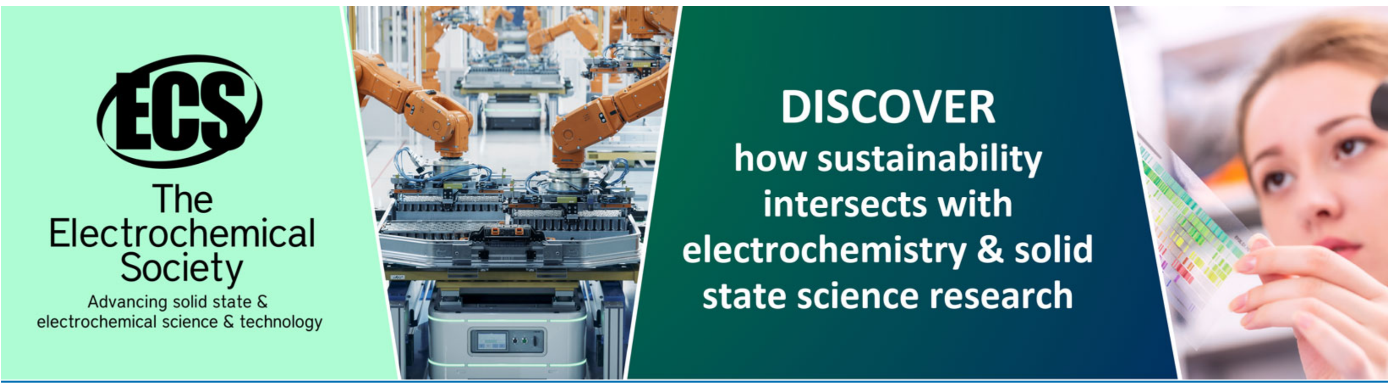
Journal of Physics: Conference Series

Stellar atmospheres in the Gaia era

To cite this article: Alex Lobel 2011 *J. Phys.: Conf. Ser.* **328** 012027



Journal of Physics: Conference Series **328** (2011) 012027 doi:10.1088/1742-6596/328/1/012027

Stellar atmospheres in the Gaia era

Alex Lobel

Royal Observatory of Belgium, Ringlaan 3, 1180 Brussels, Belgium

E-mail: alobel@sdf.lonestar.org; Alex.Lobel@oma.be

Abstract. Highlights of the meeting on *Stellar Atmospheres in the Gaia Era: Quantitative Spectroscopy and Comparative Spectrum Modeling* (http://great-esf.oma.be) held on 23-24 June 2011 in Brussels, Belgium are emphasized. New research results are summarized and a record of the scientific discussions during the meeting is provided, as well as important open questions for future research.

1. Introduction

About two years ago in November 2009 the Working Group B4 for Stellar Atmospheres was formed during the third GREAT Plenary meeting in Nice, France. At the meeting I was asked to become co-facilitator for WGB4, but rather hesitantly accepted. The GREAT Programme (Gaia Research for European Astronomy Training[1]) is a pan European science driven research infrastructure which facilitates, through focused interaction, the fullest exploitation of the ESA-Gaia 'cornerstone' astronomy mission. It brings together relevant scientific expertise by promoting topical workshops, training events, exchange visits, conferences and so forth with the aim of addressing the major scientific issues that the Gaia satellite will impact upon.

Since its kick-off meeting in Nice the Stellar Atmospheres Working Group has steadily grown, currently involving over 30 scientists from 20 research institutions. My initial hesitation stemmed from the fact that contemporary stellar atmospheres research covers a very wide variety of science topics that are often difficult to unite under the same banner. Perhaps a more appropriate common denominator is "Advanced Analyses and Interpretation of Light from Stellar Objects", but that sounds somewhat awkward.

Stellar atmospheres research is likely one of the oldest and richest fields of modern astrophysics. 150 years have passed since Gustav Kirchhoff produced the first detailed map of the solar spectrum, thereby introducing stellar physics research. Wonderful discoveries came our way since that time (the Sun is a nuclear fusion reactor, the Andromeda nebula is an independent Galaxy, radio waves from stars, the Universe expands, space and time were born together, and many more), and yet much remains unknown about the Sun and stars. The Gaia (expected launch May 2013) census of the Milky Way will observe over one billion stars with three instruments to collect astrometric, photometric, and spectroscopic data down to the $20^{\rm th}$ visual magnitude. The satellite will observe $\sim$150 million spectra of stars brighter than the $17^{\rm th}$ visual magnitude (but fainter than $V\!\sim\!6^{\rm m}.0$).

The goal of the Gaia mission is ambitious: to unravel the structure and formation history of the Galaxy with a 6-D (or 5-D) position-velocity map. The astrometric accuracies are a

[1] http://www.ast.cam.ac.uk/ioa/GREAT/

Journal of Physics: Conference Series **328** (2011) 012027 doi:10.1088/1742-6596/328/1/012027

hundred times more precise than the Hipparcos catalog, while the spectra will provide reliable radial velocity values of a staggering amount of stars. It is therefore safe to say that we should expect the unexpected astrophysics with Gaia data, although the current preparations for the data processing and analyses are quite a challenge. The confrontation of these data with theoretical models will drastically advance our understanding of the physics of stellar atmospheres. For example, new stellar populations such as previously unknown emission line stars will be discovered, and fundamental questions such as the basic scenarios of stellar evolution will be addressed with Gaia data.

The meeting is summarized here in five major topics emphasizing important points and new research results presented in the 23 oral and 10 poster presentations. I only mention the name of the speaker and of the first author of the poster, as the complete list of authors of the contributions can be consulted in this Volume. A record of the four main Discussion sessions following the Morning and Afternoon Sessions is added to the relevant topic. The record is probably incomplete but provides a concise overview of interactions between the participants that stimulated further debates. I also add a number of personal comments and views about important open questions for future stellar atmospheres research.

2. Radiation transport codes

The presentations and discussions at the meeting identified key areas for the improvement of model spectra from various modern spectral synthesis codes required to determine reliable physical parameters of hot and cool stars. The presentations of the first day highlighted new results with the Phoenix, Marcs, and Moog spectral synthesis codes for cool stars, but also included a presentation about advanced future spectroscopic instrumentation. The second day focused on new results with the Atlas, Tlusty, and Cmfgen synthesis codes applied for modeling the spectra of hot stars. A substantial number of presentations also addressed very recent research initiatives, showing some preliminary results, for large ground-based spectroscopic sky surveys to support and/or complement future Gaia data analysis.

2.1. Cool stars

After an introduction about the Gaia satellite design and current development status, Ulrike Heiter presented results of the GREAT-ESF Stellar Atmospheres Workshop on Comparative Spectrum Modeling in Vienna of August 2010. Observed and simulated spectra of cool giants were modeled by 14 research groups with different atmospheric models and analysis approaches. For example, for the observed spectrum of α Tau the resulting spread of computed atmospheric parameters ($T_{\rm eff}$, log g, and [Fe/H]) is larger than the estimated error bars, although most of the parameter values agree within 2-σ. The differences in the synthetic spectra are largest in the blue wavelength region and decrease towards the near-IR. The normalized central absorption line depths can differ by 0.4 around 5000 Å, while averages around 0.1 are measured around 6600 Å [1]. There do not appear to be clear trends in the computed parameter values that depend on specific assumptions of the modeling method. However, the main cause for the differences in atmospheric parameter values can be attributed to the atomic input data (adopted oscillator strengths and damping constant), and to the choice of the modeled wavelength regions. I conclude that the 'comparative modeling experiment' for cool giants should be repeated for other types of stars, including hot stars for which atomic input data of the higher ions is less well-tested compared to cool star spectra. The results for cool giants also show that one should first homogenize a number of assumptions in the modeling method for pinpointing a specific cause of the different parameter values. For example, utilize the same 1-D atmosphere model grid for exposing possible differences in the methods and data to compute the stellar continuum fluxes, or for example, caused by missing/incomplete molecular opacity (for cool stars) and differences in the adopted equation of state.

Of central importance for the ongoing preparations of Gaia data processing is the development of codes that properly classify all observed objects (stars should be separated from galaxies, quasars, solar system bodies) and determine the astrophysical parameters (APs), which also include reddening, α-element enrichment, radial- and projected rotation velocity, activity. Rosanna Sordo presented an overview of high-resolution synthetic spectral libraries of model spectra computed with a large variety of spectrum synthesis codes [2]. The model girds will be utilized to compute stellar parameters with the Discrete Source Classifier Algorithms currently under development in Gaia DPAC-Coordination Unit 8 (CU8). They are implemented in the Stellar Population Code to train the codes for the classification of many different types of hot and cool stars; FGK & M stars, OB stars, white dwarfs, red supergiants, peculiar A and B stars, carbon stars, ultra cool dwarfs, various types of emission line stars, Be stars, Wolf-Rayet stars, etc. An important point is that more sophisticated spectral grids computed with 3-D atmosphere models will unlikely tackle the basic problems that such an extensive compilation of training data must deal with. Apart from the large computational expenses in 3-D to cover the full ($T_{\rm eff}$, log g, [Fe/H])-range for hot and cool stars, the model 'gridpoints' have to be interpolated for continuous coverage of the APs space. The interpolation procedures yield errors of $\sim$10 % in the Gaia RVS region, while for libraries with 0.1 nm wavelength sampling they can amount to $\sim$4 % for $T_{\rm eff}$=5000 K.

The application of input libraries from different spectral synthesis codes for training the DPAC-CU8 codes introduces in the computed APs errors that should be quantified at some point. Detailed comparisons of MARCS, PHOENIX, and ATLAS spectra for $T_{\rm eff}$= 4000 K, log g=4.0, and [Fe/H]=0.0 reveal mean flux differences to $\sim$10 % below 5000 Å. For $T_{\rm eff}$=8000 K they decrease and overall agreement improves, although with rather different spectral energy distribution (SED) slopes in the blue. Bertrand Plez very eloquently pointed out major flux differences between the three synthesis codes by comparing $T_{\rm eff}$ and $V-K$ color, and color-color diagrams for 2500 K $\leq T_{\rm eff} \leq$ 9000 K, for log g=0.5 (giants) and 4.5 (dwarfs). The codes agree well above 4000 K because the opacity sources are almost identical. Below 4000 K ATLAS dwarf models are too blue in the near-IR for currently unknown reasons. For $T_{\rm eff}$ below 4000 K considerable differences in the blue between MARCS and PHOENIX fluxes should also be investigated.

An important conclusion of the meeting is that SED differences between the synthesis codes for cool stars ($T_{\rm eff}\leq$10 kK) are not attributable to (small) differences in the 1-D atmosphere model structures. For example, differences in log($\tau_{\rm Ross}$) versus gas kinetic temperature (T) computed with ATLAS9 and ATLAS12 are limited, although the opacity treatment (ODFs versus opacity sampling) is rather different [3]. Comparisons of spherical ATLAS models and PHOENIX NEXTGEN models for cool giants [4] reveal almost identical T-structures that cannot account for the large SED differences in the emergent flux spectra. Plez shows similar good agreement between models computed with MARCS and ATLAS (using new ODFs) for dwarfs, giants, and supergiants. This is also the case by comparing with (spherical) PHOENIX-ACES models (using an extended EOS), except perhaps for the limited differences that occur at small optical depths of log($\tau_{\rm Ross}$)≤ -2 for $T_{\rm eff}\leq$3000 K. The flux differences in the spectra are therefore likely the result of appreciable differences of the input background opacity sources, for example due to different strengths of broad TiO and FeH molecular bands. I also add that the partition functions of the most important hydrides and oxides require further improvements.

More detailed comparisons of the shapes of the Ca II near-IR triplet lines (in the Gaia RVS wavelength range) reveal that the line wings predicted with MARCS are somewhat broader than with PHOENIX, which can be reconciled by adopting the same line damping and broadening constants in both codes. I remark that detailed line profile comparisons with observed spectra of large signal-to-noise ratio also require a proper treatment of isotopic line splitting (in log(gf)-components) and, if possible, hyperfine splitting for a number of important elements such as Mn and Co. Hyperfine splitting broadens the wings of absorption lines and causes remarkably flat central line cores. Much progress is likely to come from detailed comparisons with high-resolution observed spectra of stars having model-independent $T_{\rm eff}$- and log g-values, for example obtained from accurate angular diameter and bolometric flux measurements, or from comparisons with seismologic surface gravity values (see Section 4.1).

New results with PHOENIX for brown dwarfs ($T_{\rm eff}$=1800 K and 2000 K) were presented by Peter Hauschildt. The new models include the formation/destruction of dust grains depending on the location (depth) of the convection zone. They incorporate the feedback of dust nucleation & growth and dust gravitational settling on the overall atmospheric structure PHOENIX computes (in dust-drift mode) for a stationary solution. The theoretical SEDs very closely fit the observed SEDs of brown dwarfs (log g=5.5) and of metal-poor cool giants ($T_{\rm eff}$=1600 K, log g=3.0, [Fe/H]=−1.0). The PHOENIX (v16) package is a versatile suite of codes for computing 1-D or 3-D atmosphere models and the emergent flux spectra in non-LTE. It can include velocity fields (of winds, supernovae) and chemical equilibrium calculations. PHOENIX has been optimized for massively parallel processing. For example, ongoing tests show overall good agreement for fully line blanketed 1-D synthesis calculations compared to 3-D (using spherical coordinates) for UV and optical spectra of stars with $T_{\rm eff}$=3000 K, 5700 K (solar type), and 9000 K. 3-D spectrum synthesis calculations are currently computationally rather expensive. However, they will become very important for testing a large variety of physical processes in cool star atmospheres with the fast increases of compute power.

2.2. Hot stars

The determination of accurate APs of OB stars with Gaia photometry and RVS spectra will be challenging. In hot stars the small RVS wavelength region is dominated by a handful of broad H Paschen series lines from P13 to P16. Ground-based spectroscopic surveys of hot stars will therefore become very important to test and verify the APs obtained with Gaia data using various other wavelength intervals that can also yield reliable elemental abundance values for these stars. Norbert Przybilla presented an overview of quantitative spectrum modeling of hot dwarfs and giants from B4 to O9 (15 kK $\leq T_{\rm eff} \leq$ 35 kK). He compares the results of three spectrum synthesis codes: ATLAS/SYNTHE in LTE, TLUSTY/SYNSPEC in non-LTE, and a hybrid approach that combines LTE atmosphere models (from ATLAS9) with non-LTE line transfer calculations using DETAIL/SURFACE, called 'ADS' [5]. For $T_{\rm eff}$ below 22 kK 1-D atmospheric structures and SEDs computed in LTE and non-LTE are very similar ($\Delta T/T \leq$1 %). Above 22 kK non-LTE effects become more important in the cores and wings of H Balmer lines and He I/II absorption lines. In detailed line profile modeling the non-LTE effects generally become stronger towards larger $T_{\rm eff}$, and differences of line fluxes computed with the three codes increase towards smaller log g-values. Non-LTE line spectra computed with relatively simple atomic structures (e.g., H I, He I/II, and Mg II) yield reliable APs, but which is not valid for more complicated species. A remarkable conclusion of Przybilla's code comparisons is that advanced non-LTE computations which employ simplified model atoms (but in fact too simplified or outright inappropriate) often yield wrong results that can largely exceed the systematic errors of (simple) LTE line approximations. He finds that the (carbon, nitrogen, silicon, iron) model atoms of TLUSTY require extensive revision and updates for comparison to observed OB spectra. It is my opinion that the study profoundly and thoroughly demonstrates the enormous impact of missing or inadequate atomic input data on quantitative stellar spectroscopy. Garbage in, garbage out, whatever the amount of megaflops and number of processor threads used. It underscores the demand for new and *tested* atomic input data (both laboratory and astrophysical), and the great care we must take when using them.

In case the energy density in the spectral lines formation region of a stellar atmosphere is dominated by the ambient radiation field the detailed atomic balance (e.g., ionization and excitation rates and the resulting population fractions) can very far depart from local TE conditions. The local gas state (T, ρ, $P_{\rm el}$) must be coupled to the atomic rate equations for computing the line opacity and emergent fluxes. These overall non-LTE conditions occur in the atmospheres of stars with $T_{\rm eff} \geq$ 30 kK. In massive O-type stars the stellar atmosphere also expands due to radiative forces. The radiation-driven winds of O stars rapidly accelerate to highly supersonic velocities within one stellar radius above the stellar surface. It determines the transport of radiation because the line formation physics (line opacity and scattering) in the expanding wind is influenced by the Doppler effect, requiring a rather sophisticated calculation of the line source function. The spectral lines adopt a characteristic horn shape or P-Cygni profile. These 'wind' lines dominate the UV spectra of massive hot stars with many resonance transitions of N, C, and Si ions. They are however also observed in the optical spectra of several types of OB supergiants, such as Luminous Blue Variables (LBV) and Wolf-Rayet (WR) stars.

Jose Groh discussed the determination of APs with the CMFGEN code for these stars [6]. CMFGEN can solve the transfer equation in spherical symmetry for a user-specified radial monotonic velocity field using the co-moving frame prescription (e.g., opacity and emissivity are isotropic). It can compute a hydrostatic atmosphere structure to just below the sonic point in the wind, which incorporates full line blanketing due to metals with Z up to 30. Back-warming is mainly caused by iron. The $T_{\rm eff}$ is classically computed from the ionization balance with detailed fits to diagnostic spectral absorption lines such as He I λ4471 & He II λ4542 for O stars, and He I λ4471, λ4713/5876/6678 & He II λ4686 or optical Si II/III lines in LBVs. Important stellar wind parameters such as the mass-loss rate ($\dot{M}$ or $\dot{M}/\sqrt{f}$) and the volume-filling factor (f) for modeling the inhomogeneity or (micro-)clumping of the wind can be obtained from fits to Hα and He II λ4686, while UV wind lines or strong H Balmer lines provide the terminal wind velocity (v_∞). The effective atmospheric acceleration of OB dwarfs with log $g \geq$3.0 can be constrained from the pressure-broadened Hδ and Hγ absorption lines. In LBVs and WR stars, however, the H Balmer and Paschen lines are filled in by wind emission and adopt P Cygni profiles, generally preventing an accurate determination of log g-values for these stars. Interestingly, Groh also showed that surface abundances of nitrogen and carbon can be determined from optical NIII/IV and C III/IV lines. Diagnostic lines of the same species are less affected by model details, although they may require simultaneous fits to absorption and emission profiles (i.e., N III). New versions of CMFGEN are currently tested with time-dependent co-moving frame transfer solutions for monotonic spherical outflow. Relativistic effects are included and one can hence expect exciting new results with CMFGEN by comparing with the SNe atmosphere models of PHOENIX.

2.3. Other radiative transfer codes

For completeness I also mention the MOOG, MAFAGS, and STEPAR LTE spectrum synthesis codes that were employed for computing APs of FGK stars in a number of presentations at the meeting. Non-LTE abundance determinations in cool stars were also presented using the MULTI2.3 code, while quantitative analyses with the FASTWIND code were presented for O-type stars (see Section 5). All radiative transfer codes can be separated depending on the numerical method for solving the radiative transfer equation; either a discrete ordinate method (short, long, or mixed characterisitcs) or a Monte Carlo method is implemented. A plethora of codes have been developed for modeling radiative transfer in Earth's atmosphere. A small literature search reveals the names of various other spectrum synthesis and line modeling codes actively used in the stellar physics community such as CLOUDY, SPECTRUM, MALI, ATA, COSSAM, XSPEC, and many more. Most of them solve the transfer equation, while some employ approximative methods such as photon escape probability. I apologize to everyone whose pet code is not listed or was not discussed at the meeting (but am delighted to learn about them, so contact me). There are also codes for solving radiative transport in dusty envelopes and discs around stars, such as Dusty, 2-Dust, radcm, to name a few.

The longevity of transfer codes depends on much needed resources (financial and personnel) for new science applications. It requires new code updates and a proper understanding of how a code works internally. The development of a code is different from its application, but experienced users usually become developers provided they are helped (e.g., document your code) and are given sufficient time to become familiar with them. For example, as an undergraduate I worked with a transfer code called Scan originating from Kees de Jager and co-workers at Utrecht, The Netherlands, for studying microturbulent broadening in the spectra of cool super- and hypergiants. Almost two decades later I still employ a more advanced version (Scanspec) for computing the detailed spectra of cool stars and for testing the quality of the atomic input data. Astrophysical $\log(gf)$-values are collected in an on-line spectral database called SpectroWeb[2] [7]. Later I adapted spherical and molecular versions of the well-known Multi code for investigating self-reversed emission lines formed in the chromospheres of cool supergiants such as Betelgeuse, including the effects of partial frequency redistribution in the lines. More recently I developed a transfer code (Wind3D) for modeling internal wind structures of hot stars using the dynamic spectra of wind lines. My point with these examples is that many transfer codes are initially developed by one (or a small group) of person(s) for modeling a given type of feature or property observed in stellar spectra. It is reassuring that these long-term radiative transfer code developments by many research groups worldwide will now benefit the entire stellar astrophysics community interested in the Gaia mission and its data products.

3. Radiation hydrodynamics codes

3.1. 3-D stellar atmosphere models

Two presentations at the meeting addressed very recent developments in 3-D hydrodynamic modeling of the atmospheres of late-type stars. Remo Collet showed that the convective pattern of large granules in Stagger-Code simulations of red giants yield density and temperature inhomogeneities (with correlations to macroscopic velocity fields) at the stellar surface that can profoundly alter the profiles and strengths of spectral lines compared to 1-D atmosphere models [8]. Interestingly, he pointed out that differences between the temperature stratifications in the upper atmosphere ($\log\,\tau_{5000}\leq-2$) of 1-D and 3-D models can amount to $\sim$1000 K, which severely affect the excitation, ionization, and molecular equilibria in those layers. In 3-D hydro models of metal-poor stars the physical cause is related to a reduced efficiency of radiative heating due to line opacity for balancing the adiabatic cooling rate compared to 1-D models. LTE transfer calculations of the detailed profiles and strengths of temperature-sensitive Fe I lines (hence with a large fraction of their line contribution function below $\log\,\tau_{5000}=-2$) in cool giants yield abundance differences of -0.5 dex or more, compared to the 1-D line transfer. The computed 3D$-$1D LTE abundance differences increase (they become more negative) with decreasing [Fe/H]- and $\log g$-values. The grid resolution and non-grey radiative transfer (i.e., the opacity wavelength resolution or binning) may also have profound effects on these differences, but the importance of 3-D hydro and transfer modeling for reliable determinations of the APs of cool-type spectroscopic (metal-poor) standard stars is clear. Andrea Chiavassa investigated surface convection in K-giants by combining the Stagger-Code with the radiative transfer code Optim3D. He finds convective Doppler shifts of up to 0.75 $\mathrm{km\,s^{-1}}$ for spectral lines in the Gaia RVS wavelength range. For a *star-in-a-box* model of red supergiant Betelgeuse from the CO^{5}BOLD code, the convective blue-shifts of the Ca II near-IR triplet lines can increase to ~-8 $\mathrm{km\,s^{-1}}$ [9]. He also finds that significant excursions of the Gaia G-band photocenter of RSGs can amount to $\sim$3 % of the optical stellar radius during the 5 years of the Gaia mission. It results from brightness fluctuations, with spots of up to 50 times brighter than dark surface

[2] `http://spectra.freeshell.org`

regions on the RSG, over time-scales of weeks.

3.2. Astrophysical microturbulence

Current *box-in-a-star* hydro-simulation research ought to provide more profound and valuable information for unraveling the physics of astrophysical 'microturbulence'. It is not sufficient to point out that spectral synthesis using 3-D atmosphere models does not require any microturbulence broadening without addressing the basic physical properties (or underlying mechanisms) of the atmospheric velocity fields that increase the line EWs. It is paramount for stellar astrophysics because it is impossible by means of classical spectroscopic methods to reliably determine APs (such as [Fe/H]) without considering microturbulence broadening. Astrophysical microturbulence is therefore often called a 'fudge-factor', an ad-hoc individual-to-the-star, free parameter for non-thermal line broadening that applies to spectral lines formation in hot stars as well. It is an AP that urgently requires a firm physical foundation. 3-D atmosphere models can address a number of long-standing pertinent astrophysical questions. What is the energy spectrum (e.g., the typical length scales of the velocity fluctuations with energy) of local atmospheric movements in 3-D hydro models that match traditional 1-D microturbulence velocities (ζ_μ)? Mean bulk velocities, or the velocity dispersion, in the lines formation regions of 3-D models of spectroscopic standard stars (Procyon, Arcturus, Canopus, etc.) can be compared to the 'observed' 1-D values, including depth-dependent models. An informed guess is that the energy spectrum adopts a (Kolmogoroff) power-law known for hydrodynamical turbulence, but advanced 3-D atmosphere models (e.g., properly resolved hydro-simulations) ought to provide a quantitative answer as to how it scales with the local thermodynamic conditions in stellar atmospheres. Why are microturbulence velocities in supergiants observed to exceed the local speed of sound? Is supersonic microturbulence signaling shock wave propagation or do the large values result from the 1-D thermodynamic model structure in the lines formation region? Do microturbulence velocities depend on the local gas kinetic temperature, in other words, do the non-thermal velocity fluctuations result from the balancing of local atmospheric heating and cooling mechanisms? The physical properties of astrophysical microturbulence are presumably different from plasma microturbulence modeled and observed at much larger gas kinetic temperatures in tokamaks, but how different?

Discussion session I

Workshop Question 1: *Do you think it is possible to define a standard format for (exchange of) model atmosphere data? How could we start to define such a standard? This would make comparisons and tests of different implementations of model physics and numerical approaches easier.*

Answer by Ulrike Heiter: I think it is worth a try to define a "stellar atmosphere data model". With that I mean a definition of physical and other quantities, with detailed description, units and keywords, that should be included in every model atmosphere file. One could start by doing a "model atmosphere user survey", asking users what they need for their calculations. These could be spectrum synthesis calculations, but also limb darkening (e.g., for interferometric angular diameters), boundary conditions for stellar evolution models, or non-LTE calculations.

Answer by Remo Collet: On the practical side, one possibility would be to share the data using "self-describing" file formats (i.e., NetCDF), which allow to easily add documentation and description of variables to the files. A more fundamental issue to consider when exchanging model atmospheres or synthetic spectra is the one of consistency. One should bear in mind that, in general, erroneous results and conclusions may be derived when spectra are computed with an equation-of-state and opacities that are inconsistent with the ones assumed for the model atmospheres. When exchanging model atmosphere data, one should consider using variables that are less sensitive to this problem.

Answer by Maria Bergemann: It is necessary to provide more data relevant to the equation-of-state (EOS) used to compute model atmospheres. Common experience says that the equation-of-state used in the latter and in spectrum synthesis packages adopted by a user are inconsistent. In the case of 1-D versus 3-D this inconsistency may be fatal. Individual partial pressures for as many elements as possible can be used to cross-check for this. Besides, some spectrum synthesis codes demand partial pressures as input.
Answer by Leo Houziaux: Is it workable to define a standard format? Letting aside the usual trinity $T_{\rm eff}$, log g, [M/H], it seems necessary to decide on 1-D or multi-D, (N)LTE, various velocity fields, $v\sin i$, dust around the object, to say nothing about the influence of magnetic fields on the structure of the atmosphere that nobody mentioned. Inevitably, I think we will have to cope with various codes.
Answer by Bertrand Plez: In Montpellier we have set up the Pollux database of theoretical spectra. It contains spectra for O to M stars calculated for CMFGEN, ATLAS, and MARCS models (SED and high-resolution spectra). The database if fully Virtual Observatory (VO) -compliant and can be addressed through tools such as VO-Spec. It uses the VO format and data descriptors defined by VO. More spectra will be added in future releases.

Workshop Question 2: *We computed 1-D* MARCS *models for AGB stars. Although we made a lot of assumptions (such as LTE, hydrostatic, homogeneous layers, etc.) far from reality, the synthetic spectra fit the observed spectra fairly well, and computed colors match very good to observed colors (both in the optical and infrared). Is this just a coincidence, or does this show that 1-D models suffice for the moment to compute atmospheric parameters for AGB stars?*
Answer by Bertrand Plez: It is true that 1-D LTE models often fit observations pretty well, although not fully (the more and better observations we get, the more "details" don't fit). The only way to know if 1-D hydrostatic LTE models can be used to analyze observations is to try with non-LTE, 3-D, and look at the differences. If it turns out that we can use simple models and methods combined with tabulated corrections, that is very well! Otherwise we will have to do it the hard way!
Answer by Leo Houziaux: In this respect, Robert Kurucz showed about forty years ago that in the case of the solar spectrum most of the features, even very tiny ones, could be reproduced with a sort of "stone age" theory of line formation: hydrostatic equilibrium, plane-parallel atmosphere, LTE, radiative equilibrium. We know now that all these hypotheses are subjects of discussion.
Answer by Remo Collet: I think it is definitively important to pursue 3-D modeling: current 3-D models of late-type stellar atmospheres actually show that there are large systematic differences between, e.g., abundances derived with 3-D and with 1-D models, especially at low metallicities. Furthermore, predictions concerning other observables (e.g., center-to-limb variations) also differ between 1-D and 3-D calculations.
Answer by Maria Bergemann: Matching observed colors of a star to a model is very simple, and it doesn't tell much about the physics of stellar atmospheres. Models are usually computed to cover a broad range of observational data (colors or SEDs), so it is no surprise that one or a few from your grid accidentally match observed colors. The problem here is deeper: the model is far too simple to describe complex phenomena in stellar atmospheres. Especially for low-gravity cool stars, systematic errors caused by extension/LTE/1-D approximations are large. There is a large amount of studies describing these problems.

Workshop Question 3: *In coming years new 3-D hydrodynamic atmosphere model grids will become available. For example, in metal-poor cool stars oxygen abundances can be substantially overestimated with 1-D models. Should we decide when to use 3-D instead of 1-D modeling for determining atmospheric parameters, also for Gaia data? Is it feasible for very large datasets,*

Journal of Physics: Conference Series **328** (2011) 012027 doi:10.1088/1742-6596/328/1/012027

e.g. survey data?
Answer by Andreas Korn: That has to be the ambition! One has to realize the following: 3-D and non-LTE are the *current challenges* in cool stars modeling. Only by going to this new level of modeling sophistication can we hope to uncover and address *new challenges* in the physics of stars (e.g., atomic diffusion, rotation and mixing) or in the modeling (fully self-consistent 3-D non-LTE, with non-LTE feedback on the model; non-steady-state statistical equilibrium). We are still far from exploiting the full information encoded in stellar spectra!
Answer by Remo Collet: Once the grid of 3-D models will be complete, one possibility is that we directly provide the 3-D – 1-D corrections to oxygen abundances computed for different indicators and for all 3-D models and make them available to the community for direct application to abundances derived with classical 1-D methods.
Another possibility would be to directly use the average 3-D models which we will make available to the community as a substitute for classical 1-D models. This may yield results in closer agreement with "full 3-D" calculations, but at a lower computational cost and easier implementation for users of classical 1-D models.
Answer by Leo Houziaux: For Gaia spectral data, which are very limited both in wavelength range and in signal-to-noise ratio, 1-D models including microturbulence seem appropriate. 3-D models are certainly more realistic, provided the necessary atomic and molecular parameters are accurately known, especially the electronic collision cross-sections. On the other hand, oxygen abundance is very delicate to determine, not only because it is present in several molecules, but even as an atomic species, it presents well-known fluorescence mechanisms with H(Lyβ) and even with H(Lyα). In addition, care should be taken to use an appropriate Stark broadening theory for the higher lines of the H Paschen series, as the energy levels get very close to each other.

Discussion session II
Question by Remo Collet to Ulrike Heiter and Bertrand Plez: *You have reported that the GREAT-ESF workshop on comparative spectrum modeling (for cool giants in Vienna of Aug. 2010), for some of the test cases, the various participating groups derived significantly different stellar parameters from the same spectrum. Did you investigate the reasons why the different analysis strategies led to different results? Would it be possible to identify an optimal strategy using the ones that were considered?*
Answer by Ulrike Heiter: No. We did no see any clear relation between parameter differences and type of model or analysis method. We did a comparison of spectra computed with different codes for the same set of atmospheric parameters and found differences of the same order of magnitude as the differences between best-fit model and observations. This means that the modeling differences play a certain role. It would be good to repeat the experiment, letting every participant use the same strategy for parameter determination.
Answer by Bertrand Plez: One way to identify the source of errors/differences is to use (i) a single parameter determination, with spectra from the different groups, that will give us the impact of differences in modeling (due to line lists, equation of state, etc.), and (ii) use spectra from a single model to test the various fitting approaches.

Question by Bertrand Plez to Remo Collet: *What is the meaning of depth-dependent microturbulence? Why do you use the velocity dispersion from 3-D simulations as an estimate of it? Isn't microturbulence related to turbulence at microscopic (inter-atomic) scales?*
Answer by Remo Collet: In late-type stars, the so-called "microturbulent" broadening adopted in classical 1-D calculations is most likely due (mainly) to turbulence occurring on microscopic scales comparable with the inter-atomic distances, as the name seems to suggest. The microturbulence parameter in late-type stellar atmospheres is actually related more to the distribution of relative bulk velocities in the line formation region at scales of the order of the mean free

path of photons which can be quite large at the optical surface and above it. The value of the (depth-dependent) micro-turbulence for a given stellar atmosphere could be estimated by looking at the dispersion of the bulk velocities at various optical depths as predicted by 3-D hydrodynamic simulations (discussed in recent publications). As Maria Bergemann showed in her talk, such a choice of micro-turbulence removes the trends of derived iron abundances with equivalent widths of Fe I and Fe II lines in non-LTE calculations using average 3-D models. This suggests that present simulations are already resolving the important scales and velocity fields that contribute to micro-turbulence broadening.

Question by Ulrike Heiter to Remo Collet: *On the question of 1-D vs. 3-D hydrodynamic models for cool stars: 1-D models can be calculated for spherical geometry, while 3-D "box-in-the-star" models are plane-parallel. What are the prospects for 3-D spherical models and is this important?*
Answer by Remo Collet: Based on the experience from 1-D models, I think we can say that the "box-in-the-star" approximation is safe for models with log $g >\sim 1.5$ (cgs units) and that sphericity effects can be neglected to first order. For lower gravities, it would be in principle better to switch to the "star-in-the-box" mode.

4. Atmospherical parameters, abundance, metallicity, and chemical tagging studies

The workshop provided an overview of research activities for determining astrophysical parameters; the effective temperature, surface gravity, metallicity (e.g., surface abundances), mean microturbulence velocity, α-enrichment, radial velocity, projected rotation velocity, and macroturbulence velocity, from the spectra of cool and hot stars. Other parameters such as the stellar mass-loss rate, wind acceleration (β), terminal wind velocity, wind clumping factor, and the number fraction of helium over hydrogen, were also discussed for luminous hot stars.

4.1. Cool star parameters

The three APs $T_{\rm eff}$, log g, and [Fe/H] are traditionally determined from 1-D LTE spectrum synthesis calculations in FGK stars. Maria Bergemann described results of non-LTE transfer calculations with DETAIL and MULTI2.3 of Fe I and Fe II lines in FGK dwarfs and giants [10]. The iron model atom is very advanced with 296 energy levels of Fe I and 112 levels for Fe II, where 16207 permitted bound-bound transitions are considered, and assuming complete frequency redistribution in the lines. She finds lower number densities of Fe I compared to LTE, whereas Fe II lines are hardly affected by NLTE. It yields the weakening of Fe I lines compared to LTE, therefore requiring a larger iron abundance for fitting observed spectral lines. The computed "NLTE abundance corrections" for Fe I lines do not exceed $\sim$0.05 dex for solar metallicity dwarfs, but they can increase to 0.6 dex in metal-poor giants. The Fe I NLTE corrections increase with decreasing [Fe/H]- and log g-values, thus the assumed LTE ionization balance yields progressively underestimated surface gravities and metallicities. A database is under construction to provide the NLTE abundance corrections online.

Nadya Gorlova determined the APs of post-AGB F-type giant BD+46 442 with a dust disc, and finds $T_{\rm eff}$=6250±250 K, log g=1.5±0.5, [Fe/H]=−0.7±0.2 dex (slightly metal-poor), and ζ_μ=4.0±0.5 km s^{-1} [11]. She compares individual line abundances computed with the LTE spectrum synthesis codes WIDTH9 and MOOG, using EW-values of weak and medium-strong lines observed in high-resolution Mercator-HERMES spectra. She concludes that the dominant source of the abundance errors is the uncertainty in the model $T_{\rm eff}$ and log g, followed by the uncertainty in the EW measurements, and the employed line oscillator strengths. Both transfer codes yield very similar metal abundance values (with differences smaller than $\sim$0.03 dex). A comparison between the original ATLAS9 atmosphere models and the new ODF ATLAS9 models (from Fiorella Castelli) yields, however, abundance differences to −0.16 dex for 7 N I lines with

35 mÅ<EW<110 mÅ, and to −0.11 dex for Fe I and Fe II lines. Effects of the adopted 1-D atmosphere models may therefore be non-negligible for element abundance measurements, provided the LTE assumption is appropriate. A study of [Fe/H] in a sample of FGK stars with and without dusty debris discs by Jesús Maldonado reveals (using WIDTH9 and ATLAS9) a lack of correlation between the presence of debris discs and large metal abundances [12]. These metal abundance studies can provide important clues for planet formation because the formation of planetary cores is favored in discs with high-metal content. Gaia is expected to detect 10 000 exoplanets. Giancarlo Pace presented an interesting literature study to assess abundance differences between dwarfs and giants in open clusters [13]. He warns that reported [Fe/H] differences should be closely scrutinized because they can result from the adopted measurement procedures (i.e., LTE versus NLTE modeling) and spectral line lists. For example, is the lack of giants with [Fe/H]>0.2 dex compared to dwarfs in the solar neighborhood the result of comparing two different classes of objects? Actual abundance differences between dwarfs and giant have profound theoretical implications for planet formation rates and the chemical evolution of the Galaxy.

David Montes presented a study of APs and chemical tagging of nearby FGK stars. It is based on high-resolution spectra observed with a large number of spectrographs, and also collected from various telescope archives. $T_{\rm eff}$, log g, [Fe/H], and ζ_μ are computed with the STEPAR code using EW-values of some 300 Fe I and Fe II lines. STEPAR (a combination of MOOG and ATLAS9) determines the excitation equilibrium, while the ionization equilibrium is imposed by log(ϵ(Fe I)) = log(ϵ(Fe II)). Differential abundances (Δ[Fe/H]) are then used to study candidate membership of stars to i.e., the Hyades Supercluster, with respect to [Fe/H] of a known cluster member. This permits to investigate the stellar kinematics of various groups. For example, field-like stars are associated with the Galaxy spiral structure or with dynamical resonances (bar), whereas young co-eval stars with debris of star-forming aggregates in the disc. Chemical tagging studies (the analysis of Fe, Na, Mg, Al, Si, Ca, Sc, Ti, V, Cr, Mn, Co, and Ni) of possible Hyades members show 41% homogeneity of the abundances. An investigation of the metallicity and Li abundance of the Hyades Stream compared to Hyades Cluster was presented by Alain Jorissen. He finds that the Hyades Stream has a metallicity excess of 0.2 dex compared to the thin disc, and that the Stream is possibly a 4:1 resonance of the spiral pattern.

In a study of S stars Sophie Van Eck presented a grid of 3522 synthetic spectra computed with TURBOSPECTRUM for 2700 K $\leq T_{\rm eff} \leq$ 4000 K, C/O = 0.5, 0.750, 0.899, 0.925, 0.951, 0.971, 0.991, [s/Fe] = 0.0, +1.0, +2.0 dex, [Fe/H]=0.5 and 0.0 dex, and log g = 0, 1, 2, 3, 4, 5. From a comparison of color-color diagrams of observed and synthetic spectra she finds that for a given $V-K$-value, the $T_{\rm eff}$-range of models with different C/O ratios can be as large as 400 K. The application of the usual $T_{\rm eff}$-scale for M-stars (traditionally based on the $V-K$-color index) can therefore yield $T_{\rm eff}$ errors for S stars of up to 400 K [14]. The Tc, Zr, and Fe abundances of S stars are determined with the grid by Pieter Neyskens. He compared the Tc/Zr abundances (as a function of [Zr/Fe] overabundances) computed with the STAREVOL code for AGB stellar evolution models of different stellar masses and sizes of the partial mixing zone, with Tc abundances from optical Tc I lines [15]. The computed [Zr/Fe] overabundances are in good agreement with the AGB stellar evolution model predictions, while the Tc/Zr abundances are slightly over-predicted. The study helps to constrain nucleosynthesis and mixing mechanisms in AGB stars.

Alejandra Recio-Blanco presented an overview of research results for classifying FGK stars in the Gaia Data Processing and Analysis Consortium (DPAC-CU8). The Generalized Stellar Parametrizer spectroscopy group develops and tests various algorithms for automated AP determinations with Gaia RVS spectra. She compared internal errors of APs computed with the MATISSE (projection method) & DEGAS (oblique decision tree method), Nelder-Mead, and artificial neural network classification codes using spectral signal-to-noise ratios S/N≤150. She finds for S/N=50 that $\Delta T_{\rm eff}\sim$100 K, Δlog $g\sim$0.2–0.3 dex, Δ[M/H]$\sim$0.15 dex, and $\Delta[\alpha$/H]$\sim$0.1 dex. For cool dwarfs the Ca II near-IR triplet lines in the RVS wavelength domain do not provide sufficiently accurate log g-values. The development and (combined) application of these codes will also be important for the planned Gaia-ESO large public survey with the Giraffe-UVES/FLAMES instrument of VLT. Thierry Morel discussed an interesting study for improving log g-determinations of late-type stars, and hence the accuracy of elemental abundance values, based on a sample to $\sim$40 G-type dwarfs and red giants. The sample provides accurate *seismic* log g-values computed from $T_{\rm eff}$ and the frequency of the maximum oscillation power obtained from ground-based observations, and the *CoRoT* and *Kepler* missions. The log g-values computed from traditional spectroscopic methods agree remarkably well with the seismic values, showing systematic differences below 0.04 dex with 1-$\sigma\leq$0.19 dex [16]. The model-independent methods are important for parameterizing benchmark stars that will be utilized to calibrate the automated AP algorithms currently under development for Gaia and large spectroscopic surveys.

4.2. Hot star parameters

A very interesting study of CNO abundances in OB main sequence stars was presented by Maria-Fernanda Nieva with remarkable new results. She finds from spectral synthesis calculations with the SURFACE code, combined with NLTE level populations from DETAIL and atmosphere models from ATLAS9, a much larger degree of chemical homogeneity of C/O and N/O abundances with respect to the O/H abundance for a sample of 64 B-type stars, compared to previous analyses. In the past the enormous scatter in B-star abundances was difficult to reconcile with data from solar-type stars. The presented analysis accounts for all spectroscopic indicators, e.g., Balmer, helium lines, and metal ionization equilibria, and yields substantially smaller systematic errors for the APs and chemical abundances [17]. The large increase of accuracy and precision of this method for determining the APs of early-type stars is important for future analyses of the Galactic abundance gradient, i.e., with high-resolution and large S/N ratio spectra of the planned Gaia-ESO public survey.

Laurent Mahy modeled the spectra of O-type stars in young open cluster NGC 2244 of the Rosette Nebula. He determined stellar and wind parameters with NLTE synthetic spectrum fits of CMFGEN to UV and optical spectra. The atmosphere models from TLUSTY are combined with a β wind velocity law for O-type dwarfs. The analysis yields systematically smaller mass-loss rates derived from UV P Cyg profiles compared to Hα, possibly due to wind 'vorocity', or the micro-clumping of the expanding wind that can be modeled with a volume filling factor. He also finds a clear trend of N enrichment (from optical N III absorption lines) with larger stellar luminosity or mass [18].

Thomas Dall presented a nice study of the effects of non-spherical and non-homogeneous stellar surfaces on synthetic spectrum calculations. The visible stellar surface is divided into (nearly) equal geometrical sectors ('tiles') for which the emergent spectra are calculated with classical atmosphere models (ATLAS, MARCS, etc.) and summed up to a theoretical spectrum. Preliminary results for FK Com (and Altair) show rather small differences with traditional spherical synthetic spectrum calculations. The new code is however very flexible for assessing spectroscopic effects of various stellar properties, such as star-spots, fast rotation, variable temperature, gravity, and abundances across the stellar surface [19].

Discussion session III

Workshop Question 4: *How to define accuracy with which we determine atmospheric parameters? Should we make a clear distinction between internal and systematic errors? Systematic errors can be due to different modeling methods, LTE vs. non-LTE, 1-D vs. multi-D, inaccurate or incomplete line lists, etc. Internal errors can result from differences in best fit*

methods, for example spectral synthesis fits vs. classical equivalent line width (EW) methods.
Answer by Ulrike Heiter: Yes, internal and systematic errors should be analyzed and estimated separately. Nowadays, authors are doing a good job citing internal errors resulting from the numerical accuracy of their method, but systematic errors are usually poorly characterized. Total uncertainties in atmospheric parameters and abundances seem to be underestimated.
Answer by Alex de Koter: In the hot stars community, we indeed try to tackle systematic errors due to different fitting approaches. In particular, we compare a grid based method with a genetic algorithm method. The methods show very good agreement. In those remaining cases where significant discrepancies occur we can explain why these occur and have ideas how to resolve them.
Answer by Maria Bergemann: It is absolutely necessary to make a careful assessment of errors associated with missing/unrealistic physics in the models used for the Gaia stellar parameter pipeline. Furthermore, systematic errors must be accommodated in the input parameters characterizing synthetic spectra, which are used in the numerical algorithms ("nearest neighbor", "neural network", etc.) developed for Gaia Radial Velocity Spectrometer (RVS) spectra.
Answer by Leo Houziaux: The main question is that we do not really know the noise generated by the location of the Gaia instrument in the vicinity of the Earth. It is quite likely that cosmic rays etc. will lower the signal-to-noise ratio for a lot of objects. What is important is that error limits (both internal and systematic) be indicated by the members of the various consortia.
Answer by Remo Collet: I think the only feasible approach is to use a set of standard stars for which high-quality spectra and photometric data as well as measurements of parallaxes, radii, etc., are available to validate theoretical model atmospheres and synthetic spectra. One should try to reproduce with the same suite of models as many observables as possible for standard stars, in a consistent way (i.e., making sure that different indicators of effective temperature, surface gravity, etc., yield the same results).

5. Large spectroscopic surveys

A large number of presentations at the meeting discussed several techniques for measuring the abundances of various chemical elements from stellar spectra. The methods are important for ongoing developments and testing of automated & supervised algorithms for determining detailed chemical composition and tagging studies in large (chemo-dynamical) spectroscopic surveys planned to complement the Gaia (astrometric and kinematic) census of the Galaxy. The Gaia-ESO public survey (GES) will observe ∼100 000 stars, and the LAMOST survey possibly millions of stars. Smaller spectroscopic surveys of hot stars (Tarantula Survey, VLT-X-Shooter, VLT-CRIRES, IACOB project, Be-star survey, Low Dispersion Sky plate surveys) were also extensively discussed, including quantitative analyses for determining APs and advanced spectral classification methods.

Ronny Blomme provided an overview of the preparations for observing O, B, and A-stars in GES (PIs are Gerry Gilmore and Sofia Randich). It is currently estimates that ∼1500 hot star spectra will be observed with Giraffe ($R{\sim}15\,000$), and about 600 with UVES ($R{=}47\,000$) using VLT FLAMES over 300 nights during 5 years (2011–2016). The number of spectra of FGK stars is estimated more than an order of magnitude larger (10^5 Giraffe and ∼6000 UVES spectra). The definition of GES work packages is ongoing and the hot stars work package (GES-WP13) involves cluster selection and the coordination of spectrum analyses with a variety of transfer codes discussed at the meeting [20]. About 60 old star clusters will be observed as part of GES (these are defined as having an age larger than 100 Myr), and 40 young clusters. All stellar populations in the clusters will be observed by GES. Among the young clusters, 13 were selected for their massive-star content. A large variety of science topics will be addressed with GES data of hot stars. To name a few; constraining the upper part of the Initial Mass Function, the possible correlation of N abundance with $v\sin i$, modeling of micro-clumping in massive hot star winds, and the flattening of the Galactic abundance gradient for B-stars in clusters for studying thin disc formation. Note that the first GES observations are planned for December 2011.

Alex de Koter presented preliminary results for (automated) analyses of VLT FLAMES Tarantula Survey spectra. The survey is possibly the largest homogeneous study of O and early-B stars to date and consists of multi-epoch spectroscopy of ∼1000 massive stars in 30 Dor [21]. It will allow for comprehensive tests of the theory of massive star evolution. Long-standing problems such as the discrepancy between spectroscopic and evolutionary masses of O stars will be addressed. He described test results with a genetic algorithm (GA) fit method using simulated spectra of the NLTE FASTWIND radiative transfer code for atmospheric hydrogen & helium composition $Y_{\rm He}$ (N abundance is to be included). The analysis method for O-type stars incorporates spherically outflowing wind models. The fit results for a sample of 24 O-type dwarfs and supergiants are very accurate, and appear free of systematic offsets in $T_{\rm eff}$, log g, $\dot{M}$, β, $Y_{\rm He}$, and ζ_μ. The analysis results will establish empirical relations between the mass-loss rate and the Eddington factor (Γ) in massive stars, investigate rotationally induced mixing (i.e., N surface abundance versus $v$sin$i$), the effects of angular momentum loss through wind mass-loss, and important aspects of the binary fraction of massive stars, the binary period distribution and evolution. Frans Arjen Stap showed results of the automated GA fitting method to hydrogen and helium line profiles in the J, H, K, and L-band of 5 bright O-type dwarfs. The near-IR high-resolution profiles are observed with VLT-CRIRES (R∼50 000). He compares the best fit parameters with the results of optical spectrum analyses, and finds $T_{\rm eff}$ differences within a spectral subtype and Δlog g<0.2 dex [22]. The near-IR and optical spectra yield differences of computed mass-loss rates of 0.2–1.0 dex, that may possibly be reconciled using differential micro-clumping in the wind models.

Sergio Simon-Diaz presented results of the IACOB project, a grid-based automatic tool for determining stellar and wind parameters of O-type stars. The grid consists of ∼192 000 models computed with FASTWIND for $T_{\rm eff}$>25 kK and 2.6 dex ≤ log g ≤ 4.3 dex. It employs a χ^2-minimization method and uses the detailed profiles of Balmer H and He I/II (absorption) lines and the line equivalent widths as input values [23]. The stellar evolutionary mass can also be computed from evolutionary tracks. The tool is very fast and provides graphics output. It will certainly benefit the analysis of large O star samples observed in current and future ground-based surveys. Yanping Chen discussed a new library of ∼600 stars that will be observed with VLT X-Shooter for all spectral types. The spectra cover the complete wavelength range from 300 nm to 2500 nm with R≃10 000. Since the library will cover a wide range of $T_{\rm eff}$-, log g-, and [Fe/H]-values of stars observed in the LMC, SMC, and the Galactic disc and bulge, it will provide reliable stellar population models for studying galaxy formation and evolution. The X-Shooter spectra will also be calibrated in absolute fluxes and corrected for absorption in Earth's atmosphere [24]. A study of ∼150 Be star spectra observed with the Coudé spectrograph (R=12 000) of the Ondřejov 2 m telescope was presented by Pavel Koubsky. He showed that the P13 to P16 Paschen emission lines are proxies for normalized Hα emission line fluxes exceeding 2.5. The Gaia RVS spectra, which will include these Paschen lines, will hence provide independent information about the Hα line [25]. Several thousands of Be stars will be observed by Gaia, and the study of their emission lines provides important information about the physical properties of Be-star discs.

Rene Hudec provided an overview of various low-dispersion spectroscopic sky surveys. The data have been observed with objective prisms on photographic plates and are compared to simulated low-dispersion observations of the Gaia BP/RP photometers. He develops algorithms for the automated classification of digitized spectra from the photographic plates. It includes, among other things, searches for spectroscopically variable objects, strong and wide spectral emission features in cataclysmic variables, PNe, white dwarfs, carbon stars, QSOs, AGN and peculiar galaxies, and studies of the continuum flux distribution of objects at high redshift [26].

Teresa Aparicio Villegas investigated the capabilities of the ALHAMBRA photometric system for estimating APs and stellar classification. She presented a fit method based on BaSeL models for reliably estimating $T_{\rm eff}$-, log g-, [Fe/H]-, and E($B-V$)-values of a wide variety of spectral types (O to M stars) and luminosity classes, including hot white dwarfs and chemically peculiar stars. Three extinction laws were investigated yielding differences that are not significant to decide if one law should be preferred over the other [27].

Jiannan Zhang and Ali Luo presented the comparison of synthetic LTE spectra computed with the ATLAS9 (new ODFs) and MAFAGS-OS 1-D atmosphere models. The latter models are computed with opacity sampling and convection using a convective efficiency parameter. The ATLAS9 model grid is calculated with opacity distribution functions and mixing-length theory. The comparison of both synthetic spectrum grids for dwarf and giants of 5000 K $\leq T_{\rm eff} \leq$ 15 kK, based on photometric color indexes, absorption line indexes, and the complete spectra, shows appreciable differences for $T_{\rm eff}$<6000 K [28]. The reported differences can systematically influence planned AP determinations of large spectroscopic sky surveys such as LAMOST and Gaia.

Andreas Quirrenbach discussed concepts and plans for future massively parallel spectroscopic instruments that can provide huge numbers of stellar spectra. It is obviously important to match the properties and capabilities of such instruments to the requirements of quantitative spectroscopic modeling efforts. He discussed the 4MOST project proposed as a large international collaboration to go 2–3 magnitudes fainter than Gaia. It involves multi-fibre spectroscopy (300 fibers for R=20 000, and 1500 fibers for R=3000 (red) to R=5000 (blue)) of millions of stars with S/N=20, using large facilities such as NTT and VISTA. 4MOST is approved for study by ESO. Very large surveys are important for unraveling the role of stellar migration for the formation of the Galactic thick and thin disc.

6. New atomic database

Nicholas Walton presented ongoing developments of the Virtual Atomic & Molecular Data Centre (VAMDC), a new atomic database that will become online available by late 2012. The database will provide advanced and cost-effective access methods to the current 'best' fundamental atomic and molecular data. It will provide access infrastructure to a wide range of users (astronomy, nuclear, climatology, biology) in academia and industry. The new database will be important for astrophysics for improved interpretation of the huge spectral datasets that will be generated by the Gaia mission and complementary large ground-based surveys.

Discussion session IV

Workshop Question 5: *A number of large surveys are under way. What additional surveys would be needed to substantially advance our knowledge of stellar atmospheres (both for cool and hot stars)?*
Answer by Elena Pancino: In the area of surveys, it becomes more and more important to define a set of "calibrators" or "calibrating fields" of stars with known parameters and abundance ratios, well studied with high-resolution and high signal-to-noise ratios, and analyzed with different methods, to serve as a means to compare the results of different surveys and eventually combine them. The Gaia-ESO survey is trying to do this in coordination with Hermes and Apogee, but at some point this should become a community-wide effort.
Answer by Bertrand Plez: When planning surveys, including asteroseismology fields are very important so that we get additional independent constraints on stellar parameters.

Workshop Question 6: *What are the most important atomic and molecular data that should be improved or determined for realistic modeling of hot and cool star spectra? Which species and/or which type of data, e.g. level energies, transition probabilities, line broadening parame-*

ters, etc.; what wavelength region?
Answer by Alex de Koter: One (of the many) problems the analysis of hot star atmospheres may suffer is poorly known line broadening parameters and/or assumptions in the description of the broadening theory. This may have significant impact on the gravity determinations, which may be part of the reason why we find discrepancies between spectroscopically determined masses and those following from comparison to to evolutionary predictions.
Answer by Norbert Przybilla: Near-IR spectroscopy will gain in importance in the future, in particular with the upcoming generation of extremely large telescopes. In order to use their full potential, observations will depend on adaptive optics, which is technologically best feasible in the near-IR domain. Pioneering high-resolution spectroscopic surveys like CRIRES-POP show that there is an enormous lack of atomic data at near-IR wavelengths. Even line-identifications face severe problems, requiring laboratory measurements of energy levels and wavelengths for many transitions, both atomic and molecular. Quantitative analyses will require all kinds of data, ranging from transition probabilities to line-broadening data, which in the latter case are in part lacking even for hydrogen and helium.
What is currently mostly needed for non-LTE modeling are more collisional data for electron-ion impact excitation, for a large number of ions/elements. This is in contrast to the situation of data for radiative processes, where the Opacity Project and the IRON Project have provided a large quantity of data already.

Workshop Question 7: *Do the standard models used for spectroscopic analysis of massive hot stars (1-D, spherical symmetric, stationary wind, full line blanketing) provide sufficiently accurate stellar and wind parameters? Are we neglecting important physical mechanisms, such as micro- and macro-clumping, radiative instabilities, non-spherical winds?*
Answer by Artemio Herrero: We have to implement new physical phenomena both in 1-D and 3-D. As it has been shown in this conference many times, only after a more sophisticated calculation can we say whether a given effect will be important for a given type of star. Therefore we cannot anticipate whether it is more important to consider a 3-D geometry or to include more opacity sources, just to mention two possible improvements. We have to keep improving our models, because we can not be sure which is the reason for a failure in fitting the observations until we calculate it.

Question by Alex Lobel: *We have not heard much about mass-loss properties in cool stars at the meeting? Would somebody want to comment on mass-loss research for cool stars as well?*
Answer by Alex de Koter: Concerning the study of mass-loss properties of cool stars, Asymptotic Giant Branch stars, and Red Supergiants; the HIFISTARS project uses HIFI/Herschel to probe the (sometimes time-dependent) outflows using molecular line diagnostics (e.g., CO, H_2O). The goal is to model different rotational transitions – formed in different parts of the outflow – consistent with the thermal emission of grains formed in the wind. This allows to constrain the gas-to-dust ratio (from the gas mass-loss rate and the dust mass-loss rate), a fundamental quantity if one wants to understand these cool outflows. So, this is a very active field of research!

7. Summary
The GREAT-ESF workshop on Stellar Atmospheres in the Gaia Era held at the Vrije Universiteit Brussel in June 2011 has considerably improved communication and helped to establish new science collaboration between researchers and students of the hot and cool stars communities, and among members of the GREAT WGs and the Gaia DPAC for the development and application of advanced spectrum modeling codes. It addressed and identified key areas for the improvement of model spectra from various modern spectral synthesis codes required to

determine reliable physical parameters of hot and cool stars. Its outcome can form the basis for future improvements in advanced spectrum synthesis calculations. The results represent a new milestone towards accurate stellar parameters of cool and hot stars that Gaia will observe, and for Gaia follow-up programmes.

Acknowledgments
I would like to express my sincere thanks for financial support from the European Science Foundation (GREAT-ESF) and the Research Foundation - Flanders. I specially thank Jean-Pierre De Greve, Walter van Rensbergen, and Merel Fabré of the LOC for help with organizing the meeting at the Vrije Universiteit Brussel, and with editing of the Proceedings volume. The Royal Observatory of Belgium is gratefully acknowledged for help with the conference grants management, transportation, and administration. I would like to thank all workshop participants for their valuable contributions and lively discussion interactions that resulted in a truly successful scientific meeting.

References

[1] Heiter U and Lebzelter T 2011 Gaia spectroscopy overview and comparative spectrum modeling for cool giants *J. Phys.: Conf. Series this Volume*
[2] Sordo R, Vallenari A, Tantalo R, Liu C, Smith K, Allard F, Blomme R, Bouret J-C, Brott I, de Laverny P, *et al* 2011 Stellar libraries for Gaia *J. Phys.: Conf. Series this Volume*
[3] Plez B 2011 Cool star model atmospheres for Gaia : ATLAS, MARCS, and PHOENIX *J. Phys.: Conf. Series this Volume*
[4] Lester J B and Neilson H R 2008 *A&A* **491** 633–641 (*Preprint* 0809.1870)
[5] Przybilla N, Nieva M-F and Butler K 2011 Testing common classical LTE and NLTE model atmosphere and line-formation codes for quantitative spectroscopy of early-type stars *J. Phys.: Conf. Series this Volume*
[6] Groh J H 2011 Modeling the wind and photosphere of massive stars with the radiative transfer code CMFGEN *J. Phys.: Conf. Series this Volume*
[7] Lobel A 2011 *Can. J. Phys.* **89** 395 (*Preprint* arXiv:astro-ph/1012.5243)
[8] Collet R, Magic Z and Asplund M 2011 The StaggerGrid project: a grid of 3-D model atmospheres for high-precision spectroscopy *J. Phys.: Conf. Series this Volume*
[9] Chiavassa A, Bigot L, Thévenin F, Collet R, Jasniewicz G, Magic Z and Asplund M 2011 3-D hydrodynamical model atmospheres: a tool to correct radial velocities and parallaxes for Gaia *J. Phys.: Conf. Series this Volume*
[10] Bergemann M, Lind K, Collet R and Asplund M 2011 NLTE effects on Fe I/II in the atmospheres of FGK stars and application to the abundance analysis of their spectra *J. Phys.: Conf. Series this Volume*
[11] Gorlova N 2011 Abundance analysis of post-AGB stars *J. Phys.: Conf. Series this Volume*
[12] Maldonado J, Mora A, Montesinos B, Villaver E and Eiroa C 2011 Spectroscopic properties of stars with debris discs *J. Phys.: Conf. Series this Volume*
[13] Pace G 2011 The metallicity scale of dwarf and giant stars *J. Phys.: Conf. Series this Volume*
[14] Van Eck S, Neyskens P, Plez B, Jorissen A, Edvardsson B, Eriksson K, Gustafsson B, Jørgensen U G and Nordlund Å 2011 A grid of S stars MARCS model atmospheres *J. Phys.: Conf. Series this Volume*
[15] Neyskens P, Van Eck S, Plez B, Goriely S, Siess L and Jorissen A 2011 Accurate abundance determinations in S stars *J. Phys.: Conf. Series this Volume*
[16] Morel T, Miglio A and Valentini M 2011 Using seismic targets as benchmarks for spectroscopic analyses of cool stars *J. Phys.: Conf. Series this Volume*
[17] Nieva M-F, Przybilla N and Irrgang A 2011 High-precision atmospheric parameter and abundance determination of massive stars, and consequences for stellar and Galactic evolution *J. Phys.: Conf. Series this Volume*
[18] Mahy L, Martins F, Hillier D J and Rauw G 2011 A quantitative study of the O stars in NGC 2244 *J. Phys.: Conf. Series this Volume*
[19] Dall T H and Sbordone L 2011 Visualization and spectral synthesis of rotationally distorted stars *J. Phys.: Conf. Series this Volume*
[20] Blomme R 2011 Hot stars in the Gaia-ESO Survey *J. Phys.: Conf. Series this Volume*
[21] de Koter A, Sana H, Evans C J, Bagnoli T, Bastian N, Bestenlehner J M, Bonanos A, Bressert E, Brott I, Cantiello M, *et al* 2011 The O stars in the VLT-FLAMES Tarantula Survey *J. Phys.: Conf. Series this Volume*

[22] Stap F A, Sana H and de Koter A 2011 Quantitative near infra-red spectroscopy of massive stars *J. Phys.: Conf. Series this Volume*
[23] Simón-Díaz S, Castro N, Herrero A, Puls J, Garcia M and Sabín-Sanjulián C 2011 The IACOB project: A grid-based automatic tool for the quantitative spectroscopic analysis of O-stars *J. Phys.: Conf. Series this Volume*
[24] Chen Y, Trager S, Peletier R and Lançon A 2011 XSL: The X-Shooter Spectral Library *J. Phys.: Conf. Series this Volume*
[25] Koubský P, Kotková L and Votruba V 2011 Hα and Gaia-RVS domain spectroscopy of Be stars and interacting binaries with Ondřejov 2m telescope *J. Phys.: Conf. Series this Volume*
[26] Hudec R and Hudec L 2011 Tests of simulated Gaia BP/RP spectra with LDS (Low Dispersion Spectroscopy) photographic sky surveys *J. Phys.: Conf. Series this Volume*
[27] Aparicio Villegas T, Alfaro E J, Cabrera-Caño J, Moles M, Benítez N, Perea J, del Olmo A, Fernández-Soto A, Cristóbal-Hornillos D, Aguerri J A L, *et al* 2011 Stellar physics with the ALHAMBRA photometric system *J. Phys.: Conf. Series this Volume*
[28] Zhang J, Luo A, Song Y and Zuo F 2011 Comparison between MAFAGS-OS spectra and Kurucz-ODF spectra *J. Phys.: Conf. Series this Volume*