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THE PHOENIX MODEL ATMOSPHERE GRID FOR STARS

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Abstract. We present a new project for a 1D static though full NLTE model atmosphere grid ranging $T_{\rm eff} = 15,000$ to 1500 K in 100K steps, surface gravities ranging from $\log g = -0.5$ to 6.0 in steps of 0.25 dex, and metallicity ranging from [M/H]=-2.5 to +0.5 in steps of 0.25 dex accounting for alpha element enrichment of $[\alpha/\mathrm{H}]= +0.0$, +0.2, +0.4 and C/O enhancement.

Keywords: stars, red dwarfs, M Dwarfs, Very Low Mass stars, model atmosphere, spectroscopy

1 Introduction

The PHOENIX model atmosphere code has been created in 1994 in Phoenix, Arizona from merging the M Dwarf model atmosphere code (Allard 1990, molecules in equilibrium chemistry, molecular opacities, convection) with the supernovae radiative transfer code (Hauschildt 1991, spherical symmetry radiative transfer with scattering, full NLTE, Opacity Sampling, Expansion Velocity treatment). The resulting PHOENIX code has been since then developed for additional atmospheric physics such as radiative diffusion (Leblanc & Monin 2005), Quasi-molecular Alkali line profiles (Allard et al. 2007), non-local chemical equilibrium (NLCE) (Barman et al. 2011), and cloud formation(Allard et al. 2001, 2003a, 2011; Allard & Homeier 2012; Allard et al. 2012, 2013b,a; Allard 2014; Allard et al. 2014). More recently, a 3D version of PHOENIX has been developed that include all this complexity (Hauschildt & Baron 2014).

M dwarfs were the last stars to be fully understood due to an SED dominated by molecular opacities (MgH, CaOH, CaH, TiO, VO, FeH, H_2O, CO) and cloud formation below 3000 K. But recently, Rajpurohit et al. (2012, 2013, 2014, 2016) and Baraffe et al. (2015) have demonstrated that the most up-to-date code version reproduce for the first time the overall spectral energy distribution (SED) of M dwarfs down to the hydrogen burning minimum mass. The revised temperature scale has been confirmed by independent research based on interferometry Mann et al. (2016). And Veyette et al. (2016) have demonstrated the importance to account for carbon enhancement for the thermal structure of M Dwarfs. The revised solar abundances and the possibility to use all the lines of complete and accurate molecular line lists made also the difference.

Time as come to provide detailed and uniform model atmosphere grids for the analysis of the GAIA survey, in preparation of the PLATO 2.0 mission, and for the CARMENES and SPIRou survey among others. I present here the 2017 PHOENIX model atmosphere grid project.

2 Model description

In recent years the possibility to model the atmospheres of stars with Radiation HydroDynamical (RHD) simulations and 3D radiative transfert has progressed for Red Supergiant stars (Chiavassa et al. 2016) and main dwarf stars (Asplund 2014; Ludwig & Steffen 2016) improving our knowledge on stars and revised solar abundances (Asplund et al. 2009; Caffau et al. 2011) in time for the GAIA survey.

However, most of the parameter determination is still done using more available and rapid to compute 1D static model atmospheres avec iSpec (Blanco-Cuaresma et al. 2014) ou encore les services en ligne de bases de donnes POLLUX (http://or.lcpc.fr/pollux/) par exemple. The most important is to take into account the findings of the afore mentioned 3D work in doing so. However, all these codes are not NLTE codes, and NLTE has proven difficult if not impossible in the frame of 3D work. The role of full NLTE codes such as `PHOENIX` is

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therefore to provide control on the question of the importance of NLTE effects, to provide thermal structures to the large variety of radiative transfer codes being operated, and provide large uniform model atmosphere grids also for the transcription of the predictions of interior and evolution models in the observational plane.

`PHOENIX` also includes the hyperfine structure for some NLTE atoms and solves the radiative transfer in spherical geometry that is mandatory for extended atmospheres. Instead of using a fixed microturbulence velocity, mixing length, radius and mass throughout the computation of the grid, our use of `PHOENIX` is therefore to interpolate these informations for each model of the grid from RHD simulation studies (Ludwig et al. 1999, 2002; Ludwig 2006; Ludwig et al. 2006; Freytag et al. 2010b, 2012) and interior and evolution model (Baraffe et al. 2015, 2003; Chabrier et al. 2000; Baraffe et al. 1998, 1997).

This is the intention of the current project, to use the multi-purpose `PHOENIX` code in its full NLTE capacity and compute a complete and uniform model atmosphere grid with parameters ranging from $T_{\rm eff} = 15,000$ to 1500 K in 100K steps, surface gravities ranging from $\log g = -0.5$ to 6.0 in steps of 0.25 dex, and metallicity ranging from [M/H]=-2.5 to +0.5 in steps of 0.25 dex accounting for alpha element enrichment of $[\alpha/\mathrm{H}] = +0.0$, +0.2, +0.4 and C/O enhancement.

In `PHOENIX` atmosphere models, a trial atmospheric profile is applied (usually using a previously calculated model), the equations of hydrostatic and radiative transfer are solved, and the solution is tested until convergence is reached. The model is considered converged when the energy is conserved within one tenth of a percent from layer to layer. At each of the model iterations, a spectrum with typically over 30,000 points is generated which samples the bolometric flux from 0.01 to 500 μm with a step of 0.01 to 2 Å in the region where most of the flux is emitted (i.e. 0.1 to 50 μm). When the model is converged, a final spectrum is generated with maximum sampling of around 0.01 Å throughout the SED. The final spectrum must be degraded to the instrumental resolution and applied rotation and macroturbulence corrections before being compared to spectroscopic observations.

The `PHOENIX` version 15.5 model atmospheres developed by Allard & Hauschildt (1995); Allard et al. (1994, 1997, 2001, 2003b, 2007, 2011); Allard & Homeier (2012); Allard et al. (2012, 2013b,a); Allard (2014); Allard et al. (2014) are characterized by the following parameters: (i) the surface gravity, $\log(g)$, (ii) the effective temperature, $T_{\rm eff}$, (iii) the mixing length to scale height ratio, α/H_p, (iv) the micro-turbulent velocity ξ, and (v) the initial element abundances, ϵ_i. Cloud formation is based on the Rossow (1978) cloud model and used the results of RHD simulations of M-L-T dwarfs atmospheres by Freytag et al. (2010a) and Freytag et al. (2017, in prep.) to calibrate the mixing length, the overshoot, the dynamical velocity and micro-turbulence, and the diffusion coefficient. We also use the most recent solar abundance composition by Asplund et al. (2009) and Caffau et al. (2011). The most important opacities that have been updated since Allard et al. (2001) are: i) all atomic lines are now included from hydrogen to uranium (Kurucz database 2006), ii) we have migrated from the AMES (Partridge & Schwenke 1997; Langhoff 1997) to the BT2 (Barber et al. 2006) water vapor and (Plez 1998) TiO line lists, ii) the VO, MgH, and CaH line lists by (Plez 1998) replace the remaining JOLA approximations, iv) NH_3 opacities from the ExoMol project (Yurchenko et al. 2011), v) All bands of H_2-H_2 CIA tables (Borysow 2002; Abel et al. 2011), H_2-H CIA tables (Gustafsson & Frommhold 2003), and He-H CIA tables (Gustafsson & Frommhold 2001) for the most recent version implemented, vi) polarizability wavelength distributions have been added for several additional types of grains bringing our database from 30 to 43, vii) 5 different grain size distributions to choose from have been added, viii) a cloud model has been added, and finally ix) we include detailed profiles for most of the important alkali lines based on the unified theory of collisional quasi-molecular broadening Allard et al. (2007, and references therein). The CE calculations are treated as in Allard et al. (2001) with additional condensates added to serve low temperature brown dwarf atmospheres. See Ferguson et al. (2005) for a detailed description of our opacity database and its application to Rosseland and Planck mean calculations.

3 Model grids already available

We have been posting on our online web site (https://phoenix.ens-lyon.fr/simulator/) several model atmosphere grids reflecting the evolution in the development of `PHOENIX` version 15.5 code version since the original publications to the more recent developments of the BT-Settl grids thanks to funding by the Agence Nationale de la Recherche (Projects Extrasolar planets 2005-2009, GUéPARD 2010-2014). These are :

- NextGen (Allard et al. 1994; Hauschildt et al. 1997) : breakthrough opacity sampling model atmospheres,
- AMES-Cond/Dusty (Allard et al. 2001; Chabrier et al. 2000; Baraffe et al. 2003): first complete dust condensation model atmospheres i.e. models with dust in equilibrium with gas phase while the Cond

models neglect the dust opacity to simulate full sedimentation,

- BT-NextGen (Allard 2010; Allard et al. 2011, 2012): NextGen models with revised modern molecular opacities (Ferguson et al. 2005) and the BT2 water vapor line list bu Barber et al. (2006),
- BT-Cond/Dusty (Allard 2010; Allard et al. 2011, 2012): same as former AMES-Cond/Dusty, but with revised opacities as above,
- BT-Settl GNS93 (Husser et al. 2013): first extremely extended grid of model atmospheres (a former version to that published) with modern opacities,
- BT-Settl AGSS2009 (Allard et al. 2011; Allard & Homeier 2012; Allard et al. 2012): using the Asplund et al. (2009) solar abundances,
- BT-Settl CIFIST2011(Allard et al. 2011; Allard & Homeier 2012; Allard et al. 2012): using the Caffau et al. (2011) solar abundances and adding the computation of the supersaturation on-the-fly rather then using a fixed value suggested by Rossow in the cloud model,
- BT-Settl CIFIST2011b (Allard et al. 2013a,b) : accounting also for a calibration of the mixing length based on RHD simulations by Ludwig et al. (1999, 2002); Ludwig (2006); Ludwig et al. (2006),
- BT-Settl CIFIST2011bc (Allard et al. 2013b,a; Allard 2014; Allard et al. 2014) : accounting for the calibration of the mixing length, overshoot and diffusion coefficient based on RHD simulations by Freytag et al. (2010b, 2012) and account of the grain size distribution and nucleation in the cloud model,
- BT-Settl CIFIST2011c (Allard 2014; Allard et al. 2014) : Aditonnal adjustments of the calibration of the MLT, overshoot, and diffusion coefficient based on RHD simulations by Freytag et al. (in prep.),
- BT-Settl CIFIST2011_2015 (Allard et al. (en prep.), Baraffe et al. 2015) : The MLT equations were revised from (or MLT, see Kippenhahn & Weigert 1994) to the formulation according to Mihalas et al. (1978) (See also Mihalas 1978).

These models are available via the PHOENIX web server (https://phoenix.ens-lyon.fr/simulator/) and the OSU Archive (http://osubdd.ens-lyon.fr/phoenix/).

Since the model atmospheres are using spherical radiative transfer the interior+atmosphere problem becomes iterative, and future versions of the synthetic spectra grid will use the radius and the lithium abundance of the current evolution models.

4 Conclusions and propectives

Model atmosphere grids accounting for full NLTE, the calibration of the mixing length, and cloud formation are already available via the Phoenix Web Server (https://phoenix.ens-lyon.fr/simulator), but there exist at this point no comprehensive version including all the recent developments. With the mission GAIA, the need for a complete and comprehensive and uniform grid of models is high.

The PHOENIX model atmosphere project will provide a uniform grid ranging over $T_{\rm eff} = 15,000$ to 1500 K in 100K steps, surface gravities from $\log g = -0.5$ to 6.0 in steps of 0.25 dex, and metallicity from [M/H]=-2.5 to +0.5 in steps of 0.25 dex accounting for alpha element enrichment of [α/H]= +0.0, +0.2, +0.4 and C/O enhancement, and of synthetic spectra valid across the HR diagram down to the substellar regime. This corresponds to more then 500,000 models to calculate, each with 10h or computing time per cpu, or over 5 million CPU hours of computation.

Our priority in term of future development of the models is the molecular opacity upgrade. Since the ExoMol project has revised most of the molecular opacities important for the atmospheres of stars, we are planing the integration of all the molecular opacities of the ExoMol project and from other authors in a later revision of this model atmosphere grid that will be performed on the *Pôle Scientifique de Modélisation Numérique* (PSMN) and on national computing centers.

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