atlas.lester: a Unix Implementation of ATLAS9 and SYNTHE

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CCP7 User Note 15.0

1 Introduction

atlas9 is a program written by Bob Kurucz to calculate plane-parallel line-blanketed model atmospheres in LTE for stars with effective temperatures between 3500 K and 50,000 K and a wide range of metallicities, surface gravities and microturbulent velocities.

synthe is a suite of programs written by Bob Kurucz to calculate LTE synthetic spectra for the above stellar atmospheres using very extensive linelists.

The programs as distributed by Kurucz on CD-ROM currently run under VAX/VMS and require some effort to implement on other systems (particularly Unix). John Lester (Toronto) has made an extensive rewrite of Kurucz' programs in extended Fortran 77 and Fortran 90. He has kindly made these available to CCP7.

To facilitate their use, CCP7 has provided additional scripts so that they can be installed and run in a relatively transparent way. This document attempts to describe briefly how to make the implementation and run the programs, and an illustration of their use.

2 Installation

2.1 Obtaining the software

The software is packaged as a read.me file and a compressed tar file available from the CCP7 anonymous ftp server. They are located at:

`ftp://ccp7.arm.ac.uk/ccp7/Soft/atlas.lester.read.me`
: An ascii version of this document

`ftp://ccp7.arm.ac.uk/ccp7/Soft/atlas.lester.tar.Z`
: A tar file containing John Lester's distribution with CCP7 additions

The distribution tar file does not include the linelists required by **synthe** or the opacity distribution functions required by **atlas9**, but these are also available from the CCP7 ftp server. The CCP7 additions are entirely contained in a subfolder to that cotaining John Lester's distribution.

2.2 Installing atlas9 and synthe

The prospective user may elect to use only John Lester's distribution. After unpacking the tar file, the executable images can be installed using the `make` utility.

2.3 Automatic ftp and installation

If the CCP7 additions are required it is advisable to place the tar files in a standardized folder structure. This can be constructed by creating a root folder for the CCP7 library (*e.g.* ~/ccp7). `cd` to this folder and get the file

`ftp://ccp7.arm.ac.uk/ccp7/build.ccp7`

from the CCP7 ftp server. Check the permissions and execute the command `> build.ccp7`. This establishes the CCP7 folder structure and collects some subroutine libraries (in practice these are not required for **atlas9** and **synthe**). Executing `> source ./etc/login` sets the environment variable `$CCP7` to point to the root folder for the CCP7 library.

atlas.lester is then retrieved by anonymous ftp and installed by executing the single command `> build.ccp7 atlas.lester`[1].

The linelists necessary for running **synthe** are distributed separately. After installing the CCP7 standard folder

[1]The installation procedures have so far only been tested on Sun systems running Solaris 2.x.

structure and **atlas.lester** with the CCP7 extensions, you can then obtain the linelists in one of two ways.

2.4 Linelists from automatic ftp

Five of the most important linelists are stored in the correct format as a compressed tar file on the CCP7 ftp server. These are `bell_heavy, bell_light, nlte, iron, labiron`. They are stored in the package **lines.lester**, with the URL

`ftp://ccp7.arm.ac.uk/ccp7/Data/lines.lester.tar.Z`

From the CCP7 root folder, simply issue the command `> build.ccp7 lines.lester`. Since the files are big, the ftp could take a considerable time.

2.5 Linelists from CD-ROM

Alternatively, utilities are provided for loading the linelists from KURUCZ CD-ROM No. 18 into direct access binary files in the user's current folder. For use with the CCP7 scripts, this folder should be `$CCP7/lines/lester`, and it is simply necessary to issue the command `> Get_lines` to load all the linelists, or `> get_lines [list]` to recover an individual linelist. The scripts are:

`$CCP7/atlas/lester/ccp7/Get_lines`
: A general script for reading all the CD-ROM 18 linelists.

`$CCP7/atlas/lester/ccp7/get_lines`
: A compilation of **get_nlte, get_iron** etc. ...into one script requiring a single argument.

3 Access

atlas.lester has been set up in a standard way, integrated with other ccp7 library items, so that all users on a distributed system can run the package without having to create local versions of the programs, scripts or standard data files. However it is necessary to ensure that your environment contains a few definitions, so that programs and data files can be located correctly. This is achieved by executing the command

`> source $CCP7/etc/login`

either in your `.cshrc` file or from your shell. `$CCP7` must point to the root folder for the CCP7 library installation on your system.

4 Execution

The steps required to generate a synthetic spectrum, with the names of the relevant programs in the package in parentheses, are as follows

– obtain or generate a model atmosphere (**atlas9**)

– calculate population numbers for said model atmosphere (**moldeck**)

– calculate other model-dependent quantities (**xnfpel**)

– generate a linelist for the spectral region required (**synbeg**)

– combine linelist and model atmosphere (**synthe**)

– generate emergent spectrum (**specsyn**)

For each of the above steps, the programs written by Kurucz and Lester require several input files, but the user in general needs only to be concerned with a few of these. In order to reduce file housekeeping, we have written a series of C-shell scripts that provide an interface to the individual fortran programs. The following provides a prescription for the use of these scripts.

Atlas[2]. – not yet implemented

it is assumed that a model exists (e.g. ap00t20g45k2.dat)

Moldeck [model.atmosphere] [label]

the model atmosphere is specified and a label is required to identify the output (moldeck.[label])

[2]The current version of atlas9 assumes that Kurucz opacity distribution functions (odfs) are to be read directly from CD-ROM where they are stored as VAX/VMS binaries. These binaries have a different byte order to that understood by Unix programs, so byte-swapping is done 'on the fly'. The CCP7 ftp server carries odfs available in compressed 'ascii' form. It is hoped to rationalize these various systems so that **atlas9** can be used together with the on-line odfs

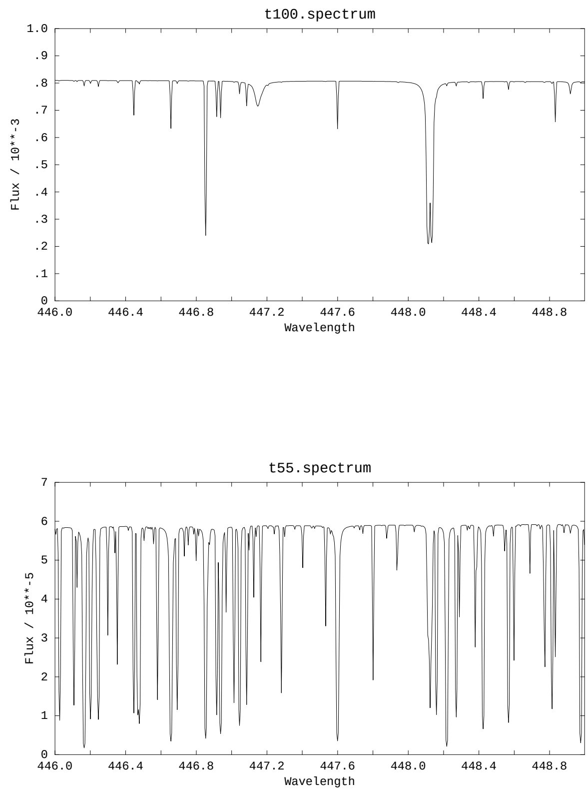

Figure 1: Emergent fluxes for model stellar atmospheres with $[Fe/H] = 0.0, T_{\rm eff} = 10\,000$K (top), 5 500 K (bottom), $\log g = 4.0$, $v_{\rm t} = 2$km/s, in the interval $\lambda = 446 - 449$ nm calculated with a resolution $R = 100\,000$

Xnfpel moldeck.[label]

take the populations from moldeck and calculate various model dependent quantities. The results are stored for use by Synthe (xnfpel.file20)

Synbeg [synbeg.input]

synbeg.input specifies the wavelength range and which linelists are to be polled. The results are stored for use by Synthe (synbeg.file22, synbeg.file23)

Synthe [synthe.input]

synthe.input specifies a few properties such as required resolution and additional microturbulence for the emergent spectrum. Synthe assumes other required input is in the files specified above (current folder). The output (synthe.file30) is required by Specsyn.

Specsyn moldeck.[label]

computes the final emergent spectrum. Either fluxes or intensities can be generated, but at present only fluxes are implemented. Kurucz provides utilities for instrumental and rotational broadening, again not implemented. The output is formatted (specsyn.spectrum) to give wavelength (nm), physical flux, continuum flux and residual flux. The spectrum starts on line 9 of the output file.

5 Example calculation using synthe

The distribution includes some limited example calculations, the necessary input files being as follows:

`$CCP7/atlas/lester/ccp7/ap00t100g40k2.dat`

Model atmosphere $[Fe/H] = 0.0, T_{\rm eff} = 10\,000$K, $\log g = 4.0$, $v_{\rm t} = 2$km/s.

`$CCP7/atlas/lester/ccp7/ap00t55g40k2.dat`
: As above with $T_{\rm eff} = 5\,500$K.

`$CCP7/atlas/lester/ccp7/synbeg.sample`
: Extract lines $\lambda = 446 - 449$nm from lists `bell_heavy, bell_light, nlte, labiron`

`$CCP7/atlas/lester/ccp7/synthe.sample`
: Synthesize spectrum $R = 100\,000$ with no additional $v_{\rm t}$

Install **atlas.lester** and **lines.lester** as already directed, copy the above files to the folder where you want to run **synthe** and issue the following commands.

```
> Moldeck ap00t100g40k2.dat test
> Xnfpel moldeck.test
> Synbeg synbeg.sample
> Synthe synthe.sample
> Specsyn moldeck.test
```

Several output files are created, the prefix indicating which program generated them. Files `*.print.*` report various stages of the calculation, and files `*.fileNN` pass data from one program to another. The final output is given in a file `specsyn.spectrum`. The resultant spectrum for our example calculation is shown in Fig. 1.

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