Software for the Spectral Analysis of Hot Stars

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Abstract. In a collaboration of the German Astrophysical Virtual Observatory (GAVO) and AstroGrid-D, the German Astronomy Community Grid (GACG), we provide a VO service for the access and the calculation of stellar synthetic energy distributions (SEDs) based on static as well as expanding non-LTE model atmospheres.

At three levels, a VO user may directly compare observed and theoretical SEDs: The easiest and fastest way is to use pre-calculated SEDs from the GAVO database. For individual objects, grids of model atmospheres and SEDs can be calculated on the compute resources of AstroGrid-D within reasonable wallclock time. Experienced VO users may even create own atomic-data files for a more detailed analysis.

This VO service opens also the perspective for a new approach to an automated spectral analysis of a large number of observations, e.g. provided by multi-object spectrographs.

1. TheoSSA – Model SED on Demand

Spectral analysis by means of Non-LTE model-atmosphere techniques has for a long time been regarded as a domain of specialists. Within the German Astrophysical Virtual Observatory (GAVO) project, we have created the VO service TheoSSA (Theoretical Simple Spectra Access).

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1http://www.g-vo.org
2http://vo.ari.uni-heidelberg.de/ssatr-0.01/TrSpectra.jsp
A VO user may use pre-calculated grids of spectral energy distributions (SEDS, in a pilot phase calculated by the *Tübingen Model Atmosphere Package* (TMAP) for hot, compact stars only) which are ready to use and it may be interpolated between them to match the user-required parameters. This is the easiest way to use synthetic SEDs calculated from Non-LTE model atmospheres.

If individual parameters are requested which do not fit to an already existing SED in the database, the VO user is guided to TMAW. With this WWW interface, the VO user may calculate an individual model atmosphere, requesting effective temperature, surface gravity, and mass fractions of H, He, C, N, and O (more species will be included in the future). For this calculation, standard model atoms are used which are provided within the *Tübingen Model-Atom Database* (TMAD). Since the VO user can do this without detailed knowledge of the programme code working in the background, the access to individually calculated SEDs is as simple as the use of pre-calculated SEDs - however, the calculation needs some time (depending on the number of species considered, the wall-clock time is ranging from hours to a few days). Standard SEDs (e.g. within wavelength ranges of $5 - 2000\,\text{Å}$ and $3000 - 55000\,\text{Å}$) of all calculated model atmospheres are automatically ingested into the GAVO database and, thus, it is growing in time. Example SEDs are shown in Fig. 1.

In case that a detailed spectral analysis is performed, an experienced VO user may create an own atomic data file tailored to a specific purpose considering all necessary species and calculate own model atmospheres and SEDs. A similar approach is in preparation, using the newly developed *HotBlast* Non-LTE code for spherically expanding atmospheres. *HotBlast* uses as an input the atmospheric structure of the static TMAP model atmospheres to simulate the atmosphere below the wind region.

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3 http://astro.uni-tuebingen.de/~rauch/TMAP/TMAP.html
4 http://astro.uni-tuebingen.de/~TMAW/TMAW.shtml
5 http://astro.uni-tuebingen.de/~rauch/TMAD/TMAD.html
Spectral analysis by means of NLTE model-atmosphere techniques requires the calculation of extended grids, varying photospheric parameters like e.g. effective temperature, surface gravity, and element abundances. Since this is far beyond our computational capacity at the Tübingen institute (IAAT), calculation of such model-atmosphere grids in the framework of AstroGrid-D is necessary.

2. **Atomic Grid Jobs – Task Farming with Globus**

*AstroGrid-D* is a research and development project that has created a Grid research infrastructure for the German astronomical community during the years 2005 to 2009. Based on the Globus Toolkit (GT4) middleware, *AstroGrid-D* connects compute cluster and storage resources with desktops and specialized hardware, e.g. robotic telescopes (Breitling et al. 2008). It resulted in several scientific applications and implements novel Grid services, such as the information service *Stellaris* (Högqvist et al. 2007).

Carrying out the *TMAP* model calculations on the compute resources of *AstroGrid-D* ensures a much better scaling to a potentially high number of requests than it would be possible on local compute hardware. Also, the grid as a whole is more reliable than a local cluster: Even when some of its resources fail, sufficient alternatives are available, given a stable network connection.

When a new model is required, the *TheoSSA* service calls a script package that independently submits jobs to computational Grid resources. This package was originally developed for a different *AstroGrid-D* use case, but is parameterized so that it can easily be adopted to other implementations of so-called *atomic grid jobs*. The label *atomic* in this context refers to a specific type of application for which all input data is transferred together with the software and there is no need for inter-process communication. The Grid is thus used as a task farming mechanism. The flexible GT4 middleware is able to perform more complex requirements, but we found task farming to be an important requirement of many scientific use cases, such as *TMAP*.

Thus transfers of the *TMAP* model-atmosphere software, input data and, upon completion, results become part of the standard job submission process in Globus Toolkit. The process is further explained in Fig. 2. We take advantage of the GT4 web services and control the process by a JSDL template (Job Submission Description Language). Whenever a new job is initiated, the template is applied to the specific case and a target machine is selected from a given list. Optionally, a Grid job broker can be used. Upon completion of the calculation, the results are passed on to the *TheoSSA* service which stores it in its database and notifies the user.

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6http://www.gac-grid.de/
7http://www.gac-grid.org/project-products/Applications/
8http://www.gridforum.org/documents/GFD.56.pdf
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Figure 2. Structural diagram: the TheoSSA VO service combined with the Atomic Grid Job package.

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