INTRIGOSS:

A Library of High Resolution Synthetic Spectra for FGK stars

M. Franchini, C. Morossi, P. Di Marcantonio

INAF-Osservatorio Astronomico Trieste, Italy

Libraries of synthetic spectra

Stellar spectra contain a wealth of information about the stars themselves as well as their progenitors. Theoretical predictions are our ultimate link between observations of stars and their fundamental physical parameters and abundances.

- **Conversion from an observed stellar spectrum to a measure of the star's chemical composition is highly nontrivial:**
  - It requires realistic **model of stellar atmospheres,** from with the stellar light originates, and accurate knowledge of the physical processes that originates the **emergent spectrum**

  The obtained abundances cannot be more trustworthy than the models employed to analyze the observations

Libraries of synthetic spectra

- **Nowadays, much work has been done to improve the realism of synthetic spectra but there are still considerable uncertainties in deriving stellar abundances depending on:**
  - different stellar atmosphere models (1D or 3D e.g. Asplund 2005, Asplund 2010)
  - inadequacies in the lines formation modelling (LTE or NLTE e.g. Asplund2005, Bergemann 2014)
  - input atomic and molecular data: completeness, accuracy of λ, log *gf* etc, Predicted Lines (i.e. transitions between levels predicted by atomic structure codes but not measured in laboratory, and affected by large uncertainties in their computed intensity and wavelength)
  - mandatory to use **atmosphere models** and **synthetic spectra** with **self-consistent abundance patterns.**

- **Nowadays, the uncertainties in stellar abundances analyses are dominated by systematic errors due to these shortcomings rather than by observational errors.**

- **Only when these shortcomings will be properly addressed, high quality data as those provided by the modern instruments, large surveys already available and/or in progress will reach their full potential**

Libraries of synthetic spectra

- **On the other hand, high quality data provided by the large surveys may be used to assess the validity of theoretical libraries in reproducing not only spectrophotometry but also high-resolution spectra**

For example in generating

INTRIGOSS (INaf-TRieste Grid Of Synthetic Spectra) for FGK stars

we took advantage of the UVES-U580 spectra of stars from **the Gaia-ESO survey (GES)** and their atmospheric parameters and abundances derived by the GES consortium to assess the validity of our library of High Resolution synthetic Normalized and Flux Surface spectra for FGK stars.

Libraries of synthetic spectra

AMBRE (de Laverney+ 2012) – **GES_Grid** – **PHOENIX (**Husser+2013) – **C14 (Coelho2014)** – **B17 (Brahm+2017)** – **etc**

- **Different Atmosphere Model CODES:**
  - Atlas9: Castelli & Kurucz 2003
  - Atlas12: Kurucz 2005
  - MARCS: Gustafsoon+ 2008
  - PHOENIX: Hauschildt & Baron 1999
  - …
- **Different spectral synthesis codes:**
  - DFSYNTHE: Castelli 2005, Kurucz 2005
  - SPECTRUM: Gray & Corbally 1994
  - PHOENIX: Hauschildt & Baron 1999
  - MOOG: www.as.utexas.edu/~chris/moog.html
  - …
- **Different adopted Solar Chemical Mixture** (Andersen & Grevesse 1989, Grevesse+ 2007, etc)
- **Different atomic and molecular line lists** (completeness, accuracy, no PLs)
- **Not all libraries provides both normalized HiRes spectra and SEDs**

INTRIGOSS

INTRIGOSS: INaf TRIeste Grid Of Synthetic Spectra

for F,G,K stars

computed with **SPECTRUM** code from the atmosphere models (**ATLAS12**)

Fully consistent

New atomic and molecular line list containing *bona fide* Predicted Lines

built by tuning log*gf* to reproduce HiRes reference spectra

Normalized SPectra (NSP) and surface Flux SPectra (FSP)

15600 HiRes spectra

$\lambda\lambda 4830$-5400Å

$\Delta\lambda = 0.01$Å ($R \lesssim 240{,}000$)

INTRIGOSS: Model Atmospheres

Atlas12 **can generates any atmospheric model since it is based on the Opacity Sampling (OS) Technique:**

➔ ***any desired individual element abundance***

➔ ***any microturbence ξ***

In particular:

- **Starting from ATLAS9 atmosphere models** calculated for the APOGEE survey (www.iac.es/proyecto/ATLAS-APOGEE) **to ATLAS12**

  T_{eff} : 3750 - 7000 K at step of 250 K
  log *g*: 0.5 - 5.0 dex at step of 0.5 dex
  [Fe/H]:-1.0 - +0.5 at step of 0.25 dex
  [α/Fe]:-0.25 - +0.5 at step of 0.25 dex (**α-el**: **O, Ne, Mg, Si, S,Ar, Ca,Ti)**

- **Microturbulence** ξ=1 and 2 km s^{-1}

INTRIGOSS: Spectral Synthesis Code

Spectrum v2.76e stellar spectral synthesis code to compute:

- ***Emergent Flux SPectrum (FSP) and Normalized SPectrum (NSP)***
- ***Local Termodynamic Equilibrium approximation (LTE)***

It requires:

- **Line list of atomic and molecular transitions**

  we used a new line list built by merging:

  1. line data used by Lobel (2011)
  2. a line list provided to us by R. O. Gray (2011, private communication),
  3. new molecular lines of CH, NH, MgH, SiH,C2 , CN, TiO from Kurucz's site
  4. atomic and molecular **Predicted Lines (**PLs) from Kurucz's site:.
- **Individual element abundances**
- **Microturbulence $\xi=1$ and 2 km s^{-1}**
- **Wavelength range and sampling ($\Delta\lambda=0.01$Å)**

INTRIGOSS: log *gf* optimization

Reliable atomic and molecular data:

➢ Several online databases:

- NIST, VALD, NORAD, Kuruz's website, etc.

  log *gf* values may be measured in laboratory or derived from theoretical calculations

  ➔ **accuracy** may vary widely from line to line from 1% (or better) to even orders of mag

➢ Possible way to reduce these uncertainties:

- ***to compare high SNR spectra of stars with their synthetic spectra:***
  - stars with well known **atmospheric parameters** (**T_{eff}, log*g*, [Fe/H],** ξ) and **abundances**
  - a **trial-and error procedure** is needed
  - Line depths depend both on stellar characteristics and on ***gf***-values:

    risk ➔ wrongly compensate with modified ***gf***-values any inaccuracies in **atmospheric parameters, abundances** and **in the modeling assumptions**.

Solution ➔ check the modified ***gf***-values in spectra of as many (and as different) as possible stars in order to disentangle the effect of incorrect **astrophysical *gf***-values from effects due to uncertainties in the assumed models and parameters.

INTRIGOSS: log ***gf*** optimization

Lobel 2011 (LO11) used Sun (5777,4.438), Procyon (6550,4.0) and ε Eri (5050,4.5):

- Solar composition assumed for Procyon and ε Eri
- Solar spectrum observed in 1981 with the NSO/KPNO FTS, degraded to R=80,000
- For Procyon and ε Eri several optical spectra with Hermes spectrometer on the 1.2m Mercator telescope at La Palma Observatory, R=80,000
- Updated the ***gf*** values of 911 neutral lines in 4000÷6000Å
- SCANSPEC synthetic spectra

Main causes of uncertainties:

- Solar composition for Procyon and ε Eri
- The use of only relatively **high temperature** ($T_{\rm eff}$ >5000K) **Main Sequence stars** which does not allow to check ***gf***-values of those atomic and molecular lines that are mainly prominent in spectra of **giants** and/or **cooler stars**

INTRIGOSS: log *gf* optimization

An *ad hoc* high SNR Solar spectrum:

- average of 59 integrated sunlight spectra as reflected by the Moon
- HARPS at 3.6m La Silla ESO telescope
- The out-of-transit sub-sample of spectra taken to detect the Rossiter-McLaughlin effect in the Sun due to the Venus transit of 2012 June 6 (Molaro+2017)
  - ➔ **SNR~4000**
- Elem. Abundances from Grevesse+ 2007

Spectra of 5 giants:

- **UVES,** 580nm setup, Gaia-ESO Survey (GES)
- **SNR** > 100
- $4500 \leq T_{\mathrm{eff}} \leq 5000$ K
- $2.0 \leq \log g \leq 3.2$ dex
- $1.0 \leq \xi \leq 1.5$ km s^{-1}
- Elem. abundances in GESiDR4 catalogue

INTRIGOSS : log *gf* optimization

Outline of our method :

1. **Use of the solar spectrum as the main reference star** to derive the astrophysical log *gf* for atomic and molecular lines that are important at solar T_{eff} and log$g$ by assuming no uncertainties in the solar parameters and in the adopted model atmosphere

   Trial-and-error procedure based on the comparison between the normalized observed and synthetic solar spectrum.

2. **Use of the 5 giants** to derive the astrophysical log *gf* for those lines that are more prominent at T_{eff} and log$g$ lower than solar:

   Trial-and-error procedure based on the comparison between the normalized observed and synthetic spectra computed using the GES atmospheric parameters, [el/Fe], $\xi, v\sin i$.

3. **Eventually, to validate our final list of astrophysical** log ***gf* over the full atmospheric parameter space covered by FGK stars, we took advantage of Gaia-ESO iDR4 release (2212 stars from GES)**

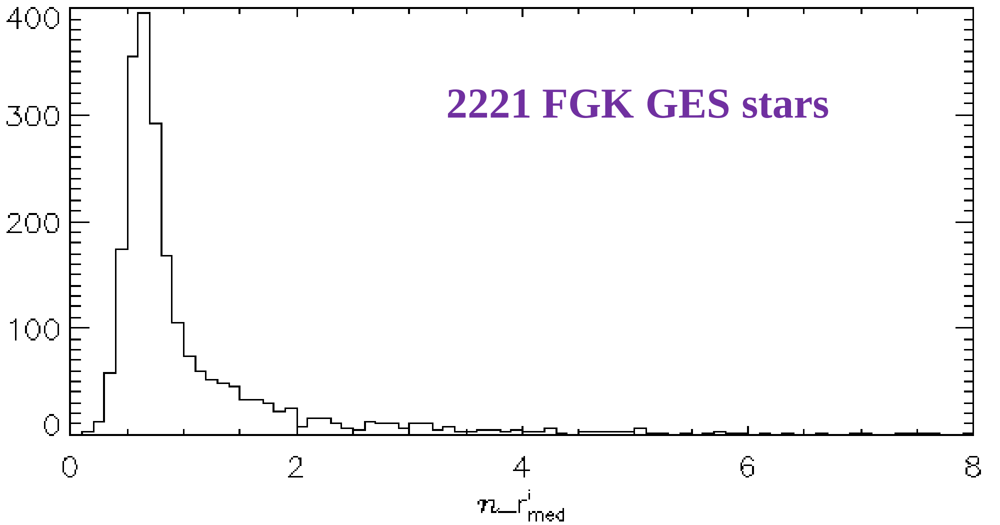
INTRIGOSS: Validity of our line list for F, G, K stars

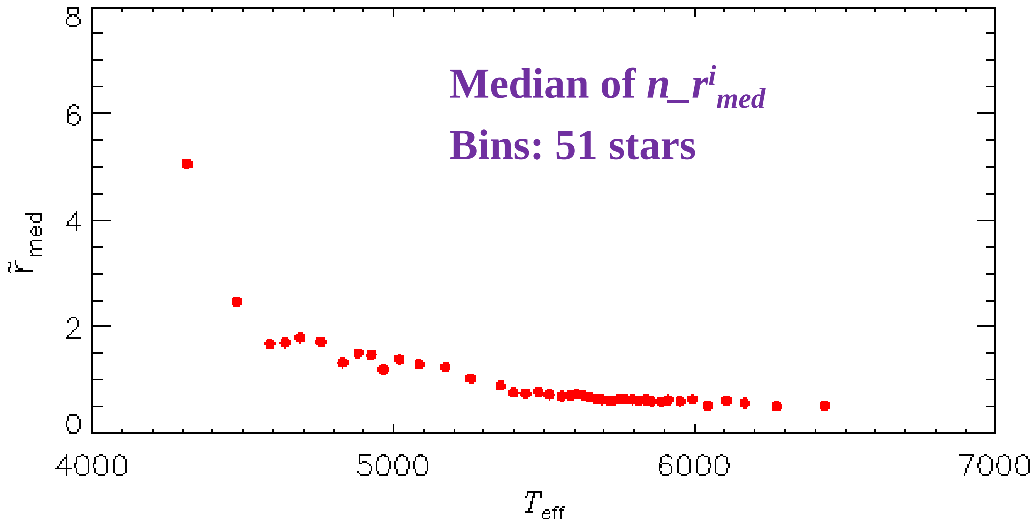
Appropriate normalized synthetic spectrum (S_i) running ATLAS12 and SPECTRUM with GES T_{eff} , log*g*, [Fe/H], ξ, *v*sin*i*, and [X/Fe], and our line list

A figure of merit to quantitatively estimate the agreement between S_i and O_i

$$n\_r^{i}_{med} = median\left[\left(\frac{O_i(\lambda) - S_i(\lambda)}{\Delta O_i(\lambda)}\right)^2\right]$$

CNAME	r_{med} **Initial**	r_{med} **Astroph**	**gain %**
00240054–7208550	2.10	1.46	**31**
00241708–7206106	1.84	1,30	**29**
02561410–0029286	1.96	1.33	**32**
00251219–7208053	1.37	0.89	**35**
03173493–0022132	1.14	0.76	**33**





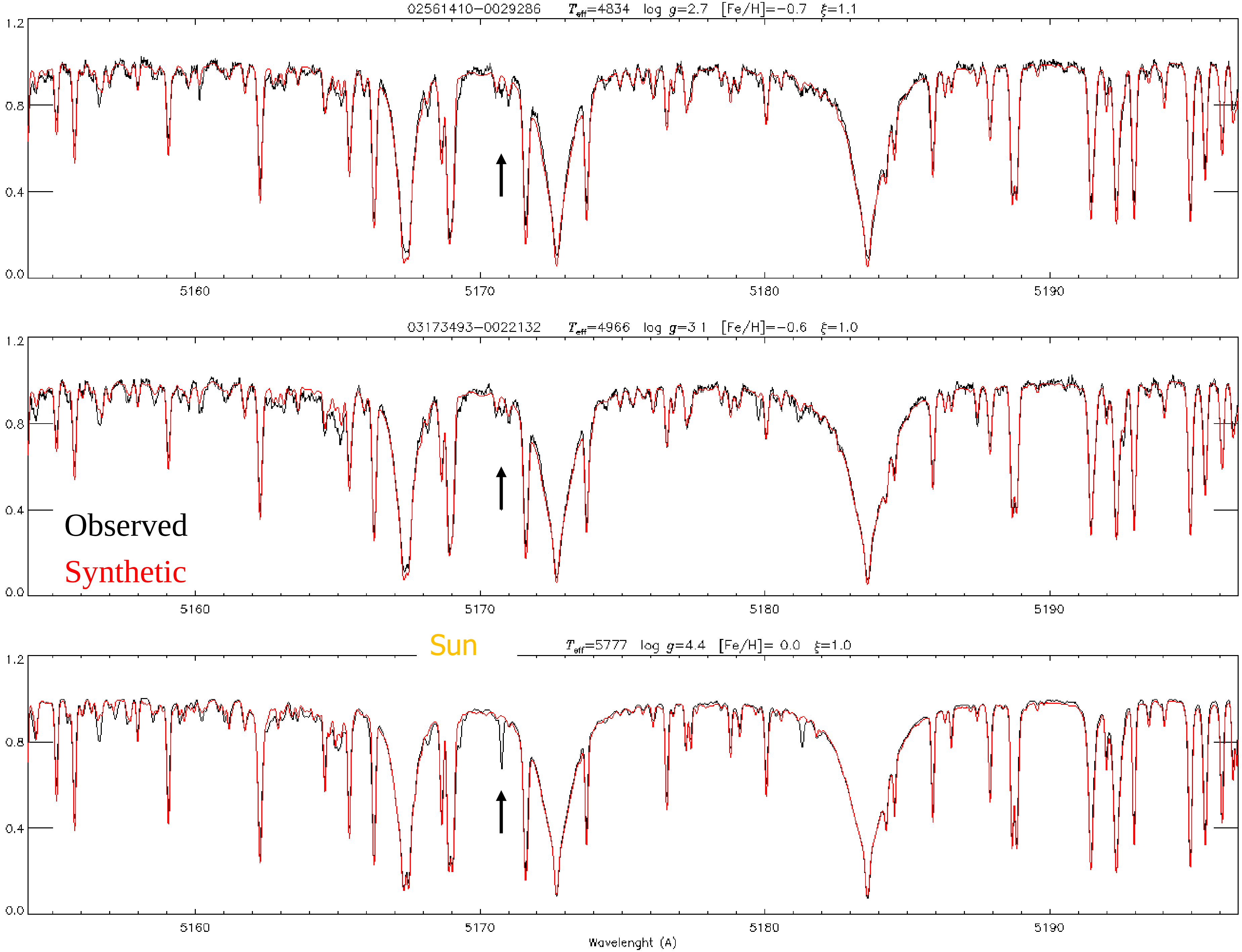
INTRIGOSS: log ***gf*** optimization

Final line-list in the 4830–5400A range includes 1427,628 entries with 16,531 (atomic), 339,652, (molecular) and 1071,445 (predicted) transitions.

We derived **astrophysical *gf*** values for
1551 atomic lines + **77** molecular lines
+
1231 Predicted Lines

The PLs allow us to minimize

- The unavoidable underestimation of blanketing in synthetic spectra if PLs are ignored
- The risk of worsening the match of synthetic spectrum with observed spectrum if PLs with incorrect intensity are used.


02561410−0029286 $T_{\rm eff}$=4834 log g=2.7 [Fe/H]=−0.7 ξ=1.1
03173493−0022132 $T_{\rm eff}$=4966 log g=3.1 [Fe/H]=−0.6 ξ=1.0
Sun
$T_{\rm eff}$=5777 log g=4.4 [Fe/H]= 0.0 ξ=1.0
Observed
Synthetic
1.2
0.8
0.4
0.0
5160
5170
5180
5190
Wavelenght (A)

Comparison with other Spectral Libraries

INTRIGOSS

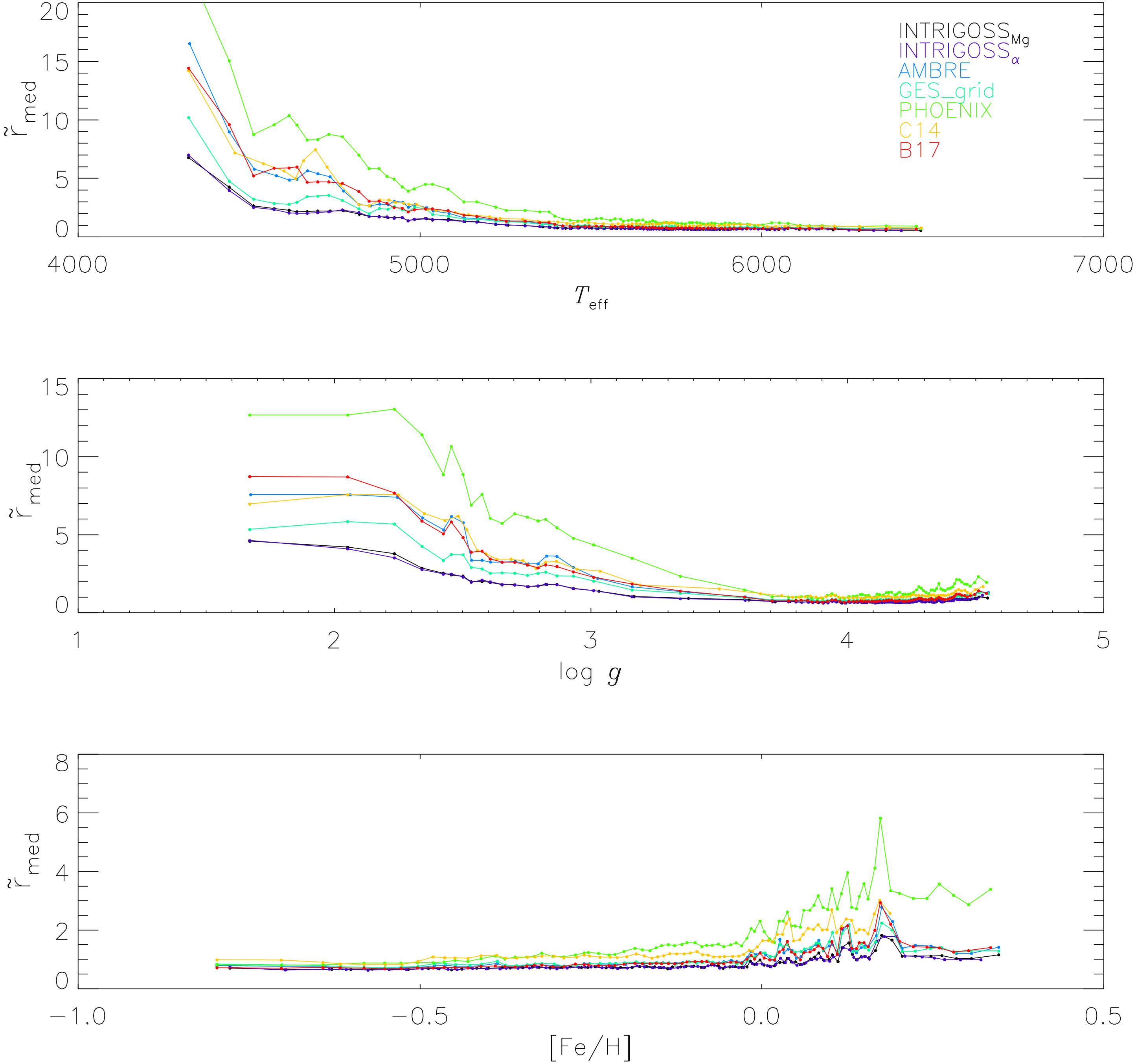
vs

AMBRE – GES_Grid – PHOENIX – Coelho14 (C14) – Brahm+2017 (B17)

⬇

For each of 2212 GES stars we computed the corresponding synthetic spectrum by interpolating at their atmospheric parameter values within the 6 libraries

Comparison with other Spectral Libraries



$$R^{j}_{med} = median\left(\frac{r^{j}_{med}}{n\_r_{med}}\right)$$

	R^{j}_{med}
INTRIGOSS$_{Mg}$	**1.043**
INTRIGOSS$_{\alpha}$	**1.025**
AMBRE	**1.313**
GES_Grid	**1.266**
PHOENIX	**2.161**
C14	**1.700**
B17	**1.289**

Interpolation among spectral library nodes

- Massive spectroscopic surveys require large numbers of models spanning a wide range of parameters and their computation can become very time consuming if you want an ad-hoc model for each star.

- In practice, the need for model spectra for many parameter combinations is often satisfied by taking a **shortcut** that avoid the actual calculation of self-consistent models. The most wide used strategy is the **interpolation** of the library models and/or spectra.

- In order to evaluate the **errors** introduced by **interpolation** procedure we computed, by using INTRIGOSS prescriptions, the intra-mesh atmosphere models and corresponding synthetic spectra of 50 representative UVES-U580 stars, i.e., by using their nominal GES T_{eff}, log g, [Fe/H], [α/Fe], and ξ, but not their individual element abundances and we compared them with the corresponding interpolated ones.

- For each star we computed the **mean value** and **the standard deviation (σ_{rd})** of the relative differences between the interpolated and the intra-mesh spectra. The mean relative differences can be used to evaluate the interpolation error introduced in the overall spectrum levels while the standard deviations can be seen as an estimate of the "noise" introduced point-by-point.

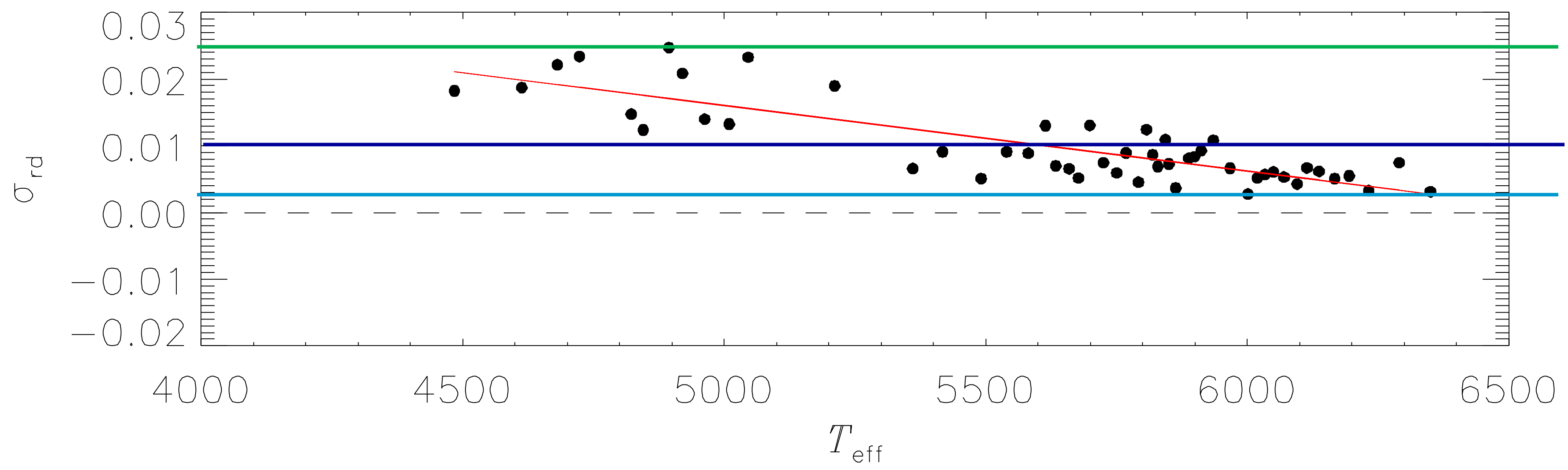
Interpolation among spectral library nodes

σ_{rd}: Errors due to interpolating INTRIGOSS in temperature:

SNR$\leq$ 40 $\sigma_{rd} \geq \sigma_{obs}(\sim 1/SNR)=0.025$ never

SNR$\geq$100 $\sigma_{rd} \geq \sigma_{obs} = 0.01$ for $T_{eff} \lesssim 5500$

SNR$\geq$ 400 $\sigma_{rd} \geq \sigma_{obs} = 0.0025$ always



INTRIGOSS is available on-line

INTRIGOSS is public and available on the web

It uses the facilities of the Italian Center for Astronomical Archive (IA2) operated by INAF

Open issues, challenges and opportunities for the near future

1. To increase the wavelength coverage:

e.g. to the whole visible + IR (?) + UV (?)

What is needed: to update the line list of atomic and molecular data with the best available data and with log *gf* optimization.

How: Using a fully automatic approach or, at least, a semi-automatic procedure since the approach adopted for INTRIGOSS would require an enormous investment of time.

➔ Joint efforts of the whole INAF community and, in particular, of the people with expertise in atomic and molecular spectroscopy and in software development is fundamental

Open issues, challenges and opportunities for the near future

2. More realistic atmosphere models:

What is needed: together with 1D Hydrostatic LTE models nowadays 3D hydrodynamical models and NLTE treatment are starting to be used more and more (e.g Asplund 2005, Bergemann+ 2019).

Currently there are a few codes used for 3D models:

- **STAGGER** (e.g. Nordlund+ 2009)
- **CO5BOLD** (e,g. Ludwig + 2009)
- **MURAN** (e.g. Vogler+ 2005)
- **ANTARES** (e.g. Muthdam+ 2009)

The last decades has been dedicated to verify the suitability of the 3D models that required months of CPU ➔ little use for practical applications to large samples of stars

NLTE calculations are still extremely challenging for atoms with complex atomic structure and because of the lack of accurate calculated or experimental atomic data.

Open issues, challenges and opportunities for the near future

2. More realistic atmosphere models:

How: most, if not all, of these fields of research are done abroad and outside of INAF. But, if we want to be competitive in the near future, we need to build expertize in this field also inside INAF.

➔ collaborations with leaders in the field (e.g. Asplund, Bonifacio, Bergemann, etc) would be useful but to foster young INAF researchers to throw themselves into these topics to acquire the needed expertize is fundamental

Open issues, challenges and opportunities for the near future

3. To expand the coverage of atmospheric parameter space:

e.g. to $T_{\mathrm{eff}} \lesssim 3750$ K and $T_{\mathrm{eff}} > 7000$ K, [Fe/H] $\ll -1$, etc

What is needed: Optimized atmosphere structure and spectrum synthesis codes for different parameter space regions (i.e. ATLAS12, Phoenix, WM-Basic, TLUSTY, etc) and a lot of computing time.

For example:

- **with our standard linux workstation (8 cores), we may need even several hours to compute an ATLAS12 converging model at $T_{\mathrm{eff}} \lesssim 4500$ K.**

- **And then, depending on the spectral range and on the adopted Resolution, also SPECTRUM is very time consuming.**

- **ATLAS12 is based on old F77 routines and is not optimized for parallel computation.**

  However, we tested successfully, thanks to OATs HPC group, the possibility to run several instances of ATLAS12 models in parallel on the HPC infrastructure at OATs and we were able to obtain more than 300 models at the same time.

Open issues, challenges and opportunities for the near future

3. To expand the coverage of atmospheric parameter space:

How: Reducing the computation time by code optimization and, where it is possible, parallelization.

➔ Use INAF expertise in optimizing and, if possible, in merging the already available codes aiming to have an “universal” one and explore the possibility of creating an ad-hoc computing facility in the framework of “Laboratorio Spettroscopia INAF”.

Thank you