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```
#####
# Mon 2007-02-19 #
#####
```

```
10.00 Information session
=====
```

```
Inside VALD - Current status of VALD-2
-----
```

```
(with written input from Nik)
```

```
** Ulrike ** Introduction and database structure
```

```
- Introduction (VALD team, goals of VALD, VALD citations)
```

```
- Data storage (data files, format, compression)
```

```
see http://www.astro.uu.se/~ulrike/Documents/Inside\_VALD\_0702\_UH.pdf
```

```
** Friedrich ** Extraction software
```

```
Preselect, Showline and Select were presented as described in "Inside VALD"
text by Nik.
```

```
see jan:~vald/development/documentation/trunk/Inside\_VALD.txt
```



**\*\* Tanya and Rimma \*\* VALD content**

The default configuration file contains data from 137 original line lists, which are combined into 75 VALD lists + 29 additional lists (commented).

Tanya's personal configuration file contains 9 additional new or corrected lists.

A problem is the citation of the original sources for data (Tanya receives complaints by producers).

Proposal: if there are new lists with improved wavelengths, change wavelengths in all "old" lists (e.g. Imperial College lists obtained via Kurucz).

About 50 new line lists are being prepared:

Ca I and II: new data, checked with NLTE calculations for different models and observations, 8 new references in total (1 of them for VdW constants: Smith G, 1981 A&A 103, 351)

Ti I: Nitz, Wickliffe, Lawler 1998, ApJS 117, 313

Ti II: Pickering, Thorne, Perez 2001, ApJS 132, 403  
(already in Tanya's personal configuration file)

Cr II: Nilsson, Ljung, Lundberg, Nielsen 2006, A&A 445, 1165 (Lund group)

Mn II (2 references)

Fe II (4 references)

Ni (2 references)

Zr II (2)

Zr III (3)

Tc, Pd

Hf II (2)

La II (2)

Ce I-III (1)

Sm II (1)

Nd II (1)

Eu I\_III

Gd, ...

Ho, ...

Th II (Lund)

Th III (calculations)

U II (Lund)

Most lists are made by Rimma, some of them are checked with calculations (e.g. Amsterdam code).

- Comparison between different data sets (log gf) show good agreement, sometimes small systematic shifts. Scatter: e.g. Fe II about 0.1 dex + a few "famous" lines in red region with large deviations (VALD-2 vs. Schnabel et al.), Raassen & Uylings, Moity, NIST.
  - Problem with non-homogeneous quality of data in one and the same source list (how do we rank them?)
  - Paul will ask Schnabel about outliers in his line list.
  - Christian: One should do comparisons (plots) for all lists included in VALD (with a script).
  - "We are certainly not worse than NIST."
-

## 16.00 Round of statements

=====

## Expectations and contributions

-----

- + ... was done at end of week (or end of stay)
- ~ ... in progress at end of week
- ... was not done

## Ulrike

- + Get a working test version of VALD-3 running (whole pipeline)
- + Some test lists in VALD-3 format available, including molecules

## Friedrich

- ~ New preselect + showline
- + Reference lists -> bibtex lists + some standard reference formats
- + Set priorities on VALD features to be made available as soon as possible
- + Discuss autoionization lines

## Tanya+Rimma

- + "Clean" VALD-2 e.g. Si list
- + Stark damping constants (Si)
- + Reconsider Kurucz NLTE line lists
- + Revision of lists for simple elements  
(remove lines which are obviously wrong)

## Rimma

- + Prepare VALD-3 lists (new data - Fe I and REE)
- + Fix final term designation

## Theresa

- + Get insight in VALD as user
- + Test user interface

## Nicole

- + Same as Theresa
- + Help with conversion and other tasks

## Christian

- + Software development (extraction tools)
- + Find way for more people to contribute to software development,  
find method for this during the workshop
- + VALD administration
- + VALD presentation (web page, ems, interface)

## Marlene

- + Learn about VALD
- + Help

## Werner

- + See VALD-3 developing, try to avoid overlap with VALD-2
- + "indirect" user of VALD
- + Expect plans of who will do what
- + Plan funding

## Eric

- + Integration of web manual and web interface
- + Update Vienna and Uppsala web interface software
- Implement personal preferences (e.g. format) with e.g. cookies
- + Synchronization: get it running and make tests
- Backup
- + Eager to see molecular line lists

## Luca

- + Feedback from "everyday" user
- + Checking VALD data on non-solar stars

Paul

- + Include new VdW data in database
- + Get feedback from everybody regarding other VdW data needed
- + Work on term designations

Oleg

- + Using VALD in projects related to magnetic stars
  - > include Lande factors, work on term designations
- + Update of predicted line lists possible?
  - if yes, contribute to it
- + Together with Nik: new version of SELECT
  - taking into account molecular equilibrium
- + Question of autoionization lines

-----

17.00 Group work: Paul, Oleg, Ulrike

=====

Term designation format

-----

Recommendation: follow NIST format

- groups separated by dots = electron configurations
- brackets around parent configurations
- the term in last group
- asterisk for odd level
- no spaces
- seniority: as in source lists (might be inconsistent -> warn users)

Flags: up to 4 characters (e.g. 'LS', 'J1J2', ...)

Example from ree\_wisc list (5797.57 La II):

LS  
5d2.a3F  
LS  
4f5d.z3G\*

5627.497 Fe II (from NIST):

LS  
3d6.(3F2).4s.a2F  
LS  
3d6.(5D).4p.z4F\*

5615.644 Fe I (from NIST)

LS  
3p6.3d6.(5D).4s.4p.(3P\*).z5F\*  
LS  
3p6.3d6.(5D).4s.(6D).5s.e5D

=====

#=====#  
# Tue 2007-02-20 #  
#=====#

14.45 Presentation

=====

Van der Waals broadening

-----

\*\* Paul \*\*

Van der Waals broadening calculations using Anstee-Barklem-O'Mara (ABO) theory

- Collisional broadening by H

From Barklem & Aspelund-Johansson 2005A&A...435..373B  
("The broadening of Fe II lines by neutral hydrogen collisions"):

"In the ABO theory, [...] a key parameter is  $E_p$ , the fixed energy debt in the Unsöld (1927) approximation to the second order interaction energy between the perturbed absorbing atom and the ground state H atom."

The  $E_p$  parameter can be approximated by  $-4/9$  au for neutrals because it is dominated by H. This is not possible for ions.  $E_p$  is calculated from C6 + ABO theory (cf.: Kurucz uses a more approximate formula for C6 + Unsöld theory).

Fe II: 24188 lines (from Kurucz lists), which have

- $\log gf > -5$
- properties such that the theory is applicable ( $n^* < 3,4$ ; exchange effects)
- observed energy levels
- $\Delta l = \pm 1$

Results: see Barklem & Aspelund-Johansson (2005)

Cr II: 2235 lines

- $\log gf > -3$  and wavelength  $> 300\text{\AA}$
- significant difference to  $E_p = -4/9$  in cross section for hundreds of lines
- mean difference to Kurucz in damping constant = 1.37

The computing time is  $\sim 2$  min. per line. The main work is setting up the identification of parent terms. No lab data is available.

Paul will send an ascii table with his data to Christian who will convert it to VALD format (done by end of week, see below).

=====

```
#=====#  
# Wed 2007-02-21 #  
#=====#
```

10.35 Discussion  
=====

Virtual Observatory  
-----

\*\* Nik \*\*

It all started with the idea to use SME for VO.  
For that, atomic data is needed, therefore VALD should be included.

Nik was approached by Jonathan Tedds et al. (UK representative on the Internal Science Team of the Euro VO DCA), who worked on the specification for a VO interface (definition/description of a "spectral line").

\*\* Werner \*\*

Werner was approached by Rudi Albrecht et al. (ESO, Munich), and further by Enrique Solano et al. (INTA, Spain, EuroVO-DCA Board member).

Under which conditions do we want VALD to become part of VO?  
Potential problems are funding and references to original sources.

Nik: We don't have to be part of VO, but must help to build an interface.

-----

11.00 Group work: Nik, Friedrich, Christian, Ulrike

=====

Linelists and software

-----

We should have a flag for the "type" of list (predicted, observed, astrophysical, ...) -> e.g. add an accuracy flag 'P' for predicted lines.

The problem of replacing wavelengths (e.g. Cr) was discussed.

There was no definitive conclusion as far as I remember.

The problem of isotopes was discussed. The conclusion was that the natural (laboratory) isotope mixture will be identified with isotope number 0, and individual isotopes by numbers 1, 2, 3, etc. The extraction tool (preselect) will handle the isotopes with an option to extract either only the lab mixture data or all individual isotopes. The implementation of the second option is not trivial, because the tool has to "look ahead" if data for isotopes exist and retain or discard the data for the mixture. Maybe one should use a flag.

It was discussed to use a portable Makefile to handle the byte-swapping option, if possible, for all VALD tools.

-----

12.30 Lunch: Nik, Oleg, Paul, Eric, Ulrike

=====

- \* Molecules: Bertrand should provide line lists with complete information for each transition (if possible during workshop).  
He will be referenced and co-author of one of the VALD-3 papers.
- \* References: The "source" field (which contains a code for the source paper from which the log gf value comes) must be taken from the list according to log gf ranking (not as it is now, the "term designation" ranking)!
- \* VALD directory structure:  
Keep the default structure and content separate from additional "tools" (like ATLAS9 etc.) and files, and keep it the same at all three servers.
- \* How to update "Inside VALD" document:  
Nik prefers that different people edit document, but we have to keep track of changes -> it is included in the version management system (see below).

-----

15.50 Discussions

=====

Organization of line lists

-----

- Number of files
- Reference system
- New species indexing system

Proposal: Group data by producer rather than element, so that each list contains lines from one particular paper.  
This will be easier to reference.

The extraction of references is not completely trivial, but the programmers will take care of it. VALD contains two "types" of references: The name of the whole list and the "source" field for each individual line. It contains a code (abbreviation) for the source of the log gf value or another parameter in the case of a replacement list. It must be checked that abbreviations for sources are unique! If the lists really strictly correspond to original sources, the "source" field would not be necessary. But e.g. the Kurucz lists will not be split up, and they are compiled from different sources.

What do we do with existing data?

-> We have to split them, except for (old) Kurucz lists.

What do we do with DREAM lists?

-> Cite one paper (the main DREAM paper).

Who will be doing it? Tanya, Rimma, Christian, Ulrike

New data - What and how much will we include in the future

Molecular data:

- TiO list from Bertrand (~10 million lines, published)  
Separate lists for each isotope  
Select can handle molecules.  
These will be included first, for testing.
- Next step: include quantum numbers for Lande factor and damping  
constant calculations. Paul will provide partition functions.
- Next: CN, CH (few 1000 lines), ZrO, C2, CaH from Bertrand (unpublished)  
(H2O: 100 million lines, not by Bertrand)

Implement switch "no molecules" in preselect etc. -> done (see below).

Model atmospheres for EXTRACT STELLAR for cool stars:

MARCS (Plez), switch to Kurucz at solar type stars.

What about data for input for model atmosphere calculations

(e.g. new predicted lines list by Kurucz)?

Bob Kurucz is positive -> ask again if he wants to be included in  
publications (see discussion on VALD papers on Thursday below).

Autoionization lines have to be flagged.

"Unofficial data" - Lists with data not officially included in VALD,  
but available to Tanya and included in her personal configuration  
file - who else is allowed to use those lists?

Was not discussed.

Who will do what (searching the literature, updating the lists, ...)?

Everyone sends new references to Tanya (preferably pdf file of paper).

Complaints concerning copyright by producers will be sent to Werner.

#####  
#=====  
# Thu 2007-02-22 #  
#=====

10.15 Morning Roundtable

=====

\* Tanya  
is working on Fe II line lists, which will be completed by the end of her  
stay in Vienna.  
It will be sent to Paul for verification/check with Schnabel.

\* Friedrich  
We should discuss software development (version management)  
-> in group with Eric, Nik, Christian, Ulrike.

\* Nik  
preselect3 is being developed.

\* Christian  
Codes for "filtering" and ascii file management are being developed.  
They should also be included in version management (done by end of week).



10.30 Group work: Eric, Christian, Ulrike, Friedrich, Nik

Version management

Discussion on version management using "subversion" program (svn).  
Eric will set it up on the Vienna server for a first trial (done).  
We need separate repositories for separate components:

- Extraction tools
- EMS
- Web interface
- Conversion tools
- Documentation

Synchronization

Eric will install rsync (done).  
Nik will inquire if Baltimore server agrees with it.

15.00 Discussion

VALD papers

**\*\* Friedrich \*\***

So far, VALD has been documented in three major publications:  
VALD-1 and VALD-2 (A&AS) and Physica Scripta paper.  
All are between 10-15 pages. The main emphasis is on new data and data comparisons. The software and database structure, service and management etc. are "add-ons".

For VALD-3, many more people will be contributing (~15).  
We will therefore split the publication in several parts (several papers), either 3-4 equal papers or one "main" paper + few smaller ones.

**\*\* Tanya \*\***

A paper on REE will be written together with different producers from Liege, Wisconsin, ... (partition function changes).

**\*\* Nik \*\***

In terms of data, there will be three new additions, therefore three papers

- REE data -> Tanya
- Fe-peak and other elements (Lund etc.) -> Tanya
- Molecular data, including technical description of VALD-3 -> Nik

Journal: A&A -> astrophysical verification/application needed:  
observations, abundance analyses, consistency checks (VALD2/3), ...  
e.g. using SME

What about involvement of Bob Kurucz?  
Nik will talk to him.

Time scales are the responsibility of the first authors.

VALD-3 should be released as soon as possible, even if the papers are not yet ready.

## 18.00 Presentation

=====

## Demo of VALD-3 pipeline

-----

**\*\* Nik \*\***

Nik constructed a test configuration file with a few atomic linelists converted from VALD-2 to VALD-3 using ukconvert2-3 and kompress3.

Note that the atomic number has been replaced by the "species index", see ~vald/data/VALD\_list\_of\_species.

Example:

```
'/VALD3/PRESELECT/gf26_obs',          23,  326,  334,3,3,3,3,3,3,3,5,  
'GFIRON obs. energy level: Fe'
```

Some TiO lists were also constructed, inserting dummy values in fields for which no information was contained in the original lists, and compressed (by factor 4.5 bin -> CVALD3).

preselect3 was shown. A new switch (no. 10) is implemented to include or exclude molecules.

The "long format" now consists of 2 lines for each transition.

The "short format" looks the same as before, except that the element code is replaced by the species index.

presformat3 and select3 were also shown, using a NextGen model atmosphere to extract molecular lines with select3.

=====

```
#=====#  
# Fri 2007-02-23 #  
#=====#
```

## 14.10 Presentation

=====

**\*\* Enrique Solano \*\***

EuroVO-DCA Board member and Work Package 6 contact person  
("Support to data centres from other European countries")

EuroVO-DCA

-----

## Outline:

- The VO - the role of science, present status
- EuroVO-DCA
- VALD and VO

\* The VO

Classical way of doing Astronomy:

Get data (new or archive) -> reduce and analyze data locally.  
-> inefficient if interoperability is needed or for large data sets,  
e.g. building SEDs.

Solutions provided by VO:

- standard semantic
- standard access protocols
- standard output formats
- standard data models
- access tools

Large data sets ("data avalanche") in VO:  
leave data where it is + remote operations.

VO is driven by science and it will become a science driver.

List of VO science cases:

- Circumstellar disks: from pre-Main Sequence stars to stars harbouring planets
- Intermediate Velocity Clouds
- Which star will go Supernova next?
- Initial Mass Function within 1 kpc: from planetary to stellar masses
- ...

see <http://www.euro-vo.org/pub/fc/cases/srm.pdf>

VO Tools: e.g. Aladin, VOSpec

see <http://www.euro-vo.org/pub/fc/software.html>

VO-Science papers:

1. Padovani et al. 2004A&A...424..545P,  
"Discovery of optically faint obscured quasars with Virtual Observatory tools" (type 2 quasars = Seyfert 2 high-power counterparts)
2. Tsalmantza et al. 2006A&A...447...89T,  
"Luminous AGB stars in nearby galaxies. A study using virtual observatory tools"
3. McGlynn et al. 2004ApJ...616.1284M,  
"Automated Classification of ROSAT Sources Using Heterogeneous Multiwavelength Source Catalogs"

see <http://www.euro-vo.org/pub/fc/papers.html>

The latest VO-Science Workshop took place as a special session (SPS3) at the IAU General Assembly in Prague (August 2006).

Science with VO:

ADS statistics ("Virtual Observatory" in title 2000-2006) results in many papers but few refereed.

\* EuroVO-DCA

The first VO projects were ASTROGRID, AVO, NVO, CVO.

The number of projects increased rapidly, therefore the International Virtual Observatory Alliance (IVOA) was created in 2002.

A European project was the AVO project (2002-2004).

EuroVO is the successor project and is co-funded by the European Commission under the Sixth Framework Programme of the European Community.

Start: 1. Sept. 2006 (28 months project).

8 partners (see <http://www.euro-vo.org/pub/general/partners.html>).

Three faces of EuroVO:

- DCA Data Centre Alliance
- FC Facility Center
- TC Technology Center

Workpackages:

- WP1 - Management
- WP2 - Definition of European DCA Strategy
- WP3 - Support to take-up and implementation of the VO framework
- WP4 - Theory in VO
- WP5 - Coordination with computational grid projects
- WP6 - Support to data centres from other European countries

see <http://www.euro-vo.org/pub/dca/workpackages.html>

\* VALD and VO

What is a Data Centre for EuroVO-DCA?

Requirements:

- willingness to provide a service to the community
- sustainability (critical mass, local financial support)
- concern for quality

EuroVO-DCA will help European data centres to integrate their data and services.

Atomic and molecular databases in the VO

- essential
- important to make data widely available
- data model for spectral lines

SLAP (Simple Line Access Protocol) is the standard protocol for retrieving spectral lines from databases. The basic parameter is wavelength. There are other extra search parameters (chem. element, energy level range, temperature).

see <http://www.ivoa.net/twiki/bin/view/IVOA/SpectralLineListsDocs>  
(main person: Marie-Lise Dubernet, LERMA, Observatory of Paris)

Standard format for output: VoTable (xml file: meta data + data).

Demo: SLAP in action

Try it yourself: <http://esavo.esac.esa.int/vospec/>

Some spectroscopic line databases are already included (e.g. NIST).

"VO science is not science fiction."

"VO is not replacing the scientist (ther will be no 'write paper' button)".

"VO has crossed the no-return point."

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Discussion

=====

VALD and VO

-----

Nik: VALD has the largest collection of atomic data in the world,  
quality control is built in.

Up to now approaches by VO to VALD have not mentioned that we have to do the work.

An important VALD feature is the extraction based on a model (includes rad. transfer calculations) - this is not yet possible to implement in SLAP.

Werner points out the potential "black box" danger.

Enrique: VO data centers (data providers) should provide highest quality data + information on quality.

Fritz: This is no problem for VALD.

Tanya: If someone was trying to identify lines for example for Przibilsky's star, and would use "EXTRACT ALL" from VALD (= PRESELECT only), this would result in completely wrong identifications.

Nik: ...

Eric points out the difference between e-mail request and web request.

Christian: Will it be possible to have a special Java interface for VALD?

Fritz: Is a delay in the response after the request a problem for VO?

Enrique: It is not a problem, the same situation for another service exists already.

Nik: It should work, we could start with "extract all".  
VO should do rerouting to the mirror sites automatically.

Ulrike: What about referencing the original sources of the data?

Enrique: Fields in the VoTable header are provided to include source information.

Fritz, Tanya: ...

Fritz: Does one have to register to use VO?

Enrique: No. Providers have to register, but at this point everybody can register (e.g. cook up a spectrum of Vega and add it).

Werner: What can VO provide for VALD?

Enrique: Many have already joined VO, many will join in future.

Werner: What happens if VALD will become overloaded due to use via VO?  
Who will pay for the necessary manpower (and hardware) to handle it?

Nik: Do you have an estimate for how many people are using VO right now?

Enrique: E.g. for spectra there are 17 services, non of them are overloaded.

Brussels can not pay for computers or infrastructure.  
Data centers must have local financial support.

WP 5 "Coordination with computational Grid projects" (INAF) can help providers if there are limits in resources to use existing computational resources (in the "grid").

Werner: Providing VALD access for VO could be used e.g. as an in-kind contribution of Austria to ESO in case Austria joins ESO.

Ulrike: Is registration of VO clients planned?

Enrique: No.

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#### 15.15 Discussions

=====

#### Future funding of VALD

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What do we need?

Funds to support Rimma, who is responsible for revision of new linelists.

VALD as part of current projects:

Vienna: FWF project "The Core of the HR diagram"

Uppsala: KVA grant, VR grant (travel)

Keep in mind future professional support needed.

Tanya: Moscow has a computer specifically for VALD.

Ulrike: There are possibilities for applications to Swedish funding agencies:

Vetenskapsrådet (VR):

- "Support for large databases", to be checked if this is applicable
- Normal project grant - a quick search in the project database of VR shows that there are many projects which contain database development.
- Travel grants
  - > grant for travel abroad (at most two months) for international collaboration
  - > grant for short visits (at most one month) for guest researchers at Swedish institutes

Swedish Foundation for International Cooperation in Research and Higher Education (STINT):

- Short term stipends (faculty at Swedish universities spending a maximum of three months at a foreign academic institution or inviting foreign faculty as visiting researchers or academic teachers at Swedish universities)

Werner: Exchange programs between Sweden and Austria (e.g. between ministries/universities/academies/research councils) should be revisited.

Enrique: On the European level there is e.g. the eContentplus programme.  
[http://ec.europa.eu/information\\_society/activities/econtentplus/index\\_en.htm](http://ec.europa.eu/information_society/activities/econtentplus/index_en.htm)

Participation of VALD team members in relevant meetings  
-----

EURO-VO workshop (21-23 March 2007, ESAC - Madrid, Spain):

\*\* Nik, Marlene, Bertrand \*\*

Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas (ASOS9, 7-10 August 2007, Lund, Sweden)

\*\* Tanya, Ulrike \*\*

Vith Serbian Conference on Spectral Line Shapes in Astrophysics  
(11-15 June 2007, Sremski Karlovci, Serbia)

\*\* Paul \*\*

[NLTE workshop, 30 July - 4 August 2007, Nice, France]

\*\* Ulrike, Oleg \*\*

[Camp on Crete in May]

Next Meeting  
-----

Nik: VALD-3 transition should be done before the summer.

There will be a meeting to finish the papers, maybe in Uppsala after the Lund meeting (see above). Maybe a smaller group (4-5 people).  
The date will be finalized in May.

-----  
16.30 Final Roundtable  
=====

Summary or presentation of work done during the week  
-----

Ulrike:

- defining term designation format
- testing extraction software
- discussing and testing version management system
- preparing for conversion of VALD-2 lists to VALD-3
- revising documentation
- taking notes during discussions and presentations

Tanya+Luca:

- comparison with recent NIST release and other sources
- Luca checked the data by determining abundances from spectra of two solar type stars.

Results for 21 Peg (Fe II):

A comparison of VALD vs. NIST, John Landstreet and Raassen & Uylings (abundances vs. lower level energy) shows that all are worse than VALD. Some lines in VALD give "wrong" abundances - they have to be checked. The same trends are visible in the second star.

- by end of next week, "VALD-3 lists will be converted to VALD-2 and made available to VALD users"

Nik:

- debugging of software tools for VALD-3  
(compression and decompression routines, etc.)  
all pipeline components have been tuned and tested (except for showline)
- ems in place

Friedrich:

- merging/homogenizing of extraction software
- references are available as a bibtex file

Christian:

- demonstration of "filter" codes which convert original source lists or VALD-2 lists to VALD-3 ascii format

Eric:

- merged web page and web interface
- set up version management system
- set up synchronization

Paul:

- Fe II list included in VALD
- Cr II calculations started (take a few weeks)
- started calculations of partition functions

Oleg:

- term designation discussion
- discussion with Bertrand Plez: molecular lines (e.g. Lande factor calculations)
- astrophysical evaluation of molecular lines
- extracted and converted new Kurucz models (Christian will import them to VALD)
- debugging spectrum synthesis code

Theresa+Nicole

- testing conversion and web interface

Marlene

- testing new web page/interface
- discussiong VO