

Spectral synthesis codes and methods of analysis : what do we have on the market

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Outline of the talk

- The codes for spectral synthesis
- Comparison between the calculations with different codes
- SME – spectral package for automatic determination of model atmosphere parameters

SYNTHE

by Robert Kurucz 1970, 1993 (CDROM 13)

<http://wwwuser.oat.ts.astro.it/castelli/sources/synthe/examples/synthenop.html>

<http://wwwuser.oat.ts.astro.it/castelli/sources/plotsynthe.html>

MOOG

An LTE Stellar Line Analysis Program

by Chris Sneden 1973

<http://www.as.utexas.edu/~chris/moog.html>

MOOG is a Fortran code designed for LTE line analysis (integrated by wavelength line intensity -equivalent width, spectral line profiles) in plane-parallel 1-D stellar atmosphere. It calculates disk-integrated flux or central intensity.

The typical task is determination of the chemical composition of a star. In many ways **MOOG** follows the formalism developed in **WIDTH** and **SYNTH** codes by R. L. Kurucz.

MOOG has 2 main options:

- *abfind* - fits previously measured observed equivalent widths to the calculated ones to derive atmospheric parameters and chemical abundances
- *synth* - computes a set of trial synthetic spectra. The user may plot observed and synthetic spectra and derive abundance either by visual inspection or by minimization of O-C diagram.

For on-line graphics **MOOG** uses SuperMongo plotting package implemented in FORTRAN codes, although it may work without graphical output.

MOOG supports different model atmosphere formats (ATLAS9, MARCS) with 'rhox' and 'tau' depth scales

MOOG uses 3 input files: Parameter file, Model atmosphere file and Line Data file. The data in the last file are entered in formatted or unformatted manner. Line Data file is produced by the user and includes wavelength, element code, line excitation potential (eV), oscillator strength, **gf** or **log(gf)**, van der Waals damping parameter, dissociation energy for a molecular feature.

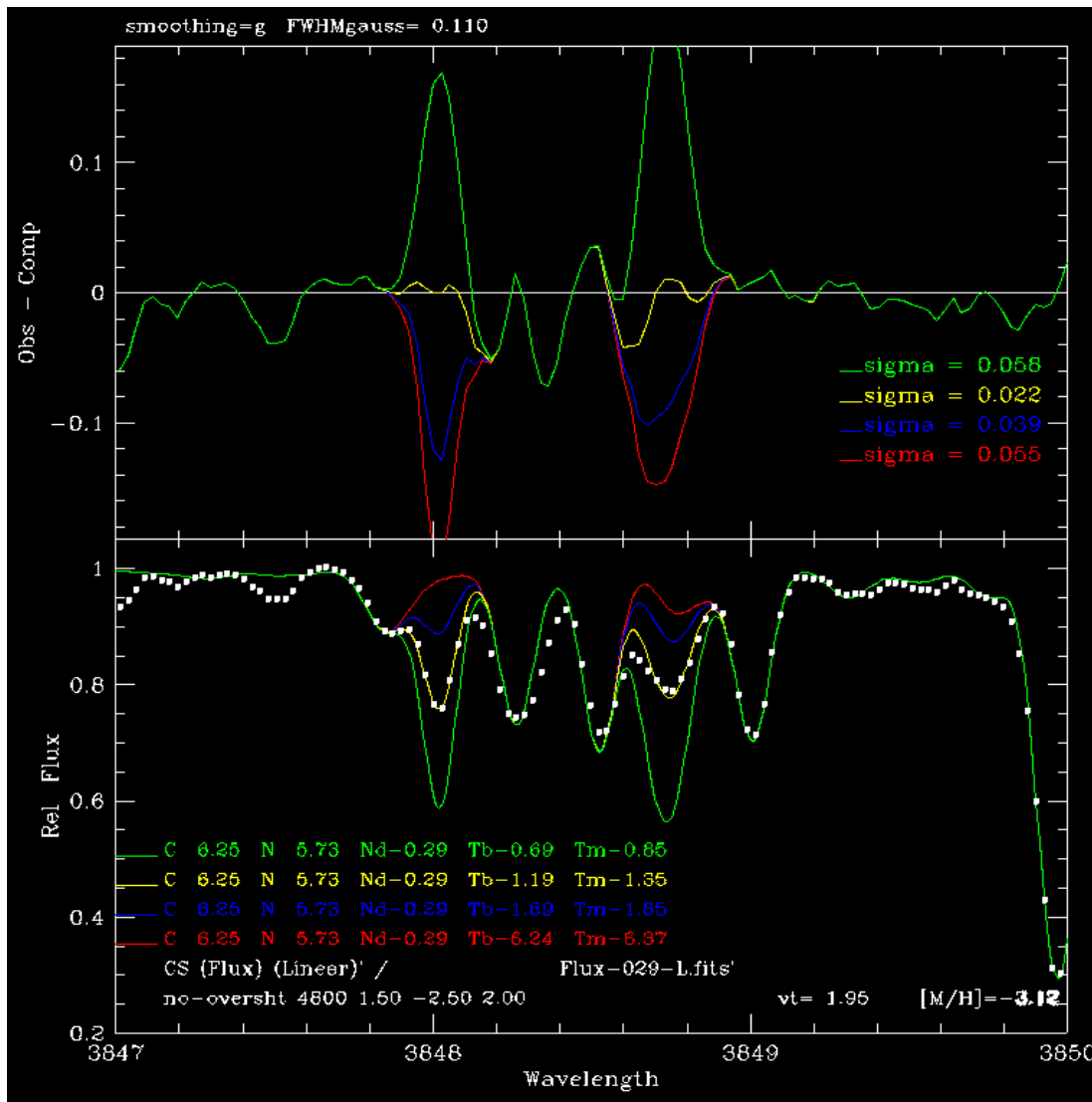
One has to specify which molecules are included in calculations, for what elements abundances are changed relative to the 'standard', etc.

WARNING ! Be careful with the oscillator strengths. Better set them in non-logarithmic form because **MOOG** interprets automatically negative numbers as **log(gf)** and all positive ones as simple **gf**-value.

2 modes of spectrum synthesis are available:

synth - varying atomic abundances

isotop - varying isotopic abundances



The plot is taken from **MOOG** webpage

Spectrum Investigation Utility – SIU

Reetz, J.K. 1991, Diploma Thesis, München University

SIU is a Fortran code built into IDL environment. Unlike **MOOG** and other codes that will be discussed later, it does not work without IDL. **SIU** calculates the emergent specific intensity or disk-integrated flux from plane-parallel 1-D stellar atmosphere both in LTE and NLTE approximations. Include continuous opacities due to bound-free transitions of H I, H₂⁺, H⁻, He I, He II, metals up to Fe, Rayleigh and Thompson scattering.

SIU is working with a grid of MAFAGS atmospheric models built into IDL shell as well as with individual models from other codes converted into special binary format which includes partial pressures for all elements in first 3 ionization stages.

All parameters (wavelength region, atmospheric parameters, spectral resolution, microturbulence, macroturbulence and rotational velocities) are specified inside IDL environment. The total line list consists of 1900 blocks by 200 lines each and is kept separately as external file in binary format. Adaptive wavelength grid is used.

The hydrogen lines calculations are performed with VCS Stark broadening tables (*Vidal et al. 1973*) limited to the temperatures $T \approx 20000$ K and to electron number densities 10^{10} cm^{-3} . Hydrogen Stark profiles are convolved with radiative and Doppler broadening profiles and the resultant profile is further convolved with the resonance broadening profile (H+H interaction). Because of the cutted tables, **SIU** is working successfully for spectrum calculations in the atmospheres of **FGK** stars of **III - V** luminosity classes only.

Abundance determinations in **SIU** are made either by visual estimates of the quality of profiles or by visual estimates of the O-C diagram produced by code on user's request.

More details about **SIU** will be given on Thursday.

Synth3

Oleg Kochukhov, 'Spectrum synthesis for magnetic, chemically stratified stellar atmospheres' 2007, in Physics of magnetic stars, eds. I.I.Romanyuk and D.O.Kudryavtsev, Nizhnij Arkhyz 2007, p.109

SYNTH3 is designed to calculate spectra emerging from the static, 1-D model atmosphere, under the assumption of LTE. These approximations are adequate for a wide range of Main Sequence objects. In practice, the code is successfully used to model stars of spectral classes from early B to late M.

In the standard mode, **SYNTH3** computes intensity by solving numerically the scalar radiative transfer equation for a set of (typically) 7 limb angles.

On the next step, an external routine **s3div** is used to produce disk-integrated flux spectrum from **SYNTH3** intensity spectra for a specified radial-tangential macroturbulent and projected rotational velocities. By default, this procedure assumes spherically symmetric star.

SYNTH3 is independent of the latter assumptions of disk integration and can supply intensity spectra for a more sophisticated disk integration procedure (e.g., modelling of spectroscopic binaries, rotationally distorted stars, stars covered by temperature/abundance spots, etc.)

SYNTH3 is able to compute spectra emergent from stellar atmospheres with a depth-dependent abundances

The format of the input file for **SYNTH3** is that of the output returned by the **VALD 'Extract Stellar'** request. The input file contains the name of the model atmosphere file in special '**krz**' format. This file is obtained by transformation of the **ATLAS9 'mod'** format with a program **KURKOL**

SYNTH3 program is written in Fortran 77, which ensures portability to all major computer platforms and straightforward interfacing with alternative software modules. The code does the following set of operations:

- Reading input model atmosphere (krz format) and atomic/molecular line list (**VALD** format). Depth-independent abundances and microturbulence are read from the line list (default) or from the model atmosphere header. Depth-dependent chemical abundance can be specified in the input model atmosphere file.
- Computation of the concentration of different ions and molecules based on the advanced equation of state solver (*Valenti et al. 1998, ApJ 498, 851*) which includes the treatment of ≈ 200 diatomic and polyatomic molecules. Calculation of continuous opacities (as in **ATLAS9**, *Kurucz 1993, CD-ROM 13*), line center opacities, Voigt function parameters. Refinement of the depth grid (adaptive grid).
- Intensity at several limb angles is computed with the help of the quadratic **DELO** radiative transfer algorithm (*Piskunov & Kochukhov 2002, A&A 381, 736*), using precomputed metallic line opacity and hydrogen line opacity evaluated according to *Barklem et al. (2000, A&A 363, 1091)*. Refinement of the line profiles is carried out by adding frequency points, until description of the spectral line shapes is deemed sufficiently precise (adaptive grid).

The codes (executables for Linux and Intel Mac computers) are available on

<http://www.astro.uu.se/~oleg/download.html>

synthV_NLTE

The author is Vadim Tsymbal.

Source files, executable for Linux, and example files are located in:

<http://vald.inasan.ru/~vadim/downloads/>

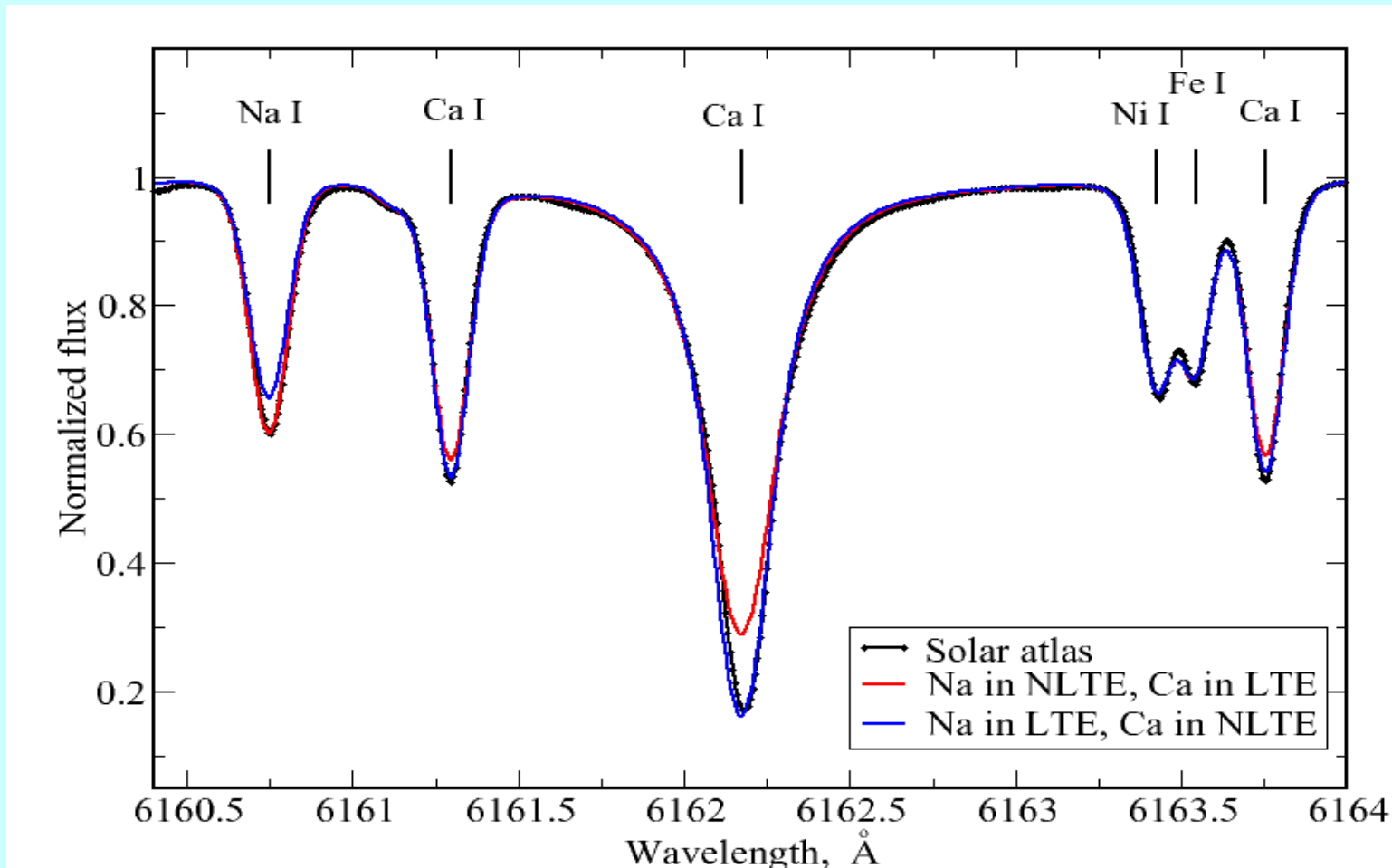
Similar to **SYNTH3 synthV_NLTE** calculates spectra emerging from the static, 1-D model atmosphere under both **LTE** and **NLTE** assumptions, and used to model stars of spectral classes from early B to late M. The format of the input linelist is the same as in **SYNTH3**. **synthV_NLTE** is also able to compute spectra for chemically stratified stellar atmospheres.

Main differences:

- **synthV_NLTE** is running with 'krz', 'mod', and MARCS model atmosphere formats
- Constant wavelength step 0.01 Å is used in spectrum calculations
- Calculation of continuous opacities and radiative transfer algorithm is the same as in Kurucz' codes, (*Kurucz 1993, CD-ROM 13*).
- Hydrogen lines and 20 He I lines are calculated with VCS (*Vidal, Cooper, Smith, 1971, JQSRT 11, 263*) Stark broadening treatment.
- 2 types of output file are possible depending on the filename extension:
 - a. if extension is '**.out**' then the code produce the output file similar to **SYNTH3** (specific intensity for 7 limb angles)
 - b. if extension is '**.prf**' then the code produce normalized disk-integrated flux spectrum

- **synthV_NLTE** requires an external file **SynthV.config**, where you put filenames with the precalculated **b-factors** (a result of **DETAIL** code). **synthV_NLTE** compares species names and wavelengths in the input linelist with the corresponding data in **DETAIL** *.pop file and calculates NLTE synthetic profiles for the lines found in *.pop file. For all other lines LTE calculations are carried out. If *.pop filenames are commented **synthV_NLTE** is working in LTE regime.

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Both **synth3** and **synthV_NLTE** are working in the following sequence:

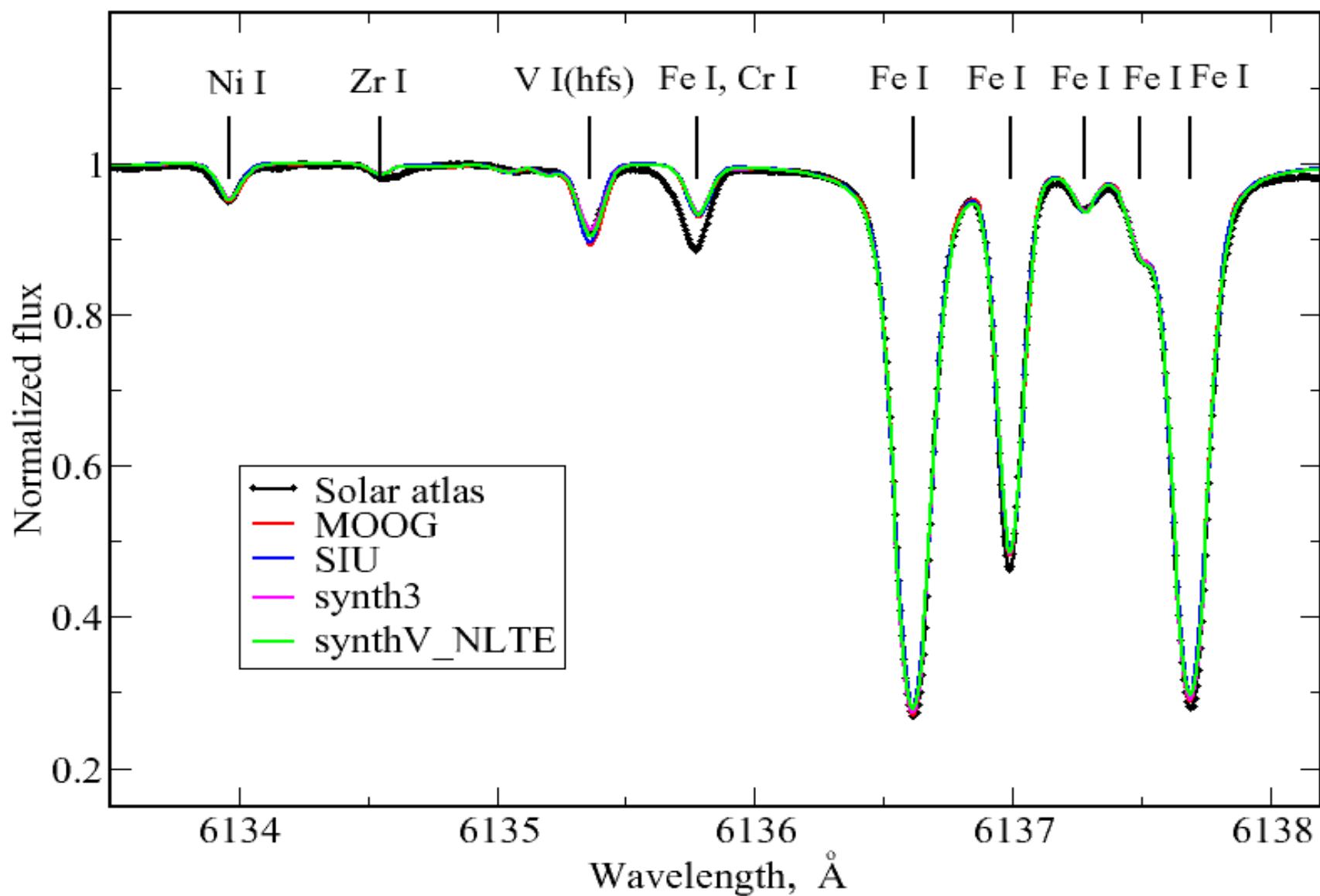
ATLAS9/MARCS(model) → **VALD3**(linelist) → **synth3/synthV_NLTE** → synthetic spectrum

ATLAS9 - model atmosphere calculations (precalculated model - model.mod)

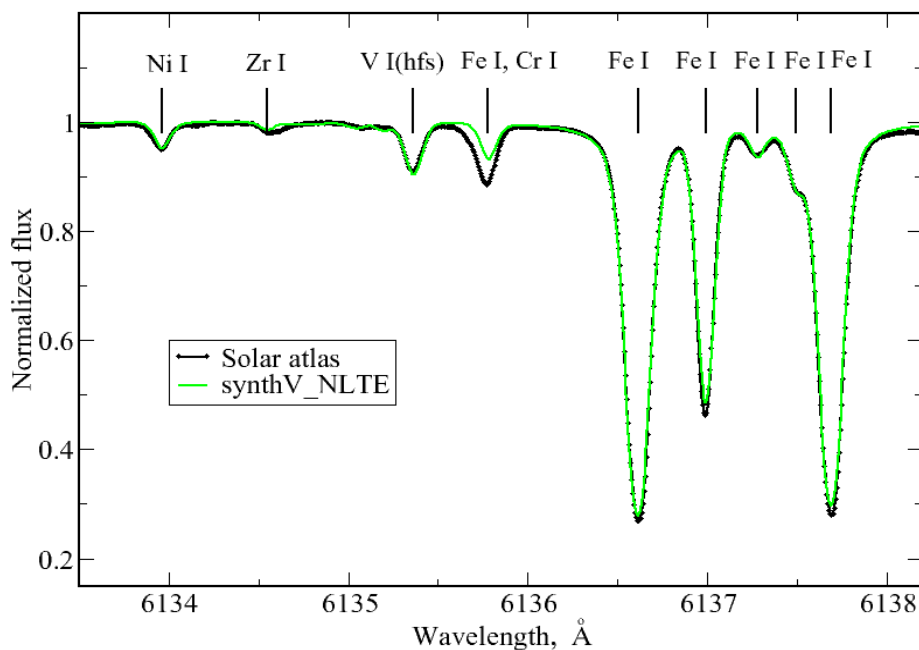
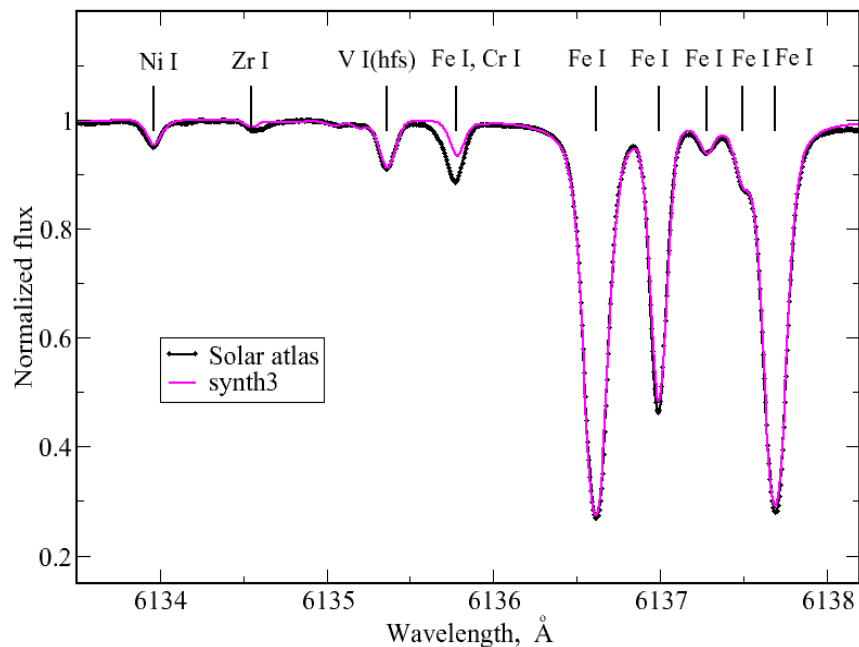
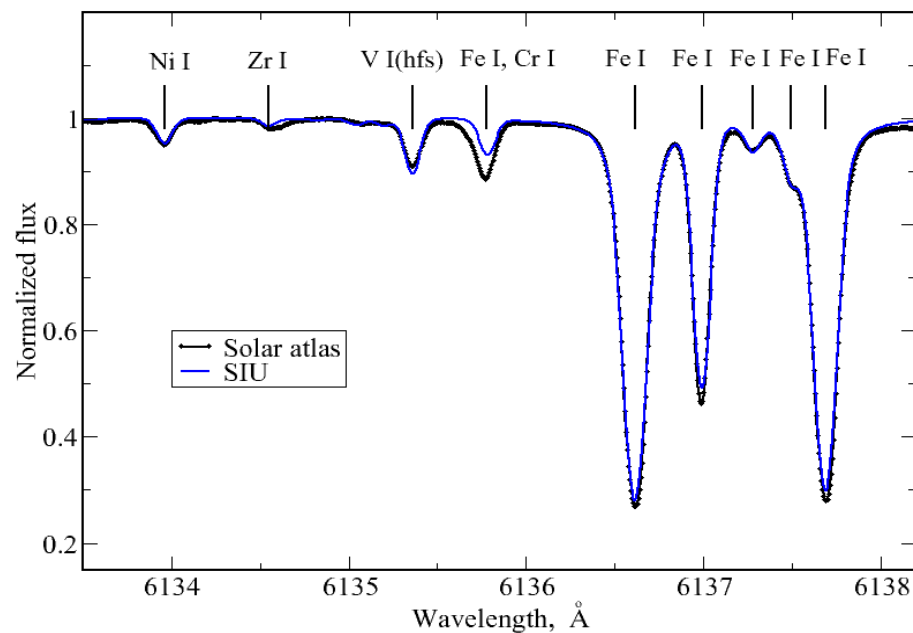
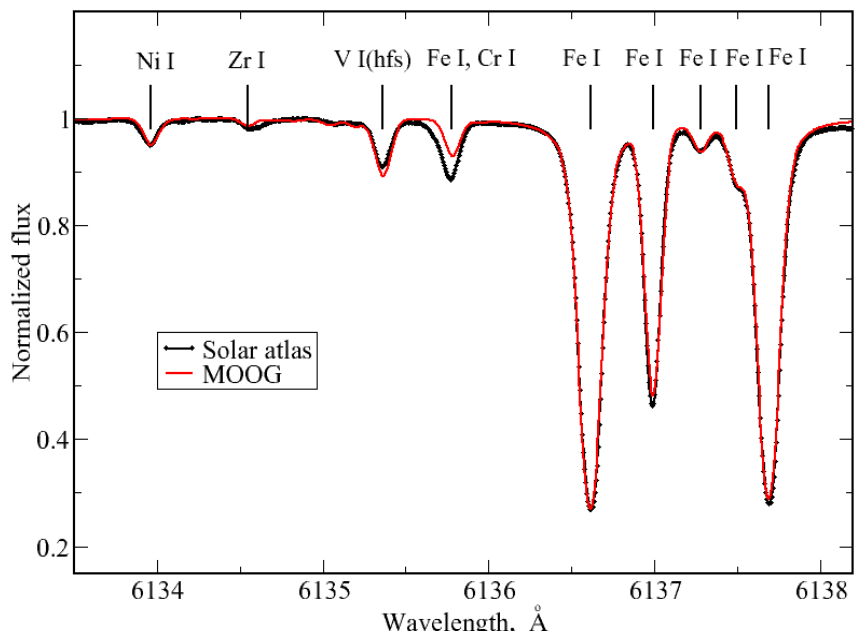
kurkol model.mod model.krz

The user should not prepare the input linelist, it is received by the standard request '**Extract Stellar**' from **VALD** database. The user may adjust this file either manually or automatically.

Comparison between different codes



Comparison between different codes



BinMag3

Oleg Kochukhov, 'Spectrum synthesis for magnetic, chemically stratified stellar atmospheres' 2007, in Physics of magnetic stars, eds. I.I.Romanyuk and D.O.Kudryavtsev, Nizhnij Arkhyz 2007, p.109

binmag3 is an IDL code designed to produce graphical comparison of the observed and computed spectra. It reads observations in *.asc and *.fits formats and synthetic spectra in *.out or *.prf (specific intensity/flux) formats. Besides simple comparison **binmag3** provides the following operations:

Parameter Fit

calculates radial velocity, rotational and macroturbulent velocities

Equivalent Width

calculates equivalent width of the line by direct integration and write in the output linelist for use in subsequent abundance calculations

Profile Fit

approximates the observed line profile by Gaussian or Doppler profiles and write the calculated equivalent width in the output linelist; for blend fits a superposition of synthetic profiles to observed (synthetic) spectrum

Show Line

shows atomic parameters of the chosen spectral line

Abundance Fit

automatically changes element(s) abundance(s) to provide the best fit to the observed line profiles; does the same changing oscillator strength and writing the corrected value to the copy of input linelist

For **Abundance Fit** operation binmag3 requires Unix-like environment and **synth3** or **synthV_NLTE** executables in the default search path. As a result the user automatically gets the abundance from the individual spectral line/blend of lines for precalculated model atmosphere. It is possible to extract an average abundance from several spectral lines. Having precalculated **b-factors** the user automatically receives **NLTE** abundance.

Up to 6 observations and 6 synthetic spectra may be loaded simultaneously.

binmag3 provides graphical (PS) and text (asc) outputs.

SME **(Spectroscopy Made Easy)**

J. Valenti & N. Piskunov. 1996, A&AS 118, 595

SME computes synthetic spectra and adjusts free parameters (T_{eff} , *logg*, *metallicity*, *Vsini*, V_{micro} , V_{macro}) 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 consists of molecular and ionization equilibrium solver **EOS**, continuous opacity package **CONTOP**, line opacity package **LINEOP** and RT solver **RTINT**

Another part of **SME** is Graphical User Interface (**GUI**), written in IDL (sme.pro). The **GUI** is used to read line data and observations, set model parameters, define fitting masks, create **SME** input and output files when the job is done. **SME** output files are standard IDL save files containing an **SME** output structure.

SME output structure is the **SME** input structure, with additional fields containing the results of job execution.

Additional IDL codes (for example, port_mask.pro) allows to copy line mask from one star to another for stars with the similar atmospheric parameters.

SME is working with the observations in (asc) or (fits) formats
The format of input linelist is the output format of VALD 'Extract Stellar' request.

SME has model libraries of Kurucz' (1993) models and latest version of MARCS models.

Ionization equilibrium solver EOS

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 10K to 8000K

Input consists of T, P and abundances. P_e can be also imposed

EOS is using rather unique solving strategy

CONTOP

Continuous opacities are from ATLAS12

Modifications: partial pressures of absorbers and their partition functions are taken from **EOS**

List of absorbers: H, H₂⁺, H⁻, He, He⁺, He⁻, Si, Si⁺, Mg, Mg⁺, Al, C, Fe, Ca⁺, N, O, Ne, S,

List of scatterers: H, H₂, He, e⁻

RTINT

Single pass short-characteristics algorithm developed for 3D radiative transfer code: fast and robust even on a sparse grid.

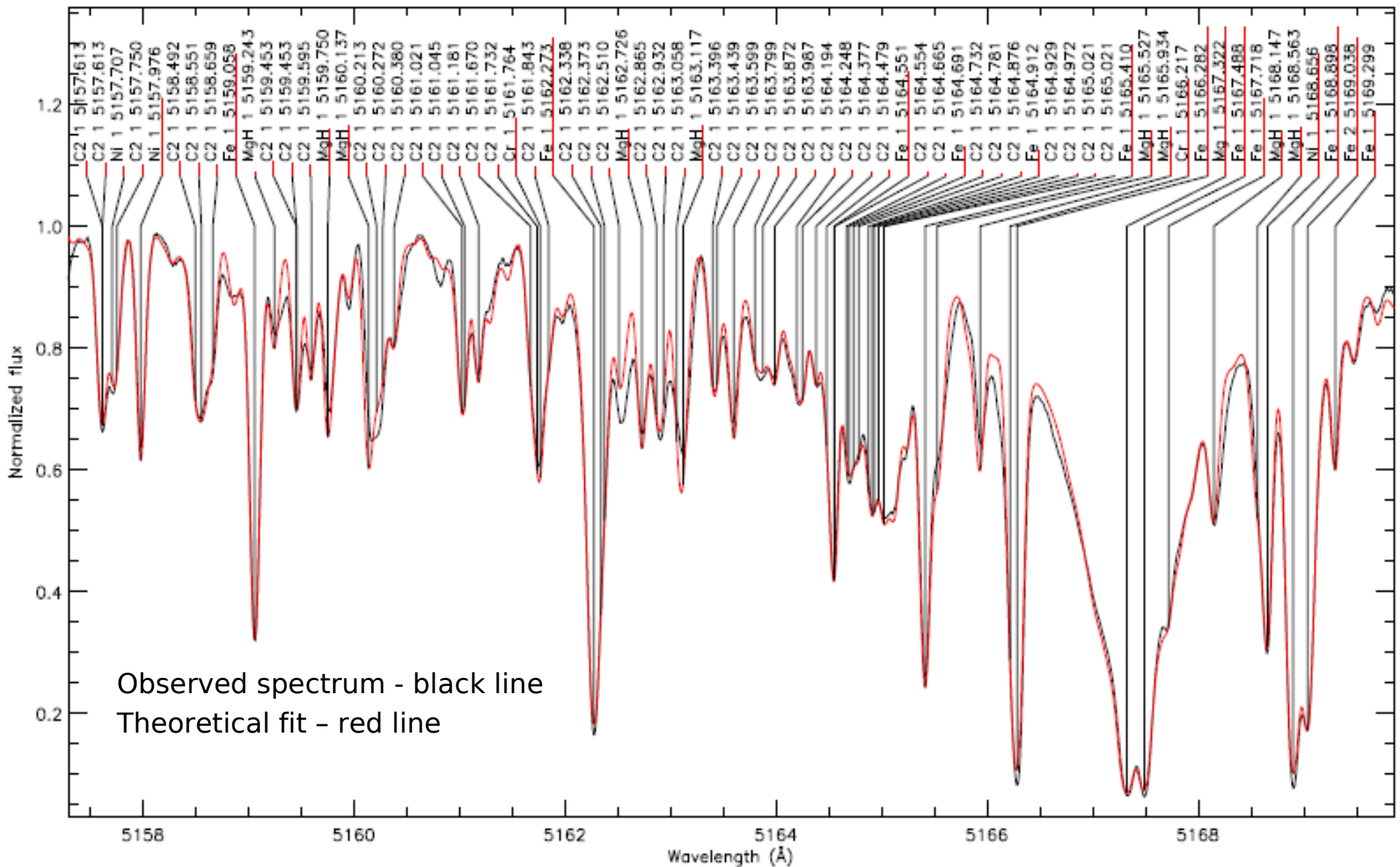
Attenuation operator with quadratic Bezier spline approximation to the source function

Bezier spline prevents overshooting

SME results: δ Eri:

Previous (interf., asteroseism): $T_{\text{eff}}=4986(57)$, $\log g=3.827(018)$, $M=+0.15$

SME: $T_{\text{eff}}=5020$, $\log g=3.79$, $M=+0.08$



SUN

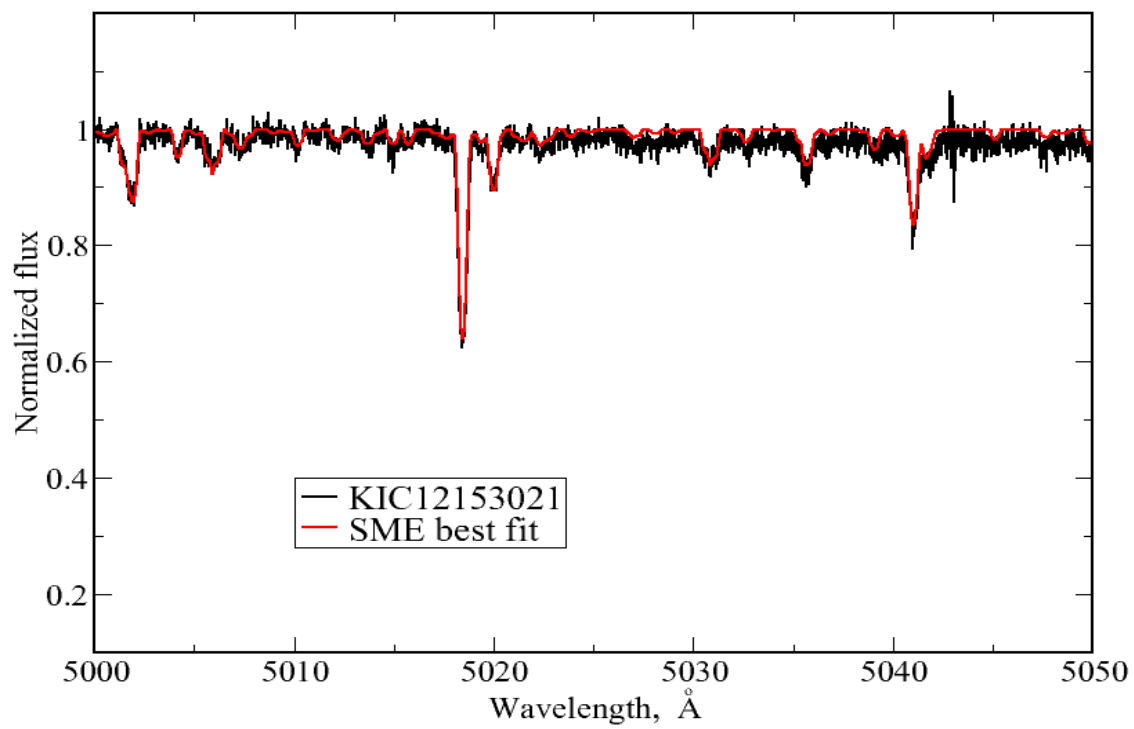
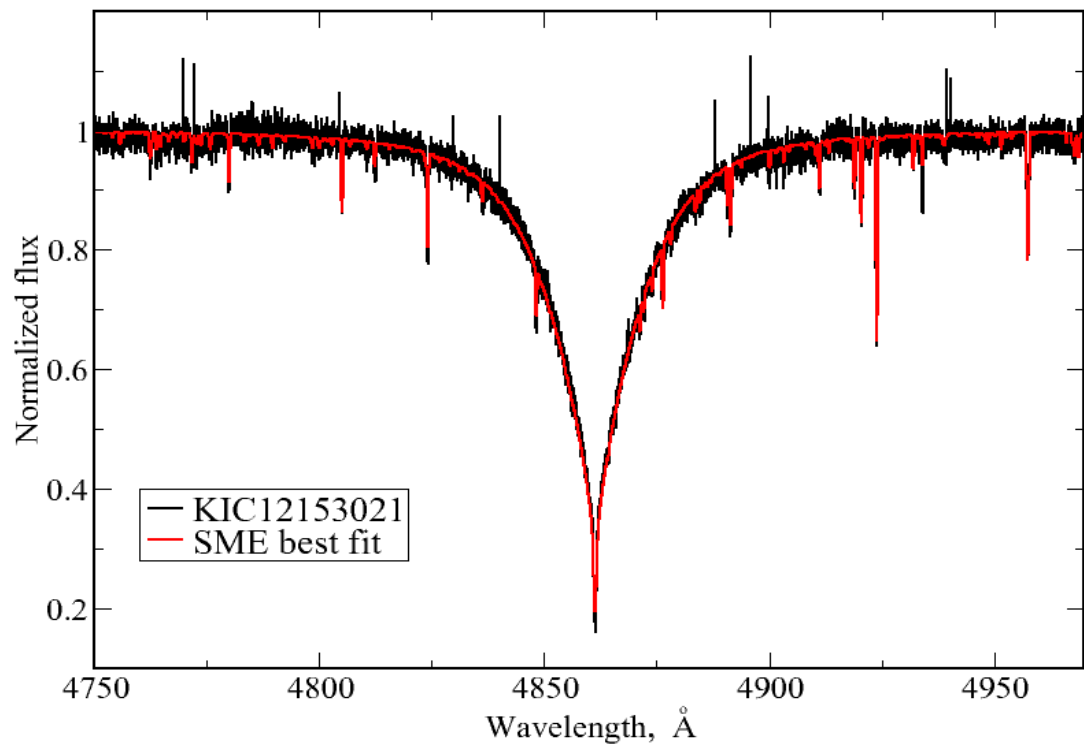
	T_{eff}	$\log g$	$V \sin i$	V_{macro}	[M/H]
Solar parameters:	5777	4.44	1.7	~3.0 -3.5	0.00

SME results

R=550000	5784	4.45		3.12	0.024
R= 69000	5797	4.47			0.000

KIC 12153021

	T_{eff}	logg	Vsini	Vmicro	[M/H]
Initial guess:	9400	3.8	18		
SME solution:	9411	3.86	19.3	2.3	0.08



KIC 04077032

	T_{eff}	logg	Vsini	Vmacro	Vmicro	[M/H]
Initial guess:	7200	4.0	15			
SME solution:	7382	3.77	13	10	3.0	0.11

