

Two semi-automated computational approaches for spectroscopic analysis of stellar photospheres: detailed characterization at high resolution and abundance determination at medium resolution

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ABSTRACT

We report on two distinct computational approaches to self-consistently measure photospheric properties of large samples of stars. Both procedures consist of a set of several semi-integrated tasks based on shell and Python scripts, which efficiently run either our own codes or open source software commonly adopted by the astronomical community. One approach aims to derive the main stellar photospheric parameters and abundances of a few elements by analysing high-resolution spectra from a given public library homogeneously constructed. The other one is applied to recover the abundance of a single element in stars with known photospheric parameters by using mid-resolution spectra from another open homogeneous database and calibrating derived abundances. Both semi-automated computational approaches provide homogeneity and objectivity to every step of the process and represent a fast way to reach partial and final results as well as to estimate measurement errors, making possible to systematically evaluate and improve the distinct steps.

Keywords: computational data analysis, stars: spectra, stars: atmospheric parameters, stars: element abundances, spectral synthesis.

1 INTRODUCTION

The physical, chemical and dynamical characterization of a stellar photosphere is made by analysing its spectrum. To achieve this astronomers need to measure the intensity and/or shape of many atomic and molecular absorption lines in high-quality optical spectrum at high resolution (resolving power $R \equiv \lambda/\Delta\lambda > 10\,000$, $\Delta\lambda = FWHM$). However, adopting mid-resolution spectra ($1\,000 \leq R \leq 10\,000$) represents an alternative either to obtain the photospheric temperature, gravity and metallicity on large surveys when associated with photometric measurements

and comparisons against other data sets ($R \approx 2\,000$) [1] or to recover multi-elemental abundances for previously characterized stars on smaller samples ($R \approx 6\,000$) [2].

The first step of any stellar spectroscopic analysis at any resolution is the spectral continuum normalization. The overall continuum shape primarily depends on the photospheric temperature but also shows particularities as a function of the wavelength due to the total local opacity (sum of all processes of light absorption and scattering integrated along the photosphere at a given frequency). The second step is to measure the intensity of each atomic absorption feature, for which the profile can be represented

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by the sum of one or more individual lines. Both steps are very time-consuming tasks that also include some level of subjectivity in the selection of continuum windows and absorption features. It is normally performed using known public programs for analysis of astronomical data such as the IRAF¹ multi-platform software and others developed by the astronomers themselves that make the features measurements faster (e.g. ARES [3]). Besides the measurements of a myriad of atomic lines, the other inputs for the spectroscopic analysis are the physical structural model of the photosphere and the physical parameters of a representative list of atomic and molecular lines to be taken into account in the theoretical spectrum computation, which is the following step and also consumes a lot of time.

In this paper we describe two semi-automated approaches developed to alleviate those issues and to objectively analyse large stellar spectral data sets. In the first one, the fundamental photospheric parameters and abundances of several elements are self-consistently derived by analysing high-resolution spectra of stars selected from the ELODIE database [4]. The other computational approach addresses the measurement of magnesium abundance in stars of the MILES spectral library [5] by inspecting the own MILES' mid-resolution spectra. The photospheric parameters of MILES' stars are previously known and were homogenized onto a uniform system from measurements of several published works [6]. The procedure presented here includes also the calibration of resulting mid-resolution Mg abundances against homogeneously scaled high-resolution measurements.

2 DETAILED PHOTOSPHERIC CHARACTERIZATION AT HIGH SPECTRAL RESOLUTION

The complete characterization of a stellar photosphere depends on the computation of a realistic model atmosphere, which is described by four fundamental parameters: the effective temperature T_{eff} , the metal content traced by the iron abundance that is usually represented in a logarithm scale relative to the solar pattern $[\text{Fe}/\text{H}]^2$, the logarithmic surface gravity $\log g$, and the micro-turbulence velocity ξ . High-resolution measurements of many optical lines of neutral and first ionized states of iron atoms (Fe I and Fe II respectively) have been historically adopted for this purpose.

In the work of Da Silva et al. (2011) [7] an automated computational procedure was developed to analyse high-resolution

spectra ($R = 42\,000$) of 172 solar-like stars collected from the ELODIE database. The method adopts the Sun's parameters as an input set ($T_{\text{eff}} = 5777\text{ K}$, $[\text{Fe}/\text{H}] = 0.0\text{ dex}$, $\log g = 4.44$, $\xi = 1.0\text{ km.s}^{-1}$) to find the best solution for the model atmosphere through an iterative process described next. This automated procedure was also applied by Da Silva & Milone (in prep.) to a wider sample of ELODIE's solar-type stars.

The abundance yielded by distinct spectral lines of an element E ($\log \epsilon(\text{E})_{\star}$ or $[\text{E}/\text{H}]$) must not be dependent on the excitation potential (χ) and equivalent width (EW). The excitation potential is the lowest energy level of the electronic transition, and the equivalent width quantifies the electromagnetic flux absorbed by the transition over the emergent photospheric spectrum ($EW \equiv \int (1 - F(\lambda)_l / F(\lambda)_c) . d\lambda$, where F_l and F_c are the line and continuum flux respectively). Also, the lines of neutral and ionised species from the same element must provide a unique abundance. T_{eff} is normally computed through the excitation equilibrium of Fe I by removing any dependence in the $\log \epsilon(\text{Fe})$ vs. χ diagram. Additionally, by removing any spurious abundance dependence on EW , ξ is estimated. Surface gravity is computed through the ionisation equilibrium between the Fe I and Fe II species, and finally $[\text{Fe}/\text{H}]$ is derived from the EW measurements of Fe I lines.

Figure 1 illustrates through a flux diagram how the photospheric parameters are determined, where δ_1 , δ_2 , δ_3 , and δ_4 are arbitrary constants as small as one wishes. If at least one of the first three conditions is not satisfied, then T_{eff} , ξ , and/or $\log g$ are changed by a given step (respectively Δ_1 , Δ_2 and Δ_3). In the fourth condition, the value of $[\text{Fe}/\text{H}]$ used as input is compared to the one provided by Fe I lines and, if they do not agree within δ_4 , the code defines $[\text{Fe}/\text{H}] = [\text{Fe I}/\text{H}]$. Therefore, the code iteratively executes several cycles until these four conditions are satisfied together. We tested the method using different sets of input parameters for distinct stars and the same solution is always reached for each star considering their uncertainties.

The computational method for obtaining the photospheric parameters is based on a Python script, which incorporates: (i) a Fortran code for interpolation in a grid of model atmospheres [8]; (ii) the execution of a spectral synthesis code (MOOG [9]) applied to the interpolated model by computing the theoretical predictions of EW for a set of Fe I and Fe II lines; and (iii) the simultaneous convergence conditions through an iterative analysis of the input/output parameters.

¹Image Reduction and Analysis Facility, IRAF, is distributed by the National Optical Astronomy Observatories, USA.

² $[\text{Fe}/\text{H}] = \log(\epsilon(\text{Fe})/\epsilon(\text{H}))_{\star} - \log(\epsilon(\text{Fe})/\epsilon(\text{H}))_{\odot}$ where $\log \epsilon(\text{Fe}) = \log(n(\text{Fe})/n(\text{H})) + 12$, $\log \epsilon(\text{H}) = 12$ and $n(\text{Fe})$ and $n(\text{H})$ are the number densities (volumetric or columnar) of iron and hydrogen atoms respectively.

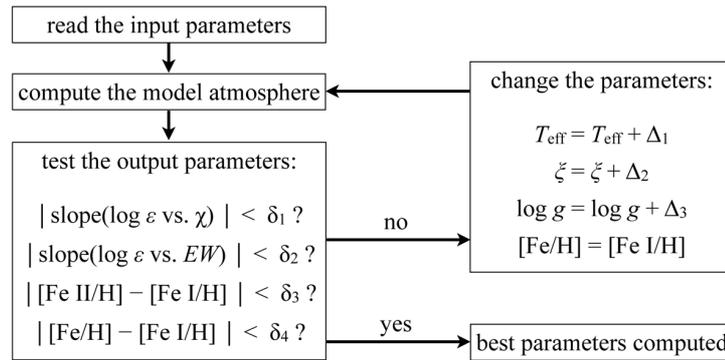


Figure 1 – Flux diagram for the spectroscopic analysis to determine the stellar photospheric parameters at high resolution.

The semi-automated element abundance determinations performed in Da Silva et al. (2011) and in Da Silva & Milone (in prep.) are based on EW_s of selected atomic lines (Na, Mg, Si, Ca, Ti, V, Mn, Fe, Ni, Cu, and Ba) as well as on spectral synthesis of C_2 , CN, C I, O I, and Na I features, where both techniques are applied with the MOOG code. The procedures were incorporated into a Python script, which includes: (i) the computation of the element abundances for each star based on their photospheric parameters and EW_s , fixing the solar gf values (these were revised to fit the solar observed EW_s because the Sun is taken as a reference); (ii) the computation of synthetic spectra for six different values of $[E/Fe]$ considering the photospheric parameters, the continuum opacity contribution, and the line-broadening corrections; (iii) a vertical shift of the synthetic spectra based on continuum windows; (iv) the computation of the rms deviation between synthetic and observed spectra within selected regions of atomic and molecular features; and (v) an iterative search for the smallest rms value, which is done by changing the six abundance values until finding a minimum in the rms vs. $[E/Fe]$ diagram.

Figure 2 presents an example of the best spectral synthesis of a C_2 feature that was reached through this computational procedure. The resulting carbon abundance is derived using a polynomial fit of the rms deviation between the synthetic and observed spectra as a function of the $[C/Fe]$ abundance ratio as illustrated in a diagnostic plot employed in the process (shown also in Fig. 2).

An error analysis for the derived photospheric parameters and element abundances was also performed in an automated way. Basically the stellar parameter uncertainties are iteratively computed through a Python script following an analogue computational procedure as that applied to determine the stellar parameters themselves (see Fig. 1). The abundance errors are

estimated considering the propagation of atmospheric parameter errors. They are automatically calculated adopting another Python script.

3 PHOTOSPHERIC Mg ABUNDANCE MEASURED AT MEDIUM SPECTRAL RESOLUTION

In the computational approach that semi-automatically runs the mid-resolution spectroscopic analysis ($R \approx 2200$) carried out by Milone et al. (2011) [10], the photospheric parameters were not determined because they were already known. The objective in that work was to measure the magnesium abundance in the stars of the MILES optical spectral library. For this purpose we first computed a large number of model atmospheres to represent the physical-chemical conditions of each photosphere. Linear interpolations of the MARCS model atmospheres [11] were applied using a public code [12], which is automatically manipulated through a C shell script. This was improved by Milone et al. (2011) to incorporate some specific procedures such as (i) reading the input list of MILES stars together with their parameters, (ii) definition of eight input models to be read from the MARCS grid, (iii) inclusion of a table of element abundances and molecular species into each model file, and (iv) transformation of the output model files into a format readable by the MOOG code. A global picture of the whole semi-automated computational approach described in this section is illustrated in Figure 3.

After the model atmospheres have been built up through interpolations, five synthetic spectra had to be computed at medium resolution in two different regions for each MILES' star inside the MARCS grid. One Mg I atomic feature was analysed per spectrum region: the strongest line of Mg b triplet at $\lambda 5183.6\text{\AA}$,

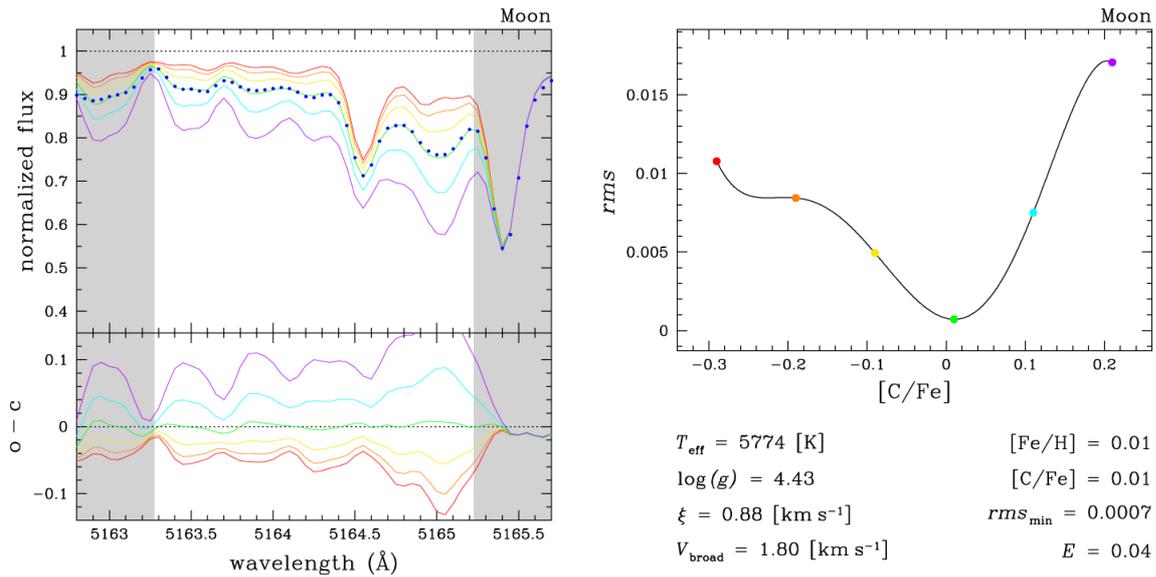


Figure 2 – Example of a spectral synthesis at high resolution of the C_2 band feature at $\lambda 5165\text{\AA}$ (left panel, from Fig. 3 of Da Silva et al., 2011) and the diagnostic plot rms of theoretical and observed spectral comparisons versus $[C/Fe]$ (right panel). The observed spectrum (blue points in the left panel) is the sunlight reflected by the Moon. The flux continuum normalization is checked in other plots.

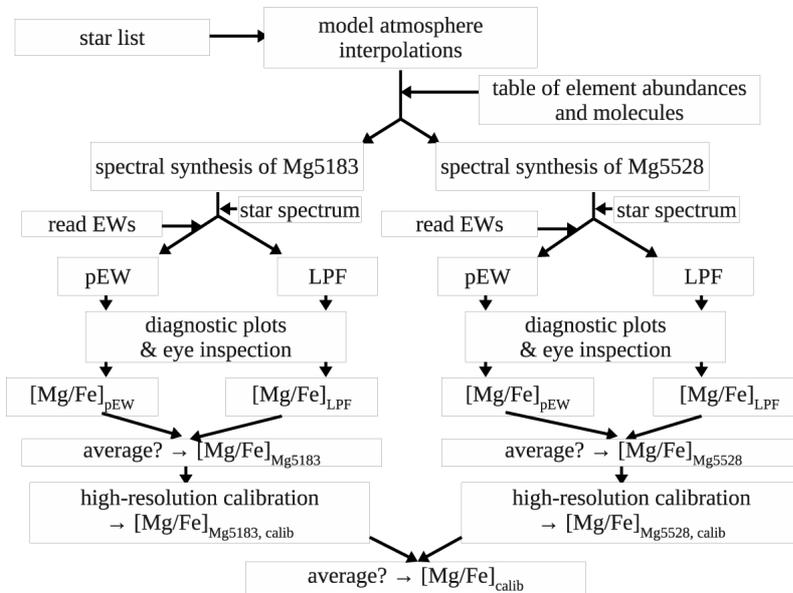


Figure 3 – Flux diagram for the spectroscopic analysis to derive the $[Mg/Fe]$ abundance ratio at medium resolution.

and the line at $\lambda 5528.4\text{\AA}$. Two element abundance determination methods were employed: the pseudo-equivalent width (pEW) and the line profile fit (LPF), both applied to each feature passband adopting two pseudo-continuum windows. Figure 4 shows an example of spectral synthesis for the Mg5183 feature in association with both methods applied to measure the Mg abundance.

843 MILES stars were analysed and 8,430 theoretical spectra had to be computed through an semi-automated process based on a very simple Expect shell script that successively runs the MOOG software thousands of times. Every synthetic spectrum incorporates a Gaussian-like instrumental broadening to reach the MILES' resolution. Their wavelength scales were re-binned to

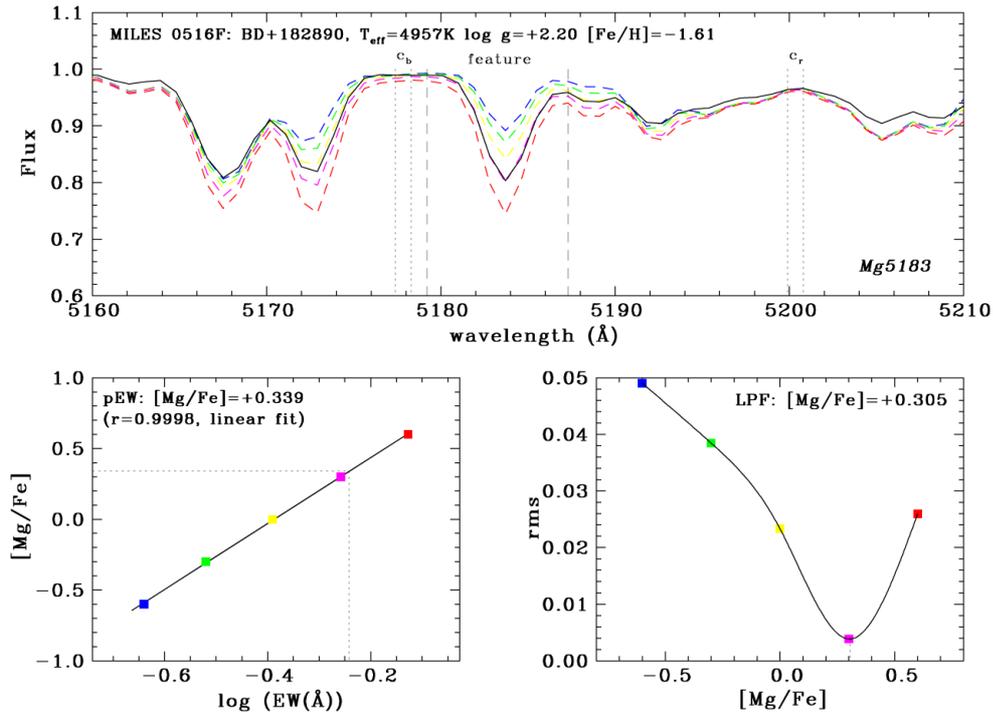


Figure 4 – Example of diagnostic plots, adapted from Milone et al. (2011), for the spectral synthesis of Mg5183 feature (top panel) and the correspondent methods employed to determine $[Mg/Fe]$ (pseudo-equivalent width in the left bottom panel and line profile fit in the right one).

exactly agree with the sampling of the MILES spectra at each observed wavelength bin. Additionally, the wavelength scales of MILES spectra were carefully shifted to the rest frame to match the model scale. To guarantee a reliable matching between the flux scales of model and empirical spectra, the latter ones had their pseudo-continuum flux locally normalized in both Mg I feature regions. All these steps were executed by C shell scripts associated to IRAF tasks (e.g. FXCOR of the NOAO Optical Astronomy Package for spectral cross-correlations and to obtain pixel fractional corrections for reaching the rest wavelength scale).

The other steps of the computational approach for recovering $[Mg/Fe]$ abundance ratios at medium resolution applied by Milone et al. (2011) can be summarize as follows (see also Fig. 3).

1. Automated measuring of EW of two Mg features over all empirical and theoretical spectra (by running the LECTOR public Fortran code, www.iac.es/galeria/vazdekis/SOFTWARE/, through C shell scripts).
2. Application of the pEW and LPP methods based on several concatenated C shell scripts, together with a macro developed by us using an interactive plotting code (SM [13]),

which employs a flexible command language. This step designs diagnostics plots of the spectral synthesis of both Mg features for each star (example in Fig. 4).

3. For each Mg feature, computation of the mean $[Mg/Fe]$ value of those obtained with the two methods after inspection by eye in the spectral synthesis plots. The average is only computed when both methods show reliable results³.
4. Linear calibration of $[Mg/Fe]_{\text{feature}}$ to a uniform scale based on our own Fortran routines, separately for each feature, via comparison with a control sample of MILES stars (for which the abundance ratios were obtained from published high-resolution analyses and previously calibrated onto a homogeneous scale), in order to provide $[Mg/Fe]_{\text{feature}}^{\text{calib}}$.
5. Simple averaging of $[Mg/Fe]_{\text{feature}}^{\text{calib}}$ combined when possible, in order to derive the final calibrated $[Mg/Fe]_{\text{calib}}$ for each star (Fortran routines from ourselves).

An error analysis was also performed along the whole process (step by step based on own codes and graphics) in order to estimate the intrinsic uncertainties from each abundance

³in some cases, only one method gives a reliable value while in others both methods fail. This gives $[Mg/Fe]_{\text{feature}}$

determination method, the uncertainties due to the error propagation from photospheric parameters, the effective internal errors of both $[\text{Mg}/\text{Fe}]_{\text{feature}}$, and the systematic or external errors of final calibrated abundance ratios $[\text{Mg}/\text{Fe}]_{\text{feature}}^{\text{calib}}$ and $[\text{Mg}/\text{Fe}]_{\text{calib}}$.

4 CONCLUSIONS

On the one hand, a stellar spectroscopic analysis at high resolution commonly offers better results than an analysis at medium resolution for determining photospheric parameters and element abundances. For instance, the typical internal uncertainties of T_{eff} , $[\text{Fe}/\text{H}]$, $\log g$, ξ and $[\text{C}/\text{Fe}]$ in Da Silva et al. (2011) are, respectively, 70 K, 0.06 dex, 0.2, 0.07 $\text{km}\cdot\text{s}^{-1}$ and 0.04 dex, while the external error of $[\text{Mg}/\text{Fe}]_{\text{calib}}$ in Milone et al. (2011) ranges from 0.10 to 0.15 dex according to the Mg feature adopted (average value of 0.12 dex). On the other hand, a medium-resolution analysis that is partially or fully automated can provide astronomers nowadays with an efficient tool to analyse large samples as done by Milone et al. (2011) to recover magnesium abundances in the stars of MILES library as well as those performed by [1] and [14] to respectively measure the stellar parameters and abundances over the SDSS/SEGUE wide survey. In [1] and [14], other techniques were also employed in automatic way such as the SDSS photometry, empirical-theoretical fitting of full spectrum, and line strength indices to help recovering the photospheric properties with more precision. The reached internal errors of T_{eff} , $[\text{Fe}/\text{H}]$, $\log g$ and $[\text{E}/\text{Fe}]$ are typically 70 K, 0.07 dex, 0.18 and smaller than 0.1 dex, while the external errors of them are 130 K, 0.11 dex, 0.21 and 0.1 dex. It is out of the scope of the current work to compare other methods found in the literature and their computational procedures against all those applied here. The techniques applied by us at high and medium resolution are fully self-consistent and the computational procedures developed here have represented an objective solution to manipulate them with reliability and efficiency.

The classical human-interactive approach performs individual analysis of each star carrying out several steps one by one in a tedious iterative and frequently subjective way (e.g. spectral synthesis of a given feature per time). The major distinctions of our semi-automated spectroscopic analyses in comparison with the classical approach are: (a) manipulation of several scripts and software written in different languages, and (b) automated execution of concatenated steps of the whole process. Their main goals are: (i) to guarantee homogeneity and a high level of objectivity in the application of each step of the process, (ii) to reach partial and final results in a fast way making possible to evaluate

the separated steps, (iii) to rapidly estimate measurement errors step by step, and (iv) to easily repeat the whole process or its distinct steps as many times as necessary to correct minor mistakes and improve parts of the process. Although the gain in CPU time is actually not improved, we have estimated that the gain in man-power time comparatively with the classical approach can reach to around a factor of 100 in the determination of the photospheric parameters, and about a factor of 10 in the application of spectral synthesis to reproduce line profiles and obtain element abundances.

We intend to make both semi-automated computational approaches publicly available when their tools are consistently integrated and documented in order to be easily installed and manipulated in any platform.

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