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DFSYNTHE: how to use it

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Abstract. The DFSYNTHE procedure written by R.L. Kurucz for computing opacity distribution functions (ODFs) is here described from the user point of view. An example suited to run the procedure under GNU-Linux is given.

Key words. Stars: model atmospheres – Stars: Abundances

1. Introduction

DFSYNTHE is a Fortran procedure written by R.L. Kurucz to generate tables of opacity distribution functions (ODFs) for given sets of abundances and given values of the microturbulent velocity ξ. The ODF tables are then used as input data for the Kurucz ATLAS9 code, which computes line blanketed model atmospheres. Only recently DFSYNTHE became available to the community, namely since it was converted by R.L. Kurucz from the Cray version to Open-VMS. Notes on DFSYNTHE can be found at the Kurucz website [1]. Just before this workshop took place, we ported DFSYNTHE from open-VMS to GNU-Linux, so that it can now be compiled and executed in a reasonable time on whichever personal computer equipped with the INTEL-Fortran compiler. An important requirement in order to speed up the whole procedure is a CPU of the order of 1 GB. In this paper we give instructions to run DFSYNTHE under GNU-Linux. Examples and source codes are available at our website[2].

2. The line opacity in ATLAS9

The method of the opacity distribution functions solves the problem of handling the line blanketing for model atmosphere computations. We recall that the problem is related with the need for computing numerous integrals over the frequency of various monochromatic quantities f(ν). These integrals are numerically solved by weighted sums over N_ν frequency intervals covering the whole integration range.

$$\int_0^\infty f(\nu)d\nu \simeq \sum_{i=1}^{N_\nu} w_i f(\nu_i)$$

In ATLAS9, as in ATLAS12, a simple trapezoidal rule is used. The weights in the sum are the widths of the intervals in which the integration range is divided, i.e., $w_i=\frac{1}{2}(\nu_{i-1}-\nu_{i+1})$.

Owing to the complex dependence of the line absorption coefficient l_ν on the frequency ν it is not so straightforward to taken it properly into account in the sums. A method is that of

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[1] http://kurucz.harvard.edu/programs/NEWDF/

[2] http://wwwuser.ost.ts.astro.it/castelli/sources/dfsynthe.html

computing a line opacity distribution function (ODF) for each $\nu_{i-1}/2 - \nu_{i+1}/2$ interval.

A description of the ODF method can be found in Kurucz et al. (1974). For a given pair T,P_{gas}, the line absorption coefficient l_ν is exactly computed in the interval $\nu_{i-1}/2 - \nu_{i+1}/2$, then it is rearranged as monotonic function of ν and is averaged over a given number of subintervals. This new function of ν is the opacity distribution function, which is accurate enough for solving integrals over frequency in model atmosphere computations. In particular for ATLAS9, the $\nu_{i-1}/2 - \nu_{i+1}/2$ interval is divided in 12 subintervals and the ODF is represented as a step function, where each step is the average of the ODF values in the subinterval. The ODF in the whole $\nu_{i-1}/2 - \nu_{i+1}/2$ interval is therefore given by a weighted sum of the step functions:

$$l(\nu_{i+1/2}, \nu_{i-1/2}) = \sum_{s=1}^{12} \omega_{s,i} l_{s,i}$$

The weights $\omega_{s,i}$ were selected as 1/10, 1/10, 1/10, 1/10, 1/10, 1/10, 1/10, 1/10, 1/10, 1/20, 1/30, 1/60 of the $\nu_{i-1}/2 - \nu_{i+1}/2$ interval. The integrals over the frequency in ATLAS9 have therefore the form:

$$\int_0^\infty f(\nu)d\nu \simeq \sum_{i=1}^{N_\nu} w_i \sum_{s=1}^{12} \omega_{s,i} f(\nu_{s,i})$$

3. ODFs from DFSYNTHE

For a given pair T,P_{gas}, a given set of abundances $\log\epsilon_i$, and a given microturbulent velocity ξ, DFSYNTHE computes a table of 12xN_f opacity distribution function $l_{s,i}$, where N_f is the number of the frequency intervals which divide the whole integration frequency range, and 12 is the number of the subintervals of each frequency interval.

To compute the $l_{s,i}$ table, the line opacity l_ν is exactly computed for resolving power R=500000 at 3507859 frequency points from λ_1=8.97666 nm to λ_f=10000 nm. The wavelength region is then divided both in 328 intervals (BIG intervals) and in 1212 intervals (LITTLE intervals). Many boundaries represent discontinuities of the opacity spectrum due to bound-free absorption edges. In each interval, l_ν is rearranged in increasing order and averaged over the 12 subintervals quoted above.

The procedure is repeated NTxNP times, where NT is the number of temperatures T and NP is the number of the gas pressure P_{gas}, which are both tabulated in such a way to cover all the T,P_{gas} values occurring in models structures for large samples of model parameters. Input tables of ODFs for ATLAS9 are the whole set of 12xN_fxNpxNT data.

Kurucz's ODFs, available in his CD-ROMs 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, were computed for NT=56 and NP=21, so that each BIG ODF table has 12x328x56x21=4628736 data, and each LITTLE ODF table has 12x1212x56x21=17103744 data. In the new-ODFs from Castelli & Kurucz (2003) NT=57 and NP=25, so that each big ODF table has 5608800 data and each LITTLE ODF table has 20725200 data.

For an ODF table, the values for T and P_{gas}, as well as their number NT and NP can be whichever the user wants. However, ATLAS9 must be modified in accordance with these values and with the dimensions related with them. In fact, because the dimensions of ODFs computed by Castelli & Kurucz (2003) are larger than in ODFs taken from Kurucz's CD-ROMs, new-ODFs can be used only with an ATLAS9 version that accounts for these larger dimensions. This means that it is different from ATLAS9 of the Kurucz website. ATLAS9 to be used with new-ODFs is available at the Castelli website[3].

In ATLAS9, the $l_{s,i}$ for a T, P_{gas}pair of an atmospheric layer, are obtained, in each frequency interval, by interpolation in the appropriate ODF table.

4. Line data for DFSYNTHE

Line data for DFSYNTHE are all the atomic and molecular lines of the line lists from Kurucz's CD-ROMs No 1, 15, 24, 26. Because the wavelengths are here codified for a spectral resolving power R=2000000, while DFSYNTHE works for R=500000, all the lines were resampled at R=500000 over the range

[3] http://wwwuser.oat.ts/astro.it/sources/atlas9.html

Table 1.

the code	input line lists	output line lists
repacklow.for	lowlines.bin	lowlinesdf.bin
repacknlte.for	nltelines.dat	nltelinesdf.bin
repackhi.for	hilines.bin	hilinesdf.bin
repacktio.for	schwenke.bin	tiolinesdf.bin
repackh2o.for	h2ofast.bin	h2olinesdf.bin

8.9766−10000 nm. The resampling codes, listed in col. 1 of Table 1, are available at the Kurucz website[1]. Cols. 2 and 3 of table 1 list the input files taken from Kurucz's CD-ROMs and the output files with the resampled data to be used as input for DFSYNTHE. The resampled files do not contain lines with λ>10000 nm. The line opacity in ATLAS9 for λ>10000 nm is obtained by assigning to 10000000 nm that for 10000 nm and interpolating at the intermediate frequencies.

5. The DFSYNTHE procedure

The DFSYNTHE procedure requires 4 codes: XNFDF, DFSYNTHE, DFSORTP, SEPARATEDF. In this procedure the line absorption coefficient:

$$l_\nu = \frac{1}{\rho}\frac{\sqrt{\pi}e^2}{m_e c} f_{ij}\frac{g_i N_J}{U_j} e^{-\chi_i/kT}\frac{1}{\Delta\nu_D} H(\frac{\Delta\lambda}{\Delta\lambda_D}, \frac{\gamma}{4\pi\Delta\nu_D})(1 - e^{-h\nu/kT})$$

is computed partly in XNFDF and partly in DFSYNTHE. The symbols have the usual meaning. In particular, N_J/U_J is the number density over the partition function of the absorbing element in the j ionization stage, ρ is the gas density, and $\Delta\nu_D$ is the Doppler shift of the transition occurring at the ν_0 frequency:

$$\Delta\nu_D = \frac{\nu_0}{c}\sqrt{\frac{2KT}{\mu m_H} + \xi^2}$$

5.1. The XNFDF code

For a given set of abundances, the XNFDF code computes the atomic and molecular number densities and the continuous opacities for all the T,P_{gas} pairs of the ODF tables. Most subroutines are the same as in ATLAS9, so that the input for XNFDF is similar to that for ATLAS9 when several models are computed in a single run. We recall that this condition is meet when each input model is put just after a BEGIN control card, while the END control card is the last one closing the whole ATLAS run.

In XNFDF there are NT input models, where NT is the number of the temperatures of the ODF tables. Each input model is directly read from unit 5. However, it is not a real model, but it is formed by NP layers with the same T and different P_{gas}, reproducing the T,P_{gas} pairs of the ODF table. The values for TEFF and LOGG of the input models can be whichever, in that they do not matter for the results. The abundances for the ODFs are those fixed in the input models.

In addition to the control cards reads from unit 5 (see the example in Appendix A), other input files are molecules.dat, which provides data for computing molecular partition functions, and continua.dat, which lists the set of frequencies ν_i where continuous absorption coefficients are computed.

Output files are two binary files, called xnfpdf.dat and xnfpdfmax.dat. The data in xnfpdf.dat are: (a) the number densities over partition function N_j/U_j for 99 atoms up to the 10^{th} ionization stage and 60 molecules; (b) the total continuous opacity κ_c at 858 frequency points, which are the borders ν_i, $\nu(i+1)$ and the middle point $(\nu_i - \nu_{i+1})/2$ of 286 intervals which divide the whole wavelength range from 1 to 50000 nm; (c) the ratio of the Doppler velocity for ξ=0 km s^{-1} to the light velocity c for all the elements, i.e., the quantity dopple= $\sqrt{(2KT/\mu m_H)}$/c.

The file xnfpdfmax.dat contains, for each of the 286 frequencies ν_i and for each ionization state of each element, the quantities xnfdopmax that will be used by DFSYNTHE to select from the line lists only those lines which contribute to line opacity at a given frequency for a given pair T,P_{gas}. The quantity xnfdopmax is defined as:

$$\text{xnfdopmax} = (\frac{1}{\rho}\frac{N_j(el)}{U_j(el)}\frac{1}{\Delta\nu_D})/(0.001\kappa_c(\text{min}))$$

where κ_c(min) is the minimum continuous opacity from those at the borders and that in the middle point of the interval ν_i, $\nu(i+1)$, and $\Delta\nu_D$ is the Doppler shift for the frequency in the middle of the interval.

Appendix A shows an example of command file for XNFDF.

5.2. The DFSYNTHE code

Input data for DFSYNTHE are the files xnfpdf.dat and xndpdfmax.dat from XNFDF and a set of NT switches iteff, where NT is the number of temperatures T for the ODF tables. There are NT runs of DFSYNTHE, namely there is a run for each temperature T fixed by setting the corresponding switch iteff to 1 and putting all the other NT-1 switches equal to zero. In each run of DFSYNTHE an ODF table for NP pairs T,P_{gas} is computed, where T (that corresponds to iteff=1) does not change, and P_{gas} assumes all the NP tabulated values.

Input lines are read from all the files listed in the last column of Table 1. Each line is checked against xnfdopmax so that it is discharged when xnfdopmax<1 for that species involved in the transition, or when

$$\frac{\sqrt{\pi}e^2}{m_e c} g_i f_{ij} \mathrm{xnfdopmax} < 1$$

or when

$$\frac{\sqrt{\pi}e^2}{m_e c} g_i f_{ij} e^{-\chi_i/kT} \mathrm{xnfdopmax} < 1$$

The line opacity spectrum is computed at 500000 resolving power, is then divided into the ODF intervals, rearranged as monotonic function in each interval, and averaged over the 12 subintervals.

In each run of DFSYNTHE five different ODF tables with the same T and NP different values for P_{gas} are computed. Each table corresponds to a different microturbulent velocity ξ = 0, 1, 2, 4, 8 km s^{-1}.

Appendix B shows an example of command file for DFSYNTHE.

5.3. The DFSORTP code

The NT runs of DFSYNTHE generate 5 x 57 (i.e 5 x NT) different binary files. Each file contains 25 matrices with dimensions 1540 (rows) x 12 (columns), where 1540 is the number of the frequency intervals resulting by summing the BIG (328) and the LITTLE (1212) intervals, 12 is the number of steps of the ODF in each interval, and 25 is the number of the tabulated P_{gas}.

The data in all the files must be reordered for the use in ATLAS9. The DSORTP code does it. It converts the 25 matrices with dimensions 1540 x 12 in 1540 matrices with dimensions 25 x 12, namely it writes 25 ODFs, tabulated as 12 steps functions, for each frequency interval. The new 5 x 57 reordered files are ascii files.

Appendix C shows an example of command file for DFSORTP applied only to files computed for ξ=2 km s^{-1}.

We remark that in the DFSYNTHE procedure for OpenVMS the rearrangement of the data is performed with the SORT utility and not with a Fortran code as DFSORTP.

5.4. The SEPARATEDF code

For each microturbulent velocity ξ, the SEPARATEDF code merges the 57 ASCII output files from DFSORTP into a single binary file and separates ODFs computed for the BIG intervals from ODFs computed for the LITTLE intervals.

The results from SEPARATEDF are the files DFxxxBIGx.bdf and DFxxxLITx.bdf, which are ready to be used as input files for ATLAS9.

Appendix D shows an example of command file for the SEPARATEDF code.

References

Castelli, F., & Kurucz, R. L. 2003, IAU Symposium, 210, 20P, (astro-ph/0405087)
Grevesse, N., & Sauval, A. J. 1998, Space Science Reviews, 85, 161
Kurucz, R. L., Peytremann, E., & Avrett, E. H. 1974, Washington: Smithsonian Institution: for sale by the Supt. of Docs., U.S. Govt. Print. Off., 1974., 37

Appendix A: An example of command file for XNFDF under Linux

This example shows how to run XNFDF to produce the input files for DFSYNTHE xnfpdf.dat and xnfpdfmax.dat when ODFs for solar metallicity are computed. This example is the same available at Kurucz's website [4] for Open-VMS, except for the number of the temperatures and gas pressures, and for the solar abundances of some elements. Here we adopted abundances from Grevesse & Sauval (1998).

```
ln -s molecules.dat fort.2
ln -s continua.dat fort.17
~/dfsynthe/xnfdf.exe<<EOF>xnfdf.out
READ MOLECULES
MOLECULES ON
ITERATIONS 1 PRINT 0 PUNCH 0
READ FREQUENCIES 1 1 1 TEST
1 1 1
TEFF 5777. GRAVITY 4.43770 LTE
TITLE TEMPERATURES AND PRESSURES FOR DISTRIBUTION FUNCTIONS
OPACITY IFOP 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 0 0 0 0 0 0
CONVECTION ON TURBULENCE OFF 0.00 0.00 0.00 0.00
ABUNDANCE SCALE   1.0000 ABUNDANCE CHANGE 1 0.9204 2 0.0783
 ABUNDANCE CHANGE  3 -10.94  4 -10.64  5  -9.49  6  -3.52  7  -4.12  8  -3.21
 ABUNDANCE CHANGE  9  -7.48 10  -3.96 11  -5.71 12  -4.46 13  -5.57 14  -4.49
 ABUNDANCE CHANGE 15  -6.59 16  -4.71 17  -6.54 18  -5.64 19  -6.92 20  -5.68
 ABUNDANCE CHANGE 21  -8.87 22  -7.02 23  -8.04 24  -6.37 25  -6.65 26  -4.54
 ABUNDANCE CHANGE 27  -7.12 28  -5.79 29  -7.83 30  -7.44 31  -9.16 32  -8.63
 ABUNDANCE CHANGE 33  -9.67 34  -8.63 35  -9.41 36  -8.73 37  -9.44 38  -9.07
 ABUNDANCE CHANGE 39  -9.80 40  -9.44 41 -10.62 42 -10.12 43 -20.00 44 -10.20
 ABUNDANCE CHANGE 45 -10.92 46 -10.35 47 -11.10 48 -10.27 49 -10.38 50 -10.04
 ABUNDANCE CHANGE 51 -11.04 52  -9.80 53 -10.53 54  -9.87 55 -10.91 56  -9.91
 ABUNDANCE CHANGE 57 -10.87 58 -10.46 59 -11.33 60 -10.54 61 -20.00 62 -11.03
 ABUNDANCE CHANGE 63 -11.53 64 -10.92 65 -11.69 66 -10.90 67 -11.78 68 -11.11
 ABUNDANCE CHANGE 69 -12.04 70 -10.96 71 -11.98 72 -11.16 73 -12.17 74 -10.93
 ABUNDANCE CHANGE 75 -11.76 76 -10.59 77 -10.69 78 -10.24 79 -11.03 80 -10.91
 ABUNDANCE CHANGE 81 -11.14 82 -10.09 83 -11.33 84 -20.00 85 -20.00 86 -20.00
 ABUNDANCE CHANGE 87 -20.00 88 -20.00 89 -20.00 90 -11.95 91 -20.00 92 -12.54
 ABUNDANCE CHANGE 93 -20.00 94 -20.00 95 -20.00 96 -20.00 97 -20.00 98 -20.00
 ABUNDANCE CHANGE 99 -20.00
READ DECK6 25 RHOX,T,P,XNE,ABROSS,ACCRAD,VTURB,CONVFRAC,VCONV
   1.000E-4   1995.  1.000E-4  0 0 0 0 0
   3.162E-4   1995.  3.162E-4  0 0 0 0 0
   1.000E-3   1995.  1.000E-3  0 0 0 0 0
   3.162E-3   1995.  3.162E-3  0 0 0 0 0
   1.000E-2   1995.  1.000E-2  0 0 0 0 0
   3.162E-2   1995.  3.162E-2  0 0 0 0 0
   1.000E-1   1995.  1.000E-1  0 0 0 0 0
   3.162E-1   1995.  3.162E-1  0 0 0 0 0
   1.000E-0   1995.  1.000E-0  0 0 0 0 0
   3.162E-0   1995.  3.162E-0  0 0 0 0 0
   1.000E+1   1995.  1.000E+1  0 0 0 0 0
   3.162E+1   1995.  3.162E+1  0 0 0 0 0
   1.000E+2   1995.  1.000E+2  0 0 0 0 0
```

[4] http://kurucz.harvard.edu/NEWDF/xnfdftest.com

```
   3.162E+2   1995.  3.162E+2  0 0 0 0 0
   1.000E+3   1995.  1.000E+3  0 0 0 0 0
   3.162E+3   1995.  3.162E+3  0 0 0 0 0
   1.000E+4   1995.  1.000E+4  0 0 0 0 0
   3.162E+4   1995.  3.162E+4  0 0 0 0 0
   1.000E+5   1995.  1.000E+5  0 0 0 0 0
   3.162E+5   1995.  3.162E+5  0 0 0 0 0
   1.000E+6   1995.  1.000E+6  0 0 0 0 0
   3.162E+6   1995.  3.162E+6  0 0 0 0 0
   1.000E+7   1995.  1.000E+7  0 0 0 0 0
   3.162E+7   1995.  3.162E+7  0 0 0 0 0
   1.000E+8   1995.  1.000E+8  0 0 0 0 0
 1
BEGIN
TEFF   5777.  GRAVITY 4.43770 LTE
TITLE TEMPERATUES AND PRESSURES FOR DISTRIBUTION FUNCTION CALCULATION
 OPACITY IFOP 1 1 1 1 1 1 1 1 1 1 1 1 0 1 0 0 0 0 0
 CONVECTION ON   1.25 TURBULENCE OFF  0.00  0.00  0.00  0.00
ABUNDANCE SCALE   1.0000 ABUNDANCE CHANGE 1 0.9204 2 0.0783
 ABUNDANCE CHANGE  3 -10.94  4 -10.64  5  -9.49  6  -3.52  7  -4.12  8  -3.21
 ABUNDANCE CHANGE  9  -7.48 10  -3.96 11  -5.71 12  -4.46 13  -5.57 14  -4.49
 ABUNDANCE CHANGE 15  -6.59 16  -4.71 17  -6.54 18  -5.64 19  -6.92 20  -5.68
 ABUNDANCE CHANGE 21  -8.87 22  -7.02 23  -8.04 24  -6.37 25  -6.65 26  -4.54
 ABUNDANCE CHANGE 27  -7.12 28  -5.79 29  -7.83 30  -7.44 31  -9.16 32  -8.63
 ABUNDANCE CHANGE 33  -9.67 34  -8.63 35  -9.41 36  -8.73 37  -9.44 38  -9.07
 ABUNDANCE CHANGE 39  -9.80 40  -9.44 41 -10.62 42 -10.12 43 -20.00 44 -10.20
 ABUNDANCE CHANGE 45 -10.92 46 -10.35 47 -11.10 48 -10.27 49 -10.38 50 -10.04
 ABUNDANCE CHANGE 51 -11.04 52  -9.80 53 -10.53 54  -9.87 55 -10.91 56  -9.91
 ABUNDANCE CHANGE 57 -10.87 58 -10.46 59 -11.33 60 -10.54 61 -20.00 62 -11.03
 ABUNDANCE CHANGE 63 -11.53 64 -10.92 65 -11.69 66 -10.90 67 -11.78 68 -11.11
 ABUNDANCE CHANGE 69 -12.04 70 -10.96 71 -11.98 72 -11.16 73 -12.17 74 -10.93
 ABUNDANCE CHANGE 75 -11.76 76 -10.59 77 -10.69 78 -10.24 79 -11.03 80 -10.91
 ABUNDANCE CHANGE 81 -11.14 82 -10.09 83 -11.33 84 -20.00 85 -20.00 86 -20.00
 ABUNDANCE CHANGE 87 -20.00 88 -20.00 89 -20.00 90 -11.95 91 -20.00 92 -12.54
 ABUNDANCE CHANGE 93 -20.00 94 -20.00 95 -20.00 96 -20.00 97 -20.00 98 -20.00
 ABUNDANCE CHANGE 99 -20.00
READ DECK6 25 RHOX,T,P,XNE,ABROSS,ACCRAD,VTURB,CONVFRAC,VCONV
   1.000E-4   2089.  1.000E-4  0 0 0 0 0
   3.162E-4   2089.  3.162E-4  0 0 0 0 0
   1.000E-3   2089.  1.000E-3  0 0 0 0 0
   3.162E-3   2089.  3.162E-3  0 0 0 0 0
   1.000E-2   2089.  1.000E-2  0 0 0 0 0
   3.162E-2   2089.  3.162E-2  0 0 0 0 0
   1.000E-1   2089.  1.000E-1  0 0 0 0 0
   3.162E-1   2089.  3.162E-1  0 0 0 0 0
   1.000E-0   2089.  1.000E-0  0 0 0 0 0
   3.162E-0   2089.  3.162E-0  0 0 0 0 0
   1.000E+1   2089.  1.000E+1  0 0 0 0 0
   3.162E+1   2089.  3.162E+1  0 0 0 0 0
   1.000E+2   2089.  1.000E+2  0 0 0 0 0
   3.162E+2   2089.  3.162E+2  0 0 0 0 0
   1.000E+3   2089.  1.000E+3  0 0 0 0 0
   3.162E+3   2089.  3.162E+3  0 0 0 0 0
   1.000E+4   2089.  1.000E+4  0 0 0 0 0
```

```
   3.162E+4   2089.  3.162E+4  0 0 0 0 0
   1.000E+5   2089.  1.000E+5  0 0 0 0 0
   3.162E+5   2089.  3.162E+5  0 0 0 0 0
   1.000E+6   2089.  1.000E+6  0 0 0 0 0
   3.162E+6   2089.  3.162E+6  0 0 0 0 0
   1.000E+7   2089.  1.000E+7  0 0 0 0 0
   3.162E+7   2089.  3.162E+7  0 0 0 0 0
   1.000E+8   2089.  1.000E+8  0 0 0 0 0
 1
BEGIN
...the same for T=2188,  2291,  2399,  2512,  2630,  2754,  2884,  3020,  3162,
                  3311,  3467,  3631,  3802,  3981,  4169,  4365,  4571,  4786,
                  5012,  5370,  5754,  6166,  6607,  7079,  7586,  8128,  8710,
                  9333, 10000, 11220, 12589, 14125, 15849, 17783, 19953, 22387,
                 25119, 28184, 31623, 35481, 39811, 44668, 50119, 56234, 63096,
                 70795, 79433, 89125,100000,112202,125893,141254,158489,177828,
                199526

END
EOF
mv fort.10  xnfpdf.dat
mv fort.11 xnfpdfmax.dat
rm fort.*
```

Appendix B: An example of command file for DFSYNTHE under Linux

This example shows the 57 runs of DFSYNTHE needed to compute preliminary tables of ODFs for ATLAS9. In each run of DFSYNTHE 5 tables of ODFs for 5 different microturbulent velocities 0, 1, 2, 4, 8 km s^{-1} are generated. Each table is formed by ODFs computed for the same T and NP=25 values of P_{gas}. T changes at each run of DFSYNTHE in accordance with the switch iteff=1 read from unit 5. For each pair T,P_{gas}, there are 1540 ODFs computed in the 1540 BIG (328)+ LITTLE (1212) intervals which divide the whole wavelength region from 8.97666 nm to 10000 nm. Each ODF is averaged over 12 subintervals.

```
ln -s ~/xnfpdf.dat fort.10
ln -s ~/xnfpdfmax.dat fort.22
ln -s ~/dflines/lowlinesdf.bin fort.11
ln -s ~/dflines/highlinesdf.bin fort.21
ln -s ~/dflines/diatomicsdf.bin fort.31
ln -s ~/dflines/tiolinesdf.bin fort.41
ln -s ~/dflines/h2olinesdf.bin fort.43
ln -s ~/dflines/nltelinesdf.bin fort.51
~/dfsynthe/dfsynthe.exe<<EOF>dfp00t1995.out
1000000000000000000000000000000000000000000000000000000000
EOF
mv fort.15 dfp00t1995vt0.bin
mv fort.16 dfp00t1995vt1.bin
mv fort.17 dfp00t1995vt2.bin
mv fort.18 dfp00t1995vt4.bin
mv fort.20 dfp00t1995vt8.bin
rm fort.*
```

```
ln -s ~/xnfpdf.dat fort.10
ln -s ~/xnfpdfmax.dat fort.22
ln -s ~/dflines/lowlinesdf.bin fort.11
ln -s ~/dflines/highlinesdf.bin fort.21
ln -s ~/dflines/diatomicsdf.bin fort.31
ln -s ~/dflines/tiolinesdf.bin fort.41
ln -s ~/dflines/h2olinesdf.bin fort.43
ln -s ~/dflines/nltelinesdf.bin fort.51
~/dfsynthe/dfsynthe.exe<<EOF>dfp00t2089.out
0100000000000000000000000000000000000000000000000000000000
EOF
mv fort.15 dfp00t2089vt0.bin
mv fort.16 dfp00t2089vt1.bin
mv fort.17 dfp00t2089vt2.bin
mv fort.18 dfp00t2089vt4.bin
mv fort.20 dfp00t2089vt8.bin
rm fort.*
...
...the same for T=2188,  2291,  2399,  2512,  2630,  2754,  2884,  3020,  3162,
                   3311,  3467,  3631,  3802,  3981,  4169,  4365,  4571,  4786,
                   5012,  5370,  5754,  6166,  6607,  7079,  7586,  8128,  8710,
                   9333, 10000, 11220, 12589, 14125, 15849, 17783, 19953, 22387,
                  25119, 28184, 31623, 35481, 39811, 44668, 50119, 56234, 63096,
                  70795, 79433, 89125,100000,112202,125893,141254,158489,177828,
                 199526
```

In each run all the switches must be zero except that which corresponds to the selected temperature. It must be set to 1.

Appendix C: An example of command file for DFSORTP under Linux

DFSRTOP rearranges the data in the output files from DFSYNTHE. In each file, 25 matrices 1540 x 12 are converted in 1540 matrices 25 x 12.
25 is the NP number of the P_{gas}; 1540 is the number of the frequency intervals BIG (328)+LITTLE(1212); 12 is the numer of the subintervals in a frequency interval.

```
ln -s dfp00t1995vt2.bin fort.1
~/dfsynthe/dfsortp.exe>dfsortp.out
mv fort.2 dfp00t1995vt2sortp.asc
rm fort.*
#!
ln -s dfp00t2089vt2.bin fort.1
~/dfsynthe/dfsortp.exe>dfsortp.out
mv fort.2 dfp00t2089vt2sortp.asc
rm fort.*
#!
...
...the same for T=2188,  2291,  2399,  2512,  2630,  2754,  2884,  3020,  3162,
                   3311,  3467,  3631,  3802,  3981,  4169,  4365,  4571,  4786,
                   5012,  5370,  5754,  6166,  6607,  7079,  7586,  8128,  8710,
                   9333, 10000, 11220, 12589, 14125, 15849, 17783, 19953, 22387,
                  25119, 28184, 31623, 35481, 39811, 44668, 50119, 56234, 63096,
                  70795, 79433, 89125,100000,112202,125893,141254,158489,177828,
                 199526
```

Appendix D: An example of command file for SEPARATEDF under Linux

This example shows how 57 output files from DFSORTP with ODFs for ξ=2 km s^{-1} are merged together and then separated in two files, the one with ODFs computed for BIG wavelength intervals and the other computed for LITTLE wavelength intervals. Output files from SEPARATEDF are ready to be used as input data for ATLAS9.

```
ln -s dfp00t1995vt2sortp.asc fort.10
ln -s dfp00t2089vt2sortp.asc fort.11
ln -s dfp00t2188vt2sortp.asc fort.12
ln -s dfp00t2291vt2sortp.asc fort.13
ln -s dfp00t2399vt2sortp.asc fort.14
ln -s dfp00t2512vt2sortp.asc fort.15
ln -s dfp00t2630vt2sortp.asc fort.16
ln -s dfp00t2754vt2sortp.asc fort.17
ln -s dfp00t2884vt2sortp.asc fort.18
ln -s dfp00t3020vt2sortp.asc fort.19
ln -s dfp00t3162vt2sortp.asc fort.20
ln -s dfp00t3311vt2sortp.asc fort.21
ln -s dfp00t3467vt2sortp.asc fort.22
ln -s dfp00t3631vt2sortp.asc fort.23
ln -s dfp00t3802vt2sortp.asc fort.24
ln -s dfp00t3981vt2sortp.asc fort.25
ln -s dfp00t4169vt2sortp.asc fort.26
ln -s dfp00t4365vt2sortp.asc fort.27
ln -s dfp00t4571vt2sortp.asc fort.28
ln -s dfp00t4786vt2sortp.asc fort.29
ln -s dfp00t5012vt2sortp.asc fort.30
ln -s dfp00t5370vt2sortp.asc fort.31
ln -s dfp00t5754vt2sortp.asc fort.32
ln -s dfp00t6166vt2sortp.asc fort.33
ln -s dfp00t6607vt2sortp.asc fort.34
ln -s dfp00t7079vt2sortp.asc fort.35
ln -s dfp00t7586vt2sortp.asc fort.36
ln -s dfp00t8128vt2sortp.asc fort.37
ln -s dfp00t8710vt2sortp.asc fort.38
ln -s dfp00t9333vt2sortp.asc fort.39
ln -s dfp00t10000vt2sortp.asc fort.40
ln -s dfp00t11220vt2sortp.asc fort.41
ln -s dfp00t12589vt2sortp.asc fort.42
ln -s dfp00t14125vt2sortp.asc fort.43
ln -s dfp00t15849vt2sortp.asc fort.44
ln -s dfp00t17783vt2sortp.asc fort.45
ln -s dfp00t19953vt2sortp.asc fort.46
ln -s dfp00t22387vt2sortp.asc fort.47
ln -s dfp00t25119vt2sortp.asc fort.48
ln -s dfp00t28184vt2sortp.asc fort.49
ln -s dfp00t31623vt2sortp.asc fort.50
ln -s dfp00t35481vt2sortp.asc fort.51
ln -s dfp00t39811vt2sortp.asc fort.52
ln -s dfp00t44668vt2sortp.asc fort.53
ln -s dfp00t50119vt2sortp.asc fort.54
ln -s dfp00t56234vt2sortp.asc fort.55
ln -s dfp00t63096vt2sortp.asc fort.56
ln -s dfp00t70795vt2sortp.asc fort.57
```

```
ln -s dfp00t79433vt2sortp.asc fort.58
ln -s dfp00t89125vt2sortp.asc fort.59
ln -s dfp00t100000vt2sortp.asc fort.60
ln -s dfp00t112202vt2sortp.asc fort.61
ln -s dfp00t125893vt2sortp.asc fort.62
ln -s dfp00t141254vt2sortp.asc fort.63
ln -s dfp00t158489vt2sortp.asc fort.64
ln -s dfp00t177828vt2sortp.asc fort.65
ln -s dfp00t199526vt2sortp.asc fort.66
~/dfsynthe/separatedf.exe
mv fort.2 p00big2.bdf
mv fort.3 p00lit2.bdf
rm dfp00t*.asc
rm fort.*
```