Program package for the analysis of high resolution high signal-to-noise stellar spectra

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Abstract. The program package SME (Spectroscopy Made Easy) (Valenti & Piskunov 1996; Piskunov & Valenti 2016), designed to perform an analysis of stellar spectra using spectral fitting techniques, was updated due to adding new functions (isotopic and hyperfine splitting) in VALD and including grids of NLTE calculations for energy levels of few chemical elements. SME allows to derive automatically stellar atmospheric parameters: effective temperature, surface gravity, chemical abundances, radial and rotational velocities, turbulent velocities, taking into account all the effects defining spectral line formation. SME package uses the best grids of stellar atmospheres that allows us to perform spectral analysis with the similar accuracy in wide range of stellar parameters and metallicities – from dwarfs to giants of BAFGK spectral classes.

1. Introduction

The first release of Gaia mission (Lindegren 2016) provides us with parallaxes and proper motions for more than 2 million stars. One needs to derive fundamental parameters of these stars – effective temperature, surface gravity, metallicity – to restore the stellar population distribution in our Galaxy. The best way to solve this task is the use of fast but robust automatic procedures for stellar spectra analysis because spectroscopy plays the main role in determination of the fundamental parameters. We briefly describe the evolution of the automatic spectral fitting package Spectroscopy Made Easy (SME) developed by Valenti & Piskunov (1996) and further upgraded by Piskunov & Valenti (2016).

2. SME

SME computes synthetic spectra and adjusts free parameters ($T_{\text{eff}}$, $\log g$, metallicity, $v_e\sin i$, $V_{\text{mic}}$, $V_{\text{mac}}$, abundances of chemical elements) based on comparison with observations. SME solver consists of the IDL routines for preparing spectral synthesis and performing optimization, and external library for synthetic spectrum calculations. The external library (SYNTH code) is written in C++ and Fortran. SME spectral synthesis includes molecular and ionization equilibrium solver EOS, continuous opacity package CONTOP, line opacity package LINEOP and radiative transfer (RT) solver. EOS
has partition functions for up to 6 ionization stages of the first 99 atoms in the periodic table and for 257 molecules (up to four atoms) fitted over the range from 10 K to 8000 K (Barklem & Collet 2016). EOS is using rather unique solving strategy. SME is working with the observations in ASCII or FITS formats. The format of input linelist is one of the output formats of VALD ‘Extract Stellar’ request (Kupka et al. 1999). Short format is used when SME is working in LTE (local thermodynamic equilibrium) regime, while for NLTE (non-local thermodynamic equilibrium) analysis a long format is needed. The current version of SME has model libraries of Kurucz’ (1993) models, the latest version of MARCS models (Gustafsson et al. 2008), and a grid of LLmodels (Shulyak et al. 2004) calculated for microturbulent velocity of 2 km s$^{-1}$. Both plane-parallel and spherical MARCS models are available.

In general, SME provides reliable estimates of the atmospheric parameters for dwarf and giant stars. For dwarfs it is justified in the papers by Ryabchikova et al. (2016), and Ryabchikova et al. (2015). For two cool giant stars the SME results are compared with other published determinations in Table 1.

### Table 1. Atmospheric parameters of the giant stars derived by different methods.

| HD     | $T_{\text{eff}}$ | log $g$ | [Fe/H] | Reference                  |
|--------|-----------------|---------|--------|----------------------------|
| 4306   | 4944(122)       | 1.95(48)| −2.80(10)| This paper (SME)          |
| 4306   | 4800( 40)       | 1.70(06)| −2.92(04)| Fulbright (2000)          |
| 4306   | 5000(100)       | 2.10(30)| −2.52(15)| Mishenina & Kovtyukh (2001) |
| 74387  | 4833( 40)       | 2.41(16)| −0.29(05)| This paper (SME)          |
| 74387  | 4840(100)       | 2.43(10)| −0.18(05)| Pakhomov et al. (2009)    |

3. **NLTE grid calculations**

SME allows us to derive not only atmospheric parameters but element abundances as well. Abundances are derived as average over all observed ions. Original SME version (Valenti & Piskunov 1996) was working with the spectral synthesis under LTE assumption. Some lines of important chemical elements were excluded from fitting procedure because of NLTE effects. The current SME version includes a possibility to use pre-calculated NLTE data in fitting. These data consist of departure coefficients $b$ (a ratio of NLTE to LTE level populations) for energy levels of an element. Calculations are performed for grids of MARCS plane-parallel models with the microturbulent velocity of 1 km s$^{-1}$ using DETAIL code (Butler & Giddings 1985). At present we have NLTE data grids for elements O I, Na I, Ca I-II, and Ba II.

**Oxygen.** NLTE oxygen calculations were performed using model atom from Przybilla et al. (2000) that includes 51 levels of O I and ground state of O II. Electron-impact excitation data from Barklem (2007) were employed.

**Sodium.** 17 levels with n$\leq$7, l$\leq$5 of Na I and ground state of Na II represent Na model atom (Alexeeva et al. 2014). Cross-sections for electron-impact collisions were extracted from Igenbergs et al. (2008) while rate coefficients for inelastic collisions with hydrogen atoms were taken from Barklem et al. (2010).

**Calcium.** Calcium model atom includes 63 levels of Ca I, 37 levels of Ca II and ground state of Ca III (Mashonkina et al. 2007).

**Barium.** For barium we used model atom developed by Mashonkina et al. (1999). It includes 35 levels of Ba II and ground state of Ba III.
Search for final atmospheric parameters and abundances is carried out by interpolation between the nodes in model and NLTE data grids as described in details in Piskunov & Valenti (2016).

Comparison of the model atmosphere structure and NLTE departure coefficients $b$ obtained by direct calculations and by interpolation process shows fairly good agreement. Even in the cases of complex dependence of $b$-factors on atmospheric depth when interpolation smooths the curves out, it does not influence too much the emergent line flux (see Fig. 1). The difference in the equivalent width of O I 7771.94 Å line does not exceed 0.2% that translates to 0.02 dex of abundance difference.

![Graphs showing comparison between $b$-factors derived by direct calculations and interpolation for O I IR-transitions](image)

Figure 1. *Top panels:* comparison between $b$-factors derived by direct NLTE calculations (full lines) and by interpolation (dashed lines) for lower (left) and upper (right) energy levels of O I IR-transitions. Calculations are made for HD 69830 ($T_{\text{eff}}=5422$ K, log $g=4.47$, metallicity=-0.04) *Bottom panel:* comparison between line profiles of O I 7771.94 Å line calculated with $b$-departure coefficients described above. Observations are shown by asterisks.

We compared abundances determined with SME and by separate fitting of carefully chosen set of spectral lines in the atmosphere of cool dwarf HD 69830. SME-derived parameters were taken from Ryabchikova et al. (2016) - ESPaDONs spectrum. The procedure of line-by-line abundance determination is given in the same paper as well. Note, that in both cases abundances were derived using different sets of spectral lines. This comparison shows fairly good agreement of both sets of abundances within the typical errors of best solar abundance determinations, ±0.04 dex.
Figure 2. Comparison between abundances derived for HD 69830 with SME and by separate fitting of carefully chosen set of spectral lines. Elements analysed under NLTE assumption are marked by open circles. Errors are shown for SME analysis.

Acknowledgments. This work was partially supported by the grant of the Leading School No9951.2016.2 and by the Russian Foundation for Basic Research (grant 15-02-06046).

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