

SYNTH - A CODE FOR FAST SPECTRAL SYNTHESIS

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ABSTRACT

We intend to describe here in full details our procedure for calculating the synthetical stellar spectrum. It features high accuracy and high computing speed. In combination with an interactive program for comparing synthetical spectrum with the observations this procedure proved to be a usefull and reliable tool for abundance analysis, spectral lines identification and other practical purposes. The computer implementation of spectral synthesis - program SYNTH - is written in F O R T R A N 77 and can be installed on several types of computers from 386 based PC/AT machine to mainframes. ROTATE -the program for comparison the results of SYNTH with the observations, is made independent from a specific graphics interface which makes it portable to a different graphical environments.

INTRODUCTION

The ultimate goal of every spectral synthesis program is to extract some astrophysical information from comparison of the synthesized spectra to the observation. Therefore the calculations must carefully approximate the process of radiative transfer through the atmosphere of the star and also account for transformation of the spectrum inside the telescope-spectrograph-detector system used in observations. And so we are going to follow the path of the light, propagating from the internals of the star "towards a computer", which produces a plot of residual intensities as a function of wavelength. At this point the comparison of the observed and computed spectra become meaningful and can provide astrophysical information.

In our synthesis procedure we consider only the absorption lines. Furthermore we treat line formation in the local thermodynamical equilibrium (LTE) approximation, which basically means that we assume the temperature of the radiation to be equal to the temperature of stellar matter in every point in the atmosphere. The whole procedure can be extended for the stars where LTE approximation is not valid, but it falls outside of the scope of this paper (for non-LTE treatment see, for example, Auer 1976, and the bibliography therein). We will also restrict ourselves with the case of plane-parallel and static atmosphere. This means that the calculations will be less accurate for giants and super giants and they are probably not applicable to the fast expanding envelopes. Another restriction arised from our disk integration

procedure which assumes no rotational broadening of spectral lines and the spherical shape of the star. The rotational broadening is important though for comparison with observations, so we included it in the code that does the comparison using the approximation, suggested by Gray (1976)

1. RADIATIVE TRANSFER

We are not going to repeat here the textbooks on the radiative transfer (see, for example, Sobolev 1960, Mihalas 1978, and the references therein). Just a few definitions:

- specific intensity I stands for the amount of energy, emmited through a unit area around a given point on the surface of the star at a given wavelength λ in a given direction. Thus I is a function of wavelength λ , and the direction of light propagation. In the case of plane-parallel atmosphere we have a symmetry relative to the radius pointing to the surface element under consideration that is why only one angle is sufficient to describe the direction. We expect the atmosphere of the star to be homogeneous, and the same model atmosphere (see below) and chemical composition are valid for every surface element. So finally we have: $I = I(\lambda, \mu)$, where: λ is the wavelength and μ is a cosine of the angle between the radius to a given point and the direction of propagation of I . As we will see soon, μ is a very convenient parameter for characterizing the direction.
- monochromatic flu F_λ is the total amount of energy radiated by the star towards the observer at a given wavelength. So F_λ can be calculated by integrating specific intensity over the visible hemisphere:

$$F_\lambda = \iint_{\text{Over visible hemisphere}} I(\lambda, \mu) \mu dM. \quad (1)$$

μdM is the projected elementary area on the stellar surface, which is getting smaller close to the limb.

- Continuous opacity coefficient K_λ is a portion of the energy which is absorbed from a beam of radiation with a specific intensity I in the elementary volume at a given wavelength λ in a bound-free and free-free transitions processes. In LTE approximation K_λ is only a function of the physical conditions inside the elementary volume (chemical composition, gas and electron pressures, and temperature) and the wavelength λ . So if the radiation with specific intensity I will cross an elementary volume with opacity K_λ , it will lose $K_\lambda \cdot I$ of its energy.

- Line opacity coefficient A_λ is the same as continuous opacity coefficient except, that the energy is absorbed in a bound-bound transition processes.
- Optical depth τ_λ is a convenient substitute for geometrical distance scale in stellar atmosphere. Optical depth between two points A and B is defined as:

$$\tau_\lambda^{AB} = \int_A^B (K_\lambda + A_\lambda) dx, \quad (2)$$

where dx is an elementary geometrical distance along the straight line between A and B . The sum $(K_\lambda + A_\lambda)$ represents the total absorption coefficient. For further convenience the direction of the positive optical depth is set so, that if we move from the surface towards the center of the star, τ_λ will increase. On the surface of the star $\tau_\lambda = 0$.

- Model atmosphere is a table of basic physical parameters, usually temperature and electron and gas density, computed along some standard depth scale in the stellar atmosphere. Model atmospheres are supposed to give an adequate description of physical conditions in the atmosphere (unfortunately, it is not always true). As a depth scale one usually use a monochromatic optical depth at a fixed wavelength (for example, $\tau_{5000\text{\AA}}$) or a column density (the total mass in a radial column with 1 cm^2 cross-section measured from the surface to a given point in the atmosphere). The state-of-the-art models have been calculated by Kurucz (see Kurucz 1971, Kurucz, Avrett and Peytremann 1974, Kurucz 1991a, Kurucz 1991b).

Now we can write the basic equation of the radiative transfer for specific intensity I :

$$\mu \frac{dI}{d\tau_\lambda} = I - B_\lambda(\tau_\lambda), \quad (3)$$

where $B_\lambda(T)$ - is a source function which in LTE approximation is equal to the Plank function and thus depends only on λ and temperature. The solution of (3) for any point M on the surface of the star ($\tau_\lambda = 0$) can be expressed in the integral form:

$$I = \frac{1}{\mu} \int_0^\infty B_\lambda(t) e^{-t/\mu} dt \quad (4)$$

and substituting (4) to integral (1) we obtain the expression for monochromatic flux radiated from the atmosphere of the star at wavelength λ (for derivation see Mihalas 1978):

$$F_\lambda = 2 \int_0^\infty B_\lambda(t) E_2(t) dt, \quad (5)$$

where $E_2(t) = \int_1^\infty x^{-2} e^{-xt} dx$ - is a second exponential integral.

We solve equation 5 numerically using an 8-th order Gaussian quadrature formula (for description of numerical integration with Gaussian quadrature see for example: Press et al. 1986):

$$F_\lambda \approx \sum_{i=1}^8 \omega_i B_\lambda(x_i), \quad (6)$$

where x_i and ω_i , shown in Table 1, are nodes and weights calculated for corresponding orthogonal polynomials. The only complication here is that x_i are given in the monochromatic optical depth scale τ_λ , but B_λ , as a function of temperature, can be obtained from the model atmosphere only in the depth scale of the model.

Table 1

Nodes	Weights
0.16134	0.27191
0.40000	0.00000
0.70000	0.00000
0.94600	0.18626
2.52410	$0.38898 \cdot 10^{-1}$
5.00660	$0.28674 \cdot 10^{-2}$
8.88090	$0.60078 \cdot 10^{-4}$
14.75900	$0.17675 \cdot 10^{-6}$

We can solve this problem and obtain the values of $B_\lambda(x_i)$ using a differential equation that links the monochromatic optical depth scale τ_λ to the "standard" scale τ_{std}

$$\frac{d\tau_{\text{std}}}{d\tau_\lambda} = \begin{cases} \frac{K_{\lambda_{\text{std}}}(\tau_{\text{std}})}{K_\lambda(\tau_{\text{std}}) + A_\lambda(\tau_{\text{std}})} & \text{if the depth scale of the model atmosphere is the standard optical depth,} \\ \frac{1}{K_\lambda(\tau_{\text{std}}) + A_\lambda(\tau_{\text{std}})} & \text{if the depth scale of the model atmosphere is the column density,} \end{cases}$$

where all the functions in the right part (K_λ , $K_{\lambda_{\text{std}}}$ and A_λ), can be found from model atmosphere and therefore are known as a functions of the model atmosphere depth scale. The initial condition for equation 7 is set on the surface where: $\tau_{\text{std}} = \tau_\lambda = 0$.

Finally we will list the steps of synthetical spectrum calculations for a single wavelength:

- Start from the surface, that is where the monochromatic optical depth $x_i = 0$;
- Integrate equation 7 from current x_i to the next x_{i+1} from Table 1 and obtain a corresponding value of τ_{std} ;
- Find the value of the Plank function $B_\lambda(x_i)$;
- Add $\omega_i \cdot B_\lambda(x_i)$ to the summ 6;
- Increment i and repeat the procedure for the next node until the deepest x_i from Table 1 is reached.

The continuous opacity and the line opacity are not given in the model atmosphere. They should be calculated using those physical parameters which are available from the model. We are going to discuss the opacities calculations in the next section.

2. OPACITIES CALCULATION

Three processes contribute to the continuous opacity: free-free and bound-free atomic transitions and scattering on most abundant particles in the atmosphere. In our calculations we include the following agents of continuous opacity: neutral hydrogen, helium, silicon, aluminium, magnesium, carbon, nitrogen and oxygen; positive ions H⁺, He⁺, Si⁺, Mg⁺, Ca⁺; negative ions H⁻ and He⁻; the scattering on free electrons, neutral hydrogen and helium atoms. We adopted formulas and interpolation tables from Kurucz (1971) with some corrections and extensions.

Line opacity is due to the bound-bound transitions in a particular ion. Several ions of different atoms can contribute to the line opacity at a given wavelength, so the total line opacity is a summ:

$$A_\lambda = \sum_{\text{Lines}} A_{\lambda_0}^l \cdot H(a, v), \quad (8)$$

where $A_{\lambda_0}^l$ is the central opacity of line l and $H(a, v)$ is the Voigt function which describes the wavelength dependence of the bound-bound absorption:

$$H(a, v) = \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{(v - y)^2 + a^2} dy, \quad (9)$$

where the parameters a and v are defined as:

$$\begin{aligned} a &= \frac{\lambda_0^2 \Gamma}{4\pi c \Delta \lambda_D}, \\ v &= \frac{\lambda - \lambda_0}{\Delta \lambda_D}, \end{aligned}$$

where: Γ is the line damping parameter and $\Delta\lambda_D$ is the Doppler width. We use the approximation of Voigt function suggested by Dobrichev (1984), which combines high accuracy and computing speed:

$$H(a, v) = \left(\Delta\lambda_V \sqrt{\log 2} \right)^3 e^{-(v\Delta\lambda_V)^2 \log 2} + \frac{a\Delta\lambda_V^2}{\sqrt{\pi}[1+(v\Delta\lambda_V)^2]} - \frac{2a\Delta\lambda_V^{4.1}}{\sqrt{\pi}} \times \\ \left[0.07e^{-0.4(v\Delta\lambda_V)^2} - \frac{1}{41 - 7(v\Delta\lambda_V)^2 + (v\Delta\lambda_V)^4} \right], \quad (10)$$

where Voigt width $\Delta\lambda_V$ is defined as:

$$\Delta\lambda_V = \frac{2}{a + \sqrt{a^2 + 4\log 2} + a/[10(\sqrt{\pi} + a^2)]}. \quad (11)$$

$\Delta\lambda_D$ includes thermal and microturbulent broadening:

$$\Delta\lambda_D = \frac{\lambda}{c} \sqrt{\frac{2kT}{m_A} + V_{\text{micro}}^2}. \quad (12)$$

The value of the damping parameter Γ in most of the cases is determined by three processes: radiative, quadratic Stark and van der Waals damping:

$$\Gamma = \Gamma_{\text{Rad}} + \Gamma_{\text{Stark}} + \Gamma_{\text{van der Waals}}. \quad (13)$$

The corresponding constants for a number of lines are available from experiments or quantum mechanical calculations. For other lines more simple approximations of the impact theory can be used (see Gray 1976).

The central opacity is proportional to the population of the lower energy level by the atoms, responsible for the line formation, N_{ion}^l , to the oscillator strength f and to the stimulated emission factor:

$$A_{\lambda_0}^l = \frac{\pi e^2}{mc} N_{\text{ion}}^l g f \frac{\lambda_0^2}{\sqrt{\pi c \Delta\lambda_D}} (1 - e^{-hc/\lambda_0 kT}), \quad (14)$$

where m and e are the mass and the charge of electron. The population of the lower energy level is obtained from Saha equation which gives the ratio of the number of atoms in two consecutive ionization stages N_{ion} and $N_{\text{ion+1}}$ as a function of the number density of electrons N_e and the temperature T :

$$\frac{N_{\text{ion+1}}}{N_{\text{ion}}} = \frac{U_{\text{ion+1}}}{U_{\text{ion}}} 2 \frac{(2\pi mkT)^{\frac{3}{2}}}{h^3 N_e} e^{-\chi_{\text{ion}}/kT} \quad (15)$$

where U_{ion} and $U_{\text{ion+1}}$ are the partition functions for two stages of ionization and χ_{ion} is the energy difference between those two stages.

3. NUMERICAL CALCULATION OF THE MONOCHROMATIC FLUX

The equation 7 is solved starting from the surface where boundary condition is set. The integration is carried using a 6-th order Runge - Kutta procedure described, for example, by Press et al. (1986) although we would not recommend to use the code from this book. Much better F O R T R A N implementation can be found in N A G and I M S L scientific software libraries. We are using a slightly modified version of a 6-th order Runge - Kutta routine from I M S L library. By using 6-th order algorithm we achieve two goals: the accuracy can be checked without extra integration with a smaller stepsize, and if the accuracy criterium is not satisfied only three more points should be added to obtain the integral for half stepsize interval.

In each point of the integration we have to compute the right part of the equation 7. The continuous opacity K_λ usually behaves quite smoothly through the atmosphere, so we calculate it in advance for each point of the model and use the parabolic interpolation during the integration of "equation 7. In our code we are using the continuous opacities subroutines from Kurucz's ATLAS-5 program (Kurucz 1971).

Line absorption A_λ may have very steep changes. To save some computing time we tabulate the number density of all neutral atoms and ions, which produce line absorption in a given spectral interval, plus the number density for hydrogen and helium, needed in van der Waals broadening calculations. The stepsize of model atmosphere is usually too big for this sort of tables, so we add extra points (sometimes up to 100 points for one step of the model depth scale) in such a way that linear interpolation provides the requested accuracy. The electron number density and, the temperature are interpolated from the original model. The partition function have been pretabulated by Kurucz and we are just using his subroutine P F S A H A (Kurucz 1971) for solving the Saha equation. The damping constants are calculated using Lindholm approximation of the impact theory (Mihalas 1978) if more accurate values are not supplied with the other line parameters. During the integration of equation 7 we compute the central opacities (equation 14) and the Voigt function (equation 10) values for each line and evaluate the total line absorption coefficient using equation 8.

After the last node in Table 1 has been reached, we can find the value of monochromatic flux using quadrature formula 6.

4. WAVELENGTH GRID SELECTION

The avoid redundancy of the calculations we use a procedure for dynamic construction of the wavelength grid inside the spectral interval. This procedure minimizes the number of mesh points by choosing the variable stepsize which provides] a fixed accuracy of linear interpolation of the synthetical spectrum for any λ inside

our interval. The procedure starts with computing monochromatic fluxes in both ends of spectral interval. Next it adds a point in the center of every spectral line. If two lines are closer than certain limit, only one central wavelength (the shorter one) is added. Then extra points are inserted in the middle of each pair of neighbouring lines. At the last stage the procedure checks every point for the accuracy of linear interpolation and adjusts stepsize, if needed, to keep the interpolation error under a requested limit. Let's see how to estimate the stepsize which provides a certain accuracy of linear interpolation. In a given wavelength λ , which falls between λ_i and λ_{i+1} , the monochromatic flux is approximated as:

$$F_\lambda = F_i + \frac{F_{i+1} - F_i}{\lambda_{i+1} - \lambda_i}(\lambda - \lambda_i) + \text{Error.} \quad (16)$$

Two errors contribute to the value of Error: the error of linear interpolation itself and the error of approximation of the first derivative of F_λ with a finite differences formula. Both of them are proportional to $\frac{\partial^2 F_\lambda}{\partial \lambda^2}(\lambda_{i+1} - \lambda_i)^2$. Now if we add a third point in the middle of $[\lambda_i, \lambda_{i+1}]$ and let h be the stepsize between λ_i and λ_{i+1} , the total error can be estimated as:

$$\text{Error} < 2 \frac{F_{i+1} + F_i - 2F_{i+\frac{1}{2}}}{h^2} \quad (17)$$

and for a given value of Error the stepsize can be found from (17).

Note that the procedure basically adds more points in places with higher curvature (for example, line cores).

5. CONTINUUM CALCULATION

In order to be able to compare the synthetical spectrum to the observations we need to normalize it to the continuum level. The integration of the continuous flux is not very different from the monochromatic flux integration. We take advantage of a small and smooth variation of the continuum level inside the synthesized interval (typically less than 100 Å) and calculate continuous flux only in the ends of our spectral interval. For all other points continuum level is obtained by linear interpolation. Another difference from monochromatic flux calculation is the equation 7 which is transformed to:

$$\frac{d\tau_{\text{std}}}{d\tau_\lambda} = \begin{cases} \frac{K_{\lambda_{\text{std}}}(\tau_{\text{std}})}{K_\lambda(\tau_{\text{std}})} & \text{if the depth scale of the model atmosphere is the standard optical depth,} \\ \frac{1}{K_\lambda(\tau_{\text{std}})} & \text{if the depth scale of the model atmosphere is the column density,} \end{cases} \quad (18)$$

because no line opacity should be included.

The procedure of wavelength grid construction, described in the previous section is applied after the normalization to the continuum level is done.

6. ACCURACY

Three parts of the synthetical spectrum calculations are crucial for the accuracy: construction of the line optical depth scale (the integration of equations 7 and 18), calculation of the monochromatic flux (equation 6) and selection of the wavelength grid, described in section 4.

Runge - Kutta algorithm, used for integration of equations 7 and 18, can be tuned to any required accuracy. We usually select $3 \cdot 10^{-5}$, which is consistent with the accuracies achieved in the other parts.

Flux integration accuracy is more difficult to check. To do it we compared our results with a direct disk integration of equation 1 and we found that the 8-th order Gauss quadrature formula provides the accuracy better than 10^{-4} for a wide range of model atmospheres with effective temperatures from 3500 K up to 20000 K.

For the wavelength selection procedure we usually put the accuracy criterium to 10^{-4} . The resulting synthetical spectrum can be interpolated to any wavelength within a given spectral interval with the accuracy better than $5 \cdot 10^{-4}$ which corresponds to signal-to-noise ratio of 2 000.

7. LIMB DARKENING CALCULATION

We also compute a continuum limb darkening coefficient, which can be used later for convolution of the synthetical spectrum with the rotational profile. To do this we integrate equation 4 the same way as we did with equation 6 and find the values of specific intensity for continuum at 3 points on the disk at 0, 0.6 and 0.95 stellar radius from the center. The limb darkening coefficient u is then found from least square approximation of the conventional formula: $I = I_0(1 - u + u\mu)$.

8. COMPARISON WITH THE OBSERVATIONS

The comparison with the observations is done with a separate program which includes an interactive graphics interface. It shows the observed and the calculated spectra on the screen and with the help of menu one can convolute the synthetical spectrum with the rotational profile, the macroturbulence profile (using the approximation formula from Gray 1976) and the instrumental profile (Gaussian). For the rotational profile we followed the approximation suggested by Gray (1976):

$$F_\lambda^{\text{rot}} = \int_{-\infty}^{\infty} G(\Delta\lambda) F_{\lambda+\Delta\lambda} d(\Delta\lambda) \quad (19)$$

where the kernel of the convolution is a function of limb darkening:

$$G(\Delta\lambda) = \frac{2(1-u) \left[1 - \left(\frac{\Delta\lambda}{\lambda} \frac{c}{V \sin i}\right)^2\right]^{\frac{1}{2}} + \frac{1}{2}\pi u \left[1 - \left(\frac{\Delta\lambda}{\lambda} \frac{c}{V \sin i}\right)^2\right]}{\pi \lambda \frac{V \sin i}{c} (1 - u/3)} \quad (20)$$

The synthetical spectrum can also be shifted in wavelength and zoomed for fine tuning of the shifts and broadenings. The equivalent width calculation simplifies the estimate of chemical abundances.

9. COMPUTER IMPLEMENTATION

Both synthetical spectrum calculation code (`SYNT`) and the program for comparing the synthetical spectrum to the observations (`ROTATE`) are written in conventional `FORTRAN 77` and we have been using them on `AT/386` type personal computer. Compiled with `NDP FORTRAN` compiler, `SYNT` takes approximately 2 seconds per one wavelength point, while computing 25 spectral lines on a 20 MHz machine. The only critical requirement was the presence of expended memory, but with 4 Mbytes of total memory size we were able to calculate 30 Å interval with 80 spectral lines. Both programs can produce colour graphics using `NDPL`OT library. To make the code less dependent on graphics package we made a simple intermediate set of interface subroutines, which include all scalings and calls to graphics library functions. So with simple substituting of these calls we had no problems running `SYNT` as batch job on the `VAX` (with no graphics) and `ROTATE` as an `XWindows` client on `Sun` workstation with all bells and whistles available there.

`SYNT` requires two sorts of input data: lines list and model atmosphere. Lines list includes the spectral interval to be synthesized and the number of lines followed by the parameters for each line. Line's parameters include the name and ionization stage of chemical element, central wavelength, excitation energy (eV or cm⁻¹), microturbulent velocity (km/s), log gf and three damping constants (radiative, Stark and van der Waals) in exponential or logarithmic form (see example below). If some of the damping constants are not known, they should be set to 0 and `SYNT` will use the approximation formula for them. Here is an example of one spectral line description:

```
'FE1', 6165.36, 33412.71, 0.5, -1.670, 7.943, -6.156, -7.833
```

The filename of the model atmosphere data is included with the lines list. Usually model atmosphere includes the chemical composition data, used during the model calculation. We rely on this abundances values as a default for spectral synthesis, but they can be changed from the lines list. For example, to change the default abundance of iron and nikel one should add the following line to the lines list:

```
'FE:-4.4','NI:-5.8','END'
```

Model atmosphere data besides the default abundances should include the optical

depth scale, temperature, gas and electron number densities and the density of stellar matter.

As the result S Y N T H produces a file, which contains the wavelength grid, the corresponding residual intensities and the limb darkening coefficient in a format suitable for R O T A T E .

R O T A T E accepts the data produced by S Y N T H and the file with observations (if any) in the same format as the synthetical spectrum.

The results of interactive fitting (rotational, instrumental and macroturbulent broadening and wavelength shift) with R O T A T E are stored in the output file, which can be used for plotting or further processing.

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