

KOALA, a new ATLAS9 database

I. Model atmospheres, opacities, fluxes, bolometric corrections, magnitudes and colours

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ABSTRACT

We present the KOALA database, a new set of LTE, line-blanketed model atmospheres calculated with the code ATLAS9, together with the corresponding Opacity Distribution Functions and emergent fluxes. The latter were used also to calculate G-band bolometric corrections and theoretical magnitudes and colours for several photometric systems, i.e. UBVRI, 2MASS, Hypparcos-Tycho, SDSS, Gaia, Euclid and Gaia DR3. With respect to the previous grids of ATLAS9 model atmospheres, we adopted the solar mixture by Caffau/Lodders and we extend the sampling in metallicity (from -5.0 to -2.5 dex with step of 0.5 dex, and from -2.5 dex to $+0.5$ dex with step of 0.25 dex) and in $[\alpha/\text{Fe}]$ (from -0.4 to $+0.4$ dex with a step of 0.2 dex). Also, we provide a finer sampling in T_{eff} for T_{eff} lower than 7000 K. This finer grid allows for more accurate interpolation of colours and in many cases it makes not necessary to compute a new model atmosphere, since one of the grid can be used directly. A total of 51663 model atmospheres and emergent fluxes have been computed. Finally, we discuss the impact of $[\text{M}/\text{H}]$ and $[\alpha/\text{Fe}]$ on the thermal and pressure structures of the model atmospheres and on theoretical colours.

Key words. stars: atmospheres

1. Introduction

model atmosphere describes how thermodynamic quantities (i.e. temperature, gas pressure, electron number density) vary as we move through the photosphere, from outer, optically thin layers to the deeper, optically thick regions where continuum photons are formed. The run of these quantities with the depth can be expressed as a function of the optical depth (in plane-parallel geometry) or of the stellar radius (in spherical geometry). These models are the backbone of the spectral synthesis and of the modelling of the spectral energy distribution of the stars, that we observe at different resolution through photometric filters or spectra. The relevance of the model atmospheres in astrophysics is multiple, being a fundamental element in the chemical abundance analysis, in the transformation of stellar tracks/isochrones into observational planes and in the modelling of the spectral energy distribution of the galaxies.

ATLAS9 (Kurucz 1970; Kurucz et al. 1974; Kurucz 2005) and ATLAS12 (Kurucz 2005; Castelli 2005) are the only publicly available codes to calculate model atmospheres, together with TLUSTY (Hubeny 1988; Hubeny & Lanz 1995; Lanz & Hubeny 2003) and TMAP (Werner & Dreizler 1999), while other codes are not publicly distributed despite the wide use of their grids of model atmospheres, for instance MARCS (Gustafsson et al. 2008) and PHOENIX (Hauschildt et al. 1997; Hauschildt & Baron 1999). With respect to other codes that are suitable for specific regions of the parameter spaces, i.e. TLUSTY for

OB stars (but usable also for cooler stars, see e.g. Hubeny et al. 2021), MARCS for FGKM stars, PHOENIX for AFGKM stars, ATLAS9/ATLAS12 allow us to calculate reliable model atmospheres over a large range of parameters. These models assume one-dimensional, plane-parallel geometry, local thermodynamic and radiative equilibrium, and the radiation/convection as the only energy transport mechanisms. The main difference between ATLAS9 and ATLAS12 is in the treatment of the line opacity. ATLAS9 handles the complex and time-consuming step of the calculation of the line opacity coefficient using the opacity distribution function (ODF) method (see Kurucz 1979, and references therein). In this approach the line opacity for a given chemical mixture and microturbulent velocity (v_{turb}) is calculated as a function of temperature and gas pressure in a number of wavelength intervals, namely 328 for the so-called big ODF (used in the model atmosphere calculation) and 1212 for the so-called little ODF (used in the emergent flux calculation).

The main advantage of the ODF method is that, after a relatively time-consuming effort to calculate big and little ODFs, any model atmosphere or emergent flux with the chemical mixture and v_{turb} of the corresponding ODF can be calculated in a very short time, adopting the appropriate T_{eff} and $\log g$. This approach is therefore suitable to calculate a large number of models and emergent fluxes for stars with similar chemical composition. For stars with peculiar chemical compositions (or with specific elemental abundances that significantly impact on the total opacity) the opacity sampling method (Peytremann 1974, and imple-

mented in ATLAS12) is recommended allowing us the proper calculation of the opacity coefficients for the parameters of the model.

The availability of extensive grids of atmospheric models (as well as ODFs and fluxes) that adequately sample the parameter space (T_{eff} , $\log g$, but also the chemical mixture) is fundamental for various aspects of astrophysics. The most used grids of ATLAS9 model atmospheres have been provided by Castelli & Kurucz (2003, hereafter CK03)¹. This grid assumes as reference solar mixture that by Grevesse & Sauval (1998) and provides metallicities $[M/H]$ between -4.0 and $+0.5$ dex, with a typical step of 0.5 dex, and two values of $[\alpha/Fe]$ $+0.0$ and $+0.4$ dex. However, the grid is not sampled in a regular way, lacking with some combination of $[M/H]$ and $[\alpha/Fe]$.

Here we present the first paper of the KOALA project, a new database of opacities, model atmospheres and emergent fluxes, calculated with the ATLAS9 software. In this paper we describe the new grid that substitutes the previous ones by CK03 and following the same physical assumptions, in particular for the adopted opacities. In the next papers we will discuss future grids testing the impact of peculiar chemical composition and of some physical assumptions.

2. The new ATLAS9 grid

We present new, wider and complete grid of ODFs, model atmospheres and emergent fluxes, calculated with the `gfortran` version of the codes DFSYNTH, KAPPA9 (Castelli 2005) and ATLAS9 (Kurucz 2005), all of them available in the F. Castelli website². With respect to the grid by CK03, we adopted a different solar chemical composition, we increase the parameter sampling in $[M/H]$ and $[\alpha/Fe]$ and we increase the sampling in T_{eff} for the cool models (see details in Section 2.1). All the products of this new release (big and little ODFs, Rosseland opacity tables, model atmospheres, emergent fluxes, G-band bolometric corrections and theoretical magnitudes) are available in a dedicated web-site³, where we will provide future, new grids of models calculated with specific chemical mixtures or testing different physical assumptions. The dataset presented here has been already used to calculate the colour-temperature transformations used to transform into observative planes the theoretical isochrones and tracks of the BaSTI-IAC database⁴ (Hidalgo et al. 2018; Pietrinferni et al. 2021, 2024).

2.1. Main features and novelties

In the following we summarise the characteristics of this new grid and the main improvements with respect to the previous one by CK03.

- The reference solar chemical mixture is composed by the solar abundances by Caffau et al. (2011) for Li, C, N, O, P, S, K, Fe, Eu, Hf, Os and Th, and those by Lodders (2010) for the other elements. This new solar chemical mixture substitutes that by Grevesse & Sauval (1998) adopted by CK03. For all the ODFs we assumed a helium mass fraction of $Y=0.2476$, following the *Planck* mission results (Coc et al. 2014). We point out that the relatively small change in He abundance due to the Galactic chemical evolution has minor effects on

the structure of the model atmospheres. For a detailed description on the effects of the He abundance on the spectra of late-type stars we refer the reader to Böhm-Vitense (1979).

- We considered different chemical mixtures in terms of α -elements (O, Ne, Mg, Si, S, Ar, Ca and Ti), namely $[\alpha/Fe]=-0.4$, -0.2 , $+0.0$, $+0.2$ and $+0.4$ dex. The grid by CK03 included only $[\alpha/Fe]=+0.0$ and $+0.4$ dex.
- For each value of $[\alpha/Fe]$, we consider 18 metallicities. The adopted metallicities range from $[M/H]=-5.0$ dex to -2.5 dex with a step of 0.5 dex, and from -2.5 dex and $+0.5$ dex with a step of 0.25 dex. This significantly extends the metallicity range and sampling of the grid by CK03, the latter adopting a sampling of $+0.5$ dex and with some lacking metallicities for $[\alpha/Fe]=+0.4$ dex. Therefore, for each $[\alpha/Fe]$ we provide a regular grid of models in terms of $[M/H]$.
- Another novelty of the new grid with respect to the grid by CK03 is the adoption of a step of 125 K in the range $3750-6000$ K (for $\log g \leq 3.0$) and in the range $3750-7000$ K (for $\log g > 3.0$), finer by a factor of 2 with respect to the previous grid. This finer grid allows for more accurate interpolation of colours and in many cases it makes not necessary to compute a new model, since one of the grid can be used directly. We add as boundary of the grid models with $T_{\text{eff}}=3750$ K even if problems in the ATLAS9 integrated colours for T_{eff} lower than 4000 K has been pointed out (see e.g. Plez 2011). For hotter T_{eff} we maintain the same step by CK03, 250 K for stars up to $T_{\text{eff}}=12000$ K, 500 K up to $T_{\text{eff}}=20000$ K and 1000 K up to $T_{\text{eff}}=50000$ K. Also for $\log g$ we adopted the same step (0.5 dex) by CK03. Fig. 1 shows the sampling of the entire grid in the $T_{\text{eff}}-\log g$ plane, compared with the extension of the MARCS (Gustafsson et al. 2008), PHOENIX (Husser et al. 2013) and TLUSTY (Lanz & Hubeny 2003, 2007) model atmospheres.

2.2. Calculation of ODFs, model atmospheres and emergent fluxes

The ODFs were computed with DFSYNTH and KAPPA9 codes (Castelli 2005), adopting the same atomic and molecular line lists used by CK03 and described in Kurucz (2011). Briefly, in the computation of ODFs we included all the atomic lines in the last release of the R. L. Kurucz dataset, together with the linelists for several diatomic molecules, i.e. H_2 , CH, NH, OH, MgH, SiH, C_2 , CN, CO, SiO, and TiO (for the latter we adopted the linelists by Schwenke 1998). The only difference with respect to the opacities used by CK3 is related to H_2O . For the latter we adopted the last version of the Partridge & Schwenke (1997) linelist as provided by R. L. Kurucz⁵, fixing a bug present in the previous release of the same linelist. In the future releases of KOALA, we plan to improve new opacity sources not included in the last release of Kurucz's database. For each chemical composition, specified by the metallicity $[M/H]$ (see Appendix A) and the α -element abundance ratio $[\alpha/Fe]$, we calculated big and little ODFs adopting five values of v_{turb} , namely 0 , 1 , 2 , 4 and 8 km/s.

Model atmospheres with $v_{\text{turb}}=2$ km/s were calculated with ATLAS9 (Kurucz 2005), adopting the big ODFs. ATLAS9 enforces Saha-Boltzmann ionization/excitation plus molecular dissociation equilibrium at each depth, together with elemental abundance conservation and charge neutrality. The code solves a coupled set of equilibrium equations for all species (atoms/ions and selected molecules), returning number densities and the

¹ <https://wwwuser.oats.inaf.it/fiorella.castelli/grids.html>

² <https://wwwuser.oats.inaf.it/castelli/sources/atlas9codes.html>

³ <https://sites.google.com/view/koala-database/>

⁴ <http://basti-iac.oa-abruzzo.inaf.it/>

⁵ <http://kurucz.harvard.edu/molecules/h2o/>

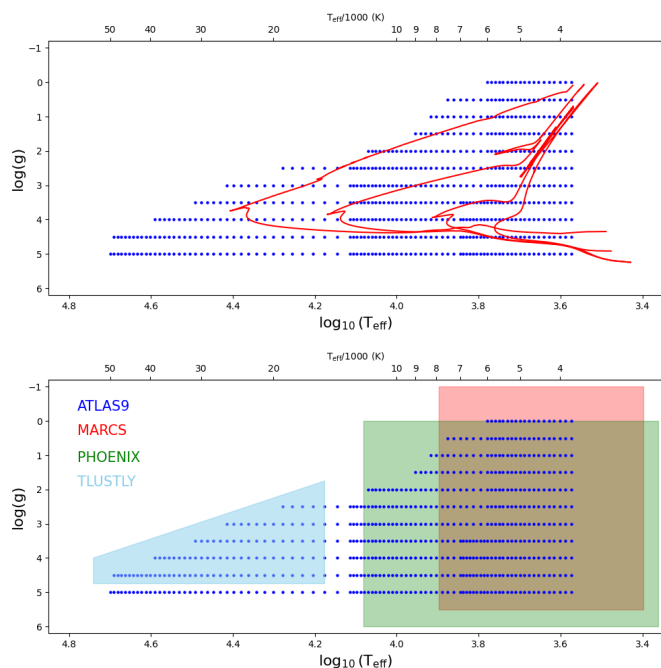


Fig. 1. Distribution of the ATLAS9 model atmospheres of the new grid (blue circles) in the $\log_{10}(T_{\text{eff}}) - \log g$ plane, superimposed (upper panel) to four theoretical BaSTI-IAC isochrones with 15 Myr, 100 Myr, 1 Gyr and 13 Gyr and solar-scaled metallicity (Hidalgo et al. 2018), and compared (lower panel) to the distribution of MARCS (Gustafsson et al. 2008), PHOENIX (Husser et al. 2013) and TLUSTY (Lanz & Hubeny 2003, 2007) model atmospheres.

electron pressure for a given temperature, pressure and composition. For additional details about the main physical assumptions and the calculation scheme adopted by ATLAS9 we refer the reader to the vast literature available on this code (Kurucz 1970; Kurucz et al. 1974; Kurucz 1979; Castelli 1988). Since a model atmosphere is calculated through an iterative numerical process starting from a guess solution, these models were obtained by choosing as the guess model the CK03 grid model closest in terms of T_{eff} , $\log g$, and $[M/H]$ to the solution to be computed. The choice of a different guess model, as long as it is close to the desired solution, has a negligible impact on the computed model, whereas using guess models that are far from the required solution can slow down the calculation or compromise the convergence of the final model.

All of the models have 72 plane-parallel layers ranging from the logarithm of the Rosseland optical depth $\log \tau_{\text{Ross}} = -6.875$ to $+2.00$, in steps of $\delta \log \tau_{\text{Ross}} = 0.125$. In the treatment of the convective flux, the classical mixing length theory (Böhm-Vitense 1953; Böhm-Vitense 1958) is adopted, with the pressure scale height equal to α times the characteristic length of a rising convective cell. Here we adopted a mixing length parameter α equal to 1.25, as done in previous grids of ATLAS9 models (CK03, Kirby 2011; Mészáros et al. 2012). We stress as the adoption of a different value impact only on the deepest layers of the coolest models, where continuum and very weak lines form. The approximate overshooting (Kurucz 1992) is switched off because, even if it is able to better reproduce some spectral features in the solar spectrum, for most of the stars it does not provide a good description of several features (Castelli et al. 1997) or introduces unphysical features in the thermal structure of the most metal-poor models (Bonifacio et al. 2009). For all the layers, local thermodynamical equilibrium is assumed (but this assumption

can become progressively less realistic for temperatures hotter than ~ 15000 K, see e.g. Lanz & Hubeny 2007).

For any model, a given layer is considered converged if its flux and flux derivative errors are less than 1% and 10%, respectively. The majority of the computed models satisfies these criteria in all the layers. In some models (especially those with low T_{eff} and $\log g$) some layers are not converged, usually the most external ones. Sometimes, small changes in the guess model atmosphere (for instance of the order of some tens of K) can be enough to solve the problems of convergence of a layer. However, possible not converged outermost layers do not affect significantly the use of the model atmosphere, because in those layers the core of strong lines formed, usually not adopted for chemical analyses because of some effects (i.e., non-LTE, chromospheric activity) are not accounted for in ATLAS models. Additionally, for some low $T_{\text{eff}} (\leq 4600)$, high $\log g (\geq 2.0-2.5)$ and low $[M/H]$ models ($[M/H] < -2.5$ dex, i.e. models corresponding to metal-poor, low Main Sequence stars, as K and M dwarfs) we found problems of convergence also in the central layers, where a significant fraction of the flux is transported by convection (in particular an unphysical discontinuity in temperature is present close to these layers). The use of different guess model atmospheres or small changes in the requested parameters were not able to fix this issue and we decide to remove these models from the grid.

The number of model atmospheres of the final grid is summarised in Table 1, according to the adopted $[M/H]$ and $[\alpha/\text{Fe}]$. A total of 51663 model atmospheres is provided. Finally, for each model of the grid described above the corresponding emergent flux (i.e. a low-resolution spectrum covering the entire spectral range) has been calculated as H_ν , energy for frequency unit.

3. Impact of the adopted solar chemical mixture

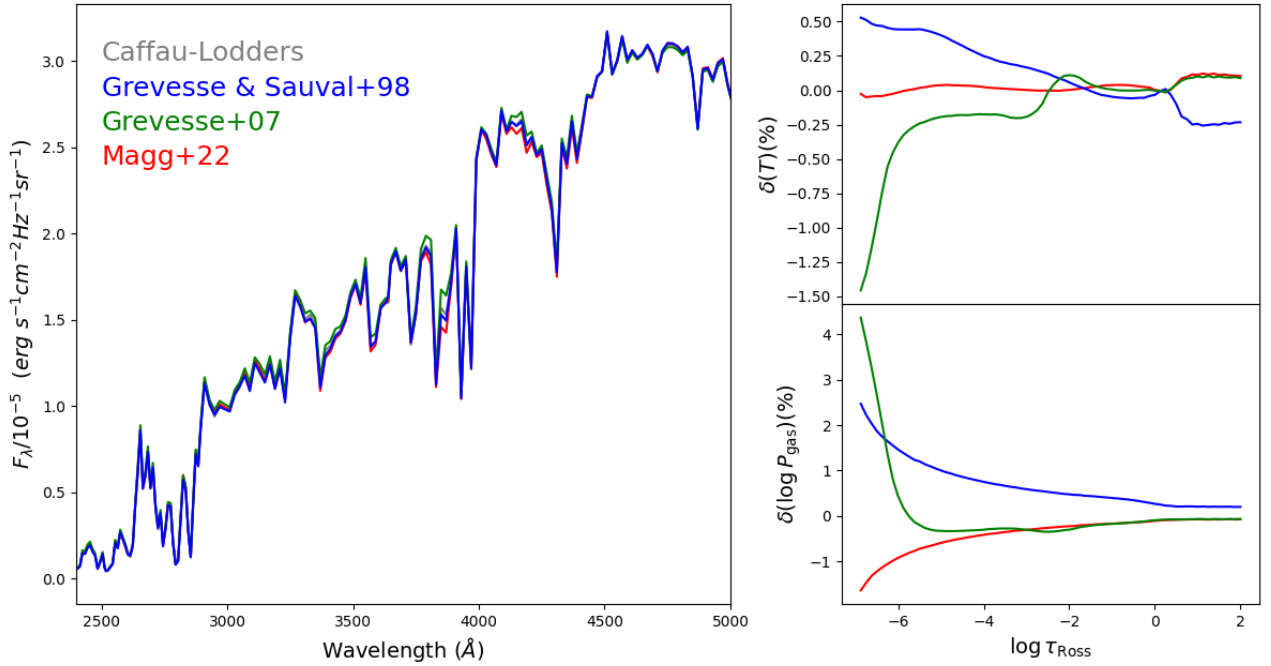
The comparison between different families of model atmospheres is not trivial because of the large number of assumptions in the recipes adopted by different codes. In order to evaluate the true impact of the different solar chemical mixtures on the model atmospheres and fluxes, we calculated additional ODFs, assuming the solar mixtures by Grevesse & Sauval (1998), used by CK03, Grevesse et al. (2007), used in the MARCS models grid by Gustafsson et al. (2008) and the recent one by Magg et al. (2022). The most significant differences among these four mixtures are for C, N and O. In Fig. 2 we compare the emergent fluxes and the thermal and pressure structures of model atmospheres for the Sun adopting these chemical mixtures. Small differences are appreciable in the outermost regions, especially for the model adopting the mixture by Grevesse et al. (2007), characterized by the lowest C, N, O abundances. This exercise suggests that the adoption of the solar chemical mixture does not significantly impact on the structure of the model atmospheres. On the other hand, the adopted solar abundances have a significant impact on the derived fluxes in the UV/blue spectral regions dominated by strong CH, NH and CN molecular bands. Checks performed for other sets of metallicity and stellar parameters lead to similar conclusions.

4. Impact of the metallicity on the model atmospheres

Fig. 3 shows how model atmospheres for a giant ($T_{\text{eff}}=4500$ K and $\log g=1.5$) and for a dwarf ($T_{\text{eff}}=6500$ K and $\log g=4.5$) star change by changing $[M/H]$. In particular, we show the run of

Table 1. Number of computed model atmospheres and fluxes according to the metallicity and $[\alpha/\text{Fe}]$.

[Fe/H] (dex)	$[\alpha/\text{Fe}]=-0.4$	$[\alpha/\text{Fe}]=-0.2$	$[\alpha/\text{Fe}]=+0.0$	$[\alpha/\text{Fe}]=+0.2$	$[\alpha/\text{Fe}]=+0.4$
+0.50	579	579	579	579	579
+0.25	579	579	579	579	579
+0.00	579	579	579	579	579
-0.25	579	579	579	579	579
-0.50	579	579	579	579	579
-0.75	579	579	579	579	579
-1.00	579	579	579	579	579
-1.25	579	579	579	579	579
-1.50	579	579	579	579	579
-1.75	579	579	579	579	579
-2.00	579	579	579	579	579
-2.25	579	579	579	579	579
-2.50	578	579	579	579	579
-3.00	575	573	576	565	568
-3.50	565	567	567	564	568
-4.00	559	559	562	561	561
-4.50	555	559	555	553	556
-5.00	554	551	550	551	555
TOTAL	10334	10336	10337	10321	10335

**Fig. 2.** Main panel: comparison among ATLAS9 fluxes for the Sun calculated with suitable ODFs adopting different solar chemical mixtures: Caffau-Lodders (this work, grey line), Grevesse & Sauval (1998, blue line), Grevesse et al. (2007, green line), Magg et al. (2022, red line). Left panels: percentage difference in temperature (upper panel) and logarithm of the gas pressure (lower panel) as a function of the Rosseland optical depth of the model atmospheres with respect to that computed with Caffau-Lodders chemical mixture (same colour-code of the main panel).

temperature, gas pressure ($\log(P_{\text{gas}})$) and electron number density ($\log(XN_{\text{elec}})$) as a function of $\log \tau_{\text{Ross}}$. It is immediately clear that models with $[\text{M}/\text{H}] \gtrsim -2.5/-2.0$ dex become increasingly distinct from each other at a fixed optical depth, while more metal-poor models are often indistinguishable or show only small differences. This justifies our choice of a finer sampling at higher metallicities, namely +0.25 instead of +0.5 adopted by CK03. As exercise, we discuss in Appendix B the properties of

a zero-metallicity ODF, representative of an ideal Population III star.

The thermal structure of the model is sensitive to $[\text{M}/\text{H}]$ in particular in deeper ($\log \tau_{\text{Ross}} \gtrsim 0.5$) and outer ($\log \tau_{\text{Ross}} \lesssim -3$) layers (with the differences more pronounced in the giant model). Fixing T_{eff} (and therefore the total flux, according to the Stefan-Boltzmann relation), a higher metallicity leads to a larger absorption from metallic lines and a higher opacity. This reduces

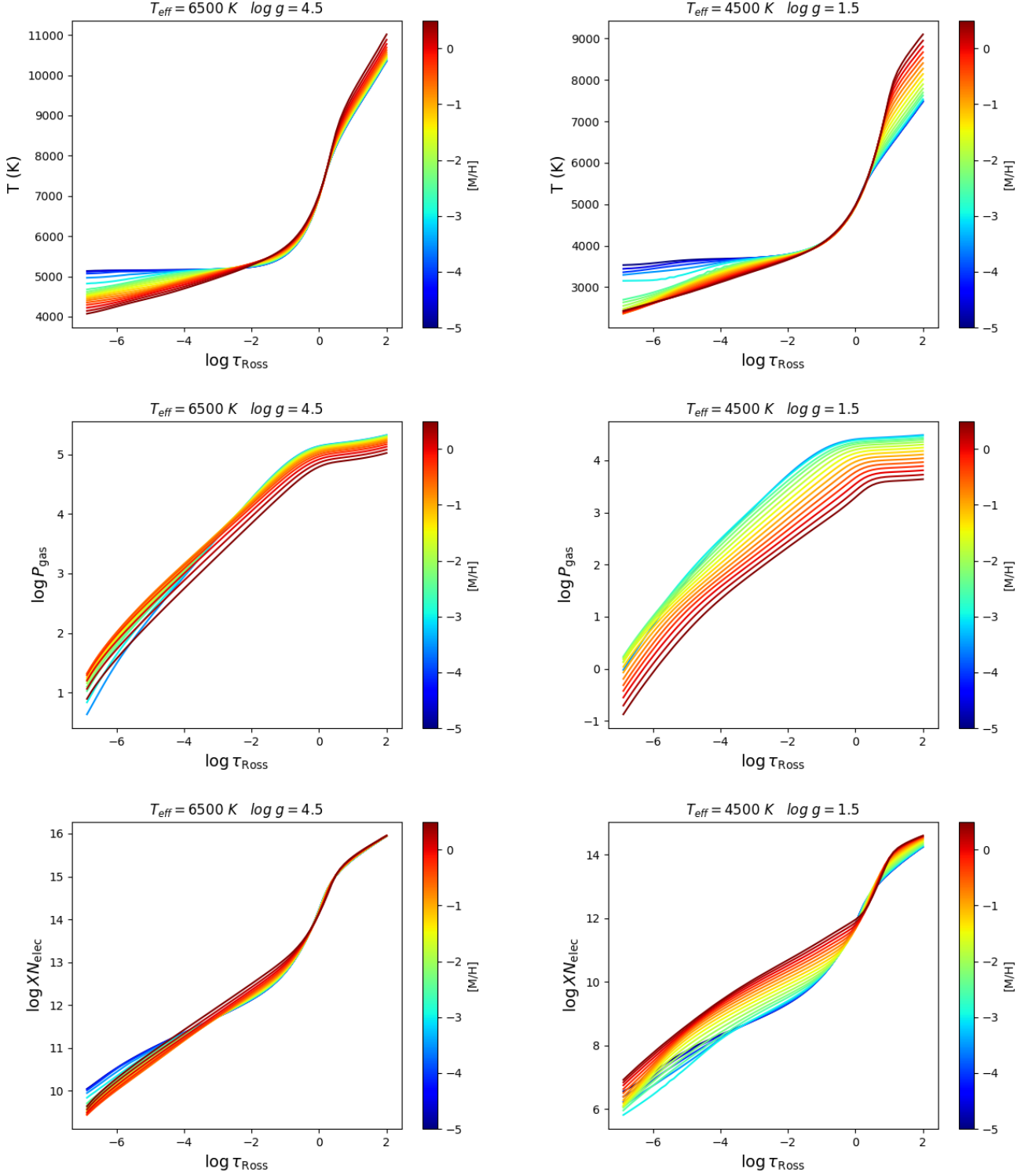


Fig. 3. Run of temperature (upper panels), logarithm of the gas pressure (middle panels) and logarithm of the electron number density (lower panels) as a function of $\log \tau_{\text{Ross}}$ for the model atmospheres of a dwarf ($T_{\text{eff}}=6500 \text{ K}$ and $\log g=4.5$, left panels) and a giant ($T_{\text{eff}}=4500 \text{ K}$ and $\log g=1.5$, right panels) star, colour-coded according to the metallicity $[M/H]$. We adopt $[\alpha/\text{Fe}]=+0.0$ dex for all the models.

the capability of the star to radiate energy and the temperature of the innermost layers must increase to make the total flux constant. On the other hand, the temperature of the outermost layers (where the atmosphere becomes optically thin) decreases because it is easier for the model to radiate (see e.g. Kurucz 1979).

Also the gas pressure and the electron number density are significantly affected by $[M/H]$ but in different and opposite ways. For $[M/H] \gtrsim -3.0/-2.5$ dex, $\log(P_{\text{gas}})$ increases by decreasing $[M/H]$ at each $\log \tau_{\text{Ross}}$, while $\log(XN_{\text{elec}})$ decreases. This occurs because, as metallicity decreases, the fraction of free electrons (provided by metals) also decreases leading to a lower

electron number density (lower panels of Fig. 3) and therefore a lower number of H^- atoms. This corresponds to a lower line opacity coefficient that increases the gas pressure according to the hydrostatic equilibrium (middle panels of Fig. 3) even if the electron pressure decreases.

For $[M/H] \lesssim -3.0$ dex, the gas pressure and the electron number density are very similar despite different metallicities in most of the model. In the outermost layers the metal-poor models have more steep gas pressures and higher electron number density. This behaviour reflects the different contributor to free electrons provided by hydrogen and metals in the outermost layers of metal-poor atmospheres. As shown in Fig. 4, showing the fraction of electrons provided by H and Mg as a function of $\log \tau_{Ross}$, in the external regions and $[M/H] < -3.0$ dex hydrogen becomes the dominant source of free electrons, while the contributor of Mg (the main electron donor for FGK stars) decreases significantly.

5. Impact of the adopted $[\alpha/Fe]$ on the model atmospheres

The approach commonly used when computing a synthetic spectrum is to vary the abundance of a given element while still using an atmospheric model that was calculated with a different abundance for that species. This procedure is legitimate and does not introduce significant errors as long as the abundance variations do not have a major impact on the atmospheric opacity or the ionization structure. Therefore, even substantial changes in the abundances of elements that contribute little to the overall opacity do not lead to inaccuracies in the resulting synthetic spectrum. On the other hand, greater caution should be exercised when varying the abundances of elements such as the α elements. Therefore, the use of model atmospheres including appropriate chemical mixtures in terms of $[\alpha/Fe]$ is recommended.

We checked the differences in the thermal and pressure structures of model atmospheres with different $[\alpha/Fe]$. We recognized a peculiar pattern in cool models with $[M/H] \gtrsim -2.0$ dex and $[\alpha/Fe] = -0.4$ dex. As visible in Fig. 5, the decrease of $[\alpha/Fe]$ at fixed $[M/H]$ mimics a decrease of $[M/H]$, with the features that we discussed above in Section 4. On the other hand, the model with $[\alpha/Fe] = -0.4$ dex is discrepant in the outermost layers, where it has a higher T_{eff} and a lower P_{gas} than the model with $[\alpha/Fe] = -0.2$ dex (we should expect the opposite behaviour following Fig. 3). This run could be explained by the peculiar chemical mixture of this model, where the extremely low $[\alpha/Fe]$ changes the budget of the free electrons. In fact, we found that the free electrons in the outermost layers of this model arise mainly from Fe and Mg, both negligible in the external regions of the other models, where the majority of the free electrons are provided by Na and Al.

A finer sampling of $[\alpha/Fe]$ in the adopted model atmospheres has an impact also on the spectral synthesis, in particular on the strength of some specific features sensitive to the adopted chemical mixture of the model atmosphere. An example of possible issues arising from use of model atmospheres with different $[\alpha/Fe]$ is visible in the analysis of the Ca II triplet lines. Fig. 6 shows the comparison between synthetic spectra of the second Ca II triplet line calculated with the code SYNTHE and using our new grid of model atmospheres. In particular, the three synthetic spectra were calculated with the same Ca abundance ($[Ca/Fe] = +0.2$ dex) but assuming three different model atmospheres in terms of $[\alpha/Fe]$ namely $+0.0$, $+0.2$, $+0.4$ dex. This means that in the spectral synthesis calculation we varied the Ca abundance of

$+0.2$, 0.0 and -0.2 dex with respect to the original abundance of the models, respectively, in order to obtain the same $[Ca/Fe]$. Despite the same Ca abundance of the three synthetic spectra, the wings of the Ca II line are different from each other. The broadening of these lines is dominated by van der Waals broadening and extremely sensitive to the gas pressure. The increase of $[\alpha/Fe]$ in the model atmosphere (despite the Ca abundance variation adopted in the spectral synthesis) leads to a decrease of the gas pressure (similar to what happens when $[M/H]$ increase) reducing the strength of the wings. On the other hand, linear/saturated Ca lines are not affected by the assumption of the $[\alpha/Fe]$ of the model atmosphere.

6. Theoretical magnitudes and colours

For each flux of the new grid described above we calculated theoretical magnitudes and colours in different photometric systems and bolometric corrections in Gaia DR3 G-band, BC(G). The procedure to calculate theoretical colours is described in details in Section C. The photometric systems that we consider are the UBVRI (Bessell & Murphy 2012), the 2MASS JHK (Cohen et al. 2003), the Hipparcos-Tycho (Bessell & Murphy 2012), the SDSS *ugriz* (Fukugita et al. 1996), the Euclid $I_E Y_E J_E H_E$ (Euclid Collaboration et al. 2022), the GALEX NUV and FUV (Morrisey et al. 2007) and the Gaia DR3 photometric system (Gaia Collaboration et al. 2023).

The behaviour of bolometric corrections and colours as a function of the parameters, i.e. T_{eff} , $\log g$, $[M/H]$, has been extensively discussed in other works (see e.g. Bessell et al. 1998; Bonifacio et al. 2018; Casagrande & Vandenberg 2018). Here we focus on their sensitivity on the adopted $[\alpha/Fe]$, the main novelty of this new dataset. The G-band bolometric correction BC(G) is basically unaffected by the adopted $[\alpha/Fe]$, but for metal-rich ($[M/H] \geq +0.0$ dex) giant models, for which BC(G) decreases by increasing $[\alpha/Fe]$. As example, Fig. 8 shows the run of BC(G) as a function of T_{eff} for $[M/H] = +0.0$ dex and different values of $[\alpha/Fe]$. The sensitivity of BC(G) with $[\alpha/Fe]$ can be appreciated at lower T_{eff} . At lower metallicities, the difference among the models, even at low T_{eff} , decreases and disappears entirely. Below $[M/H] \sim -1.0$ dex, BC(G) is completely independent of $[\alpha/Fe]$ value.

Concerning the colours, the main effects of $[\alpha/Fe]$ appear in general at low T_{eff} and high $[M/H]$. The behaviour of colours with $[\alpha/Fe]$ at fixed T_{eff} and $[M/H]$, is not univocal, as it depends on two opposing effects that affect the emerging spectrum when $[\alpha/Fe]$ varies. On one hand, a decrease in $[\alpha/Fe]$ naturally leads to a reduction in the strength of features associated with α -elements, resulting in an increase in flux within the adopted filter profile, especially in the visual region between ~ 4500 and ~ 6500 Å and at wavelengths shorter than ~ 3200 Å. On the other hand, the drop in oxygen alters the molecular equilibrium of the CNO cycle, progressively enhancing the strength of CN molecular bands (see e.g. Ryde et al. 2009), at ~ 3800 Å and beyond 6500 Å, and of the G-band CH band at ~ 4300 Å. This effect is significantly strong for models with $[\alpha/Fe] = -0.4$ dex, therefore the colours calculated with this chemical mixture are in almost all the cases the most divergent with respect to the other ones. Fig. 7 shows an example of these effects, with two emergent fluxes calculated for a K giant ($T_{eff} = 4500$ K, $\log g = 1.5$) and a K dwarf ($T_{eff} = 4500$ K, $\log g = 4.5$) star, both with $[M/H] = +0.0$ dex. In particular, the strong CN and CH molecular features are clearly visible in the emergent fluxes with $[\alpha/Fe] = -0.4$ dex. Depending on the filters involved, these two effects can lead to

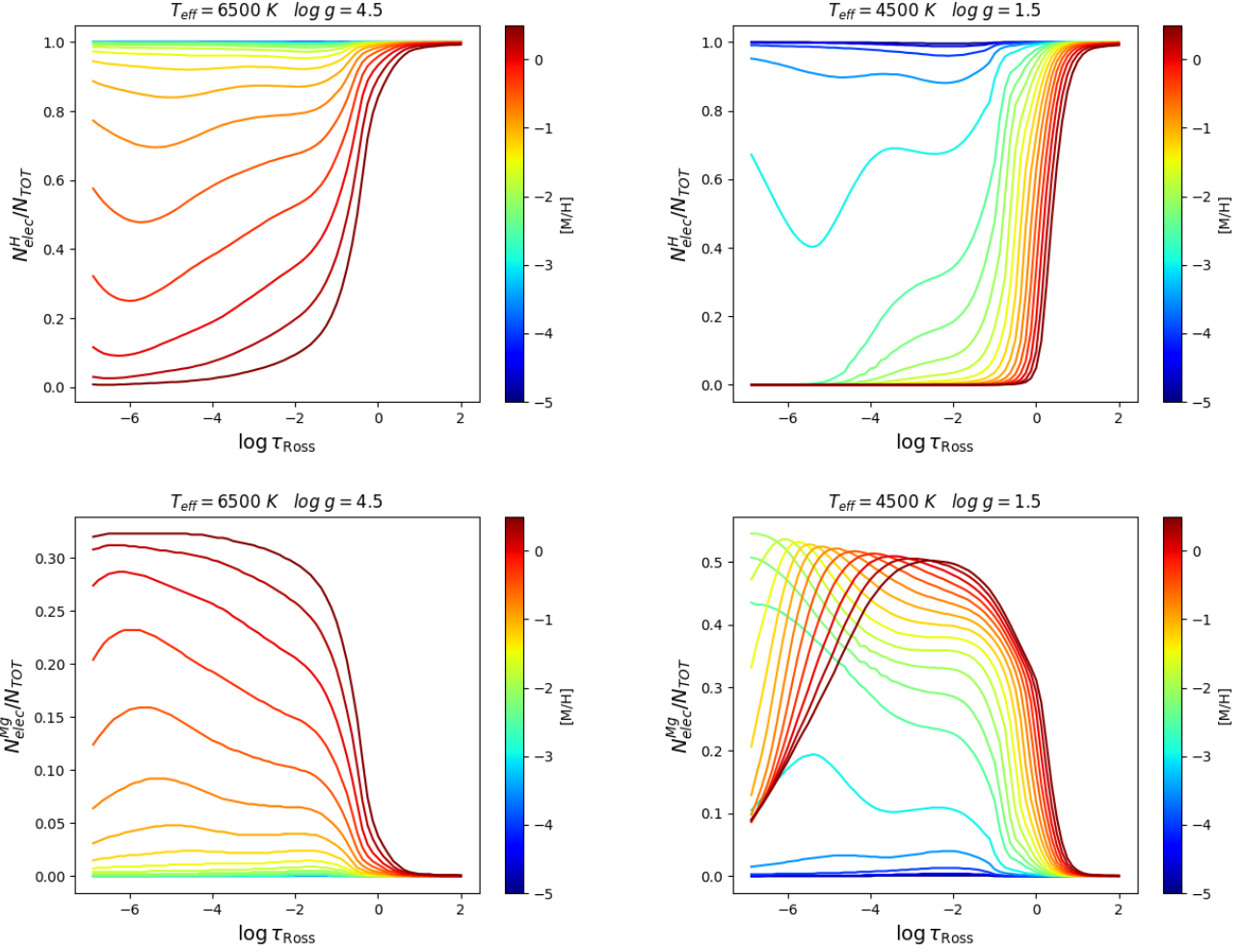


Fig. 4. Run of fraction of electrons provided by H (upper panels), and Mg (lower panels) as a function of $\log \tau_{Ross}$ for the model atmospheres of a dwarf ($T_{eff}=6500$ K and $\log g=4.5$, left panels) and a giant ($T_{eff}=4500$ K and $\log g=1.5$, right panels) star, colour-coded according to the metallicity $[M/H]$. We adopt $[\alpha/Fe]=+0.0$ dex for all the models.

either an increase or a decrease in the flux ratio as $[\alpha/Fe]$ decreases. In particular, we grouped the colours in three classes according to their sensitivity on the adopted $[\alpha/Fe]$:

- Colours directly proportional to $[\alpha/Fe]$: most of the colours become bluer by reducing $[\alpha/Fe]$, among them (r-i), (i-z), all the Gaia colours, (V-I) and (I_E-Y_E) both for giant and dwarf models, and (V-K) for dwarf stars. The run of (V-I) with T_{eff} in dwarf models is shown in lower-right panel of Fig. 8 as example of this class of colours.
- Colours inversely proportional to $[\alpha/Fe]$: other colours show an opposite behaviour, becoming redder by reducing $[\alpha/Fe]$, as (BT-VT), (Y_E-J_E) and, for dwarf stars, (U-B), (B-V), (u-g). The run of (B-V) with T_{eff} in dwarf models is shown in lower-right panel of Fig. 8. In these colours, the flux of the second filter is significantly reduced because the filter profile is dominated by the Mg b triplet (see Fig. 7).
- Colours (almost or totally) insensitive to $[\alpha/Fe]$: all the other colours have negligible or lacking dependence on the adopted $[\alpha/Fe]$. Almost all the Euclid colours have little or negligible variations with $[\alpha/Fe]$ but for the models with $[\alpha/Fe]=-0.4$ dex where the colours are significantly discrepant

with respect to other ones. Lower-right panel of Fig. 8 shows as example the run of (J-K) with T_{eff} .

7. Summary

We present a new database of ATLAS9 ODFs, model atmospheres, emergent fluxes, G-band bolometric corrections and theoretical magnitudes and colours. The latter have been calculated in different photometric filters, namely UBVRI, 2MASS, SDSS, Hypparcos-Tycho, Euclid, Gaia DR3. All the products are available in the dedicated website. The new grid of ODFs includes a finer sampling in $[M/H]$ (from -5.0 to $+0.5$ dex) and $[\alpha/Fe]$ (from -0.4 to $+0.4$ dex). We discussed the impact of $[M/H]$ and $[\alpha/Fe]$ on model atmospheres (in terms of temperature, pressure and electron number density), emergent fluxes and theoretical colours. Among the features that we discussed, the most relevant are the following:

- models with $[M/H] \gtrsim -2.5/-2.0$ dex become increasingly distinct from each other at a fixed optical depth, both in terms of thermal and pressure structures, while more metal-poor models are often indistinguishable or show only small differences. This highlights the need of a finer sampling in $[M/H]$ for model atmospheres with $[M/H] \gtrsim -2.5/-2.0$ dex;

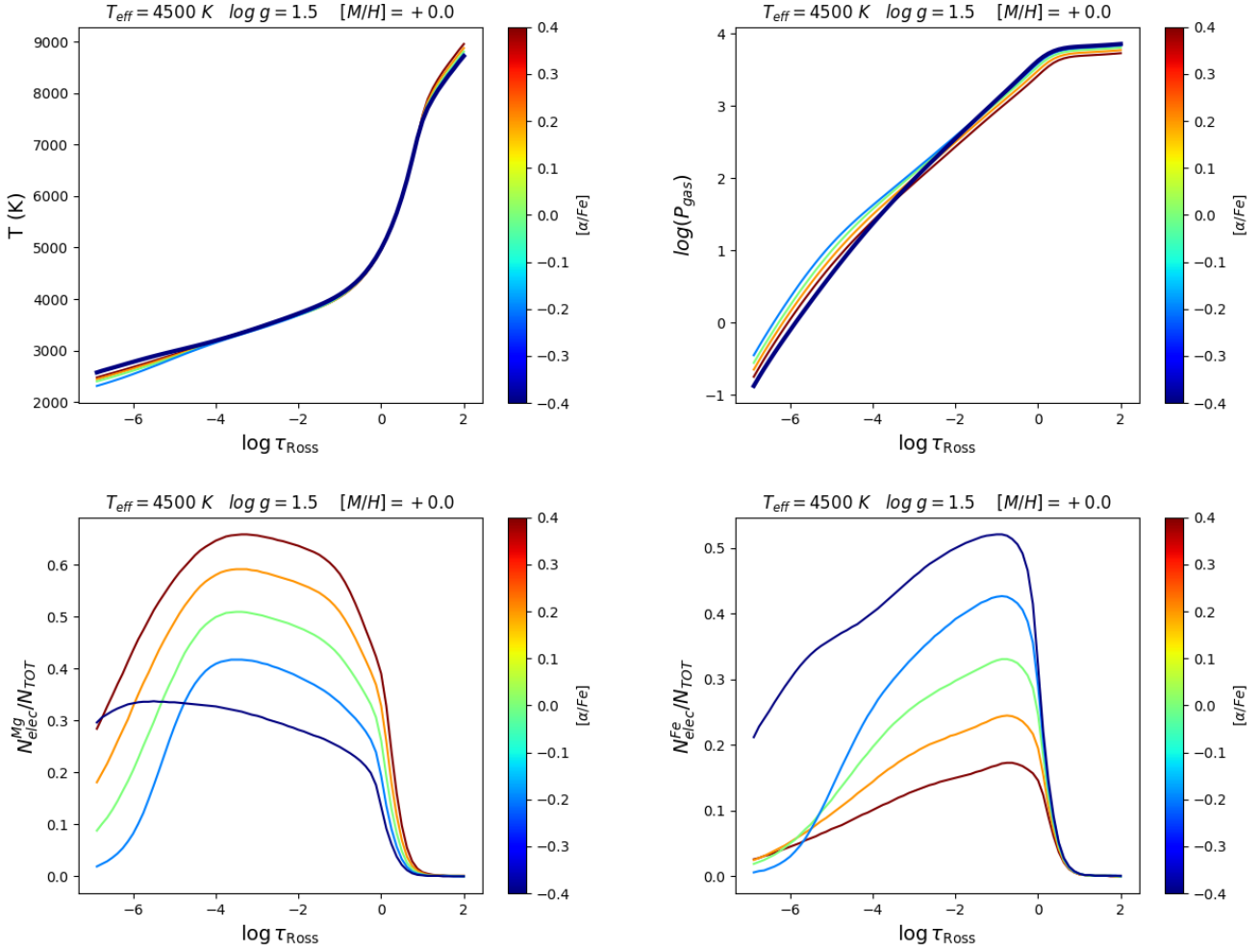


Fig. 5. Model atmospheres with $T_{\text{eff}}=4500$ K, $\log g=1.5$, $[M/H]=+0.0$ dex and different $[\alpha/\text{Fe}]$. The panels show the behaviour of temperature, logarithm of the gas pressure, fractions of free electrons provided by Mg and Fe. The model with $[\alpha/\text{Fe}]=-0.4$ dex, showing a different behaviour with respect to the other ones, is plotted with a thicker curve.

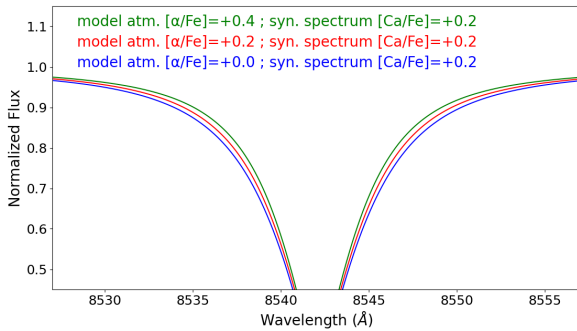


Fig. 6. Synthetic spectra for the second line of the Ca II triplet calculated with model atmospheres with $T_{\text{eff}}=4500$ K, $\log g=1.5$, $[M/H]=+0.0$ dex and three different values of $[\alpha/\text{Fe}]$. Despite the latter value, all the synthetic spectra were computed assuming $[\text{Ca}/\text{Fe}]=+0.2$ dex.

- the thermal structure of the model is sensitive to $[M/H]$ in particular in deeper ($\log \tau_{\text{Ross}} \gtrsim 0.5$) and outer ($\log \tau_{\text{Ross}} \lesssim -3$) layers. Also the gas pressure and the electron number density are significantly affected by $[M/H]$ but in different and opposite ways;

- the decrease of $[\alpha/\text{Fe}]$ at fixed $[M/H]$ impacts on the thermal and pressure structures of model atmosphere similar to the decrease of $[M/H]$. However, the models with $[\alpha/\text{Fe}]=-0.4$ dex is discrepant in the outermost layers, where it has a higher T_{eff} and a lower P_{gas} than the model with $[\alpha/\text{Fe}]=-0.2$ dex. This is due to the large contribution of Fe and Mg to the budget of the free electrons in outermost layers;
- The $[\alpha/\text{Fe}]$ in the adopted model atmosphere can affect the spectral synthesis of some features dominated by the van der Waals broadening (like the wings of the Ca II triplet lines). Generally, it is recommended to adopt for the spectral synthesis a model atmosphere with an appropriate chemical composition in terms of $[\alpha/\text{Fe}]$;
- theoretical colours can have different sensitivity to $[\alpha/\text{Fe}]$, depending on the balance between two different effects affecting the involved filter profiles: the decrease in $[\alpha/\text{Fe}]$ leads to weaker α -element features (i.e. the Mg b triplet) and stronger CN and CH features. Again, the colours calculated with $[\alpha/\text{Fe}]=-0.4$ dex are often significantly discrepant with respect to the other ones.

Acknowledgements. This work is dedicated to the memory of R. L. Kurucz, who passed away in March 2025, whose contribution to the study of stellar atmo-

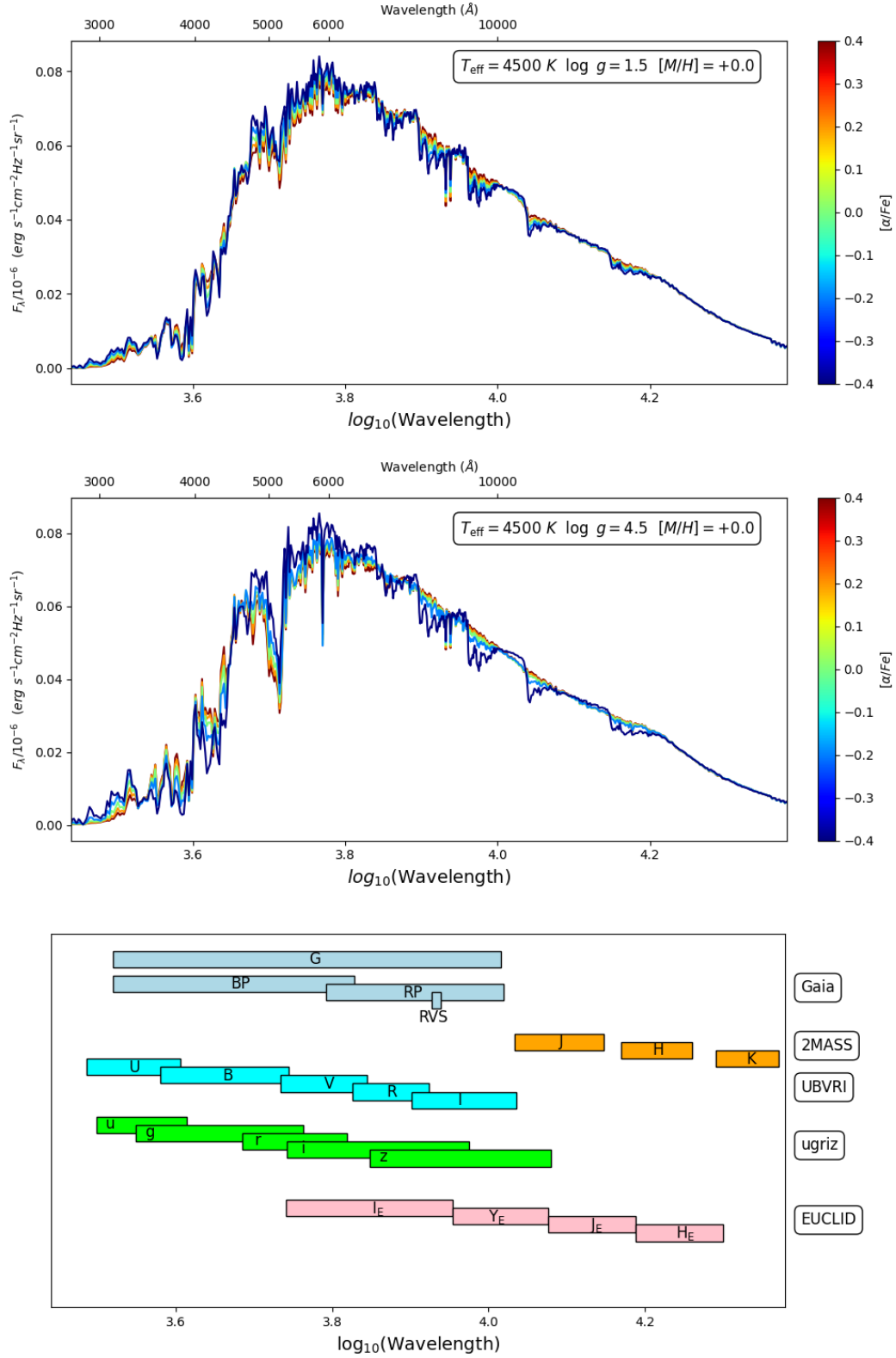


Fig. 7. Examples of ATLAS9 emergent fluxes calculated for a giant and dwarf star (upper and middle panel, respectively), calculated with different values of $[\alpha/\text{Fe}]$. The lower panel shows the log-wavelength range of the photometric filters discussed here.

spheres was fundamental. We are grateful to R. Lallement for explaining to us the details of building extinction maps and for reading a draft of our paper. A.M. acknowledges support from the project "LEGO – Reconstructing the building blocks of the Galaxy by chemical tagging" (P.I. A. Mucciarelli) granted by the Italian MUR through contract PRIN 2022LLP8TK_001.

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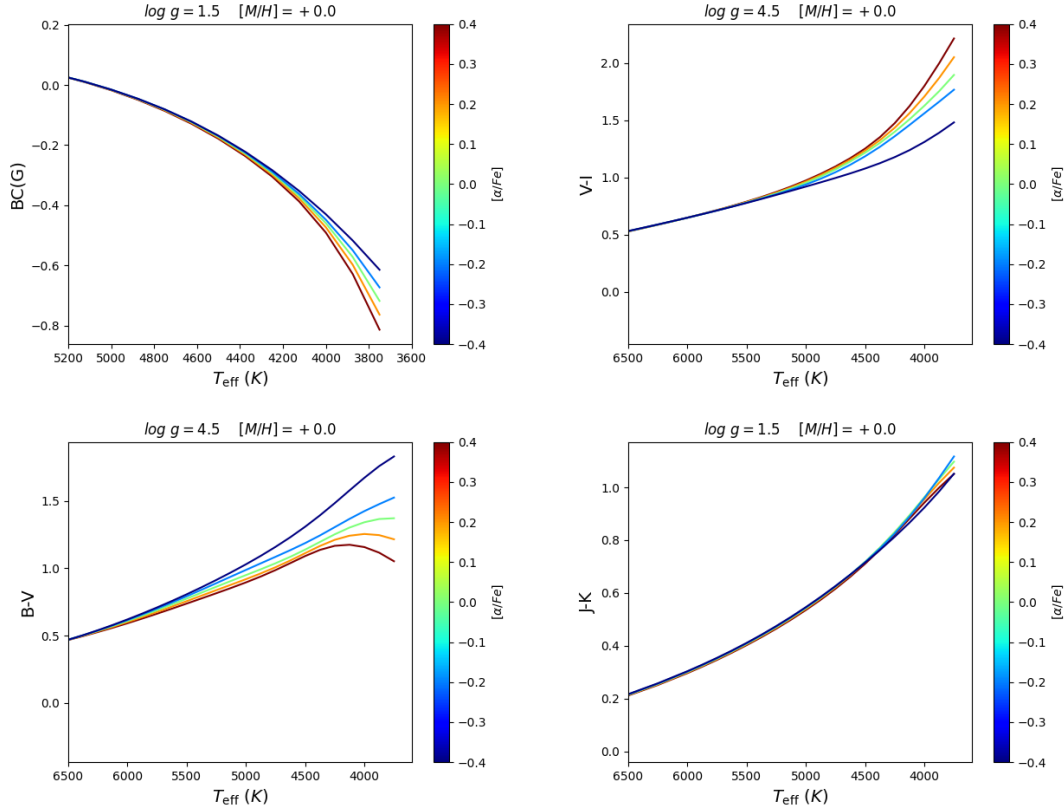


Fig. 8. Upper-left panel: run of the G-band bolometric correction as a function of T_{eff} for model atmospheres with $\log g = 1.5$, $[M/H] = +0.0$ dex and different $[\alpha/\text{Fe}]$. Upper-right panel: run of (V-I) as a function of T_{eff} ($\log g = 4.5$, $[M/H] = +0.0$ dex). Lower-left panel: run of (B-V) as a function of T_{eff} ($\log g = 4.5$, $[M/H] = +0.0$ dex). Lower-right panel: run of (J-K) as a function of T_{eff} ($\log g = 1.5$, $[M/H] = +0.0$ dex).

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Appendix A: About the metallicity in ATLAS9 model atmospheres

A model atmosphere is specified according to the effective temperature (T_{eff} , that defines the total bolometric flux that traverses the photosphere through the Stefan-Boltzmann relation, $F_{\text{bol}} = \sigma T_{\text{eff}}^4$), the surface gravity ($\log g$, that is related to the gas pressure through the hydrostatic equilibrium, $\frac{dP}{dr} = \frac{g}{k_v}$) and the chemical composition. Therefore, it is not the overall metallicity that defines the characteristics of the model, but rather the details of its chemical mixture, particularly the abundance of those elements that have a significant impact on the total opacity (for instance the α -elements).

ATLAS9 models tabulate explicitly the fraction of H and He atoms with respect to the total number of atoms ($\frac{N_{\text{H}}}{N_{\text{TOT}}}$ and $\frac{N_{\text{He}}}{N_{\text{TOT}}}$), while the metallic abundances are obtained by scaling the solar chemical composition (taken as reference) to a scaling factor (corresponding to the metallicity $[M/H]$).

In the ATLAS9 models, the abundance of the i -th metal is provided as

$$A_{\text{kurucz}}(Z_i) = \log_{10}\left(\frac{N_{Z_i}}{N_{\text{TOT}}}\right)$$

This formalism is slightly different to the traditional scale used to provide the absolute abundance of metals, namely

$$A_{\text{trad}}(Z_i) = \log_{10}\left(\frac{N_{Z_i}}{N_{\text{H}}}\right) + 12$$

and we can easily translate the Kurucz scale into the traditional one as

$$A_{\text{trad}}(Z_i) = A_{\text{kurucz}}(Z_i) + 12 - \log_{10}\left(\frac{N_{\text{H}}}{N_{\text{TOT}}}\right).$$

Appendix B: The zero-metallicity ODFs

Additionally, we compute a set of *zero-metallicity* ODFs calculated without including the contribution of the metals but only hydrogen and helium. This set is useful to calculate model atmospheres and fluxes for ideal Population III stars and provide boundaries for the photometric colours reliable for the search for very metal-poor stars. We compared some model atmospheres and corresponding fluxes for giant and dwarf Population III stars, finding that these models are indistinguishable from the most metal-poor ones of our grid. This exercise suggests that the spectral characterization of these rare, very metal-poor stars does not need additional, specific models.

Appendix C: Computing theoretical magnitudes and colours

This topic has been often reviewed, and we refer the reader to Bessell (1990); Bessell et al. (1998); Castelli (1999); Girardi et al. (2004); Bessell & Murphy (2012); Casagrande & Vandenberg (2014); Bonifacio et al. (2017, 2018) for definitions and discussion. In this appendix we detail how we computed magnitudes and colours presented in this paper.

All our codes have been derived from R. L. Kurucz's code *cousins*⁶, with one main difference, while the original code performed energy integration (eq. 3 of Bonifacio et al. 2017)

we computed all colours assuming photon counting. Energy integration is appropriate for *UBVRI* photometry obtained with photomultiplier tubes operated in energy integration mode. In the last thirty years however all photometry in any system has been obtained using photon counting detectors, including photomultipliers operated in photon counting mode (e.g. Bonifacio et al. 2000). The magnitude is computed as:

$$m - m_0 = -2.5 \log \left(\frac{\int \lambda f(\lambda) R(\lambda) d\lambda}{\int \lambda R(\lambda) d\lambda} \right) \quad (\text{C.1})$$

where $f(\lambda)$ is the flux from the star and $R(\lambda)$ is the instrument response function of the photometric band, this must include not only the filter response, but also the detector quantum efficiency and the telescope throughput. For some systems like SDSS (Fukugita et al. 1996), also the transmission of the Earth's atmosphere is included.

From equation C.1 it appears that two integrals have to be evaluated, however while for Vegamags, m_0 is a constant and the two integrals appearing explicitly in equation C.1 have to be evaluated, the situation is slightly different for AB mags, like SDSS.

In this case m_0 is the magnitude of an object that has a constant flux $F_\nu = 3631 \times 10^{-23} \text{ ergs s}^{-1} \text{ cm}^{-2} \text{ Hz}^{-1}$. Since the band-passes of the filters are provided as a function of wavelength, it is convenient to carry out the integrations in wavelength, rather than frequency. In this case $d\nu = \frac{c}{\lambda^2} d\lambda$, where c is the speed of light.

The AB magnitudes are defined as integrals over frequency, we use the above relation to transform the integral over frequency into integral over wavelengths. We follow what suggested in the Gaia DR3 documentation⁷ equations 5.42 and 5.44 and $m_0 = 56.10$.

$$m = -2.5 \log \left(\frac{\int \lambda f(\lambda) R(\lambda) d\lambda}{\int \frac{c}{\lambda^2} R(\lambda) d\lambda} \right) - 56.10 \quad (\text{C.2})$$

The two integrals that appear in the numerator and denominator of the right-hand of equation C.2 must be evaluated. One warning: for SDSS we use magnitudes and not ‘luptitudes’ as provided in the SDSS catalogue (Lupton et al. 1999), the reasons for this choice are well explained in Girardi et al. (2004). Following the original approach of R. L. Kurucz the integrals are approximated by a sum of rectangles, where both theoretical flux and instrumental response function have been rebinned at a step of, typically, 0.1 nm. The instrument response function is rebinned using the polynomial interpolation subroutine PINTER from Kurucz's original code, and the theoretical flux is linearly interpolated using the ATLAS subroutine LINTER. For some filters, like e.g. SDSS z , PINTER provides some negative values at the very edge of the response function, in this case we simply set the response function to zero. The SDSS z filter is rebinned at steps of 0.5 nm that is sufficient to recover the correct flux.

Another difference with respect to Kurucz's original code is that we adopt the approach of Casagrande & Vandenberg (2014): we compute the magnitude for every model as if it corresponds to a star of one solar radius at a distance of 10 pc. In practice we multiply the theoretical fluxes by a dilution factor $(R_\odot/10)^2 = 5.083267 \times 10^{-18}$.

⁶ <http://kurucz.harvard.edu/programs/colors/cousins.ford>

⁷ https://gea.esac.esa.int/archive/documentation/GDR3/Data_processing/chap_cu5pho/cu5pho_sec_photProc/cu5pho_ssec_photCal.html

ATLAS fluxes are provided as H_ν in units $\text{erg s}^{-1} \text{cm}^{-2} \text{Hz}^{-1} \text{sr}^{-1}$, we transform this to F_λ so we need to insert a factor 4π and since we express wavelengths in nm, we transform the units to $\text{Wm}^{-2}\text{nm}^{-1}$ in practice for each wavelength WAVE(NU) in the theoretical flux HNU(NU) we use this fragment of FORTRAN code to perform the transformation

```
FREQ=2.99792458E17/WAVE(NU)
HLAM(NU)=1.e-3*HNU(NU)*FREQ/WAVE(NU) * DIL *(4*PI)
```

where DIL is the above-defined dilution factor, PI is π and HLAM is F_λ .

The theoretical fluxes are also useful to define the extinction coefficients in the various bands. The relationship between the intrinsic magnitude of a star and the magnitude observed by us is:

$$m_i = m + 5 \log \left(\frac{R_*}{d} \right) - A \quad (\text{C.3})$$

where m_i is the intrinsic magnitude, m is the observed magnitude, R_* is the stellar radius, d is the distance of the star and A is the total extinction. If the magnitudes are monochromatic at wavelength λ A is the extinction at that wavelength. If the magnitudes are defined over a band, A is the integral of the monochromatic extinction over the band. Equation C.3 can also be interpreted as *definition* of total extinction. It is clear by combining equation C.1 and equation C.3 that A is a function of the flux distribution of the star. This means that the light of stars of different T_{eff} , $\log g$ and metallicity going through the same interstellar medium will have a different A . Since, in general, the angular diameter of stars is not known it is convenient to express extinctions as ratios with respect to extinction at a given wavelength or in a given band. The two, by far, most common choices for reference extinctions are A_V , the extinction in Johnson's V band and A_0 , the monochromatic extinction at 550 nm. There are many 2D (e.g. Schlafly & Finkbeiner 2011) and 3D Galactic maps (e.g. Schlafly et al. 2014; Vergely et al. 2022) that provide extinction as a function of position on the sky (2D) or position on the sky and distance (3D). The map of Vergely et al. (2022) is derived from the reddening estimates of a large number of stars, obtained with different methods, both photometric and spectroscopic. In a first step the derived A_0 for any of the stars is indeed a function of the stellar parameters. In a second set all the different estimates are inter-calibrated and combined with the basic assumption that for the stars in a small space volume. The third, and quite complex, step in making an extinction map is the geometric computation to convert all sun-star integrated quantities to local values, this process is called inversion (Lallement et al. 2014; Vergely et al. 2022). The properties of the dust are the same (or equivalently that this volume is homogeneous) and from this process one determines a value of A_0 that is only a function of the spatial coordinates and not of the stellar type. All reddening maps need to make an assumption of this type, that is some homogeneity of the dust in a small volume of space. Once the inversion is made and maps are computed, they provide an estimate of the extinction (e.g. A_0) in each point in three dimensional space that is fully independent of target star properties, provided that the individual determinations have used correct assumptions on stellar parameters/spectra. However, it is only the value of the extinction at the exact wavelength used for the mapping which is a property of the interstellar dust. If, for a given observed star, one wants to use a map value, e.g. if one wants to use A_0 , but would like, also, to have estimates of the extinction at other wavelengths or in a photometric band, one should be

aware that only the extinction at other wavelengths depends on the stellar properties.

If one wants to correct for reddening the photometry of a star, one should know the parameters of the star. Either one uses a method independent of photometry to determine the stellar parameters, or one uses an iterative procedure such as described, for example, in Bonifacio et al. (2019) or Lombardo et al. (2021). Since in reality the extinction coefficients do not have a strong dependence on the stellar parameters, the strongest one being on effective temperature (see e.g. Danielski et al. 2018), it is often acceptable, to use a single extinction coefficient for all the stars. This is usually the approach adopted in dereddening the photometry of star clusters and dwarf galaxies.

In this paper for any synthetic band, X provided we also provide the ratio AX/A_0 , if T_{eff} , $\log g$, metallicity and $[\alpha/\text{Fe}]$ of the star are known, even approximately, it is straightforward to interpolate in our tables to determine the appropriate extinction, that can be combined using a value of A_0 obtained from maps or otherwise. Since several maps are provided in terms of A_V or $E(B - V)$, we also provide the ratio A_V/A_0 that can be used to convert between the two extinctions.

In order to compute the extinction coefficients we had to assume a Galactic extinction law and we assumed that of Fitzpatrick et al. (2019) corresponding to $R(55) = 3.02^8$. The extinction cast into flux units, using

$$b = 10^{-\frac{k+3.02}{2.5}} \quad (\text{C.4})$$

for any wavenumber, then the wavenumbers were transformed in wavelengths and each vector sorted. The value of b_0 at 550 nm was obtained with a Hermite spline interpolation (subroutine INTEP, Hill 1982) and we then computed $A_0 = -2.5 \log(b_0)$. For any filter the extinction law was rebinned with PINTER on the same mesh as the filter response function. For each filter we computed

$$A = -2.5 \log \left(\frac{\int \lambda f(\lambda) R(\lambda) b(\lambda) d\lambda}{\int \lambda f(\lambda) R(\lambda) d\lambda} \right) \quad (\text{C.5})$$

what is provided in the tables is A/A_0 .

One final comment, all our synthetic photometry is provided with six significant figures (five decimal places), not because we believe that this is its accuracy, but because this helps to minimise interpolation errors when using these tables.

⁸ $R(55) = \frac{A(55)}{E(44-55)}$, the value 3.02 corresponds to $R(V) = \frac{A_V}{E(B-V)} = 3.1$.