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ATLAS12: how to use it

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Abstract. The Opacity Sampling (OS) ATLAS12 code written by R.L. Kurucz for computing stellar model atmospheres is here described from the user's point of view. An example suited to run ATLAS12 under GNU-Linux is given.

Key words. Stars: model atmospheres – Stars: Abundances

1. Introduction

Among the several methods which handle line opacity in stellar atmosphere models, the Opacity Distribution Function (ODF) technique and the Opacity Sampling (OS) technique are those most commonly used. They are extensively described by Carbon (1984). Among codes written for computing LTE blanketed model atmospheres, the ATLAS code from Kurucz is one of the most popular (Kurucz 1970). ATLAS9 is the last version for computing models with the ODF method, while ATLAS12 is a version for computing models with the OS method. Except for the treatment of the line opacity the two codes are identical, in principle.

The different line opacity treatments imply different advantages and disadvantages in the two cases.

Models from ATLAS9 are limited to abundances and microturbulent velocities used for computing the pretabulated line opacity. Once the ODF tables are computed with the DFSYNTHE code (Kurucz 2005; Castelli 2005) the advantage is the short time required to compute a single model (few minutes).

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Models from ATLAS12 can be generated for whichever individual abundances and microturbulent velocity are given in input. The disadvantage is the long time required to get a single model (from half an hour to several hours, depending on the CPU and on the amount of the line blanketing).

Kurucz has always made public his codes, but it may happen that sometimes they are not very friendly for users, mostly owing to the poor documentation of the software. The ATLAS9 code and its previous versions ATLAS5 and ATLAS8 have been documented in a few papers (i.e., Kurucz 1970; Castelli 1988; Jauregi 2005). The ATLAS12 code was presented by Kurucz at several meetings (i.e. Kurucz, 1992b,1996), but instructions about its use are available only at the Kurucz website [1]. We give in this paper a few more details about ATLAS12 collected by reading the Kurucz papers and by studying the source code. We also give an example of command file to execute ATLAS12 under GNU-Linux operating system. The GNU-Linux version of ATLAS12 is available at our website [2] The hope is that this

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

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

paper can be helpful for ATLAS12 inexpert users.

2. Line Opacity in Model Atmospheres

The problem of the line opacity in model atmospheres is related to the need of computing numerous integrals over the frequency of various monochromatic quantities f(ν). They are generally solved by weighted sums:

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

The quantity f(ν) (or f(ν_i)) is some complex function of the continuous and line opacities.

A typical example is the integral over the monochromatic flux to get the total flux. The monochromatic flux at the ν frequency is:

$$F_\nu(\tau_\nu) = 2\int_{\tau_\nu}^\infty S_\nu(t_\nu)E_2(t-\tau_\nu)dt_\nu - 2\int_0^{\tau_\nu} S_\nu(t_\nu)E_2(\tau_\nu - t_\nu)dt_\nu$$

In this example, the line absorption coefficient l_ν is present both in

$$\tau_\nu = \int_0^{\tau_{ross}} \frac{\kappa_c+l_\nu+\sigma_\nu}{\kappa_{ross}} d\tau_{ross}$$

and in

$$S_\nu = \frac{\kappa_c+l_\nu}{\kappa_c+l_\nu+\sigma_\nu}B_\nu + \frac{\sigma_\nu}{\kappa_c+l_\nu+\sigma_\nu}J_\nu$$

Line opacity requires a very large number of points to describe the spectrum properly. They are carefully taken into account when a synthetic spectrum is computed. In fact, in this case, the computation is feasible in that only the emergent flux (i.e., that for τ_ν=0) is considered and no iterations are needed. Instead, for model atmospheres, several integrals over the frequency, like that for the total flux,

$$F_{tot}(j) = \int_0^\infty F_\nu(\tau_\nu)d\nu$$

have to be computed for each depth j in the atmosphere; furthermore, these computations are repeated in all the iterations needed to get a convergent model. This process is so time consuming that it is impracticable even with modern computers. The problem was solved by handling the line opacity with statistical methods, like the ODF or the OS methods.

3. The Opacity Sampling (OS) method

The Opacity Sampling method was first adopted by Peytremann (1974) for computing a set of ATLAS model atmospheres. It was then developed and studied over the years. One of the last reviews is from Jorgensen (1992). The method consists in selecting at random a sufficiently large number of frequency points for the integration (for the sum). In fact, as long as the errors on the integration scheme are at random about a correct mean value, these errors cancel out. It was shown by Ekberg et al. (1986) that 5000 points are enough to obtain an accurate model structure in carbon stars.

At each layer, for each selected frequency ν_i, the total absorption coefficient $\kappa_{tot}(\nu,\tau)$ is exactly computed by adding the contribution at that frequency of all relevant atomic and molecular lines $l_{tot}(\nu,\tau)$ (line blanketing), of all bound-free continuous opacities $\kappa_c(\nu,\tau)$ (true absorption), and of all free-free opacities $\sigma(\nu,\tau)$ (scattering). Namely,

$$\kappa_{tot}(\nu,\tau) = l_{tot}(\nu,\tau) + \kappa_c(\nu,\tau) + \sigma(\nu,\tau)$$

where:

$$l_{tot}(\nu,\tau) = \sum_{n=n_1}^{N_{lin}} l_n(0)V(\mathrm{v}_n,\alpha_n)(1-e^{-h\nu/kT})$$

here $l_n(0)$ and V(v_n, α_n) are the line absorption coefficient in the line center and the Voigt function, respectively, for each contributing line n lying between n_1 and N_{lin}. It is:

$$V(\mathrm{v},\alpha) = \frac{1}{\sqrt{(\pi)}\Delta\nu_D}H\left(\frac{\Delta\lambda}{\Delta\lambda_D}, \frac{\gamma}{4\pi\Delta\nu_D}\right)$$

where $\Delta\nu_D$ or $\Delta\lambda_D$ is the Doppler shift:

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

and

$$\Delta\lambda_D = \frac{c}{\lambda^2}\Delta\nu_D$$

4. The OS method in ATLAS12

In ATLAS12 the integrals over the frequency are numerically solved by means of the trapezoidal rule. This means that they are replaced by weighted sums over a set of frequency

Table 1. Integration intervals as function of $T_{\rm eff}$ for the integrals over the frequency in ATLAS12

$T_{\rm eff}$(K)	λ_1 (nm)	$\log\lambda_1$	λ_N(nm)	$\log\lambda_N$
≤ 50000	10	1	10000	4
< 30000	22.788	1.358	22782.43	4.357
< 13000	50.431	1.703	50419.67	4.703
< 7250	91.180	1.960	91159.09	4.960
< 4500	144.577	2.160	144544.0	5.16

points ν_i, where the weights are the widths of the intervals in which the integration range is divided, i.e. $w_i=\frac{1}{2}(\nu_{i-1} - \nu_{i+1})$. The sum is made over 30000 frequency points in the wavelength range λ_N-λ_1, where λ_1 and λ_N are the first and the last wavelength of the integration interval. The length of the interval is such that $\log\lambda_N-\log\lambda_1=3$. As required by the OS method, the frequency points are placed at random with respect to the lines in that they are evenly spaced in logarithm with step $\Delta\log(\lambda_n)=0.0001$. The value of λ_1 (and therefore that of λ_N) depends on the effective temperature $T_{\rm eff}$ of the model. The limits of the integration interval are listed in Table 1.

5. Opacity in ATLAS12

5.1. Continuous Opacity

Continuous opacities are computed in ATLAS12 both at 344 frequencies and at the 30000 sampling frequencies. The first 337 frequencies of the 344 ones are those adopted in ATLAS9 for frequency integration when BIG ODFs are used. In ATLAS12 six more frequencies were added, so that the whole wavelength range from 9.09 nm to 400000 nm is covered. The 344 continuous opacities form a continuum which is used only to extract from the line lists the lines stronger than 0.001 times this continuum at any depth using the specific abundances of the model.

Continuous opacities are the same as in ATLAS9. They are: H I, H^-, H_2^+, He I, He II, He^-; low temperature absorbers C I, Mg I, Al I, Si I, Fe I, CH, OH; intermediate temperature absorbers, N I, O I, Mg II, Si II, Ca II; high temperature absorbers C II-CIV, N II-V, O II-VI, Ne I-VI; electron scattering, H-Rayleigh scattering, H_2 Rayleigh scattering, He I Rayleigh scattering, and the absorption due to the short-lived “super-molecular” H_2-H_2, H_2-He (CIA) which is effective in metal poor, high gravity stars, with $T_{\rm eff}$≤4000 K (Borysow et al. 1997).

5.2. Line Opacity

The line opacity is computed starting from all the atomic and molecular lines of line lists from Kurucz’s CD-ROMs. The line lists used by ATLAS12 are the binary files listed below. Here the filenames are those we adopted in our website[3]

1. nltelines.bin – lines of H I, He I, He II, C I, C II, O I, Na I, Mg I, Mg II, Al I, Si I, Si II, K I, Ca I, Ca II. This file is the binary version of the ASCII file NLTELINE.DAT of Kurucz’s CD-ROM No 1.
2. lowlines.bin – lines of all the elements in the first 5 stages of ionization. The lines of nltelines.bin are not included. It is the file LOWLINES.DAT of Kurucz’s CD-ROM No 1.
3. highlines.bin – atomic lines of elements in ionization stages n>5 up through Zn. It is the file HILINES.DAT of Kurucz’s CD-ROM No 1.
4. diatomicsiwl.bin – lines of diatomic molecules ordered by increasing wavelength. It is the file DIATOMIC.DAT of Kurucz’s CD-ROM No 16. The molecules considered are: CH, NH, OH, MgH, SiH, CO, SiO, CN, C_2. More details about bands and isotopes can be found in Kurucz (1992a,1994)
5. schwenke.bin – TiO lines from Schwenke (1998). It is the binary file SCHWENKE.BIN of Kurucz’s CD-ROM No 24.
6. h2ofast.bin – H_2O lines from Partridge & Schwenke (1997). It is the binary file H2OFAST.BIN of Kurucz’s CD-ROM No 26.

[3] http://wwwuser.oat.ts.astro.it/castelli/linelists/

Table 2. Units for input-output for the first run of ATLAS12

file	unit
Input	
data for molecular partition functions	2
starting input model	3
lowlines.bin	11
highlines.bin	21
diatomicsiwl.bin	31
schwenke.bin	41
h2ofast.bin	51
Control Cards	5
Output	
the whole printout	6
preselected lines	12

6. How to run ATLAS12

ATLAS12 computes a model atmosphere in two steps, namely two runs of ATLAS12 are needed. In the first run, all the line files, except nltelines.bin, are used to extract the relevant lines for the given model parameters and the given abundances. In the second run the model is computed by using the preselected lines and the nltelines.bin file. Standard ATLAS12 models are computed for 72 depths from τ_{ross}=1.33.10^{-7} to τ_{ross}=100 at steps of 0.125 in $\log_{10}(\tau_{ross})$.

The starting input model and the line files are assigned to fixed units, while the input data for the specific model are supplied by control cards exactly as in ATLAS9. Table 2 and Table 3 list the input and output units for the first run and respectively for the second run of ATLAS12.

7. The Control Cards

As in all the Kurucz codes, also in ATLAS12 control cards are read from unit 5 in order to fix the free parameters for the model. Most of the control cards required by ATLAS12 have the same meaning as in the other ATLAS versions (for ATLAS8 see Castelli (1988)). However, while some previous options are not longer needed for ATLAS12, some other options were added. Control cards useful for ATLAS12 are listed below:

- TEFF
- GRAVITY
- OPACITY
- ITERATIONS
- MOLECULES
- ABUNDANCE
- PRINT

Table 3. Units for input-output for the second run of ATLAS12

file	unit
Input	
data for molecular partition functions	2
starting input model	3
nltelines.bin	19
preselected lines	12
Control Cards	5
Output	
the whole printout	6
the model	7

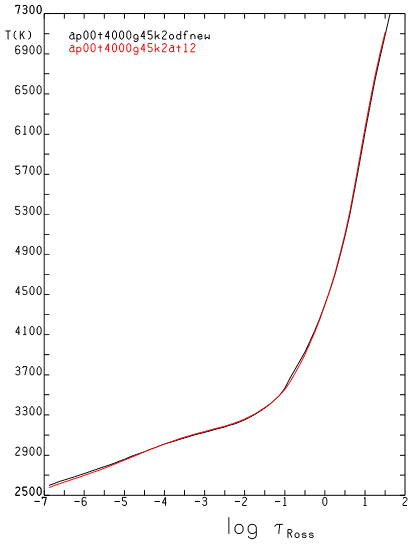

Fig. 1. Comparison of T$-\log_{10}(\tau_{ross})$ relations from ATLAS9 (red) and ATLAS12 (black) for $T_{\rm eff}$=4000 K, log g=4.5, [M/H]=0.0, ξ=2 km s^{-1}

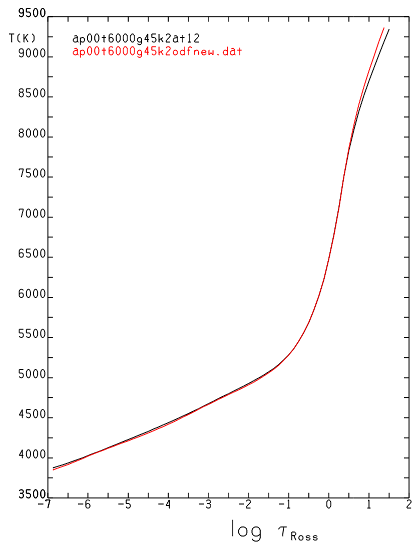

Fig. 2. Comparison of T−$\log_{10}(\tau_{ross})$ relations from ATLAS9 (red) and ATLAS12 (black) for $T_{\rm eff}$=6000 K, log g=4.5, [M/H]=0.0, ξ=2 km s^{-1}

- PUNCH
- READ
- LTE
- NLTE
- BEGIN
- SCATTERING
- END
- CONVECTION
- TURBULENCE
- CHANGE RHOX
- TITLE
- SURFACE
- PRESSURE
- CORRECTION
- SCALE MODEL
- CALL
- VTURB
- SMOOTH

We briefly comment here only some particular control cards.

7.1. READ

Control cards starting with READ tell to ATLAS12 which files have to be read in input.

The are:

READ PUNCH —-> Read the file with the input model

READ MOLECULES —> Read the file with data for molecular Partition Function (PF). These data will be used by ATLAS12 only if the control card MOLECULES ON is also present.

READ LINES —> Read the files with the line data except for nltelines.bin. This control card is used in the first run of ATLAS12. The file nltelines.bin will be read in the second run, provided that the control card OPACITY ON XLINES is present.

7.2. OPACITY

This control card fixes the opacity of the model. It has the form (see Castelli (1988)):

```
OPACITY ON names
OPACITY OFF names
OPACITY IFOP switches
```

ATLAS12 adopts the switches of the OPACITY IFOP card read from the input model. To change the opacities of the input model, an OPACITY card must be put after the READ PUNCH card.
In particular:

```
OPACITY ON XLINES
OPACITY ON LINES
```

have to be put for the second run of ATLAS12. They tell to the code to read the file nltelines.bin and, respectively, the file with the preselected lines.

7.3. ABUNDANCE

This control card fixes for each element iz the abundance xabund(iz), given by:

xabund(iz)=abund(iz)+xrelative(iz)

where abund(iz) is the abundance of the

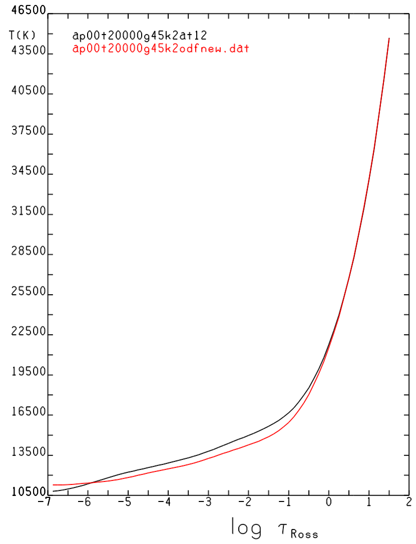

Fig. 3. Comparison of T−$\log_{10}(\tau_{ross})$ relations from ATLAS9 (red) and ATLAS12 (black) for T_{eff}=20000 K, log g=4.5, [M/H]=0.0, ξ=2 km s^{-1}

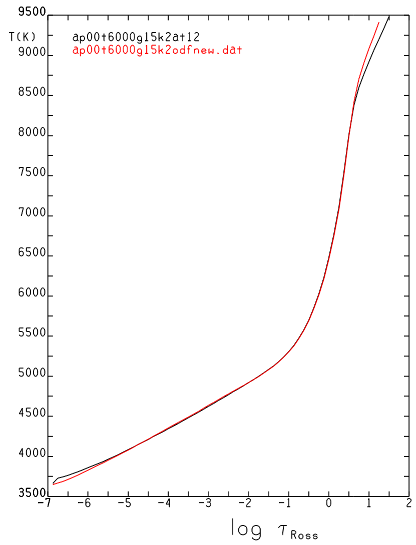

Fig. 4. Comparison of T−$\log_{10}(\tau_{ross})$ relations from ATLAS9 (red) and ATLAS12 (black) for T_{eff}=6000 K, log g=1.5, [M/H]=0.0, ξ=2 km s^{-1}

iz element **before** scaling and xrelative(iz) is the scale factor.

Starting abundances are those of the input model. If it is an ATLAS12 model both abund(iz) and xrelative (iz) are read from the set of data listed by ABUNDANCE TABLE. If the input model is an ATLAS9 model only abund(iz) is given in input and all the xrelative(iz) values are zero.

To change input abundances one or more ABUNDANCE cards have to be put after the READ PUNCH card. The data abund(iz) and xrelative(iz) can be read by means of the cards:

```
ABUNDANCE CHANGE iz abund(iz)
ABUNDANCE RELATIVE iz xrelative(iz)
ABUNDANCE TABLE  followed by a table of data
abund(iz) and xrelative(iz)
for all the 99 elements.
```

The absolute abundance is read with:

ABUNDANCE ABSOLUTE iz xabund(iz)

Only if the input model is an ATLAS9 model the card:

ABUNDANCE SCALE xscale

scales by xscale the whole set of ATLAS9 abundances abund(iz) from iz=3 (Li) to iz=99 (Es). **This last option is not available in the original Kurucz code**, but it was implemented in our version available at our website[2].

7.4. CONVECTION

This control card fixes the convection in the model. It has the form:

```
CONVECTION OFF
CONVECTION ON   n1
CONVECTION OVER n1 overwt (nconv)
```

No convection is computed with CONVECTION OFF.
With CONVECTION ON the convective flux is calculated with the local mixing-length theory, where the mixing length to the pressure scale height is l/H_p= n1. In this case, an approximate overshooting at the top of the

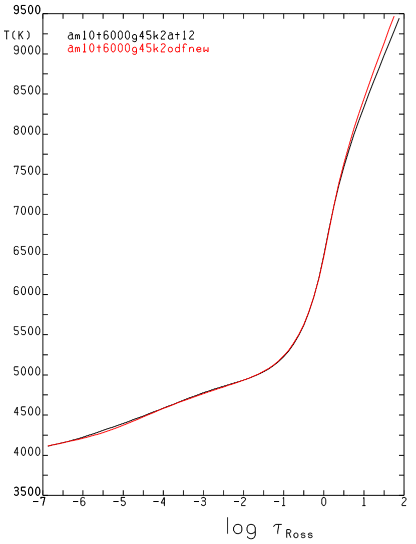

Fig. 5. Comparison of T$-\log_{10}(\tau_{ross})$ relations from ATLAS9 (red) and ATLAS12 (black) for $T_{\rm eff}$=6000 K, log g=4.5, [M/H]=−1.0, ξ=2 km s^{-1}

convection zone is adopted by default.
The control card CONVECTION OVER controls the amounts of the overshooting by means of the weight overwt, whose values range from 0 (no overshooting) to 1 (full overshooting) (Castelli 1996). Therefore, the card

CONVECTION OVER 1.25 0

gives rise to a convective flux computed with L/H_p=1.25, but with no overshooting (overwt=0).

We added in the version available at the website[2] the further parameter nconv, which indicates the layer j in the atmosphere where numerical results related with the Schwarzschild criterion can be assumed as reliable. In the original ATLAS12 code, nconv is fixed inside the code at j=36. While this value is pretty good for all the models with $T_{\rm eff}$>4000 K, it may indicate a too deep layer for cooler models where convection may occur above j=36. This constraint for convection was put to avoid numerical artifacts which affect the computational accuracy of the Schwarzschild criterion in the uppermost layers.

8. Energy distributions from ATLAS12

It is computed when the control card

SURFACE FLUX

is given in input. However, this flux is not accurate enough to be compared with the observations. In fact, it is only computed at the 30000 sampling points, with gaps that increase with increasing wavelengths (sect. 4). As a consequence, the details between two consecutive points are lost. Energy distributions for ATLAS12 models should be computed with the SYNTHE code at a resolving power of 500000, using the same line lists that were used for the model calculation. The high resolution spectrum should then be instrumentally broadened at the resolution of the observed energy distribution.

9. Comparison of T$-\log_{10}(\tau_{ross})$ relations from ATLAS9 and ATLAS12

We have compared the T$-\log_{10}(\tau_{ross})$ relations from ATLAS9 and ATLAS12 for different choices of the model parameters. The cases examined have shown that the differences increase with increasing $T_{\rm eff}$ (Figures 1, 2, 3) but, for a given $T_{\rm eff}$, they are the same for different gravities (Figures 2 and 4) and different metallicities (Figures 2 and 5).

10. An example of command file for ATLAS12 under Linux

ATLAS12 was written and is currently developed by R.L. Kurucz in Fortran under Open-VMS. Because this operating system has become rather obsolete, several efforts have been done recently for porting Kurucz's codes to operating systems nowadays more popular than Open-VMS. For instance, Sbordone et al. (2004) and Sbordone (2005) have ported ATLAS9 and SYNTHE to GNU-Linux equipped with INTEL-Fortran, a compiler highly compatible with Open-VMS Fortran. Bischof (2004, 2005) has ported ATLAS12 to UNIX, using the Fortran g77 compiler, and also to Ada95, an object-oriented parallel language.

The following example shows a command file, here named atlas12tot.com, that can be executed under GNU-Linux, once ATLAS12 is compiled with the INTEL-Fortran for Linux. In this case, the command for executing atlas12tot.com is: source atlas12tot.com.

The aim of this example is to compute an ATLAS12 model with parameters $T_{\rm eff}$=5500 K, logg=4.5, ξ=1 km s^{-1}, [M/H]=−1.0 for all the elements, except for iron for which the abundance log(N(Fe)/N_{tot})=−4.25 (i.e. −3.25 − 1.0) is assumed instead of −5.54 (i.e. −4.54 − 1.0). The file atlas12tot.com is:

```
#
#           FIRST RUN
#
# molecular data for PF
ln -s molecules.dat  fort.2
# input model
ln -s am10t5500g45k1odfnew.dat  fort.3
# input lines
ln -s lowlines.bin   fort.11
ln -s highlines.bin  fort.21
ln -s diatomicsiwl.bin  fort.31
ln -s schwenke.bin   fort.41
ln -s h2ofast.bin    fort.51
# execution, printout, and CONTROL CARDS
/atlas12.exe<<EOF>am10t5500g46k1at12a.out
MOLECULES ON
READ MOLECULES
READ PUNCH
READ LINES
ITERATIONS 1
PRINT 1
PUNCH 0
ABUNDANCE CHANGE 26 -3.25
BEGIN
END
EOF   #closes the input data from unit 5
# the output: the preselected lines
mv fort.12 sellinm10t5500g46k1.bin
#
#          SECOND RUN
#
# molecular data for PF
ln -s molecules.dat  fort.2
# input model
ln -s am10t5500g45k1odfnew.dat  fort.3
# input lines
ln -s nltelines.bin fort.19
# input of preselected lines from STEP 1
ln -s sellinm10t5500g46k1.bin fort.12
# execution, printout, and CONTROL CARDS
/atlas12.exe<<EOF>am10t5500g46k1at12b.out
MOLECULES ON
READ MOLECULES
READ PUNCH
ABUNDANCE ABSOLUTE 26 -4.25
OPACITY ON LINES
OPACITY ON XLINES
CONVECTION OVER 1.25 0 30
ITERATIONS 17
PRINT 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
PUNCH 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
SCALE MODEL 72 -6.875 0.125 5500 4.6
BEGIN
END
EOF  #closes the input data from unit 5
# the output: the resulting model !
mv fort.7 am10t5500g46k1at12.dat
rm fort.*
```

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