README: Theoretical Grids of Star Spectra

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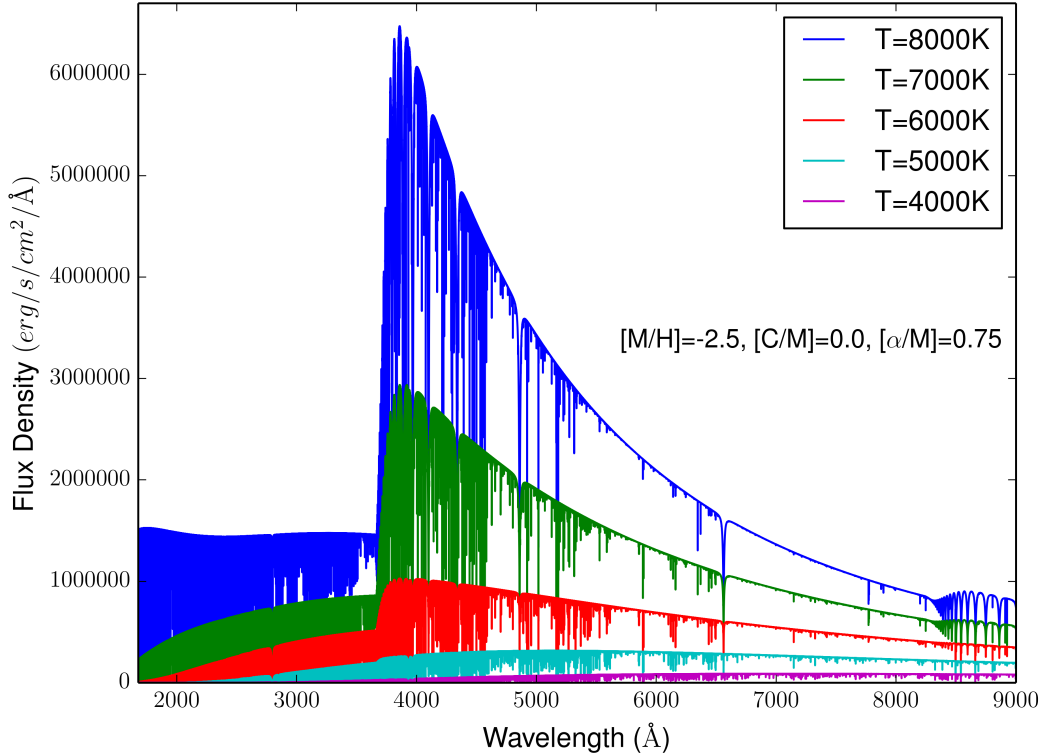

Figure 1: Example temperature sequence from the lowest metallicity, highest [α/Fe] abundance stars generated in our theoretical stellar spectral grid. [M/H]=[Fe/H] in this plot.

1 Introduction

These data are for three theoretical grids of stellar spectra, generated by A.T. Knowles in work for his thesis (Knowles A.T., 2019, PhD thesis, UCLan). The spectra are produced using ATLAS9 code to create model atmospheres and opacity distribution functions (described in [5][1]) and ASSET radiative transfer code [4] to create resultant star spectra. The details of computation are presented in A.T. Knowles' thesis and are similar to those described in [2].

Star spectra are computed for a large range of effective temperatures, surface gravity, metallicity ([M/H])[2], as well as abundances of elements formed by the capture of α particles ([α/M])[3] and abundances of carbon

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[1]See also : http://www.iac.es/proyecto/ATLAS-APOGEE/

[2][M/H] $= \log[n(M)/n(H)]_* - \log[n(M)/n(H)]_\odot$, where $n(M)$ is the number abundance of element M relative to solar values. [M/H] here is defined as a scaled-metallicity in which most metals are scaled by the same factor from the solar mixture (e.g. [M/H]=0.2=[Fe/H]=[Li/H]). This definition means [α/M]=[α/Fe] and [C/M]=[C/Fe].

[3]The α elements we included are: O, Ne, Mg, Si, S, Ca and Ti.

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&SYNTH
SYNTHFILE_INTERNAL = '3500RawGrid.dat'
ID = '3500Grid'
N_OF_DIM = 5
N_P = 7 5 3 11 11
LABEL(1) = 'METALS'
LABEL(2) = 'O Ne Mg Si S Ca Ti'
LABEL(3) = 'C'
LABEL(4) = 'TEFF'
LABEL(5) = 'LOGG'
LLIMITS = -2.5 -0.25 -0.25 3500 0.0
STEPS = 0.5 0.25 0.25 250 0.5
NPIX = 146497
WAVE = 1677.1 0.05
LOGW = 0
 /
2.90652877766e-07 1.64888803056e-07 2.78591272718e-07 1.95505364786e-07 2.44667717197e-07 2.9
```

This is the input FERЯE data file name.

This is the ID assigned to the input FERЯE data file.

Figure 2: Extract of 3500-6000K FERRE grid data file header and start of spectral data.

([C/M], relative to metal abundances. The atomic and molecular line lists used are those described in the thesis of A.T. Knowles and in [2]. Any star above 6000K is computed with the same line list as lower temperatures but with TiO molecular transitions removed. Spectra are computed with different resolving powers, dictated by the microturbulence and thermal Doppler width, but binned to a common wavelength sampling of $\delta\lambda=0.05$Å with a wavelength range of 1677.1Å to 9001.9Å.

The grid is split into three sub grids in effective temperature: The main grid (from 3500-6000K - named **Main-Grid.dat**), the intermediate grid (6000-8250K - named **IntermediateGrid.dat**) and the high grid (8000-10000K - named **HighGrid.dat**). A separate smaller grid is also computed with calcium tracking iron ([Ca/Fe]=0 - **CaFeGrid.dat**), as seen in some early-type galaxies.

The microturbulence of each star, in the range of effective temperature from 3500-6000K is based on a relation described in A.T. Knowles' thesis as is given by:

$$\text{vturb (km/s)} = 0.998 + 3.16 \times 10^{-4}(\text{T}_{\text{eff}} - 5500) - 0.253(\log \text{g} - 4)$$
$$-2 \times 10^{-4}(\text{T}_{\text{eff}} - 5500)(\log \text{g} - 4) + 0.165(\log \text{g} - 4)^2 \quad (1)$$

Stars with effective temperatures above 6000K are assumed to have the same microturbulence as stars at 6000K.

2   Data

In Figure 1, I show an example spectral sequence in effective temperature of the star data files described above.

The data files here are presented as text .dat files, for use in FERЯE interpolation and fitting code (e.g. illustrated in [1] and publicly available at [4]), with the flux densities in a spectrum, and one spectrum per line, after the headers. In Figure 2 I give the start of an example FERЯE input file and explain the headers.

The 4th line gives the number of grid dimensions – in these data this is the 5 dimensions of effective temperature, surface gravity, metallicity [M/H], [α/M] and [C/M].

The 5th line gives the number of steps in each dimension, in the order of the subsequent LABEL lines. In this example we have 7 steps in [M/H], 5 in [α/M], 3 in [C/M], 11 in effective temperature and 11 in surface gravity.

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[4]http://hebe.as.utexas.edu/ferre/

The 11th line gives the lower limits of each grid dimension. In this example, we start at [M/H]=-2.5, [α/M]=-0.25, [C/M]=-0.25, T_{eff}=3500K and log g=0.0.

The 12th line gives the grid steps in each dimension. Here we have steps of in [M/H] of 0.5 dex, steps in [α/M] of 0.25 dex, steps in [C/M] of 0.25 dex, steps in effective temperature of 250K and steps in surface gravity of 0.5 dex.

The 13th line gives the number of wavelength points (NPIX)

The 14th line gives both the starting wavelength value and the sampling. For the theoretical spectra provided, the starting wavelength is 1677.1Å with a sampling of $\delta\lambda$ =0.05Å.

The 15th line specifies if the sampling is in log or linear wavelength. We sampled here in linear wavelength.

With the looping structure described above the first flux values that appear on line 17 are for a spectrum of a star with parameters [M/H]=-2.5, [α/M]=-0.25, [C/M]=-0.25, T_{eff}=3500, log g=0.0. The 18th line would be for a spectrum with [M/H]=-2.5, [α/M]=-0.25, [C/M]=-0.25, T_{eff}=3500K, log g=0.5.

Flux is given as a flux density measured at the stellar surface (in units of erg/s/cm^2/Å)

3   Files

Several files are provided, which totals to $\approx$ 50GB when unzipped. I describe each of these files below.

- **MainGrid.dat** - This is the main grid of theoretical stellar spectra with the following parameter coverage:

    - Effective Temperature Range: 3500 – 6000K in steps of 250K
    - Surface Gravity Range: 0 to 5 dex in steps of 0.5 dex
    - [M/H] Range: -2.5, -2.0, -1.5, -1.0, -0.5, 0.0, 0.5
    - [C/M] Range: -0.25, 0.0, 0.25
    - [α/M] Range: -0.25, 0.0, 0.25, 0.50, 0.75
    - Number of Models = 12705
    - Size of File = 23 GB

- **IntermediateGrid.dat** - This is the intermediate temperature grid of theoretical stellar spectra, with the following parameter coverage:

    - Effective Temperature Range: 6000 – 8000K in steps of 250K
    - Surface Gravity Range: 1 to 5 dex in steps of 0.5 dex
    - [M/H] Range: -2.5, -2.0, -1.5, -1.0, -0.5, 0.0, 0.5
    - [C/M] Range: -0.25, 0.0, 0.25
    - [α/M] Range: -0.25, 0.0, 0.25, 0.50, 0.75
    - Number of Models = 8505
    - Size of File = 14 GB

- **HighGrid.dat** - This is the high temperature grid of theoretical stellar spectra, with the following parameter coverage:

    - Effective Temperature Range: 8000 – 10000K in steps of 250K
    - Surface Gravity Range: 2 to 5 dex in steps of 0.5 dex
    - [M/H] Range: -2.5, -2.0, -1.5, -1.0, -0.5, 0.0, 0.5
    - [C/M] Range: -0.25, 0.0, 0.25
    - [α/M] Range: -0.25, 0.0, 0.25, 0.50, 0.75
    - Number of Models = 6615

- Size of File = 9.7 GB

- **CaFeGrid.dat** - This is a separate smaller subgrid, at $[\alpha/M]=[C/M]=0.25$, which is computed with $[Ca/Fe]=0.0$, with the following parameter coverage:

  - Effective Temperature Range: 3500 – 6000K in steps of 250K
  - Surface Gravity Range: 0 to 5 dex in steps of 0.5 dex
  - [M/H] Range: -2.5, -2.0, -1.5, -1.0, -0.5, 0.0, 0.5
  - [C/M] Range: 0.25
  - $[\alpha/M]$ Range: 0.25 (excluding Ca)
  - Number of Models = 847
  - Size of File = 1.6 GB

- **3500_6000K_Grid_Order.txt** – The order that the spectra appear in the MainGrid.dat file after the headers.

- **6000_8000K_Grid_Order.txt** – The order that the spectra appear in the IntermediateGrid.dat file after the headers.

- **8000_10000K_Grid_Order.txt** – The order that the spectra appear in the HighGrid.dat file after the headers.

- **CaFe_Grid_Order.txt** – The order that the spectra appear in the CaFeGrid.dat file after the headers.

- **FERRE_to_fits_Full.py** – A python code to extract spectra from the .dat files and produce .fits files for each spectrum (requires Astropy).

  This code should be placed in the same directory as the unzipped .dat files. It can be run on individual .dat files as specified by the user (e.g. one of MainGrid.dat, IntermediateGrid.dat, HighGrid.dat or CaFeGrid.dat). The code will produce a directory (e.g. Main, Intermediate, High or CaFe) and will create one dimensional .fits[5] files, one per spectrum, in that directory with labels that match the order provided in the corresponding _Order.txt files. This can be done for all four grids with the option 'All'. Example Format in a Linux terminal: $python FERRE_to_fits_Full.py (and then reply to the prompt for which grid you want to extract from).

- **FERRE_to_fits_single.py** – A python code to extract a single spectrum from the .dat files and produce a .fits file for the spectrum (requires Astropy).

  This code should be placed in the same directory as the unzipped .dat grid files. The user specifies the effective temperature, surface gravity, metallicity ([M/H]), α-abundance ($[\alpha/M]$) and carbon abundance ([C/M]) of the spectrum they wish to extract. The parameters must be on a grid point in one of the four existing grids outlined above or the code will fail. Example Format in a Linux terminal: $python FERRE_to_fits_single.py (and then reply to the prompts to specify the parameters of the spectrum you want to extract). This will then create a spectrum with the format TxxxxgxxxMHxxAMxxCMxx.fits, in the directory with the name of the grid it was extracted from (e.g. if the user specified T=3500K, log g=4.0, [M/H]=0.0, $[\alpha/M]$=0.0, [C/M]=0.0 this will create a file : T3500g4.0MH0.0AM0.0CM0.0.fits in the directory /Main).

The python codes **FERRE_to_fits_Full.py** and **FERRE_to_fits_single.py** have been created and tested with Python version 2.7.15. Some modifications may be required if earlier or later versions of Python are used. These python codes also require the Astropy package to be installed in order to run. Astropy is included in the Anaconda distribution of python, which can run on Windows, macOS or Linux operating systems. The python codes are commented, for further information.

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[5]Note: Due to the large wavelength range (1677.1-9001.9Å) and fine sampling ($\delta\lambda = 0.05$Å), each .fits file will be approximately 1 MB in size.

4   Use of these files

Whilst these theoretical spectra are made publicly available for anyone to download and use, this is at the users own risk. The author does not guarantee that they are free from errors. If you make use of these data please acknowledge Knowles A.T, 2019, PhD thesis, UCLan. These are purely theoretical stellar spectra. For a comparison with real star spectra see [3] and A.T. Knowles' thesis.

References

[1] C. Allende Prieto, T. C. Beers, R. Wilhelm, H. J. Newberg, C. M. Rockosi, B. Yanny, and Y. S. Lee. A Spectroscopic Study of the Ancient Milky Way: F- and G-Type Stars in the Third Data Release of the Sloan Digital Sky Survey. *ApJ*, 636:804–820, Jan. 2006.

[2] C. Allende Prieto, L. Koesterke, I. Hubeny, M. A. Bautista, P. S. Barklem, and S. N. Nahar. A collection of model stellar spectra for spectral types B to early-M. *A&A*, 618:A25, Oct. 2018.

[3] A. T. Knowles, A. E. Sansom, P. R. T. Coelho, C. Allende Prieto, C. Conroy, and A. Vazdekis. Stellar spectral models compared with empirical data. *MNRAS*, 486(2):1814–1832, Jun 2019.

[4] L. Koesterke. Quantitative Spectroscopy in 3D. In I. Hubeny, J. M. Stone, K. MacGregor, and K. Werner, editors, *American Institute of Physics Conference Series*, volume 1171 of *American Institute of Physics Conference Series*, pages 73–84, Sept. 2009.

[5] S. Mészáros, C. Allende Prieto, B. Edvardsson, F. Castelli, A. E. García Pérez, B. Gustafsson, S. R. Majewski, B. Plez, R. Schiavon, M. Shetrone, and A. de Vicente. New ATLAS9 and MARCS Model Atmosphere Grids for the Apache Point Observatory Galactic Evolution Experiment (APOGEE). *AJ*, 144:120, Oct. 2012.