Deriving stellar parameters with the SME software package

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Photometry and spectroscopy are complementary tools for deriving accurate stellar parameters. Here I present one of the popular packages for stellar spectroscopy called SME with the emphasis on the latest developments and error assessment for the derived parameters.

1 Introduction

Spectroscopy and photometry are complementary tools for derivation of accurate stellar parameters. Spectroscopy is better suited for measuring those parameters directly related to the radiation field, such as temperature and abundances. Photometric monitoring of stellar variability (pulsations) is sensitive to the vertical distribution of mass. Comparison of results derived with the two techniques is regarded as a robust test for quality of stellar parameter determination. Finding the solution consistent with both photometric and spectroscopic data thus becomes the ultimate goal of stellar studies. Here I focus of the latest development of the Spectroscopy Made Easy (SME) package. The original SME was written in 1995 and presented in Valenti & Piskunov (1996). Since then most parts of the package were improved or replaced. The description of the latest version can be found in the paper by Piskunov & Valenti (2017). Below I list the most important changes and additions, discuss the uncertainty analysis and cite some recent examples of SME applications.

2 SME concept

SME is a tool for fitting the observed spectra with spectral synthesis. Thus it requires atomic (and molecular) data, a grid of model atmospheres, observations (a spectrum and its wavelengths), the properties of the instrument (e.g. instrumental broadening) and the initial guess for stellar parameters. The fit process uses the Marquardt-Levenberg algorithm and numerical partial derivatives over free parameters. All possible free parameters are divided into global ($T_{\rm eff}$, $\log g$, metallicity and microturbulence), non-global (individual abundances, oscillator strengths and van der Waals broadenings) and those that do not require recomputing the spectral synthesis (radial velocity, rotational broadening and instrumental broadening). Clearly, some of these parameters are degenerate and cannot be fitted simultaneously. The user must consider if the data provide enough orthogonal sensitivity to selected free parameters and not be surprised with peculiar results if it doesn't. The concept of "mask" assigning to spectral pixels an attribute of "bad", "good" or "continuum" adds some flexibility for balancing the sensitivity to various free parameters (Fig 1). The 20-year

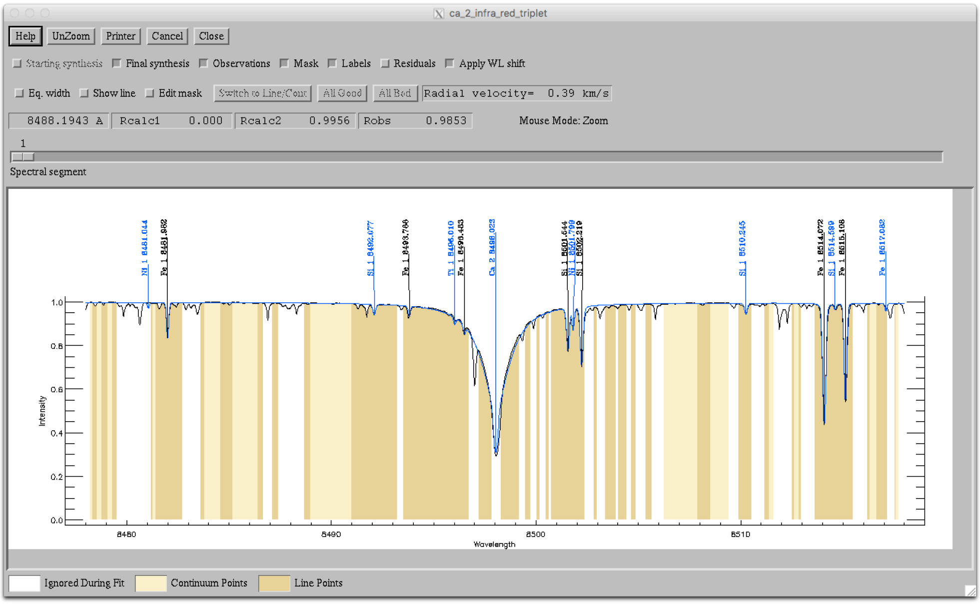

Fig. 1: The use of a mask for marking sensitive parts of the spectrum as well as continuum points.

legacy of using SME allows to formulate some general guidelines and good practices in doing certain types of fit. This are also presented in Piskunov & Valenti (2017).

3 SME changes since 1995

SME has seen many changes in the last 20 years. Here is a list of the most important upgrades:

- A molecular-ionization equilibrium solver has replaced the simple Saha equation. This now allows to have a consistency between abundances and partial number density of all constituent species for a given temperature-pressure combination. The new solver is a robust one for a large range of pressures and temperatures and its use is particularly important for cool atmospheres where different molecules compete for the same atoms.

- A new Besiér spline attenuation operator radiative transfer solver (de la Cruz Rodríguez & Piskunov, 2013) is fast, accurate and robust even on occasionally coarse depth grids given in model atmospheres. The solution for the vertical scale is done using the column mass rather than the optical depth. This decouples the individual abundances used for computing the model and the best-fit abundances found by SME.

- For giant and supergiant stars spherical model atmospheres are now consistently complemented with the spherical radiative transfer treatment.

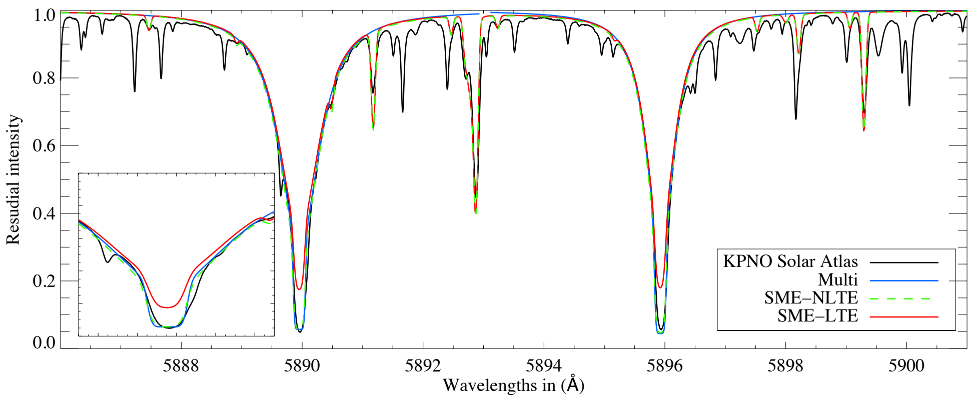

Fig. 2: Comparison of NLTE and LTE calculations of the Sodium lines in the solar spectrum. Various colours show the observed spectrum, NLTE synthesis with SME and with MULTI codes, and LTE calculations with SME.

- An improved optimization procedure has good convergence properties despite using numerical derivatives.
- A better continuous opacity package extended to hot and cool stars.
- The Balmer line opacity is computed using the occupational probability formalism of Stehlé & Hutcheon (1999) further developed by Barklem et al. (2000b).
- Broadening of atomic lines by collisions with neutral atoms of Hydrogen and Helium is computed using the Barklem, O'Mara and Piskunov approximation (Barklem et al., 2000a) producing much better fit to the observed line shapes.
- In addition to the Kurucz model atmosphere, SME is now distributed with MARCS (Gustafsson et al., 2008) and LL (Shulyak et al., 2004) atmospheric grids. A Phoenix model grid is available on demand.
- SME can now take advantage of precomputed departure coefficient grids to include NLTE effects in spectral synthesis of selected lines. Currently we have departure coefficients for Li, C, O, Na, Mg, Al, Si, Ca, Fe, Ba and Eu computed for MARCS atmospheric grid. For some elements we also have tables for the Kurucz and LL models. Figure 2 shows an example of such calculations.
- SME is now better integrated with VALD (Piskunov et al., 1995) allowing both "short" and "long" format line data to be imported. The long format is required for level identification when performing NLTE calculations.
- For mass production, SME now runs in batch mode and even on parallel clusters.

4 Uncertainties estimate

One of the critical point when using SME is the ability to estimate the uncertainties of the derived parameters. The formal uncertainties derived from the diagonal elements of the covariance matrix always look too optimistic. This is not surprising as they do not depend of the quality of the fit. The alternative estimate presented in Piskunov

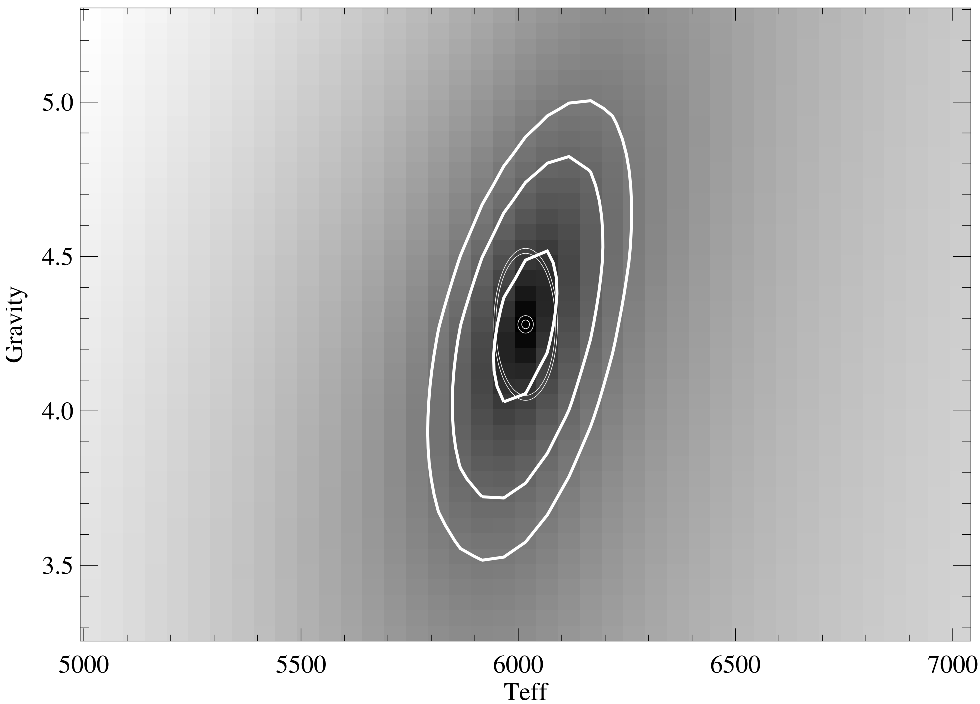

Fig. 3: Comparison of χ^2 surface constructed by scanning the $T_{\rm eff} - \log g$ parameter space with the 1 σ ellipsoid based on the SME uncertainty estimates (grey double line). Single lines show 1, 2 and 3 σ contours for the χ^2 surface. The little circle in the middle shows the quality of convergence (covariance matrix diagonal elements).

& Valenti (2017) uses the statistics of residuals and partial derivatives in all "good" pixels. The resulting estimates come much closer to what is expected from a comparison with alternative methods and when using different spectral regions and different data. The proposed method is not perfect as it does not account for a cross-talk between parameters and thus tends to give slightly too conservative numbers. Figure 3 compares the uncertainty ellipse for two global parameters with the computed χ^2 distribution.

5 Application examples

In a recent paper by Ryabchikova et al. (2016) the authors explored the effects of spectral resolution, S/N, selection of spectral features and NLTE on the derivation of the global stellar parameters ($T_{\rm eff}$, $\log g$, metallicity and microturbulence). Perhaps the most important test described in the paper is the comparison of the SME results with surface gravity and effective temperature derived from interferometry, bolometric fluxes and asteroseismology for twelve stars with such measurements. The average discrepancies of 80 K for the temperatures, 0.07 for $\log g$ and 0.06 in metallicity are very close to the new uncertainty estimates provided by SME.

Brewer et al. (2016) performed a separate analysis of components in binary systems to verify the consistency of the results in their dependence on the subset of spectral material used in fitting. The conclusion was similar to the one in the previous paper. Moreover, the authors demonstrated that the accuracy of the derived parameters can be improved further by adjusting the sensitivity of the spectral material to the free parameters of the fit.

6 Conclusions

SME is a mature tool for determination of stellar parameters with spectral synthesis technique. The physics modelled by the package is sufficiently complete to study stars from O to M spectral types, both dwarfs and giants. With good quality data SME can derive accurate stellar parameters and individual abundances and in combination with other techniques (e.g. asteroseismology) finally reach the "magic" 2 % accuracy limit, needed to constrain the evolutionary models, trace correlations with existence of planet systems etc.

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