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StarNormal synthetic spectra used by CU6 for Data Release 2

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Abstract

This Note describes the selection of the StarNormal synthetic spectra used in CU6, and the related files derived from those spectra. This Note is valid for version 19.0.3 and 20.0.2 of the files. The present Note supersedes RHB-003.

Document History

Issue	Revision	Date	Author	Comment
1	0	2017-04-21	RHB	Updated with comments from CCB
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1 Introduction

1.1 Objectives

In CU6, synthetic spectra are required by a number of modules (PointBg, DetermineAp and the various radial velocity modules in Single Transit Analysis). These synthetic spectra are stored in the MDB object StarNormal[1].

The full set of StarNormal data provided by CU8 is not used, but a selection is made. The present Note describes this selection. It also describes the creation of a number of related files that are required by the various CU6 modules. The Note describes versions 19.0.3 and 20.0.2[2].

The present Note supersedes document RHB-003, which described version 19.0.1. To ensure continuity with RHB-003, Appendix C describes versions 19.0.2 and 20.0.1.

1.2 References

[RHB-003], Blomme, R., Fremat, Y., David, M., 2015, *StarNormal synthetic spectra used in CU6*,
`GAIA-C6-TN-ROB-RHB-003`,
URL `http://www.rssd.esa.int/cs/livelink/open/3366182`

[UH-005], Heiter, U., Soubiran, C., 2017, *Minutes of the Auxiliary Data splinter held in January 2017 Sitges*,
`GAIA-CD-MN-UAO-UH-005`,
URL `http://www.rssd.esa.int/cs/livelink/open/3482942`

[HEH-004], Huckle, H., 2009, *WP620 Software Design Document - Spectra Extraction*,
`GAIA-C6-SP-MSSL-HEH-004`,
URL `http://www.rssd.esa.int/cs/livelink/open/2736766`

[OML-001], Marchal, O., Viala, Y., Blomme, R., et al., 2016, *TN describing the Extraction (DU620) module DetermineAtmParams*,
`GAIA-C6-TN-OPM-OML-001`,
URL `http://www.rssd.esa.int/cs/livelink/open/3257001`

Robin, A.C., Luri, X., Reylé, C., et al., 2012, A&A, 543, A100, ADS Link

[1] `gaia.cu1.mdb.cu8.splib.dm.StarNormal` and `gaia.cu1.mdb.cu8.splib.dmimpl.StarNormalImpl`.

[2] The only distinction between 19.0.3 and 20.0.2 is the version of the MDB data model used. In 20.0.2, all wavelength information of the StarNormal object is stored in `double` variables, while in 19.0.3 they are stored in `float` variables.

[FT-002], Thevenin, F., Korn, A., Soubiran, C., et al., 2008, *Interface Control Document for the Gaia spectral libraries*,
GAIA-C8-SP-OCA-FT-002,
URL http://www.rssd.esa.int/cs/livelink/open/2817894

[YV-002], Viala, Y., Blomme, R., Delle Luche, C., et al., 2014, *WP650 Software Design Document - Single Transit Analysis*,
GAIA-C6-SP-OPM-YV-002,
URL http://www.rssd.esa.int/cs/livelink/open/2752329

1.3 Acronyms

The following is a complete list of acronyms used in this document. The following table has been generated from the on-line Gaia acronym list:

Acronym	**Description**
AP	Astrophysical Parameters
CCB	Configuration Control Board
JIRA	issue tracking product (not an acronym, but a truncation of Gojira, the Japanese name for Godzilla)
MDB	Main DataBase
OB	Stellar spectral types O and B
RVS	Radial Velocity Spectrometer
STA	Single Transit Analysis

2 StarNormal data

A substantial number of synthetic spectra have been calculated by CU8. For the purposes of CU6, we do not use all of them, but we restrict ourselves to:

- a grid of MARCS spectra, covering $T_{\rm eff}$ = 2 500 – 8 000 K
- a grid of A-type spectra, covering $T_{\rm eff}$ = 8 500 – 15 000 K
- a grid of OB-type spectra, covering $T_{\rm eff}$ = 15 000 - 55 000 K

2.1 Data provenance

The provenance of all spectra used by CU6 is detailed in Appendix A.

The ascii version of these data is stored on
`https://gaiaweb-ope.cnes.fr/sitools/datastorage/user/CU6InitData/CU8SyntheticSpectra/`.

Plans are to move these data to a CU9 storage area (UH-005, Sect. 3).

2.2 Ascii files

The format of the ascii files is described in FT-002. Each ascii file consists of a series of two lines: the first line is a header[3] containing all parameters of the spectrum, the second line contains the fluxes. Spectra can be provided for BP/RP as well as RVS. Obviously, in CU6 we consider only the RVS spectra.

Usually, fluxes are provided as F_λ in units of $\mathrm{W\,m^{-2}\,nm^{-1}}$, but in some cases normalized fluxes have also been provided.

Any synthetic spectrum is characterized by a number of parameters. The main ones are the effective temperature ($T_{\rm eff}$), the gravity ($\log g$) and the metallicity ($[Fe/H]$). Secondary parameters include (but are not limited to): the abundance of the α elements ($[\alpha/Fe]$), and the turbulent velocity ($v_{\rm turb}$).

2.3 Selection

For the MARCS and A-star files, we chose the "abs" version of the files: these contain the non-normalized fluxes. This is consistent with previous practice in CU6. It also maintains consistency with the OB-star file, where the normalized version is not available[4].

The StarNormals are uniquely identified by their specId field. For this, CU6 uses a concatenation of the $T_{\rm eff}$, $\log g$ and $[Fe/H]$ values[5].

The MARCS spectra are available for various values of the $[\alpha/Fe]$ parameter. But as this is not

[3] The format of the header is described in `https://wiki.cosmos.esa.int/gaia-dpac/images/3/32/Simu_README_requierments.txt`.

[4] A normalized version is not available for the OB library because of the line blends – especially in B type stars. It would be useless to normalize at the computed continuum, as a similar operation cannot be performed on an observed spectrum.

[5] Specifically: specId = ($T_{\rm eff}$*1000+abs($\log g$) *10)*10000+abs($[Fe/H]$)*100. For negative values of $\log g$ and $[Fe/H]$, their highest leading 0 is replaced by 9.

coded in the specId, only the MARCS spectra with the lowest, non-negative $[\alpha/Fe]$ for a given $T_{\rm eff}$, $\log g$ and $[Fe/H]$ were selected for CU6.

Because the $v_{\rm turb}$ value is not included in the specId, we selected the OB spectra with $v_{\rm turb} = 2\ {\rm km\,s^{-1}}$ (i.e., not including the $v_{\rm turb} = 10\ {\rm km\,s^{-1}}$ spectra). This choice is consistent with the value for the cool stars[6]. Two entries are duplicated in the OB file: in those cases, we selected the first one.

The A-star and OB-star grid overlap at $T_{\rm eff}$=15,000 K. In that case, we chose the OB-star spectra, as their grid is denser.

For all spectra, we change the $[Fe/H]$ value to that compared to the solar value (for which 7.50 was adopted). The OB star file uses $[\alpha/Fe]$ that is not solar-based: we changed this by subtracting 1.62. The listed resolution of 0.003 in the OB star file was changed to 300000.0, making it consistent with the other files.

Details of the CreateStarNormal code that was used to implement the above are given in Appendix B.

Figure 1 gives an overview of the spectra that are available in the new version 19.0.3, and compares it to the old 19.0.2 version. Green symbols indicate new spectra compared to version 19.0.2, red symbols spectra that were in 19.0.2, but not in the new version. Black symbols indicate spectra that are in both versions. Although some coverage is lost (mainly in the A-type star range at solar metallicity), a substantial increase in metallicity and temperature is clearly shown.

Version 19.0.3 contains 5 256 spectra, compared to 2 933 spectra in version 19.0.2.

3 Related files

3.1 Restricted StarNormal dataset

During the first few operational cycles, we do not have any astrophysical parameters (AP) from CU8. Some stars have their astrophysical parameters set from an input catalogue. For those stars where this is not possible, a module called DetermineAP (OML-001) is used instead to determine the AP. It works by cross-correlating the observed spectrum with a restricted set of templates. The template that gives the highest cross-correlation peak provides the AP for this star.

[6] Although hotter stars are expected to have higher $v_{\rm turb}$ values.

FIGURE 1: Overview of the synthetic spectra selected for CU6. Each plot shows the $T_{\rm eff}$, $\log g$ combinations for a given $[Fe/H]$. Green symbols indicate new spectra compared to version 19.0.2, red symbols spectra that were in 19.0.2, but not in the present version. Black symbols indicate spectra that are in both versions.

A restricted dataset of 28[7] StarNormal spectra was therefore introduced for DetermineAP (HEH-004). It is also being used by PointBG (HEH-004) and TodCorHeavy (YV-002).

The following argumentation was used in the construction of this restricted StarNormal dataset:

- The set should be relatively small, so that the computation time is short.
- The steps in the APs should be chosen based on changes in morphology.
- We should consider the expected number of stars of a given spectral type/luminosity class. For this, we used the Gaia Universe Model Snapshot, described in Robin et al. (2012), specifically the tables in Sect. 3:
  - For GRVS $<$ 17 mag, the stars will be mostly main-sequence (55%), while for GRVS$<$12 mag they will be mostly giants (63%). The most frequent spectral types for GRVS$<$17 mag are G and K (32+32%). There are also 23% F stars. As a single representative type, we therefore take a G5, corresponding to T_{eff} = 5500 K, $\log g$ = 4.5 and $[Fe/H]$ = 0.0.
  - For GRVS$<$12 mag, the morphology of the spectra is important, and we use the sequence $[Fe/H]$ = 0.0 and T_{eff} = 3100, 3500, 4000, 4500, 5000, 5500, 6000, 6500, 7000, 7500, 8000, 9000, 10000, 15000, 20000, 25000, 30000 and 35000 K.
  - For the gravity for the GRVS$<$12 mag, Table 3.3 from Robin et al. (2012) suggests that most will be giants. That would be roughly $\log g$ = 3 (but it depends somewhat on T_{eff}). For the hotter stars, we keep them at their main-sequence value of $\log g$ = 4.
- A second series of cool stars with reduced metallicity ($[Fe/H]$ = -1.5) is introduced.
- Not all combinations of values we would like are available. Specifically the $\log g$ values sometimes had to be changed from 3.0 to 3.5 in version 19.0.1 (see RHB-003 for details), and this is here maintained.
- A rotational velocity = 0.0 $\mathrm{km\,s^{-1}}$ is assumed when converting these StarNormal into templates.

The parameters of the restricted StarNormal dataset are listed here:

[7] The original restricted dataset had 31 spectra. These had to be reduced to 28 when moving from version 16.0.0 to 19.0.1. See RHB-003 for details.

T_{eff} (K)	$\log g$	$[Fe/H]$	$[\alpha/Fe]$	T_{eff} (K)	$\log g$	$[Fe/H]$	$[\alpha/Fe]$
5500.0	4.5	0.0	0.0				
3100.0	3.0	0.0	0.0	3100.0	3.0	-1.5	0.2
3500.0	3.0	0.0	0.0	3500.0	3.0	-1.5	0.2
4000.0	3.0	0.0	0.0	4000.0	3.0	-1.5	0.2
4500.0	3.0	0.0	0.0	4500.0	3.0	-1.5	0.2
5000.0	3.0	0.0	0.0	5000.0	3.0	-1.5	0.2
5500.0	3.5	0.0	0.0	5500.0	3.5	-1.5	0.2
6000.0	3.5	0.0	0.0	6000.0	3.5	-1.5	0.2
6500.0	3.5	0.0	0.0	6500.0	3.5	-1.5	0.2
7000.0	3.0	0.0	0.0	7000.0	3.0	-1.5	0.2
7500.0	3.0	0.0	0.0				
8000.0	3.0	0.0	0.0				
9000.0	3.0	0.0	0.0				
10000.0	3.0	0.0	0.0				
15000.0	4.0	0.0	0.0				
20000.0	4.0	0.0	0.0				
25000.0	4.0	0.0	0.0				
30000.0	4.0	0.0	0.0				
35000.0	4.0	0.0	0.0				

3.2 Other files

Not all the modules that use StarNormal information, directly use the StarNormal file or the restricted StarNormal file. The CreateStarNormal code also creates the following related files:

- `CalibratedSpectrum-699-5-SYNTHETIC_SPECTRUM_TEMPLATES_NORMALIZED_RESTRICTED-R19.0.3.gbin` The StarNormal spectrum is passed through GenerateTemplate, to convert it into a template, which is stored in a CalibratedSpectrum object.
- `TemplateSpectrumDescription-699-5-SYNTHETIC_SPECTRA_DESCRIPTION_RESTRICTED-R19.0.3.gbin` The object TemplateSpectrumDescription that contains the parameters used to convert the StarNormal spectrum into a CalibratedSpectrum template.
- `SpectralLibrary-699-5-SYNTHETIC_SPECTRA_INDEX_RESTRICTED-R19.0.3.gbin` The SpectralLibrary[8] object contains a summary of the astrophysical parameters and specId of the restricted StarNormal dataset[9].

[8] `gaia.cu6.auxiliarydata.dm.SpectralLibrary`
[9] In version 20.0.2, there is also a file `SpectralLibrary-699-5-SYNTHETIC_SPECTRA_INDEX-R20.0.2.gbin`

- CalibratedSpectrum-699-5-SMOOTHED_TEMPLATES_CALIBRATED _SPECTRUM_FORMAT_RESTRICTED-R19.0.3.gbin The SmoothedTemplates[10] are calculated, and their information is then converted into a CalibratedSpectrum object.

Details of the CreateStarNormal code that was used to implement the above are given in Appendix B.

4 Overview of the files generated

This is a list of all version 19.0.3 files generated[11]:

- StarNormal-699-5-SYNTHETIC_SPECTRA-R19.0.3.gbin The full list of 5 256 synthetic spectra. Used by GenerateTemplate in the STA Chain.
- StarNormal-699-5-SYNTHETIC_SPECTRA_RESTRICTED-R19.0.3.gbin The restricted list of 28 synthetic spectra. Used by TodCorHeavy and PointBG.
- TemplateSpectrumDescription-699-5-SYNTHETIC_SPECTRA _DESCRIPTION_RESTRICTED-R19.0.3.gbin The template spectrum descriptions corresponding to the restricted list of 28 synthetic spectra. Used by DetermineAP and TodCorHeavy.
- CalibratedSpectrum-699-5-UNKNOWN-R19.0.3.gbin The calibrated spectra derived from the restricted list of 28 synthetic spectra. This is an intermediate result from CreateStarNormal, but it is not used by any module.
- CalibratedSpectrum-699-5-SYNTHETIC_SPECTRUM_TEMPLATES _NORMALIZED_RESTRICTED-R19.0.3.gbin The normalized versions of the calibrated spectra derived from the restricted list of 28 synthetic spectra. Used by DetermineAP.
- SmoothedTemplates-699-5-UNKNOWN-R19.0.3.gbin The smoothed templates derived from the restricted list of 28 synthetic spectra. This is an intermediate result from CreateStarNormal, but it is not used by any module.
- CalibratedSpectrum-699-5-SMOOTHED_TEMPLATES_CALIBRATED _SPECTRUM_FORMAT_RESTRICTED-R19.0.3.gbin The SmoothedTemplates information, converted into a format of a CalibratedSpectrum. Used by PointBG.

that contains the SpectralLibrary object for the full StarNormal dataset. There is no need for an equivalent of this file in version 19.0.3, as it is constructed in SP_PreProcessing/IncorporateAuxilaryInformation.

[10] gaia.cu6.auxiliarydata.dm.SmoothedTemplate

[11] For the 20.0.2 names, just replace 19.0.3 by 20.0.2 in the names listed.

- SpectralLibrary-699-5-SYNTHETIC_SPECTRA_INDEX_RESTRICTED -R19.0.3.gbin A summary of the astrophysical parameters and specId of the restricted StarNormal[12] dataset. Used by PointBG.

5 Version 19.0.2 vs 19.0.3: Effect on GlobalR2 results

The effect on GlobalR2 results of version 19.0.2 vs 19.0.3 is detailed in JIRA DCODO-11, which describes the difference between two technical tests run by CNES[13]. An edited version of this JIRA is reproduced here:

A comparison was made between the radial velocities of ground-based standards between StarNormal 19.0.2 StarNormal 19.0.3. Figure 2 shows the differences for various selections of the ground-based standards (given in the title to each plot). Each time, the left plot shows version 19.0.2 ("TC0"), the right one version 19.0.3 ("TC0_bis"). On each figure, the gray symbols give the individual velocity differences (RVS velocity from Integrator + BaryCentric-Correction - ground-based velocity) as a function of externalGRVS magnitude. The important numbers to look at are the ones in red (these are limited to isValid=true results with nbComponents=1). Each set of numbers gives the median, half of the 68.3% range, and the number of values that are outside 3 times this half range, over the total number of values. The numbers are given per interval of 2 mag, and also over the whole magnitude range (at the bottom right of each figure). For each set of numbers the one with the better median (between 19.0.2 and 19.0.3) is put in a red rectangle.

Summarizing the whole series of plots, one can say that version 19.0.2 is performing better for the higher-quality data, while version 19.0.3 is better for the lesser-quality data. But, usually the differences are not very large.

An additional test was made by comparing all radial velocities (not just the ones with ground-based values) between versions 19.0.2 and 19.0.3 – see Fig. 3. The format of the plot is similar to the previous ones, except that the gray symbols that showed individual differences have been replaced by a density plot, using a rainbow colour scale. The differences between the StarNormal 19.0.2 and 19.0.3 are minimal. The largest median difference is only -0.090 km/s for the brightest stars.

JIRA DCODO-11 then goes on to describe some problems with the error bars derived on the radial velocities. This is probably related to the errors on the wavelengths, and falls outside the scope of this Technical Note.

[12] See footnote 9.

[13] These are the TC0 and TC0_bis tests described in https://wiki.cosmos.esa.int/gaia-dpac/index.php/CU6:_Global-R2-Reprocessing_All_test_cases. They consist of running the CU6 codes on the data from revolutions [1110;1125] and [2240;2255]. The only changes between these two runs are the StarNormal and related files.

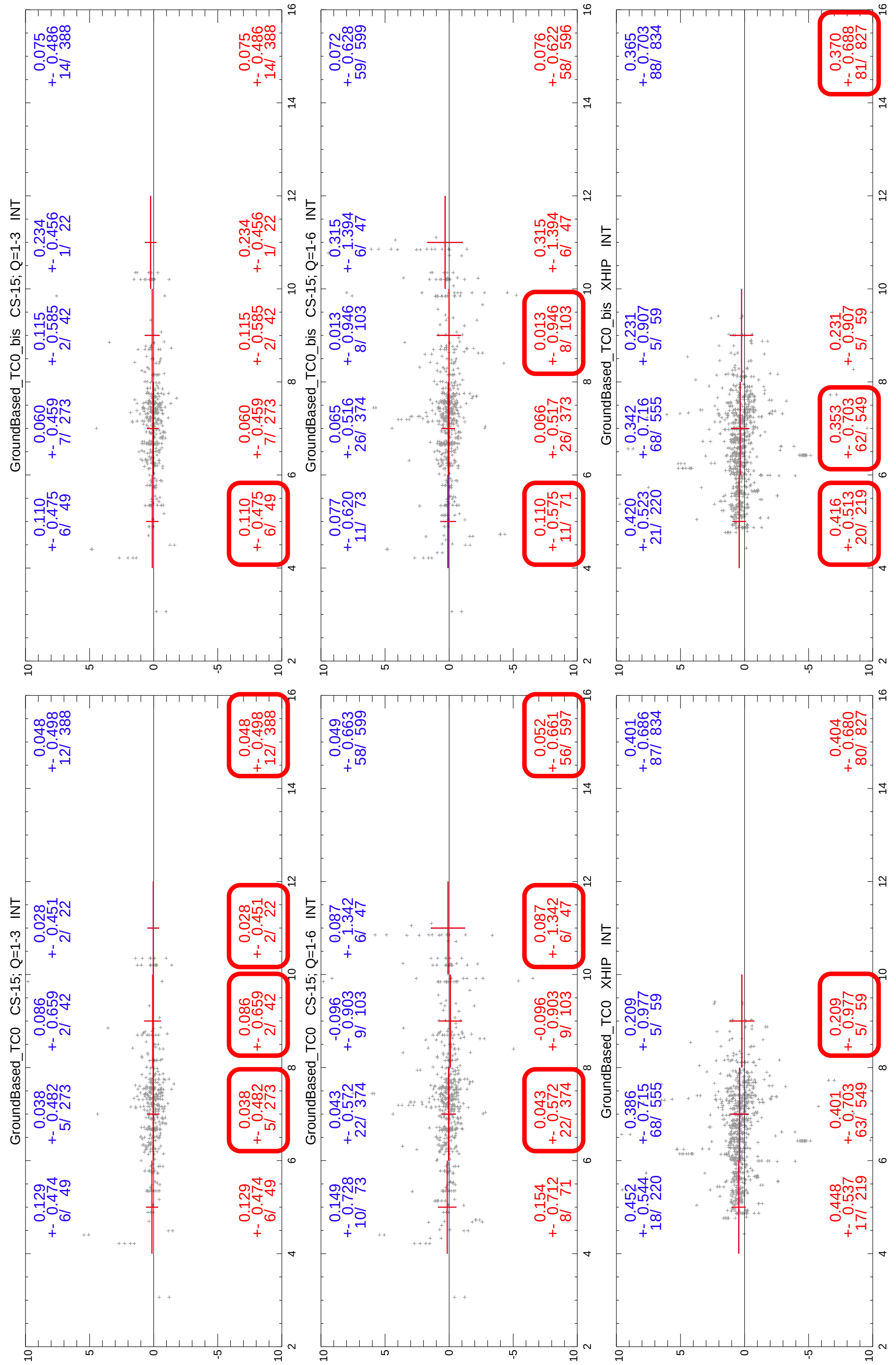

FIGURE 2: PART 1: Comparison between the radial velocities (y-axis in $\mathrm{km\,s^{-1}}$) of ground-based standards between StarNormal version 19.0.2 and version 19.0.3.

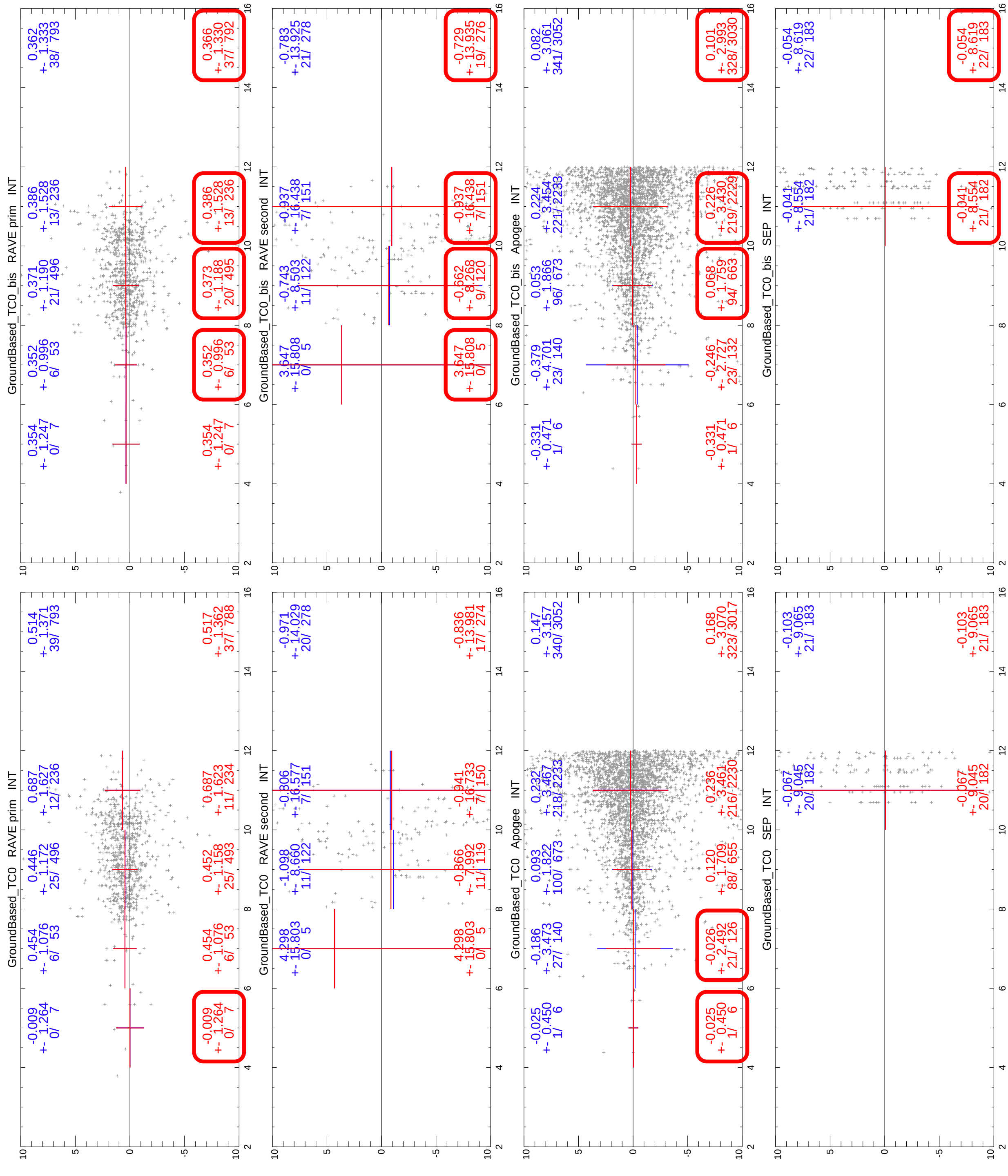

FIGURE 2: PART 2: Comparison between the radial velocities (y-axis in $\mathrm{km\,s^{-1}}$) of ground-based standards between StarNormal version 19.0.2 and version 19.0.3.

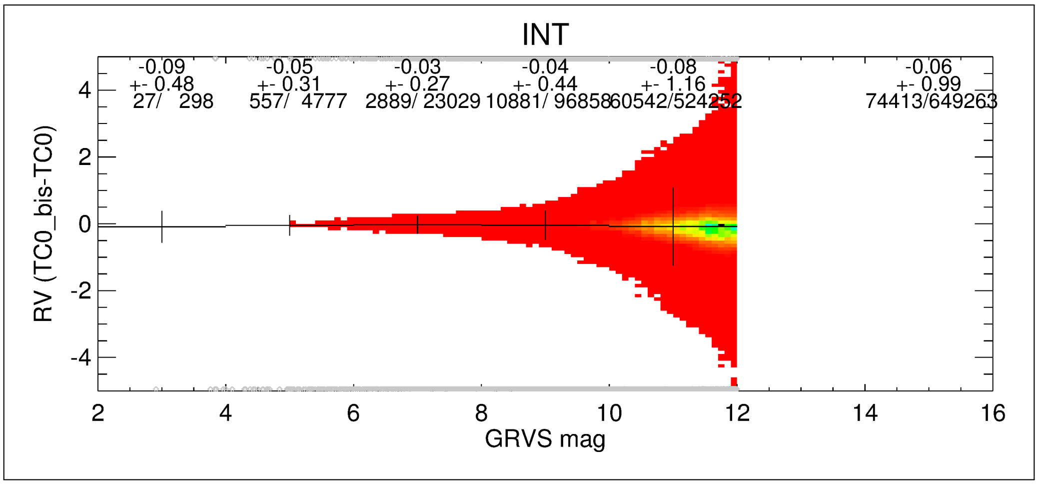

FIGURE 3: Comparison between all radial velocities (y-axis in $\mathrm{km\,s^{-1}}$), between StarNormal version 19.0.2 and version 19.0.3.

Appendix A Provenance of the synthetic spectra

A.1 ReadMe file of the full MARCS grid

```
17246 MARCS/BSYN RVS Version 3.0 spectra for GAIA 2015-12-20

0) Producers
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   Kjell Eriksson <Kjell.Eriksson@physics.uu.se>

1) Changes relative to Version 2 of the MARCS RVS spectra:
   *) Several line lists, e.g., the metal line list, have changed, see 7).
   *) The continuous opacity data treatment has been improved in that the
      the model structures were pressure integrated for the abundances used in
      the spectrum synthesis and consistent continuous opacities computed.
      In the earlier versions the pressures and opacities were adopted from the
      MARCS 2008 grid witout compensation for the different abundances.

2) Teff range:
   2500-3900 K, step 100 K.
   4000-8000 K, step 250 K.

3) log g -0.5 to +5.0, step 0.5 dex, g in units of cm/s^2.

   Note: many models and spectra are missing due to failing convergence of the
         model atmospheres.

4) Mass, Radius, Luminosity:
   a) The plane-parallel models, +3.5 <= log g <= +5.0, are massless. For
      these models the atmospheric extension is negligible relative to the
      radius, as are thus the sphericity effects. A plane-parallel model
      with a surface gravity "log g" may be used for any (astrophysically
      reasonable) mass and will have R/Rsun=SQRT(M/Msun * 10**(4.44-log g)).
      A Mass-Radius relation may be adopted, e.g., from a favourite set
      of theoretical isochrones.
   b) The spherical models, log g <= 3.0, for which the sphericity effects may
      be considerable for low masses and/or low log g, have been calculated
```

```
     for a mass of 1.0 Msun, and thus have a particular radius, see the
     equation under 4a).
   The luminosity is given by L/Lsun=(R/Rsun)**2 * (Teff/Teffsun)**4.

5) Abundance scales:
   The underlying MARCS models were calculated on the solar abundance scale by
   Grevesse, Asplund, Sauval (2007), Z=0.0122.

   From those new pressures and continuous opacities were computed by use of the
   following solar abundance scale (Z=0.0137).
   The logarithmic solar ( [Fe/H]=0.00 ) number abundances (H-U) are
  12.000  10.930   1.100   1.400   2.790   8.410   7.800   8.670   4.480   8.080
   6.330   7.580   6.470   7.550   5.450   7.330   5.280   6.400   5.120   6.360
   3.170   5.020   4.000   5.670   5.390   7.500   4.920   6.250   4.210   4.600
   2.880   3.410   2.370   3.410   2.630   3.310   2.600   2.970   2.240   2.600
   1.420   1.920 -99.000   1.840   1.120   1.690   1.240   1.770   0.820   2.000
   1.000   2.240   1.510   2.170   1.130   2.130   1.170   1.580   0.710   1.500
 -99.000   1.010   0.510   1.120   0.350   1.140   0.510   0.930   0.150   1.080
   0.060   0.880  -0.130   0.690   0.280   1.450   1.350   1.800   0.850   1.130
   0.830   1.950   0.710 -99.000 -99.000 -99.000 -99.000 -99.000 -99.000   0.090
 -99.000  -0.500

6) Abundance variations:

   Overall metallicities: [Fe/H] -5.0, -4.0, -3.0, -2.5, -2.0, -1.5, -1.0, -0.75,
                                 -0.50, -0.25, 0.0, +0.25, +0.5, +0.75, +1.0

   The MARCS MODELS were calculated for these 15 overall metallicities [Fe/H] with
   different values of [alpha/Fe]: Elements considered to be alpha elements are
   O, Ne, Mg, Si, S, Ar, Ca and Ti
     [alpha/Fe] = +0.00 for [Fe/H] =  +1.00, +0.75, +0.50, +0.25, +0.00
     [alpha/Fe] = +0.10 for [Fe/H] =  -0.25
     [alpha/Fe] = +0.20 for [Fe/H] =  -0.50
     [alpha/Fe] = +0.30 for [Fe/H] =  -0.75
     [alpha/Fe] = +0.40 for [Fe/H] =  -1.00, -1.50, -2.00, -2.50, -3.00,
                                      -4.00, -5.00
   In the calculations of SPECTRA from each MARCS MODEL four different values of
   the general alpha-element abundance were used: delta[alpha/Fe] -0.2, 0.0, +0.2,
   +0.4, all relative to the standard [alpha/Fe] values listed above.

7) Line data files:

   Hlines_RVS.list (Barklem & Eriksson)
   metals_8370-8930.list new VALD + Gustafsson et al. 2008 + astrophysical
   12CH-BX_8370-8930.list new Masseron et al. 2015, private communication
   13CH-BX_8370-8930.list new Masseron et al. 2015, private communication
   12CH-vibrotUGJ_8370-8930.list Joergensen (Hill et al. 1999 + Cayrel et al. 2004)
   13CH-vibrotUGJ_8370-8930.list Joergensen (Hill et al. 1999 + Cayrel et al. 2004)
   12C12C-Swan_Brooke_8370-8930.list new Brooke et al. via Plez
   12C12C_Fox-Herzberg_Kurucz_8370-8930.list new Kurucz (CD-ROM13)
   C12C12-BR_8370-8930.list Querci et al. 1971 (Ballic-Ramsay bands)
   C12C13-BR_8370-8930.list Querci et al. 1971 (Ballic-Ramsay bands)
   C12C12-P_8370-8930.list Querci et al. 1971 (Phillips bands)
   C12C13-P_8370-8930.list Querci et al. 1971 (Phillips bands)
   C13C13-P_8370-8930.list Querci et al. 1971 (Phillips bands)
   12C14N_Masseron_8370-8930.list new Sneden et al. 2014 via Masseron
   13C14N_Masseron_8370-8930.list new Sneden et al. 2014 via Masseron
   C12N15R_8370-8930.list Plez (see Hill et al. 1999)
   C13N15R_8370-8930.list Plez (see Hill et al. 1999)
   28SiH_A-X_electronic_Kurucz_8370-8930.list Kurucz (CD-ROM13)
   CaH_electronic_A-X_Plez_8370-8930.list Plez unpublished (See Plez 1998)
   CaH_electronic_B-X_Plez_8370-8930.list Plez unpublished (See Plez 1998)
   46TiO_electronic_Plez_2008_8370-8930.list Plez (See Plez 1998)
   47TiO_electronic_Plez_2008_8370-8930.list Plez (See Plez 1998)
   48TiO_electronic_Plez_2008_8370-8930.list Plez (See Plez 1998)
```

```
   49TiO_electronic_Plez_2008_8370-8930.list Plez (See Plez 1998)
   50TiO_electronic_Plez_2008_8370-8930.list Plez (See Plez 1998)
   VO_electronic_Plez_8370-8930.list Plez (See Plez 1998 and Plez et al. 2003)
   56FeH_Dulick_8370-8930.list new Dulick et al. 2003 via Plez
   90ZrO_electronic_Plez_8370-8930.list Plez (See Plez 1998 and Plez et al. 2003)
   91ZrO_electronic_Plez_8370-8930.list Plez (See Plez 1998 and Plez et al. 2003)
   92ZrO_electronic_Plez_8370-8930.list Plez (See Plez 1998 and Plez et al. 2003)
   94ZrO_electronic_Plez_8370-8930.list Plez (See Plez 1998 and Plez et al. 2003)
   96ZrO_electronic_Plez_8370-8930.list Plez (See Plez 1998 and Plez et al. 2003)
   H2O_Barber_cut-8_8370-8930.list new Barber et al. 2006 via Plez
   HCN_Harris_8370-8930.list new Harris et al. (2006) via Plez

   Isotope ratios used in the calculations:
      C: 98.9%   12C,    1.1%   13C
      N: 99.634% 14N,    0.366% 15N
    ( O: 99.762% 16O,    0.038% 17O,    0.200% 18O )
    (Mg: 78.99%  24Mg  10.00%  25Mg  11.01%  26Mg )
     Si: 92.23%  28Si,  4.67%  29Si,  3.10%  30Si
    (Ca: 96.94%  40Ca,  0.647% 42Ca,  0.135% 43Ca,  2.086% 44Ca, 0.187% 48Ca )
     Ti:  8.0%   46Ti,  7.3%   47Ti, 73.8%   48Ti,  5.5%   49Ti, 5.4%   50Ti
    ( V:  0.25%  50V,  99.75%  51V )
     Fe:  5.8%   54Fe, 91.72%  56Fe,  2.2%   57Fe,  0.28%  58Fe
     Zr: 51.46%  90Zr, 11.22%  91Zr, 17.15%  92Zr, 17.38%  94Zr, 2.80%  96Zr

8) Microturbulence parameter:
   1.0 km/s for plane-parallel models which all have log g >=3.5
   2.0 km/s for spherical models which all have log g <=3.0

9) Geometry
   For the log g <=3.0 spherical geometry was used with a stellar
   mass=1.0 Msun and a microturbulence parameter 2.0 km/s,
   see Heiter & Eriksson 2006, while the log g >=3.5 models are plane parallel
   and have no mass, mass=-999.000 Msun is indicated, and their
   microturbulence parameters are set to 1.0 km/s

10) The grid is not complete; models are lacking where the MARCS models do not converge.

11) References
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    Heiter U., Eriksson K. 2006, A&A 452, 1039
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12) Acknowledgments
    We thank B. Plez and T. Masseron for providing the molecular linelists.

13) The RVS vacuum-wavelength range is 840.0 - 890.0 nm.  The synthetic spectra
    were computed with a wavelength step of 0.001 nm and convolved with a
    Gaussian profile with FWHM=0.003 nm.
    The synthetic spectra are supplied in 2 versions:
    a) absolute surface flux at each wavelength bin is given in units of W/m^2/nm.
       The gzipped absolute-flux files carry '.abs' in the name.
    b) normalized flux, relative to the local continuum flux, no units.
       The gzipped relative-flux files carry '.rel' in the name.
```

```
    There are 15 files of each kind, one for each overall metallicity,
       see 15) below.

14) Data volume
    Each spectrum is formatted with one header record and one data record
    accordinmg to Thevenin et al. 2008, GAIA-C8-SP-OCA-FT-002. These have
    been concatenated in 15 files (for each the 15 overall metallicities)
    for absolute fluxes and 15 files for relative fluxes.
    There is a little less than 4 Gbytes in the delivery.

15) Deliverance

The 15 absolute flux data files and this Readme are packed in file MARCS_3_abs.tar:

  Bytes      Name
 162710632   MARCS_3_Z+0.00_abs.dat.gz
 161493797   MARCS_3_Z+0.25_abs.dat.gz
 162067919   MARCS_3_Z+0.50_abs.dat.gz
 163941486   MARCS_3_Z+0.75_abs.dat.gz
 161022174   MARCS_3_Z+1.00_abs.dat.gz
 155187306   MARCS_3_Z-0.25_abs.dat.gz
 148779203   MARCS_3_Z-0.50_abs.dat.gz
 141209293   MARCS_3_Z-0.75_abs.dat.gz
 136518209   MARCS_3_Z-1.00_abs.dat.gz
 121217484   MARCS_3_Z-1.50_abs.dat.gz
 104454083   MARCS_3_Z-2.00_abs.dat.gz
  96155955   MARCS_3_Z-2.50_abs.dat.gz
  69805178   MARCS_3_Z-3.00_abs.dat.gz
  47963636   MARCS_3_Z-4.00_abs.dat.gz
  32215834   MARCS_3_Z-5.00_abs.dat.gz

The absolute flux data files will expand by a factor of 4 when unzipped

The 15 relative flux data files and this Readme are packed in file MARCS_3_rel.tar:

  Bytes      Name
 164084753   MARCS_3_Z+0.00_rel.dat.gz
 162524164   MARCS_3_Z+0.25_rel.dat.gz
 162050816   MARCS_3_Z+0.50_rel.dat.gz
 162901469   MARCS_3_Z+0.75_rel.dat.gz
 159029936   MARCS_3_Z+1.00_rel.dat.gz
 157552774   MARCS_3_Z-0.25_rel.dat.gz
 152060439   MARCS_3_Z-0.50_rel.dat.gz
 145242816   MARCS_3_Z-0.75_rel.dat.gz
 141242102   MARCS_3_Z-1.00_rel.dat.gz
 127818429   MARCS_3_Z-1.50_rel.dat.gz
 111319941   MARCS_3_Z-2.00_rel.dat.gz
 103423015   MARCS_3_Z-2.50_rel.dat.gz
  75958023   MARCS_3_Z-3.00_rel.dat.gz
  51152474   MARCS_3_Z-4.00_rel.dat.gz
  32718321   MARCS_3_Z-5.00_rel.dat.gz

The relative flux data files will expand by a factor of 3 when unzipped
================= END ==========================================================
```

A.2 Provenance of the A-stars grid

A.2.1 Provenance file

```
These are models for A-type stars, calculated by Alex Lobel (Alex.Lobel@oma.be).
The following information is based on email exchanges (28/03/2016) with him:
```

```
There are 8 ASCII files of ~47 Mb each (hence the total download is 371 Mb)

The models have been grouped per file with suffixes m0.5 ([M/H]=-0.50),
m0.25 ([M/H]=-0.25), p0.00 ([M/H]=0.00), and p0.25 ([M/H]=+0.25).
The .rel files contain the continuum normalized fluxes, while the .abs files
are in absolute fluxes for vacuum wavelength scale.

The 81 models per file have been computed for log(g)>=2.0 to 5.0. We also
tried to converge a number of models for log(g) < 2.0 but for these high
Teffs the ATLAS9 convergency speed considerably slowed down so we did not
explore this further. This will be done later for a number of A- and B-type
benchmark supergiant in BRASS.

Ronny Blomme (Ronny.Blomme@oma.be)
03/06/2016
```

A.2.2 Additional information

```
These ATLAS9 plane parallel LTE models have been converged using MLT parameter l/H=1.25,
no turbulence pressure Pturb=0, and without overshoot.

Teff: from 8500 K to 15000 K in steps of 500 K

logg: 5 to 0.5 in steps of 0.5

[M/H]: -0.5 to +0.25 in steps of 0.25

[alpha/Fe]: fixed to 0.0 only

Vmic: 1 km/s for logg>3.5 and 2 km/s for logg<3.5

Solar abundance scale of Grevess & Sauval 1998

These Gaia-RVS specta are computed in vacuum. All tables of continuum normalized fluxes
are ASCII tar'd for one and the same
wavelength scale from 8400.00 A to 8900.00 A in steps of 0.01 A.
A fixed broadening of FWHM=0.03 A was applied to all spectra.

To ensure maximum consistency with the MARCS grid we adopted all the atomic data provided
by K. Eriksson for the RVS. This means that the same lines in the BRASS RVS lines list
have been replaced by the atomic data contained in his files. We used the same isotopic
abundance fractions for all elements. We did not change the C, N, O abundances as is
also the case in the MARCS models.

Alex Lobel (26/03/2017)
```

A.3 ReadMe file of the OB-stars grid

```
New version of the OB star library

I recomputed some of the models that were prepared by Jean Claude Bouret and
Thierry Lanz in the first version of the grid. I started from the OSTARS and BSTARS
grids that are available on TLUSTY's website:

http://nova.astro.umd.edu/

An overview (that was written by Jean Claude) of the model characteristics is given
at the bottom of this README file.
```

```
Starting from these NLTE models, I computed the synthetic spectra for three metallicity
regimes (2 x Z_Sun, 0.5 x Z_Sun and 1 x Z_Sun) and 2 values for the microturbulence (2 and 10 km/s).
The H/He ratio was supposed Solar (Solar abundances are from Grevesse & Sauval, 1998).

Physical fluxes are tabulated in MKSA units: W/m^2/nm .

The line list was downloaded from the VALD database and covers the whole Gaia wavelength range, while
hydrogen lines are treated using the Stark broadening functions computed by Stehle C. (1996ASPC..108..123S).

BP/RP and RVS fluxes were saved in one single file: fremat_OB.dat .

Do not hesitate to take contact with me if you need more information.

Y.Fremat (ROB)

Photospheric Models

Photospheric models have been constructed with the model atmosphere code TLUSTY (Hubeny & Lanz 1995).
The main assumptions of the code are a plane-parallel geometry, hydrostatic equilibrium, and radiative
equilibrium. Departures from LTE are explicitly allowed for a large set of chemical species and
arbitrarily complex model atoms. Line opacity is treated in detail by using an opacity sampling technique
with close to 200,000 frequency points over the whole spectrum. Models with a scaled-solar composition,
Z/Z = 2, 1, 1/2 have been computed. Solar abundances are from Grevesse & Sauval (1998). We also have
computed models with solar abundances as taken from Asplund et al. (2004). All model atmospheres assume
a helium abundance y = He/H = 0.1 by number and a microturbulent velocity t = 10 km s-1 and 2 km s-1
for O and B stars, respectively. A detailed synthetic spectrum is then calculated with SYNSPEC
(Hubeny & Lanz 1995), with no variation of abundances at this step. For O stars, we have updated models
from the extensive grid originally computed and described in details by Lanz & Hubeny (2003). These fully
blanketed NLTE model atmospheres include about 100,000 individual atomic levels from 45 ions (H I-II,
He I-II, C I-IV, N II-VI, O II-VII, Ne II-V, Si II-IV, P IV-VI, S III-VII, Fe III-VII, and Ni III-VII).
Lanz & Hubeny (2003) have pointed out that the omission of highly excited atomic levels of light species
in OSTAR2002 model atmospheres results in underestimating some recombination rates. We have therefore
recalculated the full set of model atmospheres with more extensive model atoms for C III and N IV to
achieve a better prediction of recombination lines seen in emission in the visible spectrum.
Concerning B stars, because of the smaller thermal Doppler width and the lower microturbulent velocity
(2 km s-1), sampling the spectrum with the same characteristic frequency step (0.75 fiducial Doppler
width) thus requires many more frequencies over the whole spectrum than in the Ostar2005 models -
typically, the Bstar2006 models consider about 380 000 frequencies.These fully blanketed NLTE model
atmospheres include about 100,000 individual atomic levels from 34 ions (H I-II, He I-II, C I-IV,
N I-V, O I-VI, Ne I-IV, Mg II, Al II-III, Si II-IV, S II-V, Fe II-V).
```

Appendix B Code details of CreateStarNormal

.

B.1 Code itself

The code to generate the StarNormal and related files, as well as the tests are available on svn: `https://gaia.esac.esa.int/dpacsvn/DPAC_tags/CU6/data/StarNormal/R_19.0.3/` and `https://gaia.esac.esa.int/dpacsvn/DPAC_tags/CU6/data/StarNormal/R_20.0.2/`

B.2 Procedure

The main program is `MakeStarNormalAndAssociatedFiles`.

Before starting this, `VersionNumberAndNames` should be checked. This contains the version number of the new files, the names of the old files, and the directory and filenames of the input data. Note that some of these names refer to specific directories on the first author's computer.

When running `MakeStarNormalAndAssociatedFiles`, a pop-up menu is presented. The standard procedure is to call `MakeStarNormalAndAssociatedFiles` a number of times, and to go through the various choices of the pop-up menu, in order. The choices are:

1. **Analysis Ascii files** Checks a number of inputs of the StarNormal. Also checks what is the lowest non-negative $[\alpha/Fe]$ value and lowest $v_{\rm turb}$ for all $T_{\rm eff}$, $\log g$, and $[Fe/H]$ combinations. Checks that every $T_{\rm eff}$, $\log g$, and $[Fe/H]$ combination has an entry with the smallest non-negative $[\alpha/Fe]$ value, and that the combination specId + smallest non-negative $[\alpha/Fe]$ + smallest $v_{\rm turb}$ is unique.

2. **Create new full StarNormal file** Reads the input files and generates the (full) `StarNormal-699-5-SYNTHETIC_SPECTRA-R19.0.3.gbin` file. Based on information from "Analysis Ascii files", some selections are hard-coded.

3. **Check new full StarNormal file against old version**. Checks if all entries in the new full StarNormal file were also in the old one, and if they agree in detail. And vice-versa: check if all entries in the old file are also in the new one. Also checks that all old restricted StarNormals are in the new file.

4. **Create new restricted StarNormal file**. Creates `StarNormal-699-5-SYNTHETIC_SPECTRA_RESTRICTED-R19.0.3.gbin`. The selection is done by hardcoding the specIds that have to be selected.

5. **Check new restricted StarNormal file against old version**. Compare the new restricted StarNormal with the old one and note the differences.

6. **Create new templates from StarNormal**. Uses GenerateTemplate and ContinuumNormPoly to create `TemplateSpectrumDescription-699-5-SYNTHETIC_SPECTRA_DESCRIPTION_RESTRICTED-R19.0.3.gbin` and `CalibratedSpectrum-699-5-SYNTHETIC_SPECTRUM_TEMPLATES_NORMALIZED_RESTRICTED-R19.0.3.gbin`. The intermediate file `CalibratedSpectrum-699-5-UNKNOWN-R19.0.3.gbin` (with the non-normalized templates) is also created, but this is not used by any of the CU6 modules.

7. **Check new templates from StarNormal** Check the new TemplateSpectrumDescription file and CalibratedSpectrum file against the old version.

8. **Check normalization new templates** Check the new (normalized) CalibratedSpectrum file against the old version by overplotting them.

9. **Create new smoothed templates** First the SmoothedTemplates are created (file `SmoothedTemplates-699-5-UNKNOWN-R19.0.3.gbin`, not used by any of the CU6 modules). Then they are then converted to a CalibratedSpectrum object (file `CalibratedSpectrum-699-5-SMOOTHED_TEMPLATES_CALIBRATED_SPECTRUM_FORMAT_RESTRICTED-R19.0.3.gbin`). Also, the SpectralLibrary is created (file `SpectralLibrary-699-5-SYNTHETIC_SPECTRA_INDEX_RESTRICTED-R19.0.3.gbin`).

10. **Check new smoothed templates** Compare the CalibratedSpectrum file and the SpectralLibrary file against the old versions.

Appendix C Versions 19.0.2 and 20.0.1

For completeness, and to ensure continuity with RHB-003, we also describe here versions 19.0.2 and 20.0.1. These use the same StarNormal spectra as described in RHB-003. The changes made from 19.0.1 to 19.0.2 and 20.0.0 to 20.0.1 are described in JIRA C6AUXD-44, which is (partially) reproduced here:

> The StarNormal object contains the fields FeRef and FeAbund.
>
> - Document FT-002 ("Interface Control Document for the Gaia spectral libraries") describes the distinction between these two fields, but it is not clear if CU6 has enough information to fill in the FeRef value. Furthermore, in contrast to FT-002, CU6 practice is to consider abundances with respect to solar, not with respect to log H=12.
> - SP_PreProcessing/IncorporateAuxilaryInformation uses the FeRef field for the Fe abundance (with respect to solar).
> - The current implementation of CreateStarNormal does not fill in the FeRef field, but only the FeAbund field (with respect to solar). It therefore does not provide the correct information that is used by SP_PreProcessing/IncorporateAuxilaryInformation.
>
> The solution (within CU6) is therefore to have CreateStarNormal fill in both the FeRef and FeAbund field (both with respect to solar).