TheoSSA on AstroGrid-D

Iliya Nickelt (AIP / GAVO),
Thomas Rauch (IAAT / GAVO),
Harry Enke (AIP / AstroGrid-D)

and the GAVO and AstroGrid-D Teams

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4th EGEE user forum / OGF 25
Catania, 5.3.2009

Introducing AstroGrid-D

- BMBF-sponsored Grid-Project to establish the infrastructure for the German Astrophysical Community
- Part of the German D-Grid initiative
- Members: AIP, ZAH, AEI, TUM, ZIB
- Middleware: GT4.0x
- ~900 nodes in clusters, ~100TB storage space,
- Special Hardware: Robotic Telescopes, soon also a 8[illegible]B “GrayWulf” type storage server
- information server StellarIS, GridWay, Portals, Data Streams,
- 10 implemented use cases of different complexity
- almost 100 registered users, Mh of CPU usage

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Introducing GAVO

- BMBF-sponsored German “Virtual Observatory” project
- part of the IVOA initiative to standardise metadata, protocols and methods of data publication
- partners: ZAH, AIP, MPA, TUM, IAAT, Univ. Bonn
- multiple projects with the German Astrophysical Community
- data center, participation in surveys, standard development
- focus on theoretical astrophysical data (Millenium database, data models)

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TheoSSA:

Science

and

Virtual Observatory

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Scientific motivation

- modelling of high temperature stars (>10,000K, white dwarfs)
- complex spectra, highly specialised field (NLTE-spectra)

→ GAVO task: Create a simple interface to access numeric simulation results of HT spectra

→ allowing for a choice of parameters for atomic data

VObs Service TheoSSA

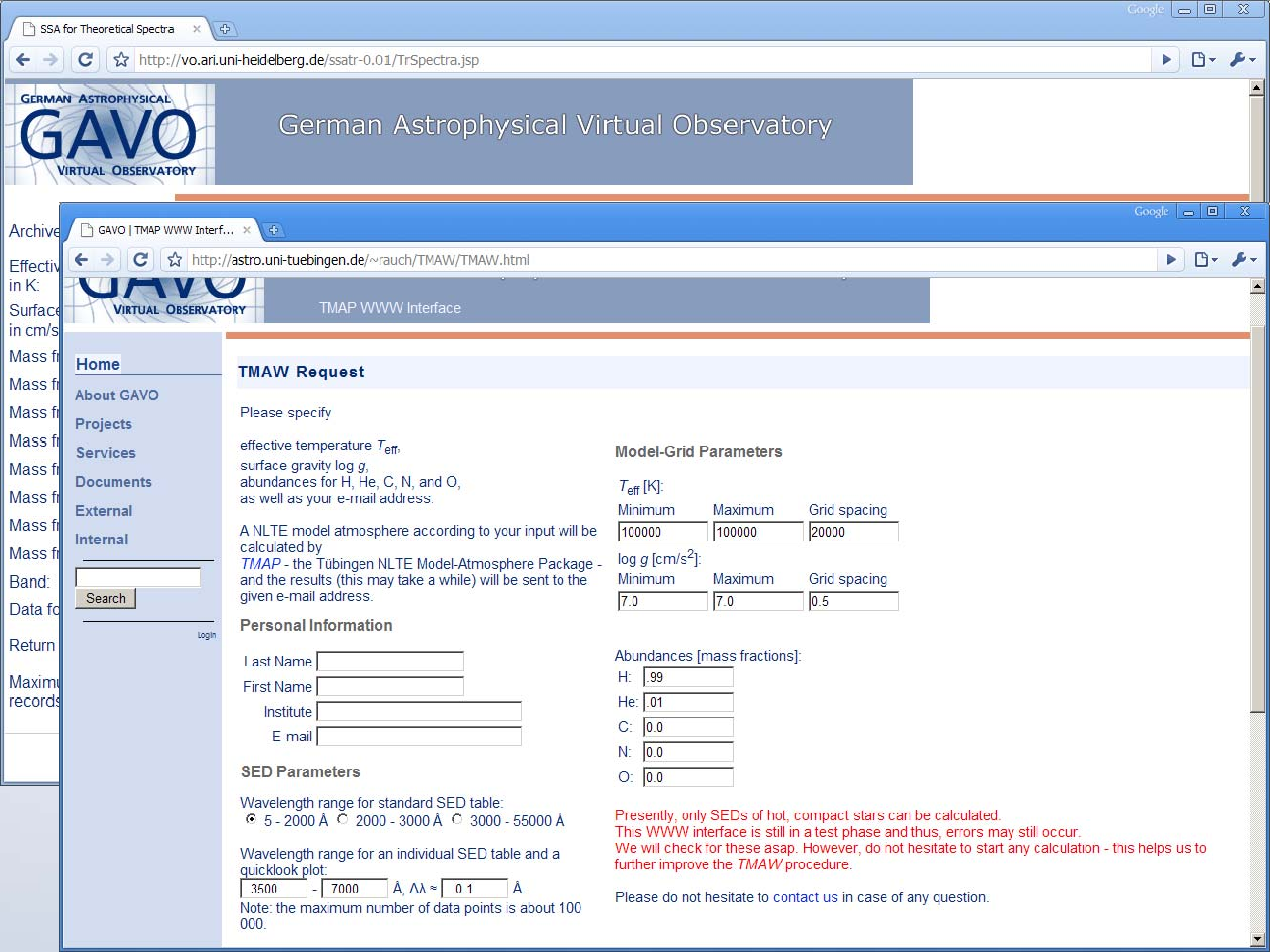
- based on the Tübingen NLTE Model Atmosphere Package *TMAP*
- provides
  - Spectral Energy Distributions (SEDs)

    TheoSSA (http://vo.ari.uni-heidelberg.de/ssatr-0.01/TrSpectra.jsp)
  - Simulation Software

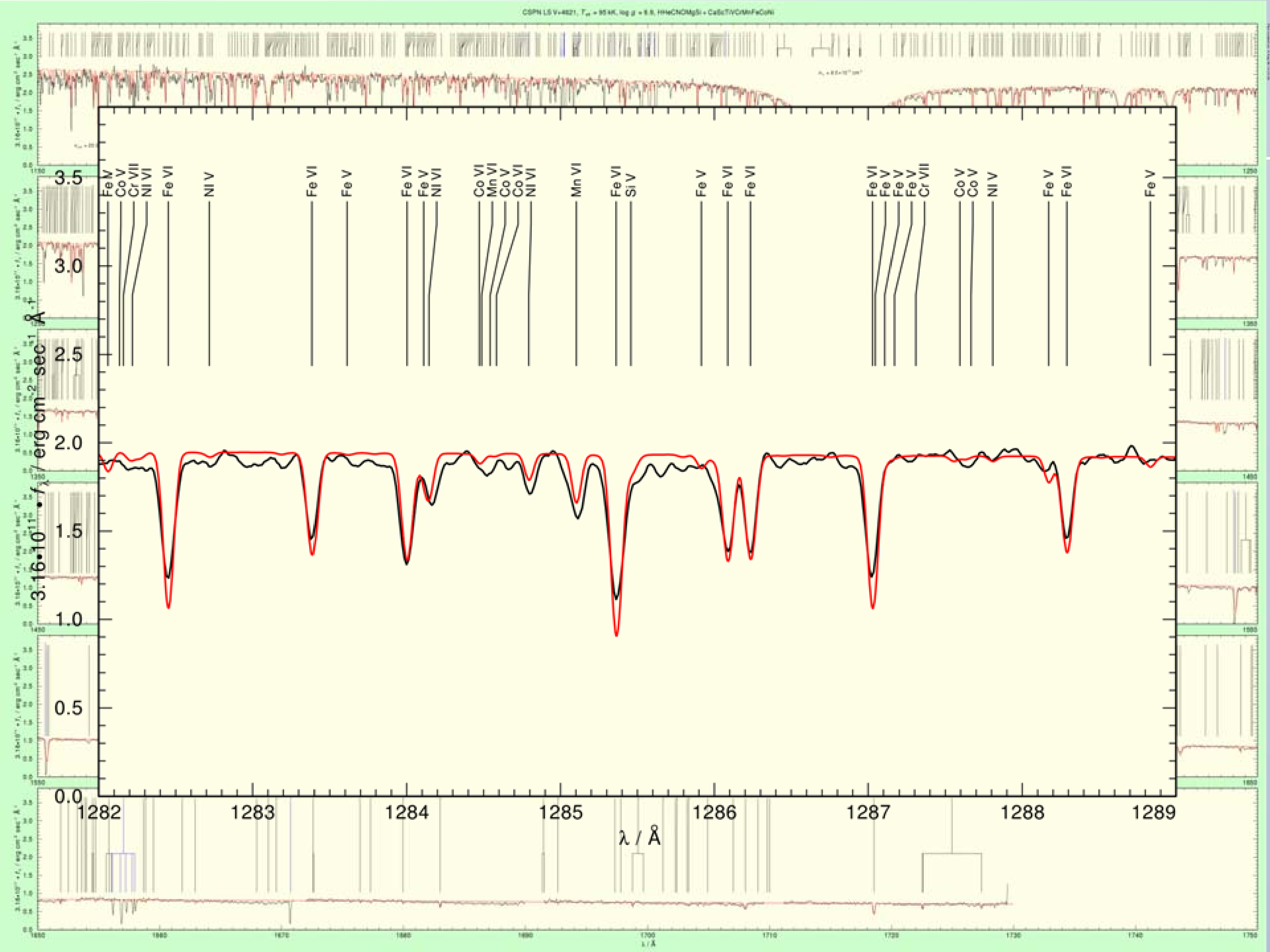
    TMAW (http://astro.uni-tuebingen.de/~TMAW/TMAW.shtml)
  - Atomic Data

    TMAD (http://astro.uni-tuebingen.de/~rauch/TMAD/TMAD.html)
- using the IVOA *Simple Spectral Access protocol* (SSAP)
- in three complexity levels depending on scientific demands

Werner & Dreizler 1999, J. Comput. Appl. Math., Vol. 109, No. 1 - 2, p. 65 - 93
Werner at al. 2003, Stellar Atmosphere Modeling, ASP Conference Proceedings, Vol. 288, p 31



SSA for Theoretical Spectra
http://vo.ari.uni-heidelberg.de/ssatr-0.01/TrSpectra.jsp
German Astrophysical GAVO Virtual Observatory
German Astrophysical Virtual Observatory
Archive
Effectiv
in K:
Surface
in cm/s
Mass fr
Mass fr
Mass fr
Mass fr
Mass fr
Mass fr
Mass fr
Mass fr
Band:
Data fo
Return
Maximu
records
GAVO | TMAP WWW Interf...
http://astro.uni-tuebingen.de/~rauch/TMAW/TMAW.html
Virtual Observatory
TMAP WWW Interface
Home
About GAVO
Projects
Services
Documents
External
Internal
Search
Login
TMAW Request
Please specify
effective temperature T_{eff},
surface gravity log g,
abundances for H, He, C, N, and O,
as well as your e-mail address.
A NLTE model atmosphere according to your input will be calculated by
TMAP - the Tübingen NLTE Model-Atmosphere Package - and the results (this may take a while) will be sent to the given e-mail address.
Personal Information
Last Name
First Name
Institute
E-mail
SED Parameters
Wavelength range for standard SED table:
5 - 2000 Å
2000 - 3000 Å
3000 - 55000 Å
Wavelength range for an individual SED table and a quicklook plot:
3500 - 7000 Å, Δλ ≈ 0.1 Å
Note: the maximum number of data points is about 100 000.
Model-Grid Parameters
T_{eff} [K]:
Minimum Maximum Grid spacing
100000 100000 20000
log g [cm/s^2]:
Minimum Maximum Grid spacing
7.0 7.0 0.5
Abundances [mass fractions]:
H: .99
He: .01
C: 0.0
N: 0.0
O: 0.0
Presently, only SEDs of hot, compact stars can be calculated.
This WWW interface is still in a test phase and thus, errors may still occur.
We will check for these asap. However, do not hesitate to start any calculation - this helps us to further improve the TMAW procedure.
Please do not hesitate to contact us in case of any question.


CSPN LS V+4621, T_eff = 95 kK, log g = 6.9, HHeCNOMgSi + CaScTiVCrMnFeCoNi
Fe V
Co V
Cr VII
Ni VI
Fe VI
Ni V
Fe VI
Fe V
Fe VI
Fe V
Ni VI
Co VI
Mn VI
Co V
Co VI
Ni VI
Mn VI
Fe VI
Si V
Fe V
Fe VI
Fe VI
Fe VI
Fe V
Fe V
Fe V
Cr VII
Co V
Co V
Ni V
Fe V
Fe VI
Fe V
3.16•10^-11 • f_λ / erg cm^-2 sec^-1 Å^-1
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
1282
1283
1284
1285
1286
1287
1288
1289
λ / Å

TheoSSA:
Grid elements

Why use a Grid?

- CPU time increases with number of considered elements (hours to weeks)
- Grid can scale according to demand
- higher reliability (backup resources)
- middleware offers additional options: Job monitoring, statistics, error handling
- TMAP is comparatively easy to compute:
  - no interprocess-communication
  - no complex compilation, all libraries supplied

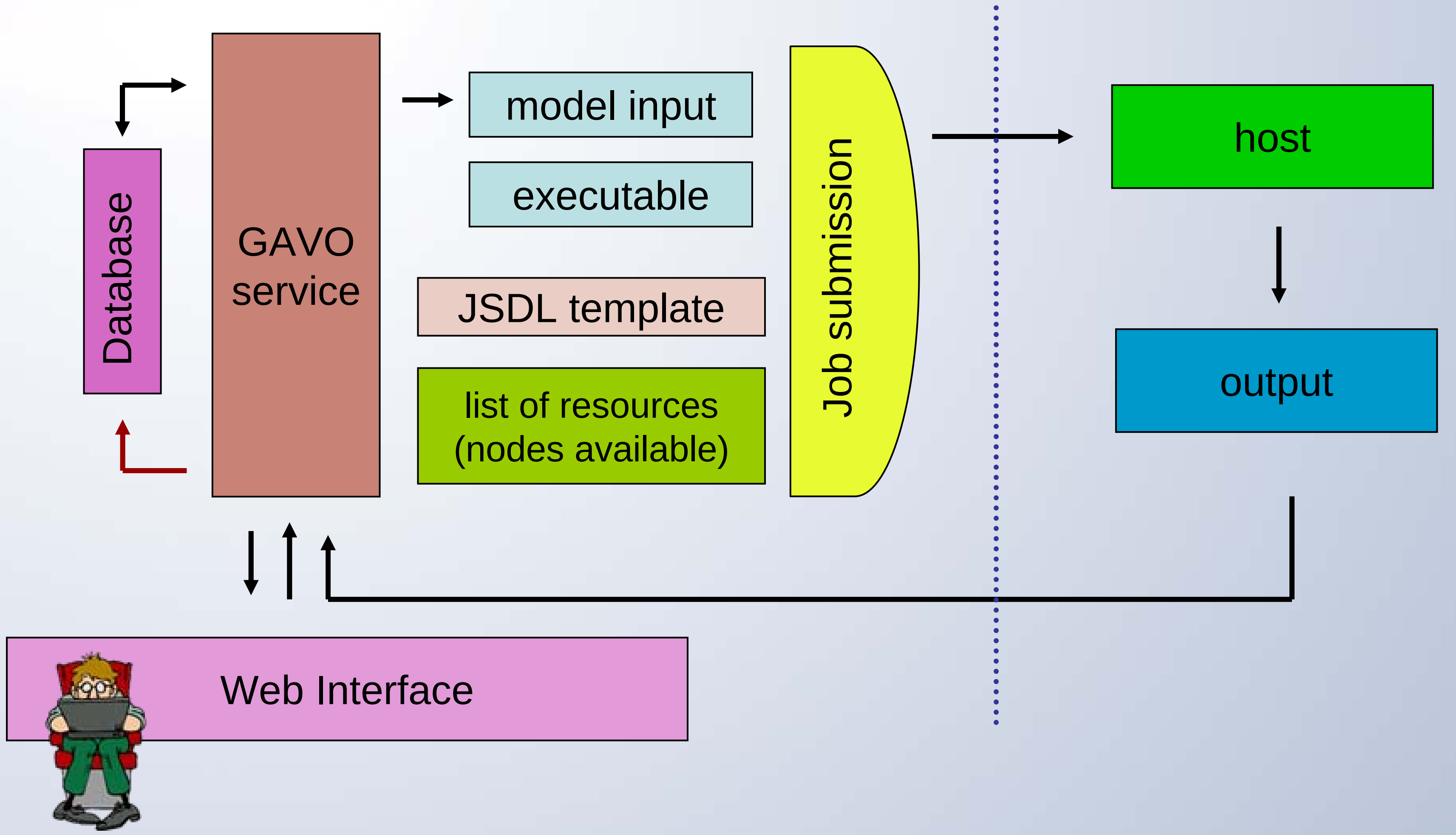
AGD “atomic job” package

- Compute resources are retrieved from the MDS (monitoring and discovery service)
- The Job is submitted using a JSDL template
- GT4.0x: with prior RSL translation via xsltproc
- Data transfer uses gsiftp, the job staging process is based on GT4 web services (globusrun-ws)
- all written in a two-page shell script

```
        <jsdl-posix:Executable>/bin/sh</jsdl-posix:Executable>
        <jsdl-posix:Argument>-c</jsdl-posix:Argument>
        <jsdl-posix:Argument>
          tar xf ${UPLOAD}.tar ;
          cd ${UPLOAD} ;
          ./${EXECUTABLE}
        </jsdl-posix:Argument>
        <jsdl-posix:Output>/dev/nul
        <jsdl-posix:Error>/dev/null
        <jsdl-posix:WorkingDirector
        <jsdl-posix:WallTimeLimit>6
        <jsdl-posix:MemoryLimit>200
      </jsdl-posix:POSIXApplication
    </jsdl:Application>

    <jsdl:Resources>
      <jsdl:FileSystem name="HOME">
        <jsdl:Description>User's ho
      </jsdl:FileSystem>
    </jsdl:Resources>
    <!-- Other well-known filesystems are: SCRATCH, ROOT and

    <!-- Stage in the tar file -->
    <jsdl:DataStaging>
      <jsdl:FileName>${UPLOAD}.tar</
      <jsdl:FilesystemName>HOME</js
      <jsdl:CreationFlag>overwrite<
      <jsdl:DeleteOnTermination>true
      <jsdl:Source>
        <jsdl:URI>gsiftp://${HOST}$
      </jsdl:Source>
    </jsdl:DataStaging>

    <!-- Stage out the output files -->
    <jsdl:DataStaging>
      <jsdl:FileName>${UPLOAD}/</js
      <jsdl:FilesystemName>HOME</js
      <jsdl:CreationFlag>overwrite<
      <jsdl:DeleteOnTermination>true
```

```
SERVICE_HOME=$(cd `dirname $0`; pwd)
HOST=`hostname --fqdn`
MACHINES=(`egrep '^[^#]' $SERVICE_HOME/machines`)     #static machine file
NUM_INPUTS=`ls -d1 $SERVICE_HOME/../input/input[0-9]* | wc -l`

until grid-proxy-info -exists -valid 0:02 > /dev/null
do
    grid-proxy-init
done

mkdir -p $HOME/.epr
rm -f $SERVICE_HOME/visualisation.data
I=0
while [ $I -lt $NUM_INPUTS ]
do
    true & EPID=$!
    MACHINE=${MACHINES[$(($I % ${#MACHINES[*]}))]}
    UPLOAD=${PROJECT}_upload_${MACHINE}_${EPID}
    RESULT=${PROJECT}_results_${MACHINE}_${EPID}

    mkdir -m 777 -p $SERVICE_HOME/$UPLOAD $SERVICE_HOME/$RESULT
    cd $SERVICE_HOME/../input
    cd input$I
    INPUTDIR=`pwd`
    cp * ../$EXECUTABLE $SERVICE_HOME/$UPLOAD
    cd $SERVICE_HOME
    tar cfz $UPLOAD.tar $UPLOAD/*
    chmod 777 $UPLOAD.tar

    eval echo $(sed "s/[\"&';<>]/\\\&/g" $SERVICE_HOME/jsdl.template) |\
        xsltproc $SERVICE_HOME/rsl.xslt - > $SERVICE_HOME/$UPLOAD/$PROJECT.rsl
    if globusrun-ws -submit -f $SERVICE_HOME/$UPLOAD/$PROJECT.rsl \
        -b -J -S -F $MACHINE -o $HOME/.epr/${PROJECT}_${MACHINE}_${EPID}.epr
        then
#           echo $MACHINE, $HOME/.epr/${PROJECT}_${MACHINE}_${EPID}.epr, $SERVICE_HOME/$RESULT, $UPLOAD, $INPUTDIR >> $SERVICE_H
        rm $UPLOAD.tar
        I=$(($I + 1))
        else
```

Task farming with Globus

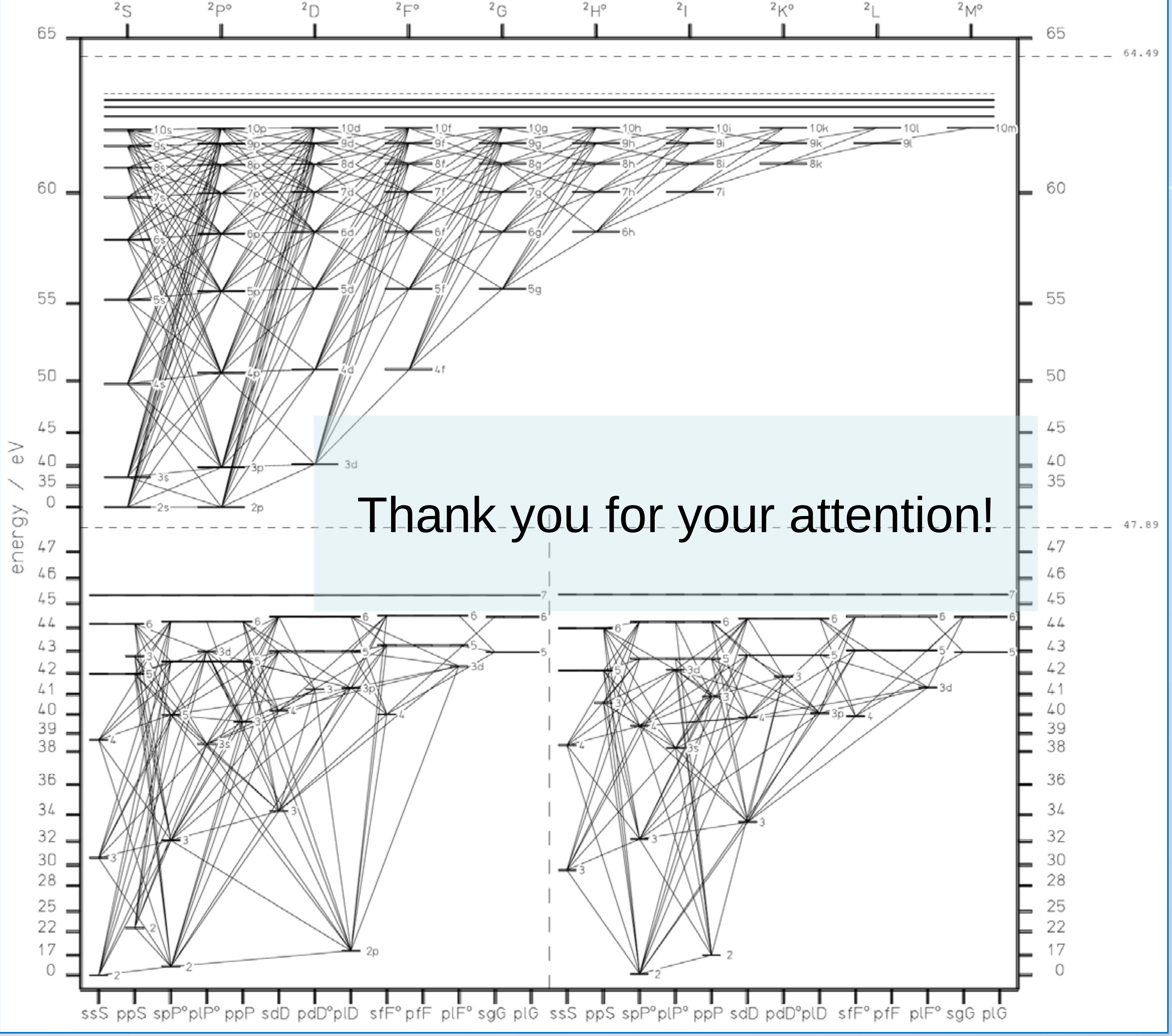


Conclusions

- TheoSSA combines advantages of a VObs standardised interface with the compute power of the Grid (“VObs on top”)
- Serves as a good example use case
- It presents SEDs of hot compact stars to the community and the VObs

Future Steps with EGEE

- AstroGrid-D project time has officially ended
- All D-Grid community projects were focused on *national* Grid infrastructure
- project is now carried by the participating institutes; ongoing applications
- interest for international collaboration
- participation in EGEE A&A Cluster (and EGI)
- gateway between AGD and EGEE
- “atomic” task farming as a test case



Thank you for your attention!