

A brief introductory guide to TLUSTY and SYNSPEC

I. Hubeny* and T. Lanz†

June 6, 2017

Abstract

This is the first of three papers that present a detailed guide for working with the codes TLUSTY and SYNSPEC to generate model stellar atmospheres or accretion disks, and to produce detailed synthetic spectra. In this paper, we present a very brief manual intended for casual users who intend to use these codes for simple, well defined tasks. This paper does not present any background theory, or a description of the adopted numerical approaches, but instead uses simple examples to explain how to employ these codes. In particular, it shows how to produce a simple model atmosphere from the scratch, or how to improve an existing model by considering more extended model atoms. This paper also presents a brief guide to the spectrum synthesis program SYNSPEC.

Contents

1	Introduction	3
2	Basic characteristics	3
2.1	TLUSTY	4
2.2	SYNSPEC	5
2.3	Associated programs	5
2.4	Why use TLUSTY?	5
2.5	Word of caution	6
3	Installing the package	6
3.1	Main file	7
3.2	Opacity table	8
3.3	Iron data	9
3.4	Line lists	9

*University of Arizona, Tucson; USA; hubeny@as.arizona.edu

†Observatoire de Côte d’Azur, France; lanz@oca.eu

4	Running TLUSTY	10
4.1	Source code files and compilation	10
4.2	Input files	10
4.3	Output files	11
4.4	Producing a model atmosphere with TLUSTY	12
4.5	Test-case model atmosphere	13
4.6	How can I tell that the model is well converged?	14
5	Running SYNSPEC	16
5.1	Source code files and compilation	16
5.2	Input files	16
5.3	Description of SYNSPEC-specific input files	19
5.3.1	File <code>fort.55</code>	19
5.3.2	File <code>fort.56</code>	21
5.3.3	Line list	21
5.4	Output files	22
5.5	Producing a synthetic spectrum for a Kurucz model	23
5.6	What chemical species and what lines are being considered? . . .	23
5.7	Test cases	24
6	Working with OSTAR2002 and BSTAR2006 grids	27
6.1	Do we need to compute a model atmosphere from scratch? . . .	28
6.2	Producing detailed spectra for grid models	28
6.3	Using SYNPRO	30
6.4	Running a B-star model	30
6.5	Interpolating model structures or predicted spectra?	33
6.6	Adding new NLTE species to existing models	34
6.7	Adding atomic energy levels to existing models	36
7	What is next?	38
	Appendix A: Treatment of line profiles in SYNSPEC	39
	Appendix B: Treatment of NLTE level populations in SYNSPEC	41
	Appendix C: Fine points of running SYNSPEC	44
	Appendix D: Auxiliary SYNSPEC output files	45
	Appendix E: Program ROTIN	48
	References	50

1 Introduction

Unlike previous manuals, this one is much more comprehensive and is consequently divided into three parts. This paper, the first part, presents a very brief manual for busy or impatient users. It shows how to work with TLUSTY and SYNSPEC on simple practical examples. In particular, it shows how to use TLUSTY to produce simple model atmospheres from the scratch, as well as to modify existing models from available grids to change basic parameters, or to extend model atoms to more complex ones. It also presents a brief guide to the spectrum synthesis program SYNSPEC and associated programs to obtain detailed predicted spectra to be compared to observations.

The second part (Hubeny & Lanz 2017b; hereafter called Paper II), presents a detailed reference manual for TLUSTY, which contains a description of basic physical assumptions and equations used to model an atmosphere, together with an overview of the numerical methods to solve these equations.

The third part (Hubeny & Lanz 2017c; hereafter called Paper III) represents a basic operational manual for TLUSTY. It provides a guide for understanding the essential features and the basic modes of operation of the program. Since TLUSTY offers great many numerical options, as well as various approximations of the basic physical description, there are also many options the code can consider, and consequently many switches and parameters which they control, Paper III is divided into two parts. The first part describes the most important input parameters and available numerical options. The second part covers additional details and a comprehensive description of all physical and numerical options, and a description of all input parameters, many of which needed only in special cases.

The user who intends to construct simple models, or perhaps more sophisticated models using samples of input data provided in the TLUSTY website by just modifying them, will obtain enough information and guidance from this Paper I. However, in case of problems, for instance a slow convergence of the iteration process, or the lack thereof, the user should consult appropriate sections of other parts. Dedicated users are encouraged to consult the full content of all three papers.

Both programs, TLUSTY and SYNSPEC, together with the utility programs PRETLUS and ROTIN, and with all the input files needed to run the test case models, are available either on the main TLUSTY website¹, or as a gzipped tar file that contains the whole distribution².

2 Basic characteristics

The present set of computer programs is a package designed to accomplish a wide range of stellar spectroscopic diagnostics studies. It can construct a

¹<http://tlusty.oca.eu/>

²<http://aegis.as.arizona.edu/~hubeny/pub/tlusty205.tar.gz>

model atmosphere either from scratch or from another model, compute a detailed spectrum on a selected wavelength range, and, if desired, convolve the synthetic spectrum with an arbitrary rotational velocity and instrumental profile of the spectrograph to obtain a predicted spectrum directly comparable to observations.

2.1 TLUSTY

The basic component of the package is TLUSTY, a program for calculating plane-parallel, horizontally homogeneous model stellar atmospheres in hydrostatic and radiative (or radiative + convective) equilibrium. Departures from local thermodynamic equilibrium (LTE) are allowed for a set of occupation numbers (populations) of selected atomic and ionic energy levels. Thanks to the flexibility and efficiency of the adopted numerical procedures, described in detail in Paper II, the number of such levels, referred to as *NLTE levels* can be essentially as large as the amount of available atomic data allows.

The code offers several global numerical schemes to solve the set of structural equations; most importantly the hybrid complete-linearization/ accelerated Lambda-iteration (CL/ALI) method, or the Rybicki reorganization scheme, both augmented by applying various mathematical acceleration procedures. The program employs the concept of superlevels and superlines, thus allowing for computing fully consistent, non-LTE metal line-blanketed model atmospheres. For cool objects for which LTE models are satisfactory, the code can use pre-calculated opacity tables that include all important atomic and molecular opacity sources.

The program is fully data oriented as far as the choice of atomic species, ions, energy levels, transitions, and opacity sources is concerned. In several cases, there are various default formulas and internal tables provided for selected cross sections and opacity sources, but in most cases the user is able to choose between several options. On top of that, there is a collection of input atomic data for a number of atoms and ions accessible from the TLUSTY website,, so users are not obliged to collect the necessary atomic data themselves.

In the past, there was a separate variant called TLUSDISK, designed to calculate vertical structure of accretion disks. Starting at version 200, both programs are contained within a single, universal code TLUSTY. The user is able to make a choice between computing a model of a stellar atmosphere or a vertical structure of an accretion disk, based on input data. In the following text, we will usually refer to a “stellar atmosphere”, but everything applies, unless specifically noted, for an accretion disk as well.

The code is written in standard FORTRAN77, making it highly portable. The current version removed outdated features of FORTRAN, and adheres to modern standards, so the program compiles on all platforms, most importantly using compilers available within the LINUX and Mac OSX operation systems.

2.2 SYNSPEC

The second basic program is SYNSPEC, current version 51, which is a program for calculating the spectrum emergent from a given model atmosphere. It was originally described in Hubeny, Lanz, & Jeffery (1994), also see Hubeny & Lanz (2011), and a detailed description and the user’s manual is available on the TLUSTY website. It has been originally designed to synthesize emergent spectra from model atmospheres calculated using TLUSTY, but may also be used with other model atmospheres as input, for instance Kurucz’s ATLAS models. The program is complemented by the program ROTIN which calculates the rotational and instrumental convolutions for the net spectrum produced by SYNSPEC.

2.3 Associated programs

Finally, there is a number of interface and utility programs. They provide a graphical interface for plotting output models, the convergence log etc. (written in IDL). Similarly, there is graphical interface SYNLOT (written again in IDL), which enables the user to perform an interactive work with SYNSPEC and its utility programs (computing the spectrum, plotting it, performing various convolutions, and identifying and annotating predicted lines). It is available online³, together with a detailed user’s manual.

There is also a program PRETLUS, distributed along the main TLUSTY code, which can be run before running TLUSTY, and which prints dimensions of the most important arrays. Its results can be used to set up the array dimensions in TLUSTY, and thus to control the overall memory consumption of TLUSTY. Its operation and function is described in detail in Paper III, §2.3.

2.4 Why use TLUSTY?

We believe that the code is useful because it was designed to be very flexible, versatile, but also easy to use. Such a goal presents a non-trivial task, because with increasing flexibility and versatility of a program, the complexity of operation and the difficulty of its usage usually increases as well.

TLUSTY can construct models ranging from the simplest ones, being computed just in seconds, and thus having a potential to be used as an interactive pedagogical tool, to the most complex NLTE metal line-blanketed models whose construction may easily take hours to tens of hours on modern computers.

TLUSTY is also extremely versatile. It can construct models for stellar atmospheres, or a vertical structure of accretion disks. As far as the range of physical conditions is concerned, TLUSTY can compute model atmospheres from extremely cool brown dwarfs or giant planets, to very hot accretion disks around solar-mass black holes. In other words, one can model structures with temperatures from a few times of 10^1 K to a few times of 10^8 K. The limit on the low-temperature side is not imposed by algorithmic or physical shortcomings, but rather by the availability of the corresponding available molecular opacity

³<http://aegis.as.arizona.edu/~hubeny/pub/synplot2.1.tar.gz>

data. On the high-temperature side, the limiting factor is the current lack of fully relativistic treatment of the Compton scattering, and a more accurate description of inner-shell transitions, pair production, and other high-energy phenomena. For densities, there is no strict limit on a low-density side; the limit on the high-density side is the total particle number density of about 10^{20} cm^{-3} , above which the multi-particle effects in the equation of state, atomic transition rates, and description of line broadening, became important.

What are the basic limitations of TLUSTY? Besides the limitations of temperature and density, which usually are not very serious for most applications, the most stringent limitations follow from the basic assumptions and approximations. It is a 1-D code that assumes a plane-parallel, horizontally-homogeneous atmosphere. It is therefore inapplicable for highly inhomogeneous media, although it can still be used to describe atmospheres with large patches with different physical conditions, provided that those patches have large enough horizontal optical depths that they are independent of the ambient atmosphere. TLUSTY is not applicable for spherical atmospheres, although its adaptation to spherical 1-D geometry would be relatively straightforward. (Actually, spherical version existed in the past, but did not propagate to later versions).

The second basic limitation is the assumption of hydrostatic equilibrium (or vertical hydrostatic equilibrium in the case of disks). TLUSTY is therefore inapplicable for instance for stellar winds, although it can still model deeper layers of a star that exhibits a wind in its outer layers. The hydrostatic models produced by TLUSTY would still be useful for the atmospheric layers where the outflow velocity does not significantly exceed the thermal velocity.

The third basic limitation is the assumption that the only external force acting on the material is gravity. Therefore, TLUSTY is inapplicable, or its results should be viewed with caution, for instance for atmospheres with strong magnetic fields, or for atmospheres of rapidly rotating stars where the centrifugal force plays an important role.

2.5 Word of caution

Although considerable effort has been devoted to eliminate errors in the code, there is by no means a guarantee that it is error free. In fact, the same warning as Bob Kurucz usually puts into his codes applies here as well: “This code is guaranteed to contain errors.” The user is thus warned against using the program as a “black box”. It would be highly appreciated if any errors detected by the user, and any comments or suggestions for improvements, are communicated to I. Hubeny (hubeny@as.arizona.edu) or T. Lanz (lanz@oca.eu).

3 Installing the package

As mentioned above, the program together with the necessary data files and the input files for several examples and test cases can be obtained either from

- the main TLUSTY site in Observatoire de Cote d’Azur in Nice,

`http://tlusty.oca.eu`,

which is a website previously located at `http://nova.astro.umd.edu`, or

- the tarball of the whole package obtained from

`http://aegis.as.arizona.edu/~hubeny/pub/tlusty205.tar.gz`.

In the following text, this site will be referred to as the *Arizona site*. When using the Nice site, one can download the programs, data, and examples individually, while by downloading and extracting the tarball obtained from the Arizona site one obtains all the files, together with a specific directory tree where the files are located.

The main website at Nice is, at the time of submitting this manuscript (June 2017), not yet fully operational. When it is, the website will contain detailed instruction for downloading. In the meantime, or as an alternative means, the potential user is encouraged to download the package from the Arizona site. One can either download the file(s) interactively, or using the LINUX command `wget`, if available. In the subsequent text, we will use the `wget` command as an example, keeping in mind that the files can also be downloaded interactively using any web browser.

Complete download proceeds in one or more steps, depending on the user's needs. The first file is the main one, required to be downloaded in any case. In addition, there are several auxiliary files which are optional. The reasons for having several files to download are several: (i) The auxiliary files are big, which may cause problems in downloading all the files together; (ii) long-time users may already have some or all of the auxiliary files; and (iii) many applications do not require these files, so for some users they would represent an unnecessary waste of memory and time for downloading. We summarize the files to download below.

3.1 Main file

The main file, which is sufficient for most purposes, is downloaded as follows (we stress again that it can be downloaded interactively using any web browser):

```
wget http://aegis.as.arizona.edu/~hubeny/pub/tlusty205.tar.gz
gunzip tlusty205.tar.gz
tar -xvf tlusty205.tar
```

That action creates directory `./tlusty205`, with several subdirectories, which we will call here the “standard TLUSTY directory”. Although the user can obviously use any location of the files, we will use in the following examples the directory tree that originates from the `tlusty205.tar` file. This directory also contains several shell scripts that work with the directory tree thus generated. In the following text, we will call this directory tree as the *standard directory tree*. If the user prefers, or has already created a different directory system, the provided script files have to be modified accordingly. In any case, the test cases can be run either individually, or all of them in one run.

The standard directory tree has the following structure: The main directory `./tlusty205` contains the shell scripts `RTlusty` and `RSynspec` for running TLUSTY, and SYNSPEC, respectively, and five subdirectories:

- **tlusty** - which contains the source file for the current version of TLUSTY, called `tlusty205.f`, together with auxiliary files `*.FOR` - see below;
- **synspec** - an analogous directory for SYNPEC. It contains the source files, plus the utility program `ROTIN`;
- **pretlus** - source files for the utility program `PRETLUS` - see Paper III, § 2.3;
- **data** - a collection of needed atomic data.
- **examples** - it contains the shell script `Runtest` that runs all the test cases, and five subdirectories for the test cases, described in detail in Paper III, Chap. 6.
 - **hhe** – a simple H-He LTE and NLTE model atmosphere - see § 4.5 here and Paper III, § 6.2.
 - **bstar** – a NLTE metal line-blanketed model of a B stars, analogous to models from the `BSTAR2006` grid (Lanz & Hubeny 2007) – see Paper III, § 6.3.
 - **optab** – an LTE line-blanketed model of a K stars, using an opacity table - see Paper III, § 6.4.
 - **cwd** – an LTE and NLTE model of a moderately cool DA (pure-hydrogen) white dwarf - see Paper III, § 6.5.
 - **disk** - a simple H-He LTE and NLTE model of a vertical structure if an accretion disk - see Paper III, § 6.6.

All subdirectories contain (i) input data for a run, and (ii) some output files obtained by running the test cases on a MacBook Pro done by the author (I.H.), which are included for comparisons with user's runs to the purposes of checking an implementation of the codes on the user's platform.

3.2 Opacity table

The users who intend to compute LTE metal line blanketed model atmospheres, using a pre-calculated opacity table whose application is shown in Paper III, § 6.4, need to download the file `absopac.dat` into directory `data`. One proceeds as follows:

```
cd ./tlusty205/data
wget http://aegis.as.arizona.edu/~hubeny/pub/absopac.dat.gz
gunzip absopac.dat.gz
```


3.3 Iron data

If the user intends to calculate NLTE metal line blanketed models for early type stars, as shown on the test case presented in Paper III, § 6.3, and using the input data stored in \$TLUSTY/examples/bstar, one needs to download detailed data for iron. One proceeds as follows:

```
cd ./tlusty205/data
wget http://aegis.as.arizona.edu/~hubeny/pub/gf26.tar.gz .
gunzip gf26.tar.gz
tar -xvf gf26.tar
```

As a results, the files gf2601.gam to gf2605.gam, and analogously for and gf26*.lin are created that represent Kurucz data files for iron levels and transitions, and from which TLUSTY generates necessary parameters for iron superlevels and superlines - see Paper II, § 3.6.

3.4 Line lists

Finally, for computing detailed synthetic spectra with SYNSPEC, one needs full line list(s). We stress that the standard "data" directory contains a sample line list for tests, with line data for wavelengths between 1390 and 1500 Å. When computing synthetic spectra for different spectral regions, one needs to obtain one of more of the following files. They should also be placed in the "data" directory, namely The user can choose from several possibilities:

- full line list between 1 Å and about 15 microns. The list contains about 5.5×10^6 lines (download is about 121 MB).

```
cd ./tlusty205/data
wget http://aegis.as.arizona.edu/~hubeny/pub/gfTOT.dat.gz .
```

- lines in the FUV region, between 880 and 2,000 Å, The list contains about 121,000 strongest lines in this region.

```
cd ./tlusty205/data
wget http://aegis.as.arizona.edu/~hubeny/pub/gfFUV.dat.gz.
```

- lines only in the visible region, between 3,000 and 7,500 Å, The list contains about 149,000 strongest lines in this region.

```
cd ./tlusty205/data
wget http://aegis.as.arizona.edu/~hubeny/pub/gfVIS99.dat.gz.
```

Other line lists (for instance the infrared region, or molecular lines) are in principle available, but are not a part of the standard distribution.

4 Running TLUSTY

4.1 Source code files and compilation

The program is distributed as one big file that contains all subroutines, plus several (8) small files that contain the `INCLUDE` statements which declare most of variables and arrays, together with array dimensions. These can be used to recompile the code to decrease or increase its memory consumption, as explained in Paper III, § 2.1. All files should reside in the same directory.

A compilation of the program is explained in more detail on Paper III, § 2.1, where the compiler instructions on different platforms are summarized. Here we only show a compilation using `gfortran`, which is available on most Mac and LINUX platforms,

```
gfortran -fno-automatic [-O3] -o tlusty.exe tlusty205.f
```

where the option `"-fno-automatic"` indicates the static allocation of memory. The level-3 optimization (`"-O3"`) should be switched on since it improves the performance of the code considerably. For more details, and several examples of compiling the program on different platforms, refer to Paper III, § 2.1.

4.2 Input files

The essential feature of the input data format is that there is only a very short standard input file, which specifies: (i) the very basic parameters, such as T_{eff} , $\log g$, chemical abundances, etc., for which no reasonable default values can be specified; (ii) the name of the file where the optional *keyword parameters* are set up; and (iii) the names of files where the atomic data for the individual ions are stored. Keyword parameters are defined as those for which the program assigns default values, which are optimum for most applications, but could be changed as required for a particular special application. They also enable one to choose among several alternative numerical schemes, or to cope with convergence problems. There are also several keyword parameters that determine the overall computational strategy. The most important ones are described in Paper III, Chap. 7, and the remaining ones in Chaps. 12 and 13, and the full list of keyword parameters together with their default values is presented in Paper III, Chap. 16.

Here is a list of basic input files.

- **fort.1** — The basic control file, containing just one single number, specifying whether one calculates a stellar atmosphere or an accretion disk model. If this number is 0, or if the file is missing altogether, a stellar atmosphere model is to be computed. Otherwise, a disk vertical structure is computed.
- Standard input file (unit 5) — Main control data. It is a short file with only the most important parameters, and filenames of other files. The

structure of the file and the meaning of the individual input parameters are explained in Paper III, Chap. 4.

- A file that specifies non-default values of the keyword parameters. Its name is specified in the standard input file.
- **fort.8** — A starting model atmosphere in the case the calculation does not start from the scratch (that is, with an LTE-gray model) - see Paper III, Chap. 8.

In the standard mode, where the opacities are computed on the fly, and where one introduces the concept of explicit ions and levels (which is mandatory for NLTE models), there is an important set of input files, namely

- Files containing atomic data for the individual ions. These files are described in detail in Paper III, Chap. 11. A collection of such files is available in the standard distribution of TLUSTY, and in the TLUSTY website.

There is another mode which uses pre-calculated opacity tables; for more details and examples, refer to Paper III, § 6.4 and 13.1. In that case, the atomic data files are not needed.

There may be many more additional input files for specific applications, such as white dwarfs, cool stars, etc. They are described in Paper III, Chap. 12.

All the input files are ASCII files to enable easy portability. All the **READ** statements use a free format. Moreover, Unit 5 may contain comment lines; TLUSTY understands a line beginning with ***** or **!** as a comment.

4.3 Output files

There are several output files. By default, all the output files are generated as ASCII files for portability. TLUSTY does not contain any explicit **OPEN** statements for the output files, so the files are generated with names **fort.nn**, where *nn* is the corresponding unit number.

Here we only list the basic output files; there are more files used for special purposes only. All the output files are described in detail in Paper III, Chap. 9.

- Unit 6 – Standard output
- **fort.7** – Condensed model atmosphere
- **fort.9** – Convergence log
- **fort.10** – Performance and error log
- **fort.11** – Mean opacities and other physical quantities for the resulting model
- **fort.12** – *b*-factors (NLTE departure coefficients) – only for NLTE models
- **fort.13** – Emergent flux in all frequency points (spectral energy distribution)
- **fort.69** – Timing log

4.4 Producing a model atmosphere with TLUSTY

Generically, the program can be run as follows:

```
tlusty.exe < [std. input file] > [std. output file]
```

A standard input file is mandatory. If the specification of the standard output file is missing, the output is directed to the screen. It is however advisable to save the standard output to a file because it contains a useful information about the performance of the code, and will help in case of problems.

Although the file names can be arbitrary, it is advantageous to use the following convention: Any name of an input or output file is composed of a *core name* that may label the basic physical parameters of a model, with an extension identifying the unit number. For example, let us take a H-He model for $T_{\text{eff}} = 35,000$ K and $\log g = 4$, in LTE. Let the core name be **hhe35lt**, so the standard input file is then **hhe35lt.5**. This file is a part of the standard distribution of TLUSTY.

The code can then be run as follows

```
tlusty.exe < hhe35lt.5 > hhe35lt.6
```

where the standard output is redirected to the file **hhe35lt.6** for further inspection. However, in this case the executable file **tlusty.exe** has to be present in (or linked to) the current directory, and also the necessary atomic data, in this case the files **./data/h1.dat**, **./data/he1.dat**, and **./data/he2.dat** have to be available. Therefore, one has to either create a subdirectory **./data** in the current directory, or to set an appropriate link to a universal directory that contains a collection of atomic data files.

An easier and safer way is to use a shell script **RTlusty**, which is based on a script **XTlusty** kindly provided by Knox Long, and which is also a part of the standard distribution of TLUSTY. It is called with one or two parameters,

```
RTlusty    model_core_name    [core_name_of_starting model]
```

The second parameter does not have to be present if the model is calculated from scratch. The executive part of the script looks like (schematically)

```
MOD=$1
if [ -e $2.7 ] cp $2.7 fort.8
ln -s $TLUSTY/data data
$TLUSTY/tlusty/tlusty.exe < $MOD.5 > $MOD.6
cp fort.7 $MOD.7
cp fort.9 $MOD.9
cp fort.69 $MOD.69
cp fort.13 $MOD.13
```

The second command checks for the existence of the file that contains the starting model, and if it does exist, copies it to **fort.8**. The third command links the general directory containing the necessary atomic data to a temporary directory

that is being referred to in the input files, and the last part runs the code and stores the most important output files to corresponding files.

Important notes

The script `RTlusty` can run a model in any directory, provided that the two following requirements are fulfilled:

- One has to set up an environment variable `TLUSTY` that specifies the main `TLUSTY` directory. For instance, using the tar files downloaded from the Arizona site, and assuming that the tarball is extracted in the home directory, the main `TLUSTY` directory is generated as `~/tlusty205`, one sets

`setenv TLUSTY ~/tlusty205`
- The universal directory containing atomic data is a subdirectory of the main `TLUSTY` directory, that is, `$TLUSTY/data`

Since the script is located in the main `TLUSTY` directory, it is advantageous to set a `path` pointing to that directory. Otherwise, one would either need to copy the script `RTlusty` to the current directory, or to call it as `$TLUSTY/RTlusty`. In the following examples, we will call it simply as `RTlusty`.

4.5 Test-case model atmosphere

The actual test case using the `hhe35lt` is run as shown above, i.e.,

```
cd $TLUSTY/examples/hhe
RTlusty hhe35lt
```

which runs the code and stores not only the standard output (unit 6) but also other important output files, all with the same core name, and with the suffix that corresponds to the unit number.

The only input files are the standard input file `hhe35lt.5` and three atomic data files `h1.dat`, `he1.dat`, and `he2.dat`, for H, He I, and He II, respectively. The structure of the standard input file is described in detail in Paper III, Chap. 6.2, and the structure of the atomic data files in Paper III, Chap. 11. The keyword parameter file is missing, so that no keywords are required. The starting model file is missing too, because the model is computed from scratch and no starting model is needed.

A continuation of the run to produce a final NLTE model is described in detail in Paper III, § 6.2. Briefly, the final NLTE model would be obtained by

```
RTlusty hhe35nc hhe35lt
RTlusty hhe35nl hhe35nc
```

As explained in Paper III, it is advantageous to proceed in three steps: first to compute an LTE model, then a NLTE model with continua only (NLTC), and finally a NLTE model with lines (NLTL). This strategy follows a standard practice of constructing NLTE models, first suggested by Auer & Mihalas (1969).

The test case presented here produces a model that is similar, although somewhat more involved, than the early NLTE model atmospheres produced by the pioneers of this field (Auer & Mihalas 1970, 1972; Mihalas & Auer 1970; Mihalas et al. 1975).

Paper III, Chap. 6, presents a number of additional test cases; their input data may be used as templates for producing similar models. All the test cases can be done by applying the script `Runtest`, which calls elementary script `RTlusty` in the individual directories after making necessary links to additional atomic data files. The user is therefore encouraged to issue the following commands:

```
cd $TLUSTY/examples
Runtest
```

The script issues messages about a completion of the individual models that are being computed, and if everything goes well, it generates appropriate models in all the five subdirectories of the directory `examples`. The user may then compare the newly created files with the template output files that are provided and named with an additional label `.orig`, e.g., `hhe35lt.7.orig`. A description of physics and numerics behind these models is explained in detail in Paper III, Chap. 6.

4.6 How can I tell that the model is well converged?

This is actually a very important question, which is however sometimes overlooked. It is therefore important to look at this issue in more detail. It should be fully realized that a model is constructed by applying an *iteration* process. There are several possibilities of which actual scheme to apply, or even which actual flavor is going to be used. They are explained from the theoretical point of view in Paper II, and their practical choice and setup is described at length in Paper III. In the present context, it suffices to say that the program contains a number of default options; therefore without specifying any additional parameters the code performs according to its default settings. The basic iteration scheme is the hybrid CL/ALI (Complete Linearization/Accelerated Lambda Iteration) method, described in Paper II, § 3.2.

The first, and the most important criterion of convergence is the magnitude of the relative changes of the components of the state vector. The latter is defined as a set of all structural parameters (temperature, various particle number densities, and the mean intensities of radiation in discretized frequency points) in a given discretized depth point. The necessary condition for convergence is that the maximum relative change of all components of the state vector in all depths is “small”, say 10^{-3} , as shown for instance on the example below. However, this is generally *not* a sufficient condition. The reason is that in some cases the maximum relative change can be “small”, but the absolute error of the solution can still be large. This is known as the “false convergence”, discussed in a similar context of solving the radiative transfer equation with a dominant scattering term in Hubeny & Mihalas (2014, § 13.2). A usual symptom of such

a behavior is that while the relative changes are decreasing from iteration to iteration, the maximum relative change decreases only very slowly, showing a decrease by an order of magnitude in 10 or more iterations.

After a completed run, it is therefore mandatory to inspect the convergence log to make sure that all the relative changes of the components of the state vector are sufficiently small. The standard distribution of TLUSTY also contains an IDL program `pconv.pro` which plots the contents of the convergence log. The program requires as an input three output files from TLUSTY, namely units 7, 9, and 69, and assumes that the file names are constructed using the above convention, that is the core names are the same. The program is called as

```
pconv, 'hhe351t'
```

It can be called also as

```
pconv
```

in which case the files are supposed to have generic names `fort.*`. If IDL is not available, the user is strongly encouraged to write his/her own graphical interface routine to display the contents of the file `fort.9`. Our experience showed that by inspecting the file solely by the eye one can easily miss significant spikes in relative changes.

A supplementary, and quite stringent criterion of the convergence of a model is based on examining the conservation of the total flux. To this end, one needs to inspect the last table of the standard output, in the present case `hhe351t.6`, that summarizes the computed model atmosphere. The last four columns of the last table show the computed total flux (radiative plus, if applicable, convective), and the ratios of the radiative, convective, and computed total fluxes with respect to the theoretical total flux, σT_{eff}^4 , respectively. Therefore, the values of the last column should be very close to unity (up to at most 1% departures from it); otherwise the model cannot be viewed as sufficiently accurate, even if the convergence log may show that the model is formally converged. Again, this would be a consequence of the false convergence of the iteration scheme.

More information on convergence properties, and an outline of various strategies to cope with convergence problems, is covered in Paper III, Chaps. 10 and 15.

Inspecting the results for the test model as suggested above shows that the total flux is conserved within 0.1% (the last table of `hhe351t.6`). Using the IDL program `pconv` to display the convergence log of `hhe351t.9`, see Fig. 1, reveals an excellent and stable convergence behavior of the run (not surprisingly, because it is a very simple model). There are six panels on the figure, the upper three display the relative changes of temperature (which is usually the most important component of the state vector), while the lower three panels show the maximum relative change of all components of the state vector. The leftmost panels show the relative change as a function of column mass in the absolute scale, and the middle panels show the same in the logarithmic scale. We display both, because the linear scale shows the sign of the relative changes

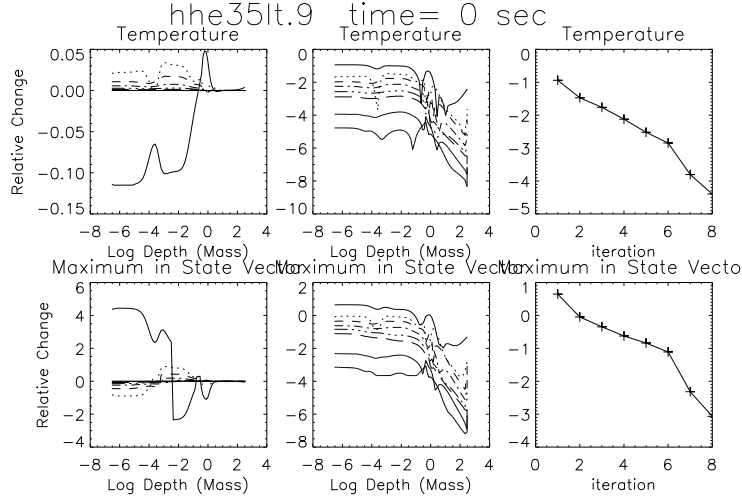


Figure 1: Convergence log for a simple LTE H-He model.

but does not properly show those that are small. These are in turn clearly seen on the logarithmic scale. The rightmost panels show the maximum relative change over all depth points. This is an indicator of the global convergence of the model. Ideally, the relative changes should gradually decrease, which was clearly the case here. A significant drop in the relative changes in the 7th iteration originated due to the Ng acceleration (see Paper II, § 3.4). The figure also contains a header that displays the core name and the total execution time. In the present case it was less than 1 s (actually 0.69 s, as shown in `hhe35lt.69`). This, and all other calculations reported below, were done on a MacBook Pro, with a 2.2.GHz Intel Core i7 CPU.

5 Running SYNSPEC

5.1 Source code files and compilation

Analogously to TLUSTY, program SYNSPEC is also distributed as one big file together with four “INCLUDE” files that declare most of the arrays and specify their dimensions. The compilation under `gfortran` is done as

```
gfortran -fno-automatic [-O3] -o synspec.exe synspec51.f
```

5.2 Input files

The basic input files used for SYNSPEC are exactly the same ones as used for TLUSTY, namely

- **fort.1** — The basic control file, containing just one single number, specifying whether one deals with a stellar atmosphere or an accretion disk model. If this number is 0, or if the file is missing altogether, a stellar atmosphere model is considered, otherwise, one ring of a disk model is considered.
- Standard input file (unit 5) — Main control data, exactly the same as used for TLUSTY to generate the model atmosphere for which the synthetic spectrum is being calculated.
- File that specifies non-default values of the keyword parameters. Its name is specified in the standard input file. Again, this is the same file as that used for running TLUSTY.
- **fort.8** — Input model atmosphere - typically given as previously computed TLUSTY model; more specifically, Unit 7 output from TLUSTY, but it can also be a Kurucz model.

Many of the input parameters do not have any meaning for running SYNSPEC, but we kept the same input files for convenience. If one computes a synthetic spectrum for a Kurucz model, one has to construct an artificial standard input file for this run. It will be described briefly in § 5.5.

In addition to these files, there are several input files specific to SYNSPEC:

- **fort.19** - atomic line list, based on Kurucz line lists. It will be described below in § 5.3.3.
- **fort.55** - additional input parameters for computing the synthetic spectrum. It will be described below in § 5.3.1.
- **fort.56** - optional file that specifies a change of chemical abundances with respect to the input model atmosphere. It is not needed for LTE models or for NLTE models in which the chemical abundances considered for the SYNSPEC run are the same as those used in constructing the input model atmosphere. The file is described below in § 5.3.2.
- **fort.57** - energy bands for superlevels. This file is needed only if the input model atmosphere is a NLTE metal-line blanketed model that treats the level structure of the iron-peak elements in terms of superlevels and superlines. It is described in Appendix B. We note that in the previous versions of SYNSPEC, this file was called **fort.13**. We changed the notation because using **fort.13** as an input file for SYNSPEC could lead to a confusion with another file **fort.13** generated by TLUSTY (a table of emergent flux) which may accidentally be present in the working directory.

It should be stressed that while the atomic data used for TLUSTY contain sufficient information for evaluating the corresponding cross sections and opacities for bound-free transitions (continua), as well as bound-bound transition (lines), SYNSPEC only takes information for bound-free transitions from the TLUSTY

input files, while the data for lines are taken from an independent, SYNSPEC-specific line list. Typically, a line list used by SYNSPEC contains “all” lines, i.e. also data for lines of the species that were not considered by TLUSTY.

Additionally, for some special purposes there are additional input files used only for some special purposes; these files are also used by TLUSTY for analogous purposes (white dwarfs; cool stars, etc.). They must have specific names listed below. They are only used if a corresponding parameter is set up – see Appendix A.

- **lemke.dat**, or **tremblay.dat**, or **hydprf.dat** - special hydrogen line broadening tables, see Appendix A, and, in the context of TLUSTY, Paper III, § 12.1.1
- **laquasi.dat**, **lbquasi.dat**, **lgquasi.dat**, **lhquasi.dat** - special hydrogen quasi-molecular data - see Appendix A
- **tsuji.molec** – a table with necessary parameters for the molecular state equation – see Paper III, § 6.4, § 7.4.1 and § 7.10.3
- **irwin.dat** – a table of Irwin partition functions – see Paper III, § 12.7

There are some other optional SYNSPEC-specific input files, not being used by TLUSTY,

- **he1prf.dat**, **he2prf.dat** - special tables for He I and He II line broadening data - see Appendix A

Finally, if required, there are one or more molecular line lists

- **fort.20** - basic molecular line list, containing data for most important diatomic molecules: H₂, C₂, CH, CN, CO, N₂, NH, NO, O₂, OH, MgH, MgC, MgN, MgO, SiH, SiC, SiN, SiO;
- **fort.21**, etc. - additional molecular line lists

This option is introduced in order to avoid working with excessively large files. For instance, in addition to the line list for basic diatomic molecules, one may have a special list for H₂O, for TiO and VO, and possibly more.

All the universal data files mentioned above are invoked by SYNSPEC by appropriate **OPEN** statements, where they are assumed to reside in the directory **./data**. Specifically, these are:

```
./data/lemke.dat, ./data/tremblay.dat, ./data/hydprf.dat, .
./data/he1prf.dat, ./data/he2prf.dat,
./data/laquasi.dat, ./data/lbquasi.dat, ./data/lgquasi.dat,
./data/lhquasi.dat,
./data/tsuji.molec, ./data/irwin.dat
```

This means that by linking the general; “data” directory to **./data** as was done before,

```
ln -s $TLUSTY/data data
```

then all these data files are automatically available, in contrast to the previous versions of SYNSPEC where all the necessary links had to be set separately.

5.3 Description of SYNSPEC-specific input files

5.3.1 File `fort.55`

The general structure of the file, using the variable names exactly as they are in the SYNSPEC source code, is as follows:

```
imode   idstd   iprin
inmod   intrpl  ichang  ichemc
iophli  nunalp  nunbet  nungam  nunbal
ifreq   inlte   icontl  inlist  ifhe2
ihydpr  ihe1pr  ihe2pr
alam0   alast   cutof0   cutoffs  relop   space
nmlist, (iunitm(i),i=1,nmlist)
vtb
nmu0    ang0    iflux
```

The parameters are read in a free format, and the last three lines of the file do not have to be present if they are not needed. In that case, `nmlist` and `nmu0` are set to 0, and `vtb` - the turbulent velocity - is given by the TLUSTY input.

Here is a brief explanation of the parameters:

- **imode** – sets the basic mode of operation:
 - = 0 - normal synthetic spectrum;
 - = 1 - spectrum for a few lines (obsolete);
 - = 2 - continuum (plus H and He II lines) only;
 - = 10 - spectrum with molecular lines.
 - = -1 an “iron curtain option”. In this case one only computes the opacity at the standard depth `idstd` (see below), but does not solve the transfer equation. It is usually used with an artificial input model atmosphere consisting of one single depth point.
- **idstd** - index of the “standard depth”, which is defined as a depth where $T \approx (2/3)T_{\text{eff}}$. Approximately, $\text{idstd} = (2/3)ND$, with ND being the total number of depth points of the model. This parameter is not critical; it only influences the selection of lines to be considered, set through the rejection parameter **relop** – see Appendix C;
- **iprin** – when > 0 increases the amount of printed information in the standard output (essentially obsolete);
- **inmod** – an indicator of the input model:
 - = 0 - the input model is a Kurucz model;
 - = 1 - the input is a TLUSTY model;
 - = 2 - the input model is an accretion disk model
- **intrpl**, **ichang** – set the change of the input model (rarely used);

- **ichemc** - if non-zero, indicates a change of abundances with respect to the input model. In this case, file **fort.56** is required;
- **iophli** - treatment of far $L\alpha$ wings (obsolete); should be set to 0;
- **nunalp**, **nunbet**, **nungam**, **nunbal** – if any of them set to a non-zero value, the quasi-molecular satellites of $L\alpha$, $L\beta$, $L\gamma$, and $H\alpha$, respectively, are considered. In that case, additional input files containing the corresponding data are needed. These have to have the following names: **laquasi.dat**, **lbquasi.dat**, **lgquasi.dat**, and **lhquasi.dat**, respectively. They are distributed along with SYNSPEC.
- **ifreq** – the choice of the radiative transfer equation solver; namely if **ifreq** ≥ 10 one uses the Feautrier scheme, otherwise the DFE scheme – see Paper II. This option is rarely used; one usually uses the default value **ifreq** = 1.
- **inlte** an auxiliary NLTE switch:
= 0 - enforces LTE: lines are treated in LTE even if the input model is NLTE.
> 0 - its actual value (1 or 2) sets the mode of evaluation of the populations of levels close to the ionization limit - see § 5.6;
- **icontl**, **inlist** – obsolete parameters, typically set to 0;
- **ifhe2** – if set to a non-zero value, He II is treated as a hydrogenic ion (see Appendix A);
- **ihydr**, **ihe1pr**, **ihe2pr** – if set to a non-zero value, these parameters invoke a special evaluation of line profiles of the respective atom/ion. In this case, additional input files with corresponding data are needed – see Appendix A;
- **alam0** – starting wavelength [Å];
- **alast** – absolute value is ending wavelength [Å],
if **alast** < 0, then all the line wavelengths are in vacuum (notice that by default, the wavelengths for $\lambda \leq 2000$ Å are in vacuum, while for $\lambda > 2000$ Å they are in the air);
- **cutof0** – cutoff parameter: the opacity of any line except H and He II is cut at **cutof0** Å from its center;
- **cutofs** – dummy variable;
- **relop** – line rejection parameter: a line is rejected if the ratio of its line-center opacity to the continuum opacity at standard depth **idstd** is less than **relop**;
- **space** – spacing parameter, which represents the maximum distance of two neighboring wavelength points at the midpoint of the considered wavelength interval, that is, $\Delta\lambda \leq \text{space}$. The actual maximum spacing is proportional to the wavelength, $\Delta\lambda \leq \text{space} \times (\text{alam0} + \text{alam1})/(2\lambda)$. For more details, see Appendix C.
- **nmlist** – number of additional molecular line lists,
- **iunitm(i), i=1, nmlist** – unit numbers of the additional molecular line lists
- **vtb** - if set, it specifies the turbulent velocity [km s⁻¹]. This parameter is only needed if the turbulent velocity for the current run of SYNSPEC is different from the value specified in the TLUSTY input;
- **nmu** – if set to a non-zero value, SYNSPEC produces not only a flux, but also

the specific intensities, $I_\nu(\mu)$ [$\text{erg cm}^{-2}\text{s}^{-1}\text{Hz}^{-1}\text{ster}^{-1}$]; μ is the cosine of the angle with respect to the normal to the surface. The value of `nmu` represents the number of the angle points, expressed as μ , and set equidistantly between `ang0` and 1;

- `ang0` – minimum angle cosine;
- `iflux` – should be set to 1 to invoke an evaluation of specific intensities;

5.3.2 File `fort.56`

File `fort.56` has a simple structure:

```
nchang
```

and then `nchang` records, each with

```
iatom abn
```

where

- `nchang` – number of chemical elements for which the chemical abundances are changed with respect to the TLUSTY input (specified in the standard input file);
- `iatom` – atomic number;
- `abn` – the modified abundance. The convention is as follows:
 - `abn > 0` – abundance by number, relative to hydrogen;
 - `abn = 0` – abundance is solar;
 - `abn < 0` – the absolute value is the ratio of the abundance to the solar one.

For all so specified chemical elements, the values of `abn` represent the current chemical abundances for the run of SYNSPEC. For explicit, NLTE, species, they are also used to multiply the NLTE level populations given by the model atmosphere input by the ratio of the “new” abundance of the corresponding chemical element (specified by the values in the file `fort.56`), and the “old” abundance, referred to in the standard input file, that were used previously by TLUSTY. This procedure is not rigorous because the NLTE line formation is not a linear process, and the modified abundances may yield a different global atmospheric structure. But this is acceptable if the abundance change concerns a minor (not very abundant) chemical species. or for a major species if the relative difference of the old and new abundances is small, say, no more than 0.2 to 0.3 dex. For larger abundance differences, it is more prudent first to recompute the model atmosphere and then to produce a synthetic spectrum.

5.3.3 Line list

The line list contains one input record for each spectral line. In fact, it could contain more records, but this option is cumbersome and is rarely used. The input record contains the following variables:

```
alam anum gf excl ql excu qu agam gs gw inext
```

and if the continuation indicator `inext` is non-zero, then the next record is

```
wgr1 wgr2 wgr3 wgr4 ilwn iun iprf
```

The meaning of these quantities is the following:

- `alam` – wavelength [nm]. One follows the convention that for $\lambda < 200$ nm the wavelengths are in vacuum, while for $\lambda \geq 200$ nm the wavelengths are in the air (they can however be modified to vacuum wavelengths by setting the parameter `alast` in `fort.55`—see above—to a negative value);
- `anum` – numerical code of the element and ion (using the Kurucz convention; e.g., 2.00 = He I, 6.03 = C IV, 26.01 Fe II, etc.)
- `gf` – $\log gf$
- `excl` – excitation potential of the lower level [cm^{-1}]
- `ql` – the J quantum number of the lower level
- `excu`, `qu` – analogous quantities for the upper level
- `agam` – $\log \Gamma_{\text{rad}}$ for radiation damping
- `gs` – $\log \Gamma_{\text{stark}}$ for Stark broadening
- `gw` – $\log \Gamma_{\text{vdW}}$ for Van der Waals broadening
- `inext` – if =1, next record is needed, where:
- `wgr1 wgr2 wgr3 wgr4` – Stark broadening values from Griem (1974) tables, values for $T = 5, 10, 20, 40 \times 10^3$ K, respectively
- `ilwn` – manual setting of the index of the lower level as used by TLUSTY
- `iun` – manual setting of the index of the upper level as used by TLUSTY
- `iprf` – if non-zero, special procedure for evaluating the Stark broadening (at present only for He I – see Appendix A).

In any of the parameters `agam`, `gs`, `gw` is set to zero, one uses an approximate formula for evaluating the corresponding broadening parameter. For details refer to Appendix A.

5.4 Output files

- Unit 6 - standard output file. It contains a log of calculations, important only in the case when something goes wrong.
- `fort.7` – synthetic spectrum. A simple table of wavelength [\AA] versus flux, expressed as the first moment of the specific intensity (Eddington flux), H_λ , in $\text{erg cm}^{-2}\text{s}^{-1}\text{\AA}^{-1}$.
- `fort.17` – An analogous table of the theoretical continuum flux.
- `fort.12` – Identification table. It contains a list of all lines that were selected by SYNSPEC to be taken into account, together with their basic parameters and an indicator of their approximate strength. This information can be used for an identification of the lines in the predicted spectrum. For more details, see Appendix D.

- `fort.16` – A list of partial equivalent widths of SYNSPEC-generated spectral regions – see Appendix D.

5.5 Producing a synthetic spectrum for a Kurucz model

As pointed out above, SYNSPEC accepts a Kurucz model structure as an input model. One has to set the parameter `inmod` in the file `fort.55` (1st number on the second line) to 0 – see § 5.3.1.

The standard input to be used is essentially any input for TLUSTY. Recall that SYNSPEC uses the standard input only to specify the continuum opacity, that is the bound-free and free-free cross sections. Which actual transitions are included is specified by the data. In hot stars where the continuum opacity is dominated by H and He, it is actually sufficient to use the sample file `hhe351t.5` as the standard input file for SYNSPEC. For cool stars, when the continuum opacity is dominated by H^- and metal opacities, one has to construct the standard input accordingly. The standard distribution of SYNSPEC contains an example of such file, called `cool.5`, which is safe to use as the standard input to SYNSPEC to produce synthetic spectra for Kurucz models with $T_{\text{eff}} \leq 10,000$ K.

5.6 What chemical species and what lines are being considered?

The choice of chemical species that are taken into account by SYNSPEC is controlled by the standard input data to TLUSTY. As explained in more detail in Paper III, § 4.2, the chemical elements can be treated either (i) *explicitly* - treated in detail and in NLTE; (ii) *implicitly* - treated in LTE; or (iii) rejected altogether. For each explicit element, a set of appropriate ionization stages, called *explicit ions* is selected, and for each explicit ion a set of *explicit energy levels* is selected. This is specified in the atomic data file, explained in detail in Paper III, Chap. 11.

The continuum opacity sources are completely specified by the standard input to TLUSTY. As explained in detail in Paper III, § 4.3, the continuum opacity is composed of all the bound-free transitions from explicit levels, and the free-free transitions of the explicit ions, plus possibly additional opacity sources specified through the specific TLUSTY input parameters – see Paper III, § 12.2. The atomic level populations that enter the evaluation of the corresponding opacities are taken directly from the TLUSTY input model.

In contrast, lines are treated differently. SYNSPEC takes into account all lines of all species that are not specifically rejected. For instance, in the test case shown in § 5.7, H and He are treated explicitly; C, N, and O are treated implicitly, Li, Be, and B are rejected, and all the species with atomic number larger than 8 are left unspecified. They are not taken into account by TLUSTY, but since they are not explicitly rejected, all the lines of such species that appear in the line list are being taken into account by SYNSPEC. The rationale for this approach is that when constructing a model atmosphere one takes into account only the important species that may influence the global atmospheric structure,

while when constructing a synthetic spectrum using SYNSPEC one is generally interested in seeing all predicted lines. It should also be stressed that while the atomic data files used by TLUSTY contain data for selected lines, SYNSPEC takes a completely independent source of line data, namely the line list – see §5.3.3.

The atomic level populations that enter the evaluation of the corresponding opacity are determined in the following way:

(i) For non-explicit chemical elements, the level populations are evaluated in LTE. Obviously, if a model atmosphere is computed in LTE, all level populations of non-rejected species (explicit and implicit) are evaluated in LTE.

(ii) For explicit species in a NLTE model atmosphere, the level populations used for evaluating the bound-free and free-free transitions are taken from the model atmosphere generated by TLUSTY. As specified above, the line list contains, for a given line, the J -values and level energies for the lower and the upper level of the corresponding transition. Based on this information, SYNSPEC makes an association of the levels being specified in the line list and the explicit levels that are specified through the TLUSTY input atomic data files. This is described in detail in Appendix B.

5.7 Test cases

Analogously to the script `Rtlusty`, we have constructed a similar script `RSynspec` that makes the necessary links, and run SYNSPEC. It resides in the main TLUSTY directory, `$TLUSTY`. The script is called with one or two or three parameters,

```
RSynspec core_name_of_input_model file_fort.55 line_list
```

The second parameter is the name of the file that is going to be linked to `fort.55`; if it is missing, it is assumed that the file `fort.55` exists in the current directory. The third parameter is the filename of the line list; again, if it is missing, file `fort.19` already exists in the current directory.

The script stores the important output files as follows:

```
cp fort.7 $MOD.spec
cp fort.17 $MOD.cont
cp fort.12 $MOD.iden
cp fort.16 $MOD.eqws
```

which represent the full spectrum continuum flux, identification table, and the equivalent width table, respectively.

The first test case is computing a synthetic spectrum for a short interval of wavelengths between 1400 and 1410 Å, for the model `hhe351t`, which is obtained as follows:

```
cd $TLUSTY/synspec/examples/hhe
RSynspec hhe351t fort.55.lin data/linelist.test
```

where the input file `fort.55.lin` has the following content


```

0      50      0
1      0      0      0
0      0      0      0      0
1      1      0      0      0
0      0      0
1400   1410   10      0  0.0001  0.01
0      0

```

The structure of the file is explained in § 5.3.1. The 6th line sets the parameters of the synthetic spectrum - first two numbers of the limiting wavelengths of the interval to be covered, and the last number the maximum spacing of the individual wavelength points, all in Å.

The standard distribution of SYNSPEC also contains a sample of a line list used for tests, called `linelist.test`, which has to be copied or linked to `fort.19`. The contents of `fort.7`, the synthetic spectrum, and `fort.17`, the theoretical continuum, are displayed in Fig.2.

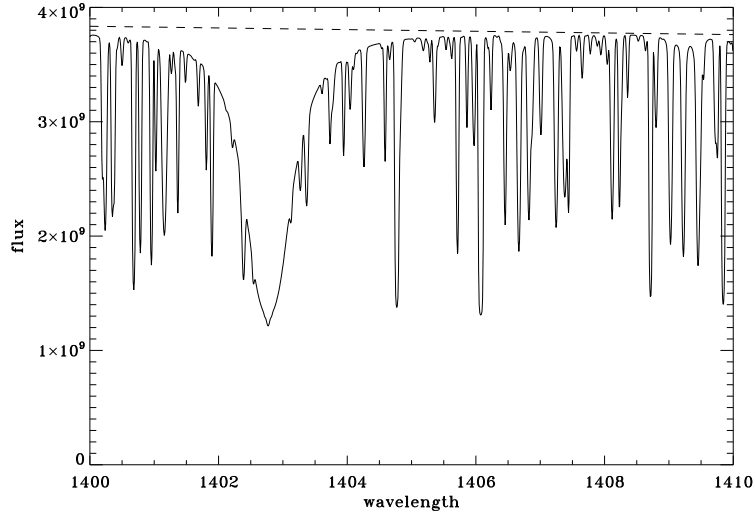


Figure 2: Example of a synthetic spectrum for a simple LTE H-He model. Dashed line portrays the theoretical continuum. The wavelength is in Å, and the flux is represented by the first moment of the specific intensity H_λ in $\text{erg cm}^{-2}\text{s}^{-1}\text{Å}^{-1}$.

Another example is the predicted continuum spectrum in the optical region. SYNSPEC defines the continuum as the true continuum plus hydrogen and hydrogenic (in this case He II) lines. File `fort.55` (stored at `fort.55.con`) is now:

```

2      50      0

```

```

1      0      0      0
0      0      0      0      0
1      1      0      0      0
0      0      0
3500   5000   10      0  0.0001  0.5
0      0

```

The continuum-only mode is set by the first number on the first line, `imode = 2`. In this case, no line list is needed. The wavelength range is now set to 3500 to 5000 Å, and the separation of the wavelength points in the middle of the interval is 0.5 Å; the wavelength spacing is proportional to the wavelength. The resulting synthetic spectrum is shown in Fig.3.

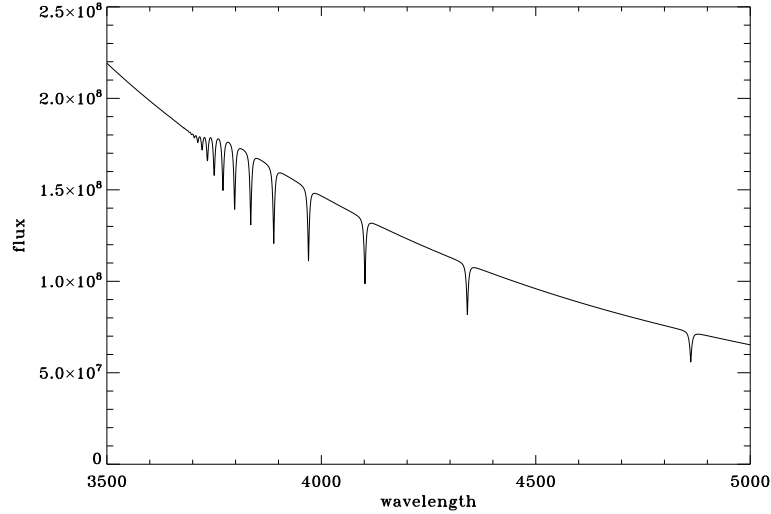


Figure 3: Example of a synthetic spectrum for a simple LTE H-He model, analogous to Fig. 2, but for the optical region and showing only continuum plus H and He II lines. In this particular case, the H and He II lines have a very similar strength. The wavelength is in Å, and the flux is represented by the first moment of the specific intensity H_λ in $\text{erg cm}^{-2}\text{s}^{-1}\text{Å}^{-1}$.

The next test case is a synthetic spectrum, in the same wavelength interval, for a Kurucz model with $T_{\text{eff}} = 9750$ K, $\log g = 4$. The necessary input files are located in directory `$TLUSTY/synspec/examples/kurucz`. A file with the model atmosphere structure, analogous to TLUSTY file `fort.7` but in the specific Kurucz format, is called `ap00t9750g40k2.dat`. The standard input file, constructed such as to provide appropriate continuum opacities as explained in § 5.5, is called `cool.5`. Because the file names do not correspond to the standard TLUSTY naming convention, one has to modify the filenames in order to be able to use the script `RSynspec`. This is provided by the script `Runtest`, located

in this directory. Without using scripts `Runtest` and `RSynspec`, the synthetic spectrum can be computed as follows:

```
ln -s -f $TLUSTY/data data
ln -s -f fort.55.lin fort.55
ln -s -f $TLUSTY/data/linelist.test fort.19
cp ap00t9750g40k2.daf fort.8
$TLUSTY/synspec/synspec.exe <cool.5 >tmp.log
```

and possibly store resulting files `fort.7`, etc., with a permanent name, as the script `Runtest` did, using a core name `kurucz9750g40`.

6 Working with OSTAR2002 and BSTAR2006 grids

Computing modern and sophisticated NLTE metal line-blanketed model atmospheres is time consuming; one model can easily take several hours to few tens of hours of computer time on a present mid-class workstation or a Mac laptop.

In many instances, it is actually not necessary to produce new models from scratch. We have constructed two extensive grids of NLTE fully metal-line blanketed model atmospheres for O-stars (Lanz & Hubeny 2003), called OSTAR2002, and an analogous grid BSTAR2006 (Lanz & Hubeny 2007) for early B-stars.

The intent was to provide more or less definitive grids of models in the context of 1D plane-parallel geometry, with hydrostatic and radiative equilibrium, and without any unnecessary numerical approximations. The essential limitation of these models is the quality and availability of atomic data which, despite recent efforts (such as the *Opacity Project*, *OPAL*, or *IRON Project*) are still incomplete (for instance, the lack of available collisional excitation cross-sections for dipole-forbidden transitions of the iron-peak elements).

The OSTAR2002 grid contains model atmospheres for T_{eff} between 27,500 and 55,000 K with the step of 2,500 K, $\log g$ between 4.75 and a value that corresponds to an approximate location of the Eddington limit, with the step 0.25, and for 10 metallicities: 2, 1, 1/2, 1/5, 1/10, 1/30, 1/50, 1/100, 1/1000, and 0 times the solar metal composition, so that the grid is useful for studies of typical environments of massive stars: the Galactic center, the Magellanic Clouds, blue compact dwarf galaxies like I Zw-18, and galaxies at high redshifts. Departures from LTE are allowed for the following species: H, He, C, N, O, Ne, Si, P, S, Fe, Ni, in all important stages of ionization. There are altogether over 1,000 (super)levels treated in NLTE, about 10^7 lines, and about 250,000 frequency points to describe the spectrum.

The BSTAR2006 grid is similar. It contains models for T_{eff} between 15,000 and 30,000 K with the step of 1000 K, $\log g$ values are set similarly to the OSTAR2002 grid, and for 6 metallicities: 2, 1, 1/2, 1/5, 1/10, and 0 times solar. The species treated in NLTE are the same as in OSTAR2002, adding Mg and Al, but removing Ni, which is less important for B stars. There are altogether about 1,130 (super)levels treated in NLTE, about 10^7 lines, and about 400,000

frequency points. The models for both grids are available online⁴.

There are two types of available files: (i) model structure – essentially three files; the standard input, `*.5`; the keyword parameter file `nst` referred to by the standard input (the same for all models), and the resulting condensed model atmosphere, `*.7`. (ii) Synthetic spectra, but with a relatively low resolution of about 1 Å. To obtain a higher resolution synthetic spectrum, one has to run SYNSPEC, as shown in §6.2.

6.1 Do we need to compute a model atmosphere from scratch?

For the range of effective temperature covered by the grids, it is advantageous not to construct a model from scratch, but rather use an existing model from the grid and possibly modify it to suit the user's purposes. In the following, we describe several useful procedures to use existing models to produce detailed spectra for the basic parameters (T_{eff} , $\log g$, chemical abundances), either for those covered exactly in the grids, or for different, but close, values of these parameters. We shall also describe several procedures for upgrading the available models by updating model atoms and/or adding new explicit chemical species.

6.2 Producing detailed spectra for grid models

The websites of the model grids already contain a synthetic spectrum, but only with a relatively low wavelength resolution of about 1 Å. For many purposes, one needs synthetic spectra of much higher resolution, or for wavelength regions not covered by the distributed files, or perhaps with somewhat different chemical abundances than those considered in the model grids. For all these purposes, SYNSPEC provides the necessary tool.

Running SYNSPEC is actually very simple. Taking an example of a sample B-star model that is contained `$TLUSTY/examples/bstar`, and also in the specific directory `$TLUSTY/synspec/examples/bstar`, namely `BGA20000g400v2` (for $T_{\text{eff}} = 20,000$ K, $\log g = 4$, $v_{\text{tb}} = 2$ km/s, and solar composition), one produces a synthetic spectrum by using the script `RSynspec`

```
cd $TLUSTY/synspec/examples/bstar
[cp superlevels fort.57]
RSynspec BGA20000g400v2 fort.55.sol data/linelist.test
```

As mentioned before, this script accomplishes a number of tasks:

- links the general "data" directory `$TLUSTY/.data` to `./data`,
- links the auxiliary input file `fort.55.sol` to `fort.55`;
- links the sample line list `$TLUSTY/data/linelist.test` to `fort.19` (notice that since the script makes the link to the "data" directory first, one can refer to this file as `data/linelist.test`;
- copies the file `BGA20000g400v2.7` (input model atmosphere) to `fort.8`;

⁴<http://tlusty.oca.eu>

- runs SYNSPEC, and
- stores important output files.

If the file **superlevels** is not copied to **fort.57**, the association of levels referred to in the line list and in the TLUSTY input is done analogously as for light elements, without taking into account the parity of the levels. If the file **fort.57** exists, an information contained in it allows for a more consistent association of levels – see Appendix B. The latter is obviously a better option.

In this example, **fort.55.sol** is analogous to that used in §5.3.1, namely

```

0      34      0
1      0      0      0
0      0      0      0      0
1      1      0      0      0
0      0      0
1400    1410    10      0  0.0001    0.01
0      0
```

which computes a short interval of spectrum between 1400 and 1410 Å, with the same abundances as those used in computing the model structure, i.e., solar. No input file **fort.56** is necessary.

Another example is an analogous spectrum, where we change abundances of the iron peak elements (Cr to Ni) to 0.5 solar, and for silicon to twice solar, one makes a slight modification of the **fort.55.sol**, which is called **fort.55.nonsol**

```

0      34      0
1      0      0      1
0      0      0      0      0
1      1      0      0      0
0      0      0
1400    1410    10      0  0.0001    0.01
0      0
```

In this case, one needs an additional file, **fort.56**, stored as **fort.56.nonsol**, which looks like this

```

6
14    -2.
24    -0.5
25    -0.5
26    -0.5
27    -0.5
28    -0.5
```

where again the negative values for abundances signify the abundances represented as ratios with respect to the solar ones. This file has to be copied or linked to **fort.56** before running SYNSPEC or invoking the script **RSynspec**.

Finally, to obtain a synthetic spectrum that is directly comparable to observations, one has to convolve the net emergent flux with a rotational velocity

of the star, and possibly with an instrumental profile of the spectrograph that produced an observed spectrum to be analyzed. To this end, one employs an additional utility program called ROTIN, which is described in more detail in Appendix E.

6.3 Using SYNPlot

For the users who have access to the IDL language, running SYNSPEC can be much more easily done through an IDL interface program called SYNPlot⁵ which sets up the input data, runs SYNSPEC and ROTIN, and produces a plot of the resulting synthetic spectrum possibly also accompanied by line identification labels, among other functions that it can perform. All that is accomplished by setting simple keyword parameters. A detailed user's guide is a part of the main distribution file. We will just mention that the above mentioned run of SYNSPEC, moreover with a subsequent convolution with rotational velocity $v \sin i = 20$ km/s, and the Gaussian instrumental profile with FWHM=0.2 Å, can be accomplished by the following simple IDL statement

```
synplot,atmos='BGA20000g400v2',wstart=1400,wend=1410, $
abund=[14,14,-2.,24,28,-0.5],vrot=20,fwhm=0.2
```

6.4 Running a B-star model

As pointed out above, constructing a fully line-blanketed NLTE model from the scratch is not trivial, for one often needs to proceed in several judiciously chosen intermediate steps – for more on this topic, refer to Paper III, Chaps. 5 and 10. Therefore, when one needs to construct a model within the range of the BSTAR2006 or OSTAR2002 model grids, it is easier to start with the closest existing model and use it as the starting model for the run.

In this section, we describe this approach in the case where the choice of explicit atoms, ions, and levels remains the same as in the original model. The case when one needs to change the structure of explicit atoms, ions, or levels, is described below in § 6.6 and § 6.7.

As an example, let us assume that one intends to construct a model with $T_{\text{eff}} = 20,500$ K, $\log g = 4.1$, and with the iron abundance being 1.5 times the solar abundance, and the Mg and Si abundance 0.6 times solar. We set up a new standard input file and call it, in analogy with the BSTAR2006 grid convention, as BGA21000g410sp.5. It is very similar to the original BGA20000g400v2.5 file. For convenience, we will show it below:

```
20500. 4.1      ! TEFF, GRAV
F F           ! LTE, LTGRAY
'nst'         ! keyword parameters filename
*
```

⁵<http://aegis.as.arizona.edu/~hubeny/pub/synplot2.1.tar.gz>

```

* frequencies
*
2000
*
* data for atoms
*
30          ! NATOMS
* mode abn modpf
  2  0.      0 ! H
  2  0.      0 ! He
  0  0.      0
  0  0.      0
  0  0.      0
  2  0.      0 ! C
  2  0.      0 ! N
  2  0.      0 ! O
  1  0        0
  2  0.      0 ! Ne
  1  0.      0
  2 -0.6      0 ! Mg
  2  0.      0 ! Al
  2 -0.6      0 ! Si
  1  0.      0 ! P
  2  0.      0 ! S
  1  0.      0
  1  0.      0
  1  0.      0
  1  0.      0
  1  0.      0
  1  0.      0
  1  0.      0
  1  0.      0
  1  0.      0
  2 -1.5      0 ! Fe
  1  0.      0
  0  0.      0
  1  0        0
  1  0        0
*
* data for ions
*
*iat  iz  nlevs  ilast ilvlin  nonstd typion  filei
*
  1   0    9    0    0    0  ' H 1' 'data/h1.dat'
  1   1    1    1    0    0  ' H 2' ' '
  2   0   24    0    0    0  'He 1' 'data/he1.dat'

```

2	1	20	0	0	0	'He 2'	'data/he2.dat'
2	2	1	1	0	0	'He 3'	' '
6	0	40	0	0	0	' C 1'	'data/c1.dat'
6	1	22	0	0	0	' C 2'	'data/c2.dat'
6	2	46	0	0	0	' C 3'	'data/c3_34+12lev.dat'
6	3	25	0	0	0	' C 4'	'data/c4.dat'
6	4	1	1	0	0	' C 5'	' '
7	0	34	0	0	0	' N 1'	'data/n1.dat'
7	1	42	0	0	0	' N 2'	'data/n2_32+10lev.dat'
7	2	32	0	0	0	' N 3'	'data/n3.dat'
7	3	48	0	0	0	' N 4'	'data/n4_34+14lev.dat'
7	4	16	0	0	0	' N 5'	'data/n5.dat'
7	5	1	1	0	0	' N 6'	' '
8	0	33	0	0	0	' O 1'	'data/o1_23+10lev.dat'
8	1	48	0	0	0	' O 2'	'data/o2_36+12lev.dat'
8	2	41	0	0	0	' O 3'	'data/o3_28+13lev.dat'
8	3	39	0	0	0	' O 4'	'data/o4.dat'
8	4	6	0	0	0	' O 5'	'data/o5.dat'
8	5	1	1	0	0	' O 6'	' '
10	0	35	0	0	0	'Ne 1'	'data/ne1_23+12lev.dat'
10	1	32	0	0	0	'Ne 2'	'data/ne2_23+9lev.dat'
10	2	34	0	0	0	'Ne 3'	'data/ne3_22+12lev.dat'
10	3	12	0	0	0	'Ne 4'	'data/ne4.dat'
10	4	1	1	0	0	'Ne 5'	' '
12	1	25	0	0	0	'Mg 2'	'data/mg2.dat'
12	2	1	1	0	0	'Mg 3'	' '
13	1	29	0	0	0	'Al 2'	'data/al2_20+9lev.dat'
13	2	23	0	0	0	'Al 3'	'data/al3_19+4lev.dat'
13	3	1	1	0	0	'Al 4'	' '
14	1	40	0	0	0	'Si 2'	'data/si2_36+4lev.dat'
14	2	30	0	0	0	'Si 3'	'data/si3.dat'
14	3	23	0	0	0	'Si 4'	'data/si4.dat'
14	4	1	1	0	0	'Si 5'	' '
16	1	33	0	0	0	' S 2'	'data/s2_23+10lev.dat'
16	2	41	0	0	0	' S 3'	'data/s3_29+12lev.dat'
16	3	38	0	0	0	' S 4'	'data/s4_33+5lev.dat'
16	4	25	0	0	0	' S 5'	'data/s5_20+5lev.dat'
16	5	1	1	0	0	' S 6'	' '
26	1	36	0	0	-1	'Fe 2'	'data/fe2v.dat'
0	0						'data/gf2601.gam'
							'data/gf2601.lin'
							'data/fe2p_14+11lev.rap'
26	2	50	0	0	-1	'Fe 3'	'data/fe3v.dat'
0	0						'data/gf2602.gam'
							'data/gf2602.lin'
							'data/fe3p_22+7lev.rap'


```

26   3   43   0   0  -1  'Fe 4' 'data/fe4v.dat'
0   0                                     'data/gf2603.gam'
                                           'data/gf2603.lin'
                                           'data/fe4p_21+11lev.rap'
26   4   42   0   0  -1  'Fe 5' 'data/fe5v.dat'
0   0                                     'data/gf2604.gam'
                                           'data/gf2604.lin'
                                           'data/fe5p_19+11lev.rap'
26   5   1   1   0   0  'Fe 6' ' ' '
0   0   0  -1   0   0  ' ' ' '
*
* end

```

Notice that the only change with respect to `BGA20000G400v2.5` is in the first line that specifies the basic model parameters, and in the appropriate entries for Mg, Si, and Fe, when the chosen non-solar abundances are specified. The same convention for coding the chemical abundances as that shown in § 5.3.1 is used here as well; that is, if a number is negative, its absolute value expresses the ratio of the current abundance to the solar one. Since the choice of explicit ions and levels remains the same as in the `BSTAR2006` grid models, the rest of the input file is unchanged.

The structure of the input files, and the meaning of the individual parameters, is explained in detail in the appropriate chapters of Paper III. For the present purposes, we mention that the first three entries of the input data for each ion represent the atomic number of the parent species, charge, and the number of explicit levels, and the last two are the label of the ion, and the filename of the atomic data file. The highest ionization stage of each chemical element must be represented by a one-level ion.

Before running `TLUSTY`, one has to check that the keyword parameter file, in this case called `nst`, is present in the current directory, or is being properly linked to the corresponding file located elsewhere. One can also make a link to the atomic data files, or simply use the script `RTlusty`, described in § 4.5. In this case, the model is run as

```

cd $TLUSTY/examples/bstar
RTlusty BGA20500g410sp BGA20000g400v2

```

This run is not considered as a test case because to fully converge the model may take several hours. This case is presented to provide a guidance to the user about how to construct new models from the models available in the `BSTAR2006` grid.

6.5 Interpolating model structures or predicted spectra?

Since the model atmosphere grids have rather densely spaced values of the basic parameters (T_{eff} , $\log g$, and chemical abundances), it is actually possible

to avoid a rather time-consuming evaluation of a model with different basic parameters, and instead to interpolate between models. Taking the above example, the existing models that bracket the desired values are `BGA20000g400v2`, `BGA21000g400v2`, `BGA20000g425v2`, and `BGA21000g425v2`. A slight complication arises due to requiring non-solar chemical abundances of Mg, Si, and Fe. However, since they do not differ significantly from the solar abundances, they can be neglected for constructing the model structure, and be taken into account only in SYNSPEC.

The question is now which of the two following procedures is more accurate:

- (i) one can construct synthetic spectra for the four bracketing models specified above, with appropriate Mg, Si, and Fe abundances, and then interpolate the resulting spectra to the desired values of T_{eff} and $\log g$, or
- (ii) one interpolates the corresponding structural parameters (temperature, electron density, all atomic level populations) from the bracketing models to the desired values of T_{eff} and $\log g$, using a log-log interpolation, and then compute a single synthetic spectrum for this new interpolated model.

This question was studied in Lanz & Hubeny (2003), who have demonstrated that it is in most cases preferable to use the second option, i.e., interpolate the models and then to compute a synthetic spectrum. It is also faster, because one computes a synthetic spectrum only once.

6.6 Adding new NLTE species to existing models

For some applications, it might be desirable to add a completely new explicit (i.e., NLTE) chemical element to the set of the original explicit species. We stress that this is an issue for NLTE models only, because for LTE models the only independent structural parameters are the temperature, the total particle number density, and the electron density, while the individual level populations are given as functions of these parameters. For NLTE models, the individual level populations have to be stored as independent state parameters, and therefore when adding new levels or new species one has to make sure that the level populations taken from the input model are properly assigned to a new system of explicit levels.

A relatively simple task is adding new NLTE species to existing models. If the atomic level structure remains otherwise unchanged, this can be accomplished easily. For example, let us assume that one intends to add argon to the set of explicit species. One has of course first construct the appropriate atomic data files. This was actually done (Lanz et al. 2008); the corresponding files are also present in the TLUSTY distribution. The standard input for calculating such model, say for $T_{\text{eff}} = 20,000$ K and $\log g = 4.0$, and with solar abundances, is very similar to `BGA20000g400v2.5`.

We will call the new file `BGA20000t400ar.5`. Here is the structure of the first block of the file:

```
20000. 4.0          ! TEFF, GRAV
```

```

F F          ! LTE, LTGRAY
'nst-ar'     ! keyword parameters filename
*
* frequencies
*
2000
*
* data for atoms
*
30          ! NATOMS
* mode abn modpf
  2  0.      0 ! H
  2  0.      0 ! He
  0  0.      0
  0  0.      0
  0  0.      0
  2  0.      0 ! C
  2  0.      0 ! N
  2  0.      0 ! O
  1  0        0
  2  0.      0 ! Ne
  1  0.      0
  1  0.      0 ! Mg
  1  0.      0 ! Al
  2  0.      0 ! Si
  2  0.      0 ! P
  2  0.      0 ! S
  1  0.      0
  2  0.      0 ! Ar
  1  0.      0
  1  0.      0
  1  0.      0
  1  0.      0
  1  0.      0
  1  0.      0
  2  0.      0 ! Fe
  1  0.      0
  0  0.      0
  1  0        0
  1  0        0
*

```

The only two changes with respect to BGA20000g400v2.5 is different keyword parameter file, **nst-ar**, and a specification of the argon being now considered as an explicit species.

Since the order of explicit ions is arbitrary, one can place the ions of argon at the end of the file, just after the record for Fe 6,

```

26   5   1   1   0   0   'Fe 6' ' ' '
18   0  71   0   0   0   'Ar 1' 'data/ar1_71lev-jK.dat'
18   1  54   0   0   0   'Ar 2' 'data/ar2_42+12lev.dat'
18   2  44   0   0   0   'Ar 3' 'data/ar3_27+17lev.dat'
18   3  26   0   0   0   'Ar 4' 'data/ar4_25+11lev.dat'
18   4   1   1   0   0   'Ar 5' ' ' '
  0   0   0  -1   0   0   ' ' ' '
*
* end

```

The keyword parameter file **nst-ar** is the analogous to **nst**, one only adds a new keyword parameter, namely

ICHANG=1

which signals that the global atomic level structure was changed (energy levels of Ar I to Ar IV were added), but that one deals with a simple change, namely adding energy levels of the new species at the end. The populations of the explicit (NLTE) levels except those of Ar are taken from the input model atmosphere, while the populations of all the argon levels are initialized to their LTE values. Again, this model is not considered as a test case because to fully converge the tmodel may take several hours, but is presented to provide a guidance to the user about how to proceed when adding new chemical elements to existing models.

6.7 Adding atomic energy levels to existing models

In some cases, one may also want to update the existing atomic data file by adding new explicit levels to an already selected explicit ion. For example, one intends to perform a detailed study of neon line formation. The standard data for Ne I and Ne II consider 35 and 32 explicit levels, respectively. One may wish to use more sophisticated model atoms, as was done by Cunha et al (2006). This study considered 79 explicit levels for Ne I, and 138 levels for Ne II. The corresponding data files are also present in the TLUSTY distribution. To run such a model, one has first to modify the input records for Ne I and Ne II to

```

10   0   79   0   0   0   'Ne 1' 'data/ne1_79lev-jK_c1.dat'
10   1  138   0   0   0   'Ne 2' 'data/ne2_138lev.dat'

```

One cannot place the new levels at the end of the file, so one has to communicate to the code that the level structure is being changed in a complex way, and to specify how to initialize the populations of the newly introduced explicit levels. To this end, one has to set the keyword parameter in the **nst** file as

ICHANG=-1

Next, one has to specify an initialization of the level populations. To this end, one has to add NLEVEL records (NLEVEL being the total number of the explicit levels in the new model) at the end of the standard input file, each representing a mode of evaluation of the initial level population. It is done as follows (a more detailed description is presented in Paper III, § 8.2):

(i) all levels of hydrogen through oxygen are unchanged, and their population is taken from the input model atmosphere. Counting these levels, one finds that there are $9 + 1 + 24 + 20 + 1 + 40 + 22 + 46 + 25 + 1 + 34 + 42 + 32 + 48 + 16 + 1 + 33 + 48 + 41 + 39 + 6 + 1 = 530$ such levels (see the listing of the file presented in § 6.4). Thus, the first 530 records that are being placed at the end of the standard input file are:

```

      1      0      0      0      0      0      1.
      2      0      0      0      0      0      1.
      . . . . .
    530      0      0      0      0      0      1.

```

which specify that the level populations of the first 530 levels are initialized as the first 530 level populations of the input model.

(ii) Next, one has to specify the initialization of the 79 levels of Ne I, so one has to set 79 records for each such level. The initialization can be done in several different ways; for simplicity we will assume here that all the populations of the Ne I levels except of the ground state are initialized to LTE populations. In this case the input records are:

```

    531      0      0      0      0      0      1.
      0      1 566      0      0      0      1.
.. and the same record 77 more times

```

Here, the first record specifies that the ground state of Ne I, with the global level index 531, is again taken from the input model, while the next 78 levels (all excited states of Ne I) are initialized to LTE. Specifically, the first number, =0, indicates that there is no equivalent level in the original model⁶; the second number, = 1, indicates LTE, and the third number specifies that the LTE is taken with respect to the ground state of the next ion (Ne II), which has a global index in the old model equal to 566 (i.e. 530 previous levels for H – O, plus 35 levels in the old model atom for Ne I, plus 1).

Analogously, for Ne II, one has altogether 138 records, again one for the ground state and 137 identical ones for the excited states,

```

    566      0      0      0      0      0      1.

```

⁶In fact, some newly specified levels can have equivalents in the old system of levels, either having an identical counterpart, or originating by a splitting of an original level composed of several actual levels, etc. TLUSTY can deal with such a situation, see Paper III, § 8.2, but since this procedure influences only the initial level populations which are going to be immediately recomputed by the code anyway, a simple procedure outlined here is satisfactory.

```

0    1 598    0    0    0    1.
.. and the same record 136 more times

```

because the ground state of Ne III has global index 598 in the input model.

(iii) The levels of the subsequent ions of Ne III - Ne V, and all ions of Mg, Al, Si, S, and Fe are unchanged. There are altogether $34+12+1+25+1+29+23+1+40+30+23+1+33+41+38+25+1+36+50+43+42+1 = 530$ such levels (which is just a coincidence with the previous unmodified 530 levels). One will thus have 530 additional records analogous to the first 530 records, namely

```

598    0    0    0    0    0    1.
599    0    0    0    0    0    1.
.....
1127    0    0    0    0    0    1.

```

because the total number of all explicit levels in the input model is $530 + 35 + 32 + 530 = 1127$.

7 What is next?

The present paper serves as a truly brief introduction to working with TLUSTY, and provides only a rudimentary information about the code. To gain a more thorough understanding of the physics and numerics involved, the user is encouraged to study Paper II. For understanding of the input parameters and many options offered by TLUSTY, Paper III provides the necessary information and guidance.

For SYNSPEC, which is conceptually much simpler, this document provides a complete guide for its operation. The only additional information relevant to SYNSPEC covered in Paper II is a description of the available radiative transfer equation solvers, and a description of the standard input file used by both TLUSTY and SYNSPEC, given in Paper III.

Acknowledgements

A more complete list of a large number of colleagues that contributed to the development of TLUSTY and SYNSPEC, or who encouraged us to implement various upgrades, is presented in Paper III. Here we would like to gratefully acknowledge a useful feedback on this paper provided by Yeisson Ossorio, Klaus Werner, Marcos Diaz, and, in particular, Peter Nemeth and Knox Long. I.H. gratefully acknowledges the support from the Alexander von Humboldt Foundation, and wishes to thank especially to Klaus Werner for his hospitality at the Institute of Astronomy and Astrophysics of the University of Tübingen, where a part of the work on this paper was done.

Appendix A: Treatment of line profiles in SYNSPEC

The treatment of line profiles in SYNSPEC is independent of that used in TLUSTY. The rationale for this approach is that in TLUSTY the main emphasis is on the global solution of the all structural equations, where often, in particular for weak lines, details of the treatment of line profiles are inconsequential. Moreover, the computer time needed to compute a model may already be quite large, so one can afford, or even should use, approximations of the line profiles of weaker lines. In contrast, SYNSPEC only computes an emergent radiation, so this should be done as accurately as possible, and consequently an evaluation of intrinsic line profiles is more involved. There is a different treatment of lines of H, He I, He II, and all the other species.

- Hydrogen: The lines of hydrogen are not included in the line list; in fact, the hydrogen lines are treated as a part of the continuum. There are several options, controlled by the parameter `ihydpr` from the input file `fort.55`:
 - if `ihydpr` = 0, then an approximate evaluation of Doppler + Stark broadening of hydrogen lines after Hubeny et al. (1994) is used.
 - if `ihydpr` = 1, the profiles are computed using Lemke’s (1997) Stark broadening tables, contained in the file `./data/lemke.dat`.
 - if `ihydpr` = 2, the profiles are computed using Tremblay & Bergeron (2009) tables, contained in the file `./data/tremblay.dat`.
 - if `ihydpr` < 0, the line profiles are computed using Schoening & Butler (1989) tables, contained in the file `./data/hydprf.dat`.

There is another possible modification of the hydrogen line profiles which can be used together with any of the above options, namely including the *quasi-molecular satellites* of the hydrogen Lyman lines and the H α line, after Allard & Koester (1992). Their inclusion is controlled by the `fort.55` parameters `nunalp`, `nunbet`, `nungam`, and `nunbal` for Lyman α , β , γ , and H α satellites, respectively. If any of these are set to a non-zero value⁷, an evaluation of the corresponding satellite opacity is switched on. The data are contained in the files `./data/laquasi.dat`, `./data/lbquasi.dat`, `./data/lgquasi.dat`, and `./data/lhquasi.dat`.

- He I: There are three options of treating these lines:
 - If nothing else is specified, the lines are treated as any other metal lines, see below.
 - If one sets the input parameter `ihe1pr` in `fort.55` (see §5.3.1) to a non-zero value, the four triplet lines, $\lambda\lambda$ 4026, 4387, 4471, and

⁷Unlike previous versions of SYNSPEC, the actual values of these parameters do not have any specific meaning; the code now uses explicit `OPEN` statement(s) that specifies the filename(s) of the file(s) that contain the corresponding table.

4921 Å, are treated using special line broadening tables, after Barnard et al. (1974) and Shamey (1969). The tables are contained in the file `./data/he1prf.dat`.

- A more cumbersome option is to change by hand the parameter `iprf` in the line list from the default value of 0 to a specific non-zero value. In this case one will use the treatment of Dimitrijevic & Sahal-Bréchet (1984), with the appropriate data already hardwired in the code. The association of the parameter `iprf` and the line is the following:

λ (Å)	<code>iprf</code>	λ (Å)	<code>iprf</code>
3819.60	1	4437.55	11
3867.50	2	4471.50	12
3871.79	3	4713.20	13
3888.65	4	4921.93	14
3926.53	5	5015.68	15
3964.73	6	5047.74	16
4009.27	7	5875.70	17
4120.80	8	6678.15	18
4120.80	9	4026.20	19
4168.97	10	4387.93	20

- He II: There are two switches that influence the He II lines, both input through the file `fort.55`, `ifhe2` and `ihe2pr`. The parameter `ifhe2` sets a general treatment of the He II opacity:
 - if `ifhe2` > 0, He II is treated as a hydrogenic ion, that is, its lines are taken into account even if they do not appear in the line list. If He II data appear in the line list, they are disregarded and replaced by analytical values for hydrogenic ions. This option is more exact, but is not adopted generally because for cool temperatures, $T < 10^4$ K, the He II ion has a very low population which can sometimes lead to numerical problems.
 - if `ifhe2` = 0, the hydrogenic property of He II is not taken into account; the He II lines are included only if they appear in the line list, and with parameters given by the line list.

Similarly to He I, there are several options to evaluate the line profiles, controlled by the parameter `ihe2pr`:

- if `ihe2pr` = 0, the He II lines are treated by the default way, i.e.
 - if `ifhe2` > 0, using the approximate hydrogenic Stark + Doppler profile after Hubeny et al. (1994);
 - if `ifhe2` = 0, they are treated as any other metal lines with the broadening parameters specified in the line list.

- if `ihe2pr` > 0, the He II line profiles are given through the Stark broadening tables of Schoening & Butler (1989), contained in the file `./data/he2prf.dat`.
- All other species: Line profiles are given by the Voigt profile, $H(a, x)$, where $x = (\nu - \nu_0)/\Delta\nu_D$, and $a = \Gamma/(4\pi\Delta\nu_D)$. Here, $\Delta\nu_D$ is the Doppler width, ν_0 the line center frequency, a is the Voigt damping parameter, and Γ is the physical damping parameter. The latter is given by

$$\Gamma = \Gamma_{\text{rad}} + \Gamma_{\text{Stark}} + \Gamma_{\text{vdW}}, \quad (1)$$

where Γ_{rad} , Γ_{Stark} and Γ_{vdW} are the natural, Stark, and Van der Waals damping parameters, respectively. They are given by the input parameters `agam`, `gs`, and `gw`, respectively, specified in the line list, `fort.19`. They are given, after Kurucz (1970), by:

- Natural broadening:

$$\Gamma_{\text{rad}} = \begin{cases} 10^{\text{agam}}, & \text{for } \text{agam} > 0, \\ 2.67 \times 10^{-22} \nu_0^2, & \text{for } \text{agam} = 0, \end{cases} \quad (2)$$

- Stark broadening

$$\Gamma_{\text{Stark}} = \begin{cases} 10^{\text{gs}} n_e, & \text{for } \text{gs} > 0, \\ 10^{-8} n_{\text{eff}}^{5/2} n_e, & \text{for } \text{gs} = 0, \end{cases} \quad (3)$$

where $n_{\text{eff}} \equiv Z_I [E_H / (E_I - E_j)]^{1/2}$ is the effective quantum number of the upper level, j , of the transition in ion I , with the excitation energy E_j and the ionization energy E_I , Z_I is the effective charge ($Z_I = 1$ for neutrals) of the ion I , E_H is the ionization energy of hydrogen, and n_e is the electron density.

- Van der Waals broadening

$$\Gamma_{\text{vdW}} = \begin{cases} 10^{\text{gw}} c_w, & \text{for } \text{gw} > 0, \\ 4.5 \times 10^{-9} (2.5 n_{\text{eff}}^4 / Z^2)^{0.4} c_w, & \text{for } \text{gw} = 0, \end{cases} \quad (4)$$

where $c_w = (N_{\text{H}} + 0.42 N_{\text{He}}) (T/10^4)^{0.3}$.

Appendix B: Treatment of NLTE level populations in SYNSPEC

As explained above, for explicit species in a NLTE model atmosphere, the level populations used for evaluating the bound-free are free-free transitions are taken from the model atmosphere generated by TLUSTY. On the other hand, the line list contains, for a given line, the J -values and level energies for the lower and the upper level of the corresponding transition. Based on this information,

SYNSPEC makes an association of the levels being specified in the line list and the explicit levels that are specified through the TLUSTY input atomic data files.

An association of levels specified in the line list, and the explicit levels specified by the TLUSTY standard input is done differently for light elements which do not use the concept of superlevels and superlines, and for the iron-peak elements which do use this concept.

Light elements

For a given line, let ℓ denote a lower level referred to in the line list, with its J -value and energy given as J_ℓ and E_ℓ , respectively, and analogously for its upper level u . The statistical weights and energies of the levels of the corresponding ion, given by the TLUSTY atomic data input, are g_i and \tilde{E}_i , $i = 1, \dots, NL$, respectively. The task is to find which of the levels i from the TLUSTY input correspond to ℓ , this level is denoted as I . The association $\ell \rightarrow I$ is done such as $I = 1$ for $E_\ell \leq \tilde{E}_2/2$, and $(\tilde{E}_I + \tilde{E}_{I-1})/2 \leq E_\ell < (\tilde{E}_I + \tilde{E}_{I+1})/2$ otherwise. The corresponding population of level ℓ is then $n_\ell = n_I(2J_\ell + 1)/g_I$, because $2J_\ell + 1$ represents the statistical weight of level ℓ . In other words, SYNSPEC selects the TLUSTY explicit level which has the closest energy to the level specified by the line list, and scales its population by the corresponding ratio of the statistical weights. Such scaling is necessary because TLUSTY often takes for a “level” a set of several actual energy eigenstates of an atom.

Finally, if $E_\ell > E_{NL}$, where E_{NL} is the energy of the highest level of the given ion considered by TLUSTY, n_ℓ is set either to its LTE value (if INLTE=1, where INLTE is specified in the file `fort.55`); or $I = NL$. i.e., all such levels have the same b -factor as level NL (if INLTE=2). A completely analogous procedure is done for level u .

Usually, the populations of the highest explicit levels are close to LTE anyway, so these two options yield essentially the same results. In the (rare) case where the highest explicit level still departs significantly from LTE, the first option, INLTE=1, may lead to wrong results that exhibit themselves by producing spurious emissions. In such a case, the second option is preferable since it usually avoids these emissions. We stress that both options are just approximations; the only exact way to deal with this problem is to improve model atoms by adding more high explicit energy levels. However, one may still face problems because necessary atomic data for such levels are usually poorly known.

The whole process is done automatically by SYNSPEC, and is thus completely transparent to the user. In rare cases when the automatic association produces wrong results (for instance, if there are many different levels with very close energies but with different multiplicity), one has to resort to the manual setting of explicit level indices as shown in § 5.3.3.

Iron-peak elements

Using the association of levels described above for the iron-peak elements may yield inaccurate results because a “level” referred to in the standard input rep-

resents a superlevel, with a generally large span of actual energy levels. Importantly, the superlevels are composed of levels with the same parity. When using an averaged energy of a superlevel to associate it to the level energy specified in the line list, an information about a parity is not used.

Therefore, a better strategy is to provide an additional input file, called **superlevels**, that contains an information about the energy limits of superlevels for both parities. This information is also contained in the atomic data files for the individual ions of the iron-peak elements treated explicitly (usually just Fe). This is explained in detail in Paper III, § 11.4. For now, the structure of the file is best explained on the following example, which provides a necessary input file when producing synthetic spectra for the BSTAR2006 model atmospheres: We display here only the beginning of the file **superlevels**, the complete file is also a part of the standard distribution of TLUSTY

```

4          ! number of ions with superlevels
26 01      ! atomic number and charge of the first such ion (Fe II)
23          ! number of even-parity superlevels
    1000.   ! upper energy limit [in cm-1] of the first superlevel
    5000.   ! analogously for higher superlevels
    1000.
    5000.
    10000.
    20000.
    25000.
    30000.
    35000.
    40000.
    45000.
    52000.
    65000.
    75000.
    82000.
    90000.
    101000.
    112000.
    131000.
    150000.
    165000.
    180000.
    200000.
    220000.
    250000.
13          ! number of odd-parity superlevels
    40000.   ! energy limits, analogous as before
    50000.
```

55000.
70000.
80000.
100000.
116000.
131000.
155000.
180000.
210000.
240000.
280000.

This section contains data for Fe II, the complete file `superlines.ener` contains analogous records for Fe III, IV, and V.

Appendix C: Fine points of running SYNSPEC

A run of SYNSPEC is composed of several basic steps:

- Initialization. The code reads the input model atmosphere and prepares a number of depth-dependent, but frequency independent quantities, such as the solution of the equation of state (i.e., total populations of the individual ionization degrees for all selected chemical species), and a number of other auxiliary quantities.
- Reading of the line list(s) and a selection of lines that are taken into account. Although one could in principle consider all lines that appear in the line list, some sort of a selection of lines is useful because the line list contains data for essentially all ionization stages of all the individual atoms, while only some ionization stages are populated enough that their lines may contribute to the total opacity.

The selection of lines is done based on two input parameters appearing in the file `fort.55`, namely `idstd` and `relop`, and is done as follows: Parameter `idstd` specifies the index of the characteristic depth, as mentioned above in § 5.3.1. The code computes a ratio of the continuum opacity at the (approximate) position of the line and the line-center opacity, $r \equiv \kappa_d^{\text{line}}(\lambda_0)/\kappa_d^{\text{cont}}(\lambda_0)$. If $r < \text{relop}$, the line is rejected. Here the subscript d , equal to `idstd`, refers to evaluating the opacities at depth `idstd`. In some special cases, for instance for atmospheres with a strong temperature rise toward the surface, the depth point with index `idstd` may have much lower temperature than that of the upper layers, and some lines which may contribute significantly to the opacity there may be rejected. In that case the cure is to lower the parameter `relop` to very low values, say 10^{-20} to 10^{-30} , in which case the code selects essentially all lines included in the line list, many of them being completely negligible,

but one can be sure that important lines contributing in the upper layers are not rejected.

- The code then proceeds sequentially through a number of analogous steps, each computing a synthetic spectrum for a small interval of wavelengths, called “set”. There are several substeps:
 - Setting the wavelength points: One goes through the list of selected lines, from the lower wavelength to higher. For each selected line, the code places a wavelength point in the line center, and in the midpoint between the current line and the next one. The code then checks whether the distance of such points is larger than the maximum allowable distance of the points set through the input parameter `space` – see § 5.3.1. If so, the code sets additional wavelength points, equidistantly between the already established points, so that their separation becomes smaller than `space`. In such a way it is guaranteed that no line center nor a window between two lines is omitted, and one still achieves a desired wavelength resolution.
 - Establishing a “set”: Once the number of such wavelength points reaches some preset value, taken by default to be 120, the setting of the wavelength points for this set is completed. Subsequently, the depth-dependent continuum opacity is computed exactly for the endpoints of the set, and is linearly interpolated for the inner wavelength points. This procedure is quite reasonable because it is faster than computing all the wavelength-dependent continuum opacities exactly, and is sufficiently accurate because the continuum opacity varies very slowly with wavelength. Moreover, since the typical value of `space` is around 0.01 Å, the length of the set is about 1 Å, the linear interpolation in wavelengths is completely satisfactory.
 - Finally, computing the synthetic spectrum: The code proceeds wavelength by wavelength, and for all depth points it computes the total line opacity, adds the interpolated continuum opacity, and solves the radiative transfer equation.

Appendix D: Auxiliary SYNSPEC output files

Here we describe in more detail two auxiliary output files from SYNSPEC that are interesting for some particular purposes. The first one is the line identification table, `fort.12`, and the second one is the equivalent width table, `fort.16`. We shall describe them in turn.

Line identification table – `fort.12`

The rationale for producing this table is a simple fact that one often needs to know which actual lines contributed to the individual features seen in the synthetic spectrum.

Let us take an example of a sample synthetic spectrum shown in Fig.2, namely a short wavelength interval between 1400 and 1410 Å, for an LTE model atmosphere with $T_{\text{eff}} = 35,000$ K, and $\log g = 4$. We show the first five records of the file `fort.12` where we skip the first two columns which contain some internal indices of lines, and which are kept for downward compatibility without having any immediate practical meaning:

1400.160	Ni III	-1.27	156852.997	1.81E-04	0.0		0	0	51
1400.160	Co IV	-2.08	182501.396	7.57E-04	0.0		0	0	51
1400.195	Ni IV	-0.64	151574.707	3.08E+00	18.1	**	0	0	47
1400.237	Fe V	0.09	195196.298	1.01E+01	25.9	**	0	0	45
1400.237	Fe V	-1.36	219486.914	1.18E-01	1.6	*	0	0	45

The individual columns represent:

- wavelength [Å]
- indication of an atom and ion
- $\log gf$
- excitation energy of the lower level [cm^{-1}]
- ratio of the line-center opacity to the continuum opacity at the standard depth
- approximate equivalent width [mÅ]
- an indication of the line strength (the more stars, the stronger the line)
- the next two numbers are the indices of the lower and upper levels of the transition for NLTE models. For LTE models, or for levels that are treated in LTE in otherwise NLTE models, they are set to 0
- the last number is the index of the depth where the monochromatic optical depth in the line center is closest to 2/3; i.e., roughly speaking, the index of the depth of formation of the given line.

The approximate equivalent width, W , is computed using classical expressions (e.g. Hubeny & Mihalas 2014, § 17.5), namely

$$W = \begin{cases} (\sqrt{\pi}/2)\beta_0[1 - (\beta_0/\sqrt{2}) + (\beta_0^2/\sqrt{3})] & \beta_0 < 1.2 \\ \sqrt{\ln \beta_0} & 1.2 \leq \beta_0 \leq 55 \\ (1/2)\sqrt{\pi a_0 \beta_0} & \beta_0 > 55. \end{cases} \quad (5)$$

where $\beta_0 = \chi_0/\kappa_c$ is the ratio of the line-center to the continuum opacity, and a_0 is the Voigt damping parameter, both computed at the standard depth.

This information can be used to identify the spectral features in the predicted spectrum. In fact, this is done in the above-mentioned IDL package SYNPLLOT. As an illustration, we present in Fig. 4 an analogous plot to Fig.2, produced with SYNPLLOT, that marks the individual predicted features, using the information from `fort.12`.

Equivalent widths table – `fort.16`

The classical concept of line equivalent width is still used in many spectroscopic studies. However, this concept is only useful if one deals with isolated lines.

1409.846	1410.000	21.9	21.9	1785.5	1785.5
----------	----------	------	------	--------	--------

The individual columns have the following meaning:

- initial wavelength of the interval λ_0 [Å]
- ending wavelength of the interval λ_1 [Å]
- equivalent width [mÅ] of this interval (EQW)
- a modified equivalent width, defined such that any emission features, which would produce a negative contribution to the equivalent width, are cut off (MEQW). Obviously, for a synthetic spectrum with only absorption lines, EQW and MEQW are identical.
- cumulative equivalent width (a sum over all previous intervals)
- cumulative modified equivalent width.

Specifically,

$$\text{EQW} = \int_{\lambda_0}^{\lambda_1} [1 - (F_\lambda / F_\lambda^{\text{cont}})] d\lambda, \quad (6)$$

and

$$\text{MEQW} = \int_{\lambda_0}^{\lambda_1} [1 - \min(F_\lambda / F_\lambda^{\text{cont}}, 1)] d\lambda. \quad (7)$$

Appendix E: Program ROTIN

This is a very simple program that performs the rotational and instrumental convolution of the original stellar spectrum. The instrumental profile is assumed to be Gaussian.

The general structure of the standard input file is, using the variable names exactly as they are in the ROTIN source code

```
fname7  fname17  fnout
vrot    chard    stepr
fwhm    stepi
alam0    alam1    irel
```

Here is a brief explanation of the input parameters:

- **fname7** – name of the file containing the detailed spectrum (output **fort.7** from SYNSPEC).
- **fname17** – name of the file containing the continuum flux (output **fort.17** from SYNSPEC).
- **fnout** – filename of the output convolved spectrum.
- **vrot** – rotational velocity $v \sin i$ in km/s.
- **chard** – characteristic distance between two neighboring wavelength points of the original spectrum - in Å.
 - if = 0, program sets up the default value of 0.01 Å.
- **stepr** – wavelength step for evaluation rotational convolution;
 - if = 0, the program sets up default (the wavelength interval corresponding to

the rotational velocity divided by 3.)

- if < 0 , convolved spectrum calculated on the original (detailed) SYNSPEC wavelength mesh.

- **fwhm** – full width at half maximum for a Gaussian instrumental profile (in Å).

- **stepi** – wavelength step for evaluating instrumental convolution (in Å)

- if = 0, the program sets up the default value of **fwhm**/10.

- if < 0 , convolved spectrum calculated on the previous wavelength mesh: used in rotational convolution.

- **alamo**, **alam1** – starting and ending wavelength for the convolved spectrum (in Å).

- **irel** – a switch for setting an evaluation of the absolute or relative spectrum:

- if = 0, an output is the absolute convolved spectrum, in the same units as the original stellar spectrum on **fname7**

- if = 1, an output is the spectrum normalized to the continuum (from input continuum flux on **fname17**).

The output file, with the name specified by the parameter **fnout**, is a simple table of wavelength (in Å) versus flux, either absolute or normalized to continuum, as specified by the input – see above.

For completeness, the convolutions for the rotational and instrumental broadening are evaluated as

$$F^{\text{conv}}(\lambda) = \int_{\lambda-\Delta\lambda_0}^{\lambda+\Delta\lambda_0} G(\lambda - \lambda') F(\lambda') d\lambda', \quad (8)$$

where F is the radiation flux, and G the corresponding kernel function. For the rotational broadening, G is given by (e.g., Gray 2008)

$$G(\Delta\lambda) = \frac{2(1 - \epsilon) \left[1 - (\Delta\lambda/\Delta\lambda_0)^2 \right]^{1/2} + (\pi\epsilon/2) \left[1 - (\Delta\lambda/\Delta\lambda_0)^2 \right]}{\pi\Delta\lambda_0(1 - \epsilon/3)}, \quad (9)$$

where $\lambda_0 = (\lambda v \sin i)/c$, ϵ is the limb-darkening coefficient, which is hardwired in ROTIN as $\epsilon = 0.6$. It would be possible to consider it as a free parameter, but we decided not to. The reason is that for evaluating an accurate rotationally broadened spectrum it is preferable to perform an integration over the stellar surface exactly, using angle-dependent specific intensities of radiation, which can also be produced by SYNSPEC, instead of flux.

For the instrumental convolution, the kernel is given by

$$G(\Delta\lambda) = c_1 \exp[-\Delta\lambda/\Delta\lambda_I^2], \quad (10)$$

where $\Delta\lambda_I = \text{FWHM}/(2\sqrt{\ln 2}) = 0.60056 \times \text{FWHM}$, and $c_1 = 1/(\sqrt{\pi}\Delta\lambda_I)$. The integration limit is formally $\Delta\lambda_0 = \infty$; for a numerical integration it is chosen $\Delta\lambda_0 = 3\Delta\lambda_I$.

References

- Allard, N., & Koester, D. 1992, A&A, 258, 464.
- Auer, L.H., & Mihalas, D. 1969, ApJ, 158, 641.
- Auer, L.H., & Mihalas, D. 1970, ApJ, 160, 233.
- Auer, L.H., & Mihalas, D. 1972, ApJS, 24, 193.
- Barnard, A., Cooper, J., Smith, E. 1974, JQSRT, 14, 1025.
- Cunha, K., Hubeny, I., & Lanz, T. 2006, ApJ, 647, L143.
- Dimitrijevic, M., & Sahal-Br  chot, S. 1984, JQSRT, 31, 301.
- Freudenstein, & Cooper, J. 1978, ApJ, 224, 1079.
- Gray, D.F., 2008, *The Observation and Analysis of Stellar Photospheres*, Cambridge Univ. Press, Cambridge, 3rd edition.
- Hubeny, I. 1988, Computer Physics Commun. 52, 103.
- Hubeny, I., Hummer, D.G., & Lanz, T. 1994, A&A, 282, 151.
- Hubeny, I., & Lanz, T. 1995, ApJ, 439, 875.
- Hubeny, I., & Lanz, T. 2011, SYNSPEC, Astrophys. Source Code Library, 1189.822.
- Hubeny, I., & Lanz, T. 2017b, TLUSTY User’s Guide II: Reference Manual, (Paper II)
- Hubeny, I., & Lanz, T. 2017c, TLUSTY User’s Guide III: Operational Manual, (Paper III)
- Hubeny, I., Lanz, T., & Jeffery, C.S. 1994, in Newsletter on Analysis of Astronomical Spectra No. 20, ed. C.S. Jeffery, St. Andrews Univ., p.30.
- Hubeny, I. & Mihalas, D. 2014, *Theory of Stellar Atmospheres*, Princeton Univ. Press, Princeton.
- Kurucz, R.L. 1979, ApJS, 40, 1.
- Mihalas, D., & Auer, L.H., 1970, ApJ, 160, 1161.
- Mihalas, D., Heasley, J., & Auer, L.H., 1975, Technical Report NCAR-TH/STR-104, Boulder, Colorado.
- Lanz, T., Cunha, K., Holtzman, J., & Hubeny, I. 2008, ApJ, 678, 1342.
- Lanz, T., & Hubeny, I. 2003, ApJS, 146, 417.
- Lanz, T., & Hubeny, I. 2007, ApJS, 169, 83.
- Lemke, M., 1997, A&AS, 122, 285.
- Schoening, T., & Butler, K. 1989, A&AS, 78, 51.
- Shamey, L. 1969, PhD thesis, University of Colorado.
- Tremblay, P.-E., & Bergeron, P. 2009, ApJ, 696, 1755.