

TLUSTY & SYNSPEC — A Brief Description

Version 160/24

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1 Introduction

The present set of computer programs is a package designed to accomplish a wide range of stellar spectroscopic diagnostics. In its maximum configuration, the user may start from scratch and calculate a model atmosphere of a chosen degree of complexity, and end with a synthetic spectrum in a wavelength region of interest for an arbitrary stellar rotation and an arbitrary instrumental profile.

The basic component of the package is TLUSTY, the program for calculating plane-parallel, horizontally homogeneous model stellar atmospheres in radiative and hydrostatic equilibrium. Departures from local thermodynamic equilibrium (LTE) are allowed for a set of occupation numbers of selected atomic and ionic energy levels. The program also allows for convection, but the current version works only for LTE convective models.

The second basic program is SYNSPEC, which is a program for calculating the spectrum emergent from a given model atmosphere. It has been written particularly to synthesize spectra from atmospheres calculated using TLUSTY, but may also be used with other model atmospheres as input (e.g. Kurucz' ATLAS models). The program is complemented by program ROTINS which calculates the rotational and instrumental convolutions for the net spectrum produced by SYNSPEC.

Finally, there is a number of interface and utility programs. They serve to prepare a part of the input data for TLUSTY (e.g. program SETFRE - for setting frequency points and integration weights in continuum); provide graphical interface for plotting output models, the convergence log etc. (written in IDL and/or Mongo); and a graphical interface for SYNSPEC (plotting spectra, identifying lines; again written in IDL).

We stress that the set of programs does not represent a rigid structure of standard programs; instead, it is a highly dynamic set in a permanent state of gradual development. The versions being described here are TLUSTY160 and SYNSPEC24. At the time of writing this Guide, the latest existing version have serial numbers 175 and 32, respectively. We intend to provide periodic updates of this manual, basically after a significant milestone has been reached. In the case of TLUSTY, this will occur when the hybrid complete linearization/accelerated lambda iteration method is worked out, and NLTE line blanketing has been fully tested and released for general use.

Considerable effort was spent on implementing both programs on a variety of different computers and operating systems. TLUSTY is currently running basically under various UNIX-based operation systems (OSF/1, Ultrix, SunOS, Unicos), as well as VMS. In version 160, there is only one single feature which depends explicitly on a computer system, namely a timing routine (run under UNIX), which has to be commented out for the use under the VMS operation system (function `ETIME`).

TLUSTY is also implemented on vector computers. The present version of TLUSTY is moderately well vectorized; subsequent versions (TLUSTY167 and later) still better so. However this has been at the cost of losing some of the modular and simple-to-understand structure which proved not to be optimum from the point of view of vectorization.

Finally, we mention that an analogous set of programs also exists for accretion disks; a program for computing the vertical structure of a disk, TLUSDISK, as well as synthetic spectra, SYNSPECU (the U stand for "universal"; in fact this program synthesizes spectra either for a model atmosphere or a disk). Program SYNSPECU also allows for calculating emergent intensities at specified angles, not only the radiation flux as is done in the standard variants. These programs are not currently distributed through CCP7, but an interested reader may directly contact I. Hubeny to obtain a copy.

2 TLUSTY

2.1 General characteristics

The basic features of the program are the following:

1. The program solves the basic equations (radiative transfer, hydrostatic equilibrium, radiative equilibrium, statistical equilibrium, charge and particle conservation) by the method of complete linearization, first introduced by Auer and Mihalas (1969). Nevertheless, not all of the basic equations have to be actually solved. The program has options for omitting some of the equations, keeping the corresponding quantities fixed. For instance, one may keep the temperature fixed and skip the radiative equilibrium equation (all the other equations being solved exactly); this corresponds to calculating the so-called semi-empirical models.
2. The program is fully data oriented as far as the choice of atomic species, ions, energy levels, transitions, and opacity sources is concerned. Furthermore, atomic transitions (lines and continua) may be treated in various degrees of sophistication. In particular, substantial computer time is saved by introducing the so-called *fixed* transitions, which are treated essentially exactly, but are not linearized. We note that we have recently improved significantly this option by treating the “fixed” transition not as truly fixed, but rather by means of the Accelerated Lambda Iteration (ALI) scheme (Hubeny and Lanz 1994).
3. The final NLTE model is usually calculated by the standard procedure which consists of calculating consecutively a series of models with increasing complexity: first an LTE-grey model, then an LTE model, then a NLTE model where all lines are assumed to be in detailed radiative balance (usually denoted as NLTE/C models; C stands for “continua-only”); and finally a model where also lines are considered explicitly. The last step may actually be composed of several partial steps, with gradually increasing number of lines considered. Except for the LTE-grey model, which is calculated from scratch, an initial estimate of the model is required. This is usually a converged model from the previous step, but it may also be a model taken from literature deemed to be a reasonable initial estimate.
4. The code is written in standard FORTRAN77, making it highly portable. In particular, the following rules hold throughout the program:
 - – names are restricted to six characters;
 - – END DO, DO WHILE are *not* used;
 - – no STRUCTURES are used;
 - – no Debugging Lines (beginning with D) are used;
 - – all comments are on separate lines starting with C.

A detailed description of TLUSTY is given by Hubeny (1988). This paper describes the basic concepts, equations, and numerical methods used. However, because the program has developed considerably since 1988, the description presented in this paper is sometimes obsolete. The new developments are virtually always downward compatible; i.e. all in the older versions are preserved in a newer version. In other words, the newer versions only add new features, but do not delete the existing ones. Below, we list the most important modifications.

- Inclusion of convection. This is done within the framework of the standard mixing-length theory described e.g. by Mihalas (1978, pp. 187-192) and Gustafsson (1971).
- Incorporation of several algorithms preventing divergences, namely the collisional-radiative switching method of Hummer and Voels (1988), and the so called rescaling method of Hubeny (1990).
- Acceleration algorithms (Kantorovich variant of the Newton-Raphson method; and the Ng acceleration), described in detail by Hubeny and Lanz (1992).
- Incorporation of the occupation probability formalism (Hummer and Mihalas 1988), and its extension to NLTE situations; a detailed treatment of the line merging near the series limits. Detailed description can be found in Hubeny, Hummer, and Lanz (1994).

- Improved treatment of the radiative equilibrium equation (Hubeny and Lanz 1994)
- A number of various coding improvements and changes.

Although considerable effort has been devoted to eliminate errors in the code, there is by no means a guarantee that it is error free. The user is thus warned against using program as a “black box”. It would be highly appreciated if any errors detected by the user, and any comments or suggestions for an improvement, are communicated to I. Hubeny (Internet address: hubeny@stars.gsfc.nasa.gov, or, more appropriately for the present purpose, hubeny@tlusty.gsfc.nasa.gov).

2.2 Compiling and linking

The program is distributed as several files. The largest is `TLUSTYnnn` where `nnn` represents the current version number. In the following text, we take 160 for the current version number. Communication between subprograms is principally carried out through labelled common blocks. To allow for the program to be scaled (re-dimensioned) easily, arrays are dimensioned by parameter constants. The arrays and parameters are defined using 'INCLUDE' files

`IMPLIC.FOR`, `BASICS.FOR`, `ATOMIC.FOR`, `MODELQ.FOR`, `ITERAT.FOR`, `ARRAY1.FOR`, `ODFPAR.FOR`

The basic parameters defining array dimensions appear in INCLUDE file `BASICS.FOR`. The 'INCLUDE' files have to reside in the same directory as the `TLUSTYnnn` file, and, under UNIX, their names *must* be in capital letters, e.g. `BASICS.FOR`.

The compilation and linking is done as follows:

- Under VMS:

```
FOR[/G_FLOAT] TLUSTY160
LINK TLUSTY160
```

The option `/G_FLOAT`, which increases the exponent range, is a recommended option to be used for compiling on VAXes, because it is in some cases crucial for a successful convergence of the modeling procedure.

- Under UNIX:

```
SunOS (Sun SPARCstations):  f77 -N1100 tlusty160.f
Ultrix (DECstations):      f77 [-O4] -static tlusty160.f
```

where the option `"-N1100"` needed for a SUN increases the number of continuation lines to 100; the option `"-static"`, which needs to be specified under Ultrix indicates a static allocation of memory. It is planned to remove this requirement in the future. The optimization (the option `-O4`) is a default at most workstations. If not, the optimization should be switched on since it improves the performance of the code considerably.

- Under Unicos (Cray YMP):

Compiling and linking may be done together by

```
cf77 -Wf"-a static" tlusty160.f
```

Again, the 'INCLUDE' file names must appear in capital letters. Another change which is recommendable is to modify the 'INCLUDE' file `IMPLIC.FOR` from

```
IMPLICIT REAL*8 (A-H), (O-Z), LOGICAL*1 (L)
```

used under VMS and UNIX, to

```
IMPLICIT REAL (A-H), (O-Z), LOGICAL (L)
```

because Cray has already a longer wordlength, and the use of `REAL*8` slows down the execution significantly. Also, it is recommended to replace the ordinary matrix inversion routine `MATINV` by a Cray-specific, highly vectorized routine `MINV` from the standard library LINPACK (or analogous), as indicated in the program.

2.3 Data required

The following input files may be required by TLUSTY; the corresponding subroutines in which they are accessed are shown in parentheses:

- Unit 5 — Main control data (`START`, `STATE`, [`LTEGR`, `CHANGE`])
- Unit 8 — Model atmosphere (`INPMOD`)

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 by `*` or `!` as comment.

Unit 5:

This file contains all the basic control parameters. They represent both the *physical* parameters (i.e. those defining the physical state of an atmosphere to be calculated), as well as the *performance flags*, i.e. parameters that control the numerical performance of the code, and enable the user to choose from a wide variety of numerical options for solving a problem defined by the physical parameters. There is an enormous range of various combinations of options, some of them being used regularly, but some non-standard combinations have never been tried. Therefore, there is no guarantee that all combinations work perfectly. In case of any troubles, it would be appreciated if the user contact the authors.

The user is encouraged to make some effort to understand the meaning of the basic parameters. Current experience with public use indicates that most users only slightly modify the benchmark tests provided, e.g. by changing the effective temperature and surface gravity. We stress that while this is a reasonable strategy for a beginner, and even then only for calculating models with close enough parameters, it may be *very* dangerous to use this option too blindly.

The unit 5 file is organized into 8 basic blocks; each block being generally composed of various numbers of records. The number of records depends on certain parameters from the previously read part of the input (as, for instance, on the number of explicit atoms, ions, levels, transitions, etc.). Also, in some cases, switching on certain flags may imply reading one or more additional input records which would otherwise be absent.

The eight constituent blocks are the following:

1. Basic input parameters
2. Frequency points
3. Turbulent velocities
4. Input parameters for individual explicit and implicit atoms
5. Input parameters for individual explicit ions
6. Input parameters for individual explicit levels
7. Input parameters for individual transitions
8. Additional parameters

The last block is a very heterogeneous mixture of both physical parameters and performance flags. Also, while the structure of the first seven blocks is quite regular, the structure of the last block depends to a large extent on input data.

A detailed explanation of the input parameters is provided as comments in the source program TLUSTY, subroutines `START` and `STATE`.

Finally, a word of caution for potential users of future versions of the program. We would like to stress that we make every effort to keep the overall structure of input files intact during the gradual development of the program. In most cases, the transition from one version to another is rather easy for a user; new options are coded by assigning a non-traditional value to a flag which is already being used. A typical example is to assign a negative value to a specified flag; the user may run the old data (containing a positive value for a flag) with a new program, and the results will be the same; however, the new features are then switched on by coding a negative value. However, in some rare cases it would be so impractical to keep the structure of data exactly the same that we were compelled to add additional records.

Unit 8: model atmosphere

In most applications, the user does not have to worry about the structure of this file because it is usually created by a previous run of TLUSTY.

2.4 TLUSTY: Output

There are several output files. We divide them into three groups, listed and described below. By default, all the output files are generated as ASCII files for an easy portability.

1. Basic output – produced always
 - Unit 6 – Standard output
 - Unit 7 – Condensed model atmosphere
 - Unit 9 – Convergence log
 - Unit 10 – Performance and error log
 - Unit 69 – Timing (Unix only)
2. Auxiliary output – produced always
 - Unit 30 – Check of the statistical equilibrium equation solution
 - Unit 39 – Check of the radiative equilibrium equation solution
 - Unit 81 – Emergent flux in fixed and explicit frequency points
3. Auxiliary output – created conditionally, depending on input
 - Unit 16 – Additional output for selected atomic transitions
 - Unit 18 – Collisional-radiative switching parameters
 - Unit 66 – Rescaling parameters

2.4.1 Basic standard output

Unit 6: Standard output.

This is a general log of the model construction procedure. It contains tables displaying the input data, some performance (and possibly error) messages, and prints several tables of the output model. In most cases, these tables are self-explanatory.

The amount of output on Unit 6 is dependent upon input parameters. For instance, in the case where an LTE-grey model is generated (`LTEGR=.true`), there is a table containing the computed LTE-grey models. Another important portion of the output are tables containing various quantities produced if convection is taken into account.

The standard part of the output on Unit 6 (always present) is generated by the following subroutines: `START`, `STATE` (tables of input parameters); and `OUTPRI` (tables of resulting model parameters). For convenience, a part of this file is repeated on different output files. It concerns the performance and error messages (Unit 10), and emergent flux (Unit 81). This is useful either for a quick look if something went wrong (Unit 10), or for easy plotting (Unit 81). The basic quantities of the model itself appear on Unit 7.

Unit 7: Condensed model atmosphere.

This is the basic output in a machine-oriented form, i.e. without any table headers, etc. It is created by subroutine `OUTPUT`. This file may serve as the model input to another run of TLUSTY as Unit 8, or to `SYNSPEC` and various interface and utility programs.

Note: Unit 6, if accidentally or intentionally deleted, may to a large extent be re-created by a simple run of TLUSTY using unit 7 output as an input (unit 8), and with a modified unit 5 in which `NITER=0` (i.e. no iterations of complete linearization) and `NLAMB=-1` (suppressing the formal solution completely). In such a case, TLUSTY only reads an input model and calculates the quantities appearing in the output tables.

Unit 9: Convergence log.

This is a very important output file, and the user is strongly encouraged to inspect it carefully after each run (there is also an IDL routine for plotting this file). The file is produced by subroutine `PRCHAN`. It contains, for each iteration of complete linearization, a table of relative changes in temperature, electron density, total particle density, and the maximum relative change of all quantities, as a function of depth. The relative change is defined as (new value - old value)/new value. The changes are printed in the order of decreasing depth index; this is because the linearized system is solved by the block-Gaussian elimination (forward elimination + backward substitution). To declare the computed model as well converged, the relative changes have to be gradually decreasing; in the last iteration they all have to drop below the prescribed value (10^{-3} being a reasonable value in most cases).

Unit 10: Performance and error log.

This file, created possibly by many different subroutines, contains messages about performance (log of accelerations, recalculation of the radiative equilibrium equation division optical depths), and all messages printed by the program when an error status occurs. These errors are either fatal (occurred when checking actual against maximum dimensions; calling various routines with inconsistent parameters; divergence of complete linearization); or warnings (slow convergence of routine `ELCOR` - a solution of the non-linear system of statistical equilibrium + charge conservation; negative opacities, etc.). All messages are more or less self-explanatory.

Unit 69: Timing.

As pointed out above, this file is produced only under Unix. The file is self-explained, and contains time spent for the formal solution (with the subroutine `RESOLV` as a driver), and linearization `SOLVE`, together with the total time elapsed from the beginning of execution.

2.4.2 Auxiliary output

- Unit 30 – check of the statistical equilibrium. Generated by subroutine `CHKSE` in the final iteration. For each explicit level, it prints the total rate in and out, and their difference divided by the rate in, for each depth. The last column should contain much lower values than the previous two columns.
- Unit 39 – Check of the radiative equilibrium. Generated by subroutine `CHKRE` in the final iteration. The table is self-explanatory.
- Unit 81 – Emergent flux. Generated by subroutine `OUTPRI` in the final iteration. It prints various quantities related to the emergent radiation, first for the “fixed frequencies” (if there are any), and then for the explicit frequencies:

2.4.3 Conditional output

- Unit 16 – Additional output for selected atomic transitions. Generated by subroutine `OUTPRI` in the final iteration. It prints, for the selected explicit transitions (line or continuum), the various interesting quantities (radiative rates, source functions, etc.)
- Unit 18 – Collisional-radiative switching parameters. Generated by subroutine `SWITCH`; print the switching parameter as a function of depths. For details, refer to subroutine `SWITCH`.
- Unit 66 – Rescaling parameters. Generated by subroutine `SETRSC`; print the rescaling parameters for each rescaled transition and depth. For details, refer to subroutine `SETRSC`, and to the original paper (Hubeny 1990).

2.5 TLUSTY: example

The basic means of obtaining program `TLUSTY` is to copy a compressed tar file (Unix) from the `CCP7` anonymous ftp account (`ccp7ftp`) or a backup saveset (VMS) from the `CCP7` VMS library (`CCP7GUEST`). Details of these library servers may be found elsewhere. Alternatively, they can be obtained as individual files or as uuencoded tar files by email from one of the authors.

The package consists of two subdirectories or folders. One contains the source code for the program itself, the 'INCLUDE' files, and command procedures to run the program. The second contains all of the files for a three stage bench test.

The benchtest files include all of the input and output files required to calculate one model atmosphere from scratch. The selected model is a moderately complex model atmosphere with solar composition and the basic parameters:

effective temperature $T_{\text{eff}} = 25000$ K
 gravity $\log g = 4$

Hydrogen and helium are considered explicitly; C,N,O are considered implicitly, i.e. for the charge and particle conservation equations. In the final NLTE model, 5 levels of hydrogen, 14 levels of He I, together with 1 level for H II and He II, are treated in NLTE (i.e. altogether 22 NLTE levels).

The calculation is done, as usual, in three steps:

- a) LTE model, starting with LTE-gray model,
- b) NLTE/C, ie. NLTE with continua only model (all lines are assumed in detailed radiative balance) - this model may be used for diagnostics of continua and weak lines, but not for the interpretation of cores of strong lines
- c) NLTE/L model, where now lines are taken into account. There are two variants, called `m25nl` and `n25nl`, which differ by a different treatment of the "fixed-option" lines. Both use model `m25nc` as input.

The files relevant to LTE model are denoted `m25lt.*`
 the files relevant to NLTE/C model `m25nc.*`
 the files relevant to NLTE/L model (1.var.) `m25nl.*`
 the files relevant to NLTE/L model (2.var.) `n25nl.*`

The directory also contains a script file `Tlusty` for running the whole set of benchmark tests under Unix; and a command file `m25.com` for the same run under VMS.

3 SYNSPEC

3.1 General characteristics

Unlike TLUSTY, this program does not have any comprehensive published description. A brief description of the program was given by Hubeny et al. (1985). Program SYNSPEC is a general spectrum synthesis program. It assumes that the model atmosphere is given; either calculated by TLUSTY, or taken from the literature, as for instance from the Kurucz (1979,1993) grid of models. SYNSPEC reads the input model atmosphere and solves the radiative transfer equation, wavelength by wavelength, in a specified wavelength range, and with a specified wavelength resolution. The wavelength points generally are not equidistant. Instead, they are calculated by the program in such a way that there is always a wavelength point at a line center, and in the midpoint between two neighboring lines. The program then adds a certain number of points, equidistantly spaced between these two, such that the interval between the points does not exceed some prespecified value (SPACE – usually about half of a typical Doppler width of a typical metal line). This procedure assures that neither any line center nor any continuum window is omitted.

The program has four basic modes of operation, controlled by a switch `IMODE`. These are as follows:

- 0 — normal synthetic spectrum (i.e. identification table and emergent flux)
- 1 — detailed profiles of a few individual lines
- 2 — emergent flux in the continuum (+ hydrogen lines) (without the contribution of metal lines)
- 1 — identification table only, ie. a list of lines which contribute to opacity in a given wavelength region, together with their approximate equivalent widths. A synthetic spectrum is not calculated.

The adopted continuum as well as line opacity is fully specified by the user. In principle, the line and continuum opacity sources used in calculating a model stellar atmosphere and in calculating the detailed spectrum should be identical. However, it is a common practice that model atmospheres, particularly those allowing for some departures from LTE, are calculated with fewer opacity sources (in particular lines) than

a subsequent calculation of a synthetic spectrum. The rationale for this approach is that the atmospheric structure (*i.e.* the run of temperature and number densities) is predominantly influenced by the strongest opacity sources, while the emergent spectrum has to be computed in detail.

The continuum opacity is calculated exactly the same way as in TLUSTY, and its evaluation is controlled by the data provided from Unit 5. The program considers the following default continuum opacity sources: i) photoionizations from all explicit levels (possibly including pseudo-continua due to dissolution of Rydberg states as described by Hubeny, Hummer and Lanz 1994); ii) free-free opacity for all explicit ions; and iii) electron scattering. The optional continuum opacity sources, included in the program and switched on by setting a corresponding flag, are the Rayleigh scattering, the H^- bound-free and free-free opacity, and the H_2^+ opacity. If SYNSPEC is used for calculating spectra for a model previously calculated by TLUSTY, the necessary data are already available from the previous runs of TLUSTY. For the use of SYNSPEC for calculating synthetic spectra for Kurucz models, the user has to set up the data set him/herself, or can use a TLUSTY data set for a model with similar basic parameters. We stress that in the latter case, the 'explicit' levels, which are originally meant to be the 'NLTE' levels, are set to LTE anyway; the only reason for them being considered as explicit is that the photoionizations from them are important continuum opacity sources.

If the input model atmosphere was calculated assuming LTE, then the source functions for all the lines and continua also have their LTE values (*i.e.* are given by the Planck function); if the input model specifies that some atomic energy levels depart from LTE, then the lines originating from these NLTE levels may be calculated, if desired (switch INLTE), with the corresponding NLTE source function. For hydrogen and helium this is done automatically and the user does not have to specify anything in the line list. For other elements the user has to specify the indices of the upper and lower levels in the line list. If only one level was taken in NLTE in the model construction, the program takes the NLTE value for this one, and an LTE value for the remaining level. Finally, for the lines originating between levels for which no precalculated NLTE population are available one may still use an approximate NLTE treatment, based on the second-order escape probability theory, as described by Hubeny, Harmanec, and Steff (1986).

The intrinsic line profiles have the form of a Voigt function and take into account the effects of natural, Stark, Van der Waals, and thermal Doppler broadening. The line broadening data are either given in the line list (see Sect. 3.3), or, if no broadening parameters are given, are assumed to be given by the classical expressions (see, *e.g.*, Kurucz 1979). The user may also choose to take the Stark broadening data from Griem (1974); in this case the line list has to contain an additional record for each such line (see Sect 3.3).

For hydrogen and helium, the user may choose from several options, ranging from approximate profiles to the use of detailed tables. For hydrogen, the best option is to use tables calculated by Vidal, Cooper, and Smith (1973) for the first four members of the Lyman and Balmer series, supplemented and upgraded recently by Butler (private communication) up to H_{10} . For higher members of the spectral series (together with an occupation probability treatment of high level dissolution), the approach described by Hubeny, Hummer and Lanz (1994) is used as default. For He I, detailed line broadening tables for the λ 4471 line are from Barnard, Cooper and Smith (1974), those for $\lambda\lambda$ 4026, 4387, and 4922 are from Shamey (1969), and those for all other lines, from Dimitrijevic and Sahal-Brechot (1984). For He II, the tables calculated by Schöning and Butler (1989) may be used. All these tables, set up in the format compatible with SYNSPEC, are provided to the interested user upon request.

In the basic mode (IMODE=0), the program proceeds first by selecting lines which may potentially contribute to the total opacity. This is done by selecting the "characteristic depth" in the atmosphere (IDSTD – see description of input file 55), which is roughly given as a depth of formation of the continuum. The program reads the line list, calculates the opacity in the line center at the characteristic depth, and rejects all lines whose central opacity is less than a selected fraction of the continuum opacity (parameter RELOP; typically 0.0001 to 0.001). The parameters for all selected lines are stored in (relatively big) arrays in the program. (Note: in the previous versions of SYNSPEC, the line list was read over and over again, to avoid large arrays which contain data for all selected lines. However, this procedure, albeit very memory-efficient, is quite time consuming. Since the memory is no longer an issue in most computers and workstations, we have chosen to apply the present time-efficient strategy.)

The program then proceeds by calculating many small intervals of spectrum, called "sets". One set is defined as 120 frequency points set up by the program as outlined above; the pure continuum opacity is calculated at the endpoints of the interval and linearly interpolated in between. The first two points of the set apply for the pure continuum radiation field, and the remaining (118) points describe the spectrum including all lines. The length of the individual sets varies because the wavelength points are set by the program, depending on the number of contributing lines and on RELOP; it is typically about 1 - 3 Å. For

each set, the program sets up a subset of lines which contribute in the corresponding interval, both those lines which are located in the interval, as well as those which are “close” and may therefore contribute through their wings. The program prints on standard output (Unit 6) for each set a list of lines which contribute in the set, plus a synthetic spectrum (absolute flux as well as the relative flux with respect to the continuum). This provides an internal identification of computed lines.

To make the identification easier, the program also calculates approximate (indicatory) equivalent widths of all selected lines, using the ratio of line-center opacity to the continuum opacity and the broadening parameter at the standard depth. The equivalent widths are calculated by means of the classical theory (see e.g. Mihalas 1978, Chapter 10.). It should be kept in mind that *these equivalent widths are meant for the identification purposes only*, and do not represent the actual predicted equivalent widths. It is impractical to calculate automatically the actual equivalent widths for all lines because virtually all predicted features are blends of several lines. Therefore, the program only calculates the total equivalent width for each set (output onto Unit 16).

The other basic modes of SYNSPEC are similar. `IMODE=1` (few lines) is almost identical to the basic mode; the only difference is that the wavelengths are selected equidistantly. Also, the program works well even if the line list contains just one line, which it is not possible in the basic mode `IMODE=0` since the program is not able to select the wavelength points properly.

`IMODE=2` calculates only opacity (and therefore emergent flux) in the continuum. However, by default, the hydrogen lines are also taken into account.

The identification mode (`IMODE=-1`) proceeds similarly as the basic mode, only does not perform the most time-consuming step - solving the radiative transfer equation and producing the synthetic spectrum. The program only produces the identification table, which may be useful for a number of purposes.

The same programming rules as for TLUSTY are adopted for SYNSPEC as well.

3.2 Compiling and linking

The program is distributed as several files. The two largest are `SYNSPECnn` and `SYN3AUX` where `nn` represents the current version number. The first file contains the main i/o and radiative transfer elements of the program, whilst the second contains subroutines for calculating partition functions and mathematical utilities. These are the *only* two programs which need to be compiled and linked together.

Communication between subprograms is principally carried out through labelled common blocks, and to allow for the program to be scaled easily, arrays are dimensioned by parameter constants. The arrays and parameters are defined using 'INCLUDE' files `PARAMS.FOR`, `LINDAT.FOR`, `MODELP.FOR`, `SYNTHP.FOR`. The parameters defining array dimensions appear in `PARAMS.FOR` and `LINDAT.FOR`.

Hints

It may be necessary to reduce the values of parameters `MLINO` and `MNLT` (in the 'INCLUDE' file `LINDAT.FOR`) in order to link the program on certain computers.

It was necessary to set `MLINO = 10000` and `MNLT = 10000` to link SYNSPEC24 on the STARLINK microVAX cluster in St Andrews, where the VMS page file quota was 40000.

3.3 SYNSPEC: Input data

The following input files may be required by SYNSPEC; the corresponding subroutines in which they are accessed are shown in parentheses:

1. Basic input

- Unit 5 — Same file as used for TLUSTY (`START`, `STATEO`)
- Unit 55 — Basic parameters for the synthetic spectrum (`START`, `INIBLO`)
- Unit 8 — Model atmosphere (`INPMOD`, `INKUR`)
- Unit 19 — Linelist (`INISSET`)

2. Additional – optional – input

- Unit 10 — Parameters for additional NLTE levels (optional: `NLTE`)

- Unit 56 — Change of chemical composition with respect to the input model atmosphere (optional: STATEO)
- Unit IBVCS — Detailed Balmer line profiles (optional: BALINI)
- Unit IHE144 — Detailed HeI 4471 line profile (optional: HE1INI)
- Unit IHE1 — Detailed HeI 4026, 4388, 4922 line profiles (optional: HE1INI)
- Unit IHE2UV — Detailed HeII line profiles calculated by Schoening and Butler, (optional: HE2INI) whose wavelengths are in the UV part of the spectrum, ie. the lines 2-3, 3-5, 3-6, 3-7, 3-8, 3-9, and 3-10.
- Unit IHE2VI — Detailed HeII line profiles (optional: HE2INI); the same for the "visible" lines, ie. 3-4, 4-8, 4-9, 4-10, 4-11, 4-12, 4-13, 4-14, and 4-15.
- Unit IHE2RE — Detailed HeII line profiles (optional: HE2INI); the same for IR and "red" lines, ie. 4-5, 4-6, and 4-7.

Note: Unit numbers IBAL, IHE447, etc., are not hard-wired in the code; instead they are specified by the user in the input file on unit 55.

Unit 5

The file is deliberately kept in the exactly same form as the standard input (Unit 5) for TLUSTY. Although not all parameters needed for TLUSTY are required for a run of SYNSPEC, this arrangement is very convenient from the point of view of the user, since it eliminates a need to create another standard input file.

The data needed for the run of SYNSPEC are basically the numbering of explicit atoms, ions, and levels, and the way the continuum opacity is calculated.

Unit 55: Basic parameters for the synthetic spectrum

The file contains fundamental parameters for evaluating the synthetic spectrum; therefore we present verbatim its detailed description as it appears in subroutines START and INIMOD.

```

C
C   IMODE      =  0 - normal synthetic spectrum
C              =  1 - detailed profiles of a few individual lines
C              =  2 - emergent flux in the continuum (without the
C                  contribution of lines)
C              = -1 - identification table, ie. a list of lines which
C                  contribute to opacity in a given wavelength
C                  region, together with their approximate equivalent
C                  widths. Synthetic spectrum is not calculated.
C
C   IDSTD      - index of the "standard depth" (ie the depth at which
C                  the continuum optical depth is of the order of unity)
C                  (for detailed explanation see the code TLUSTY)
C
C   IPRIN      - determines the amount of output:
C              =0 - "normal output" - identification table + flux,
C                  but no output on unit 36 (depths of formation)
C              =1 - as before, plus unit 36;
C              =-1 - only identification table, no flux (no unit 36)
C              <-1 - no identification table, no flux, no unit 36
C                  (suitable for very long intervals - much faster run)
C
C   INMOD      =  0 - input model atmosphere as a Kurucz model
C                  (read by procedure INKUR)
C              =  1 - input model atmosphere is a model calculated
C                  by the program TLUSTY
C                  (read by procedure INPMOD)
C
C   INTRPL     - switch indicating whether the input model has to be
C                  interpolated to the present depth scale;
C                  for details see procedure INPMOD
C
C   ICHANG     - switch indicating whether the populations from the
C                  input model have to be updated;
C                  for details see procedure CHANGE
C

```

```

C      ICHEMC      - switch indicating that new chemical composition will
C                  be read from unit 56
C      IOPHLI      - switch for treatment the Lyman line wings -see LYMLIN
C
C      ALAMO, ALAM1 - synthetic spectrum is evaluated between wavelengths
C                  ALAMO (initial) and ALAM1 (final), given in Angstroms
C      CUTOFO      - cutoff parameter for normal lines (given in Angstroms)
C                  ie the maximum distance from the line center, in
C                  which the opacity in the line is allowed to contribute
C                  to the total opacity (recommended 5 - 10)
C      CUTOFS      - the same for autoionization lines (at least =50)
C      RELOP       - the minimum value of the ratio (opacity in the line
C                  center)/(opacity in continuum), for which is the line
C                  taken into account (usually 1d-4 to 1d-3)
C      SPACE       - the maximum distance of two neighbouring frequency
C                  points fro evaluating the spectrum; in Angstroms
C
C      INLTE       = 0 - pure LTE (no line in NLTE)
C                  ne.0 - NLTE option, ie one or more lines treated
C                  in the exact or approximate NLTE approach
C                  in this case, other input parameters have to
C                  be specified - unit 10 (see procedure NLTE)
C      ICONTL      = 1 - Lyman and Balmer lines are considered as an
C                  continuum opacity source
C                  ne.1 - Lyman and Balmer lines are not considered as
C                  an continuum opacity source
C      INLIST      = 1 - line list is read in the "original" format
C                  (see procedure INISET)
C                  ne.1 - line list is read in the "new" format
C                  (see procedure INISET)
C      IFHE2       gt.0 - He II line opacity in the first four series
C                  (Lyman, Balmer, Paschen, Brackett)
C                  for lines with lambda < 3900 A
C                  is taken into account even if line list
C                  does not contain any He II lines (i.e.
C                  He II lines are treated as the hydrogen lines)
C
C      and, finally, parameters that were not present in the previous
C      version, namely ILVCS,IBVCS,IHE1,IHE447,IHE2UV,IHE2VI,IHE2RE.
C
C      IBVCS       = 0 - means that Balmer lines are calculated by
C                  approximate formulae
C                  > 0 - means that H-alpha to H-delta are calculated
C                  in detail, using the Vidal, Cooper, Smith tables;
C                  the tables are stored in file FOROxx.dat,
C                  where xx=IBVCS;
C                  higher Balmer lines are calculated as before
C
C      the meaning of other parameters is quite analogous, for the
C      following lines
C
C      IHE1        - He I lines at 4026, 4387, and 4922 Angstroms
C                  (tables calculated by L. Shamey)
C      IHE144      - He I line at 4471 angstroms; tables calculated by
C                  Barnard, Cooper, and Shamey
C
C      IHE2UV      - for the He II lines calculated by Schoening and Butler,
C                  whose wavelengths are in the UV part of the spectrum,
C                  ie. the lines 2-3, 3-5, 3-6, 3-7, 3-8, 3-9, and 3-10.
C      IHE2VI      - the same for the "visible" lines, ie. 3-4, 4-8, 4-9,
C                  4-10, 4-11, 4-12, 4-13, 4-14, and 4-15.
C      IHE2RE      - the same for IR and "red" lines, ie. 4-5, 4-6, and 4-7.

```

Unit 56: Abundance change

The file has exactly the same structure as the corresponding part of the Unit 5 file, and contains the abundance changes (see STATEO).

Unit 19: Line list

The line list has a very similar format as the original Kurucz and Peytremann (1975) tables; however we use recent Kurucz (1990) data, moreover updated and supplemented by more accurate data wherever available.

The structure of the file is very simple: for each spectral line, there are one (or two) records, which contain the following parameters; the description is again taken verbatim as appears in subroutine `INILIN`.

```
C
C  ALAM    - wavelength (in nm)
C  ANUM    - code of the element and ion (as in Kurucz-Peytremann)
C           (eg. 2.00 = HeI; 26.00 = FeI; 26.01 = FeII; 6.03 = C IV)
C  GF      - log gf
C  EXCL    - excitation potential of the lower level (in cm*-1)
C  QL      - the J quantum number of the lower level
C  EXCU    - excitation potential of the upper level (in cm*-1)
C  QU      - the J quantum number of the upper level
C  AGAM    = 0. - radiation damping taken classical
C           > 0. - the value of Gamma(rad)
C
C  There are now two possibilities, called NEW and OLD, of the next
C  parameters:
C  a) NEW, next parameters are:
C  GS      = 0. - Stark broadening taken classical
C           > 0. - value of log gamma(Stark)
C  GW      = 0. - Van der Waals broadening taken classical
C           > 0. - value of log gamma(VdW)
C  INEXT   = 0 - no other record necessary for a given line
C           > 0 - next record is read, which contains:
C  WGR1,WGR2,WGR3,WGR4 - Stark broadening values from Griem (in Angst)
C                       for T=5000,10000,20000,40000 K, respectively;
C                       and n(el)=1e16 for neutrals, =1e17 for ions.
C  ILWN    = 0 - line taken in LTE (default)
C           > 0 - line taken in NLTE, ILWN is then index of the
C                 lower level
C           =-1 - line taken in approx. NLTE, with Doppler K2 function
C           =-2 - line taken in approx. NLTE, with Lorentz K2 function
C  IUN     = 0 - population of the upper level in LTE (default)
C           > 0 - index of the lower level
C  IPRF    = 0 - Stark broadening determined by GS
C           < 0 - Stark broadening determined by WGR1 - WGR4
C           > 0 - index for a special evaluation of the Stark
C                 broadening (in the present version only for He I -
C                 see procedure GAMHE)
C  b) OLD, next parameters are
C  IPRF,ILWN,IUN - the same meaning as above
C  next record with WGR1-WGR4 - again the same meaning as above
C  (this record is automatically read if IPRF<0)
C
C  The only differences between NEW and OLD is the occurrence of
C  GS and GW in NEW, and slightly different format of reading
```

Unit 8: Model atmosphere

The program accepts either a TLUSTY model atmosphere (Unit 7 output there), or Kurucz model atmosphere in the new format (tapes distributed by R. Kurucz starting from the late 1980's and early 1990's). We stress that the first depth point in a Kurucz model is removed because it has been calculated by ATLAS incorrectly (showing a sharp decrease of temperature between the second and the first point). While this feature is likely inconsequential in the context of Kurucz's programs which use an integral method to solve the radiative transfer equation, it may sometimes cause large numerical problems in our scheme which uses the Feautrier (i.e. differential) scheme (see Mihalas 1978).

3.4 SYNSPEC: Output

There are several output files. By default, all the output files are generated as ASCII files for portability.

- Unit 6 – Standard output
- Unit 7 – Condensed synthetic spectrum

- Unit 17 – Theoretical continuum flux
- Unit 16 – Equivalent widths for all 'sets'

Unit 6: Standard output.

This a general log of the model construction procedure, It contains tables displaying the input data, some performance (and possibly error) messages, and prints several tables of the output model. In most cases, these tables are self-explanatory. The file is rather big, and is important only if something goes wrong. In most cases, it can be deleted after a successful completion of the run of the program.

Unit 7 and 17: Emergent flux

These are the basic output files. Unit 7 contains a detailed synthetic spectrum, and consists of a simple table of wavelength versus flux, for all wavelength points considered. The wavelength is expressed in Å, and the flux is expressed as H_λ , in $\text{erg}/\text{cm}^2/\text{s}/\text{Å}$. Unit 17 has an analogous format, and contains the flux for the *theoretical* continuum.

Both files may serve as an input to another program ROTINS, which performs rotational and instrumental convolutions, and sets up files for a plot.

Unit 16: Equivalent widths

As discussed in Sect. 3.1, this file contains a list of total equivalent widths for all individual 'sets', i.e. frequency intervals containing 120 wavelength points and set up automatically by the program.

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