Convection in Astrophysics
Proceedings IAU Symposium No. 239, 2006
F. Kupka, I. W. Roxburgh & K. L. Chan, eds.

doi:10.1017/S1743921307000142

ATLAS 9 and ATLAS 12 under GNU-Linux

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Abstract. We successfully ported the suite of codes developed by R. L. Kurucz for stellar atmosphere modelling, abundance determination and synthetic spectra calculation, to run under GNU-Linux. The ported codes include ATLAS 9 and ATLAS 12 for 1-D plane-parallel atmosphere model calculation, DFSYNTHE, which calculates the Opacity Distribution Functions (ODF) to be used with ATLAS 9, WIDTH to derive chemical abundances from measured line Equivalent Widths (EW) and SYNTHE to calculate synthetic spectra. The codes input and output files remain fully compatible with the VMS versions, while the computation speed has been greatly increased due to the high efficiency of modern PC CPUs. As an example, ATLAS 9 model calculations and the computation of large (e.g. 10 nm) synthetic spectra can be executed in a matter of minutes on any mainstream laptop computer. Arbitrary chemical compositions can be used in calculations (by using ATLAS 12 through opacity sampling or by calculating ad-hoc ODFs for ATLAS 9). The large set of scripting languages existing under Linux (shell, perl, python...) and the availability of low-cost multiprocessor Linux architectures (such as Beowulf) makes the port highly effective to build model farms to produce large quantities of atmosphere models or synthetic spectra (e.g. for the production of integrated light synthetic spectra). The port is hosted on a dedicated website including a download section for source codes, precompiled binaries, needed data (opacities, line lists and so on), sample launch scripts and documentation.

Keywords. Stars: atmospheres, stars: abundances, line: formation, line: identification, line: profiles, convection

1. Introduction

Across the years, one of the most popular set of tools for modelling and synthesizing stellar atmospheres has been the one developed by R. L. Kurucz. In its current form it includes codes ATLAS9 and ATLAS12 for the production of monodimensional, plane parallel atmosphere models, SYNTHE for the calculation of synthetic spectra, WIDTH for the determination of chemical abundances from the EW of spectral lines, and DFSYNTHE for producing precomputed Opacity Distribution Functions (ODFs). We will refer to them as the Atlas Suite (Kurucz 1993, 2005).

2. ATLAS9 vs. ATLAS12

Of the two atmosphere modelling codes, ATLAS9 relies on precomputed line opacities in the form of ODFs. The advantage of this approach is the very fast computational time to produce model atmospheres, at expense of flexibility: namely, the chemical composition of the calculated atmosphere must be only that of the adopted ODF. While this is satisfactory for most applications, there are cases in which an arbitrary chemical composition would be preferable, e.g. for chemically peculiar stars (CP stars). For these

needs, ATLAS12 is available. This code is essentially identical to ATLAS9, but uses the Opacity Sampling method (OS) to evaluate line opacities. Since OS computes opacities during the model calculation, arbitrary compositions are allowed, but calculation speed is much lower. For the cases when an abundance set with no available ODFs should be used for a large number of models, it might be more efficient to calculate an ad-hoc ODF once for all, and then use ATLAS9. ODF calculation is performed by the DFSYNTHE code.

3. The GNU-Linux port of the ATLAS suite

The ATLAS suite is currently maintained and developed by R. L. Kurucz at his website† under Open VMS. Open VMS is becoming gradually obsolete, and it is rarely available to researchers nowadays. Meanwhile, the increase in processing power of the mainstream PCs made them powerful enough to run such codes at a speed easily exceeding the one obtainable on Alpha class workstations. We thus decided to port the whole suite under GNU-Linux to made it available to a larger user base (Sbordone 2005; Sbordone, Bonifacio, Castelli, & Kurucz 2004; Castelli 2005A,B,C).

The ATLAS Suite has been in development for many decades, and it contains many "legacy" Fortran constructs. We then needed a compiler with a robust backward compatibility, to minimize the changes in the code. For this reason we discarded g77, not flexible enough for our purpose. Instead, we employed the Intel Fortran Compiler (IFC), a commercial software which GNU-Linux version is licensed free of charge for non-commercial research purposes. With it we ported the whole suite introducing only minimal changes to the codes. The compatibility with the VMS version of the input files (including the binary ones, such as ODF) has been fully preserved, except for the launch scripts, which have been substituted by Unix shell scripts.

Calculation times have dramatically improved: ATLAS9 models converge typically in a matter of minutes on a mainstream laptop computer. Similar times are needed for an $R = 600000$ synthetic spectrum calculation over 5 nm range, ATLAS12 models require around 20 minutes. Figure 1 is an example of computation under GNU-Linux.

4. Availability and supported systems

In principle, the ATLAS suite port should compile and run on any system under which IFC is available, namely GNU-Linux, Mac OSX (on Mac-Intel machines) and Microsoft Windows. We support GNU-Linux only, the only system for which a free IFC license is available. Users have compiled successfully the port under Mac OSX: all the scripts and utilities we provide should also work there, given OSX and Linux share the same Unix framework and scripting. We have currently no reports of compilation under Windows.

The whole port is hosted in a dedicated website‡, where users can download source codes and makefiles, precompiled, statically linked Linux binaries (which should work on most Linux distributions), a selection of ODFs, atomic and molecular line sets and other needed input data, and documentation. The DFSYNTHE port is hosted for now at Fiorella Castelli's web page¶.

R. L. Kurucz webpage remains the authoritative source of data and informations about the ATLAS suite, with extensive databases of ODFs, atomic and molecular data, model

† http://kurucz.harvard.edu/
‡ http://wwwuser.oat.ts.astro.it/atmos/
¶ http://wwwuser.oat.ts.astro.it/castelli/

https://doi.org/10.1017/S1743921307000142 Published online by Cambridge University Press

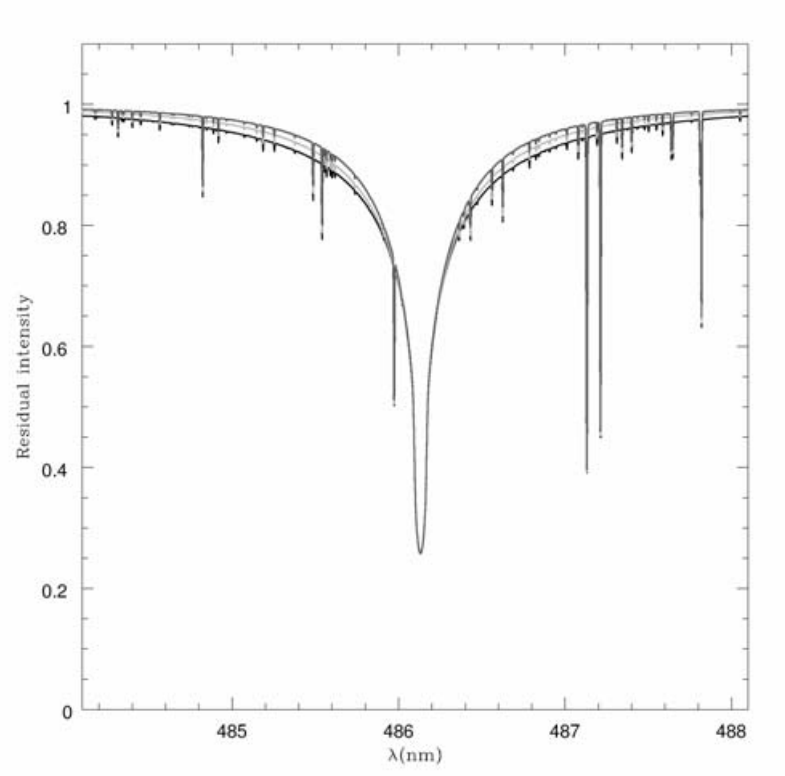

Figure 1. Effect of the convection treatment on Hβ line profile. Synthetic profiles have been calculated for an atmosphere of Teff = 6250 K, log g = 4.0, $\xi = 1$ km/s and solar-scaled [Fe/H] = −2 composition. The model atmosphere calculated with the GNU-Linux port of ATLAS 9 for mixing length parameter A = 0.5 (black), 1.25 (light gray) and 2.0 (dark gray), all without overshooting. The synthetic spectra have been derived with the ported version of SYNTHE.

grids, codes and so on. All the input files (models, ODFs, linelists) available there are supposed to work with our Linux port of the suite.

The port website also hosts tutorials and links to further documentation and web pages of related or similar projects. Users are also encouraged to subscribe to three ATLAS related mailing lists† which have been set up by Urtzi Jauregi at Ljubljana University. They are aimed at constituting the main source of user support, mutual help and exchange of opinions and news within the user community. Their archive can be browsed by users looking for previously discussed problems and solutions.

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† see `http://wwwuser.oat.ts.astro.it/atmos/Links.html`

https://doi.org/10.1017/S1743921307000142 Published online by Cambridge University Press