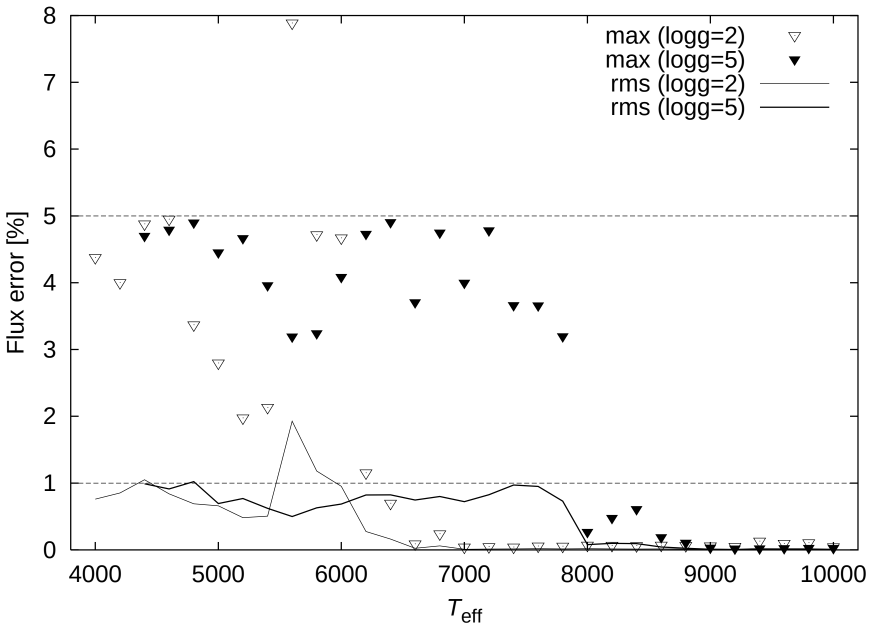

Fig. 1.— Maximum and RMS flux errors for the CGM/72 models with [M/H] = 0. The dashed lines show the limits corresponding to the primary convergence criterion.

which shows the maximum and RMS flux errors for the CGM/72 models with [M/H] = 0 and $\log g$ = 2 and 5, and the corresponding criterion limits. Problems arise in a triangular area of 4000 $\leq T_{\rm eff} \leq$ 4800 K and 3.4 $\leq \log g \leq$ 5.0 for low metallicities. For these parameters, the temperature correction algorithm used in ATLAS9 is not adequate. An additional small problematic area exists for temperatures around 6000 K and the lowest $\log g$ values for the models with denser spaced layers. The variation of the efficiency of convection with temperature and $\log g$ is demonstrated in Fig. 2 for the CGM/72 model grid.

The model grids will be useful for the characterization of potential COROT seismology target stars, for which fundamental parameters have to be derived with high precision. A more detailed description of the calculations and the effects of the different convection treatments on model structure and observable quantities will be presented in a forthcoming paper together with C. van 't Veer, F. Kupka and others.

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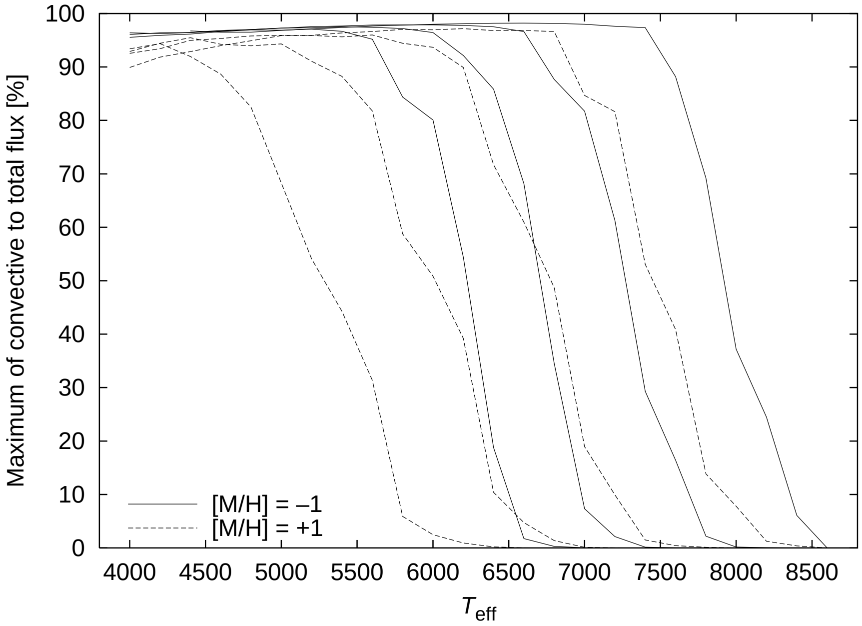

Fig. 2.— Maximum of convective to total flux for the CGM/72 models with [M/H] = -1 and +1 and $\log g$ increasing from 2 to 5 from left to right.

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