VAMDC as a Resource for Atomic and Molecular Data and the New Release of VALD

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and the **VAMDC Collaboration (P.I. M.-L. Dubernet)**

M.L. Dubernet et al. 2010, JQSRT 111, 2152

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INASAN, Moscow, Russia

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OUTLINE

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  - Node members
  - What is it ? Idea behind it ? Expected outcome ?
  - Clientele, astrophysical examples
  - Technology, available databases
- Part 2: VALD
  - The Team
  - Current status, concepts and facilities, structure
  - VALD-3 data
  - VALD-3 in action and shortcomings

VAMDC Vienna Node Team Members

Friedrich Kupka → **Institute of Mathematics**

Theresa Rank-Lüftinger → **Institute for Astronomy**

Werner W. Weiss → **Institute for Astronomy**

and until May 2011

Christian Stütz → **Computer Centre of the University**

What is VAMDC ?

The Virtual Atomic and Molecular Data Centre (VAMDC) is an international project aimed to create an interoperable interface to existing Atomic and Molecular (A&M) databases. In general, each database within VAMDC has been organised in its own way.

It consists of 8 work packages. 15 administrative partners which represent 24 teams from 6 countries within the EU (Austria, France, Germany, Italy, Sweden, and the UK) as well as from Russia, Serbia, and Venezuela have entered the VAMDC consortium.

Presently, the **VAMDC project** includes 24 A&M DBs, among others: **BASECOL, CDMS, CDSD, CHIANTI, Ethelyne, GhoSST, HITRAN, KIDA, PAH, SPECTR-W^3, StarkB, TIPbase, TOPbase, VALD.**

A detailed description of VAMDC is given by ***Dubernet et al. (2010), JQSRT 111, 2151.***

The Idea behind VAMDC

- A&M data have been collected and assessed in a various databases. They underpin a wide range of physics in applied research and industrial development.
- Many databases have been built to serve specific needs. VALD is one such example with its own advantages, special tools, and limitations.
- Various kinds of data, formats, completeness, etc. and
- specialized extraction tools exist for each of the A&M databases.
- Problems:
  - data duplication
  - different user interfaces
  - restricted access
  - often fragmentary, ...

Expected VAMDC outcomes

- Develop/extend standards for interoperability of A&M resources
- Implementation of selected databases
- Find resources easily
- Query those resources with dedicated protocols/languages
- Transfer large amounts of data asynchronously
- Create a safe environment for publishing latest sets of A&M data
- Linking producers with users

- Key benefits from using VAMDC:
  - find any type of AM data with a click, provide uniform access
  - cross-matching different data sets, wide access to latest published data

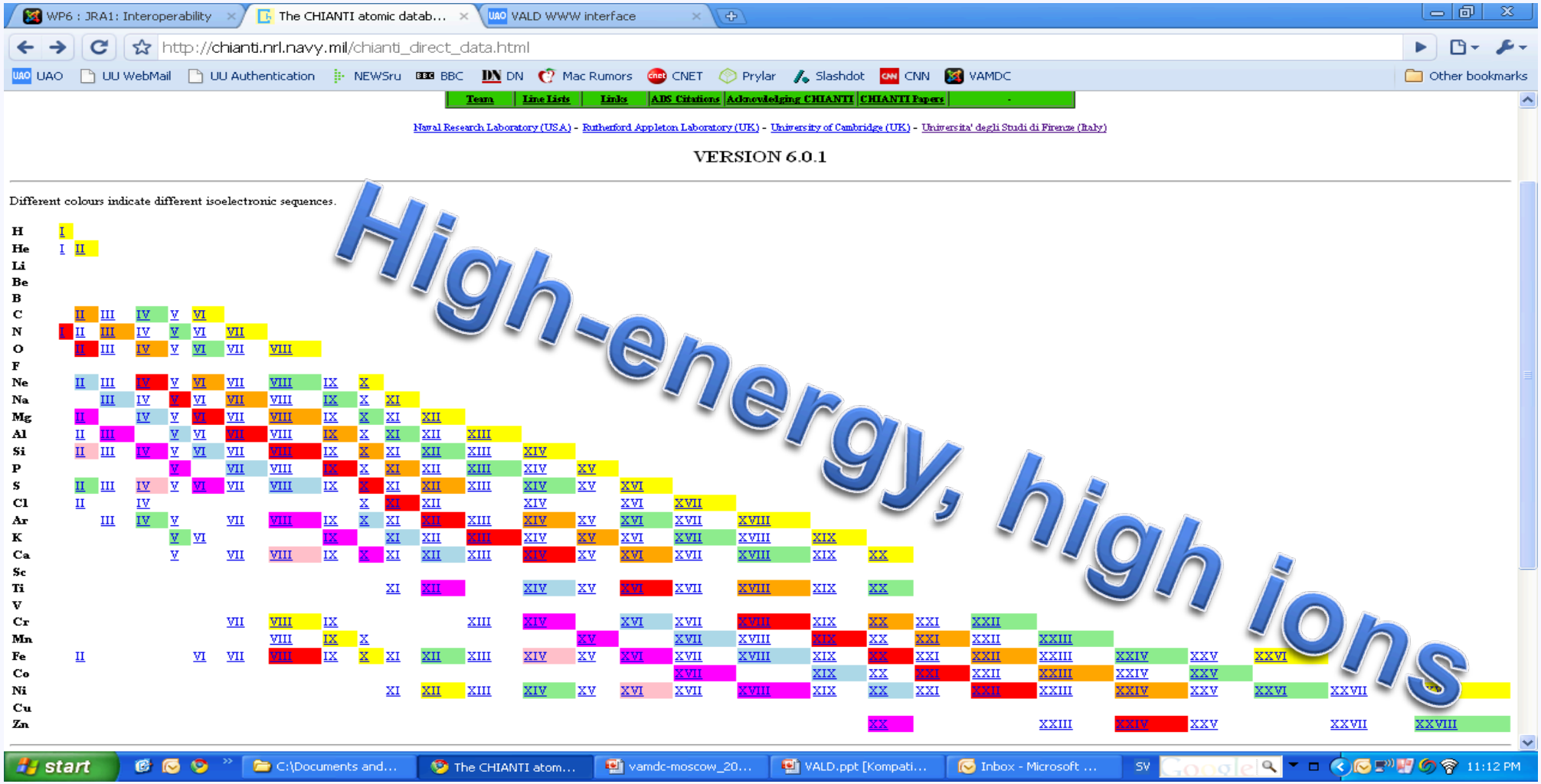
A & M Users: The VAMDC Clientele

- Astrophysics / Astronomy / Planetary Science
- Atmospheric Science
- Fusion Science
- Plasma Science
- Radiation Science

and their applications in research and industrial development

Astronomical Examples I

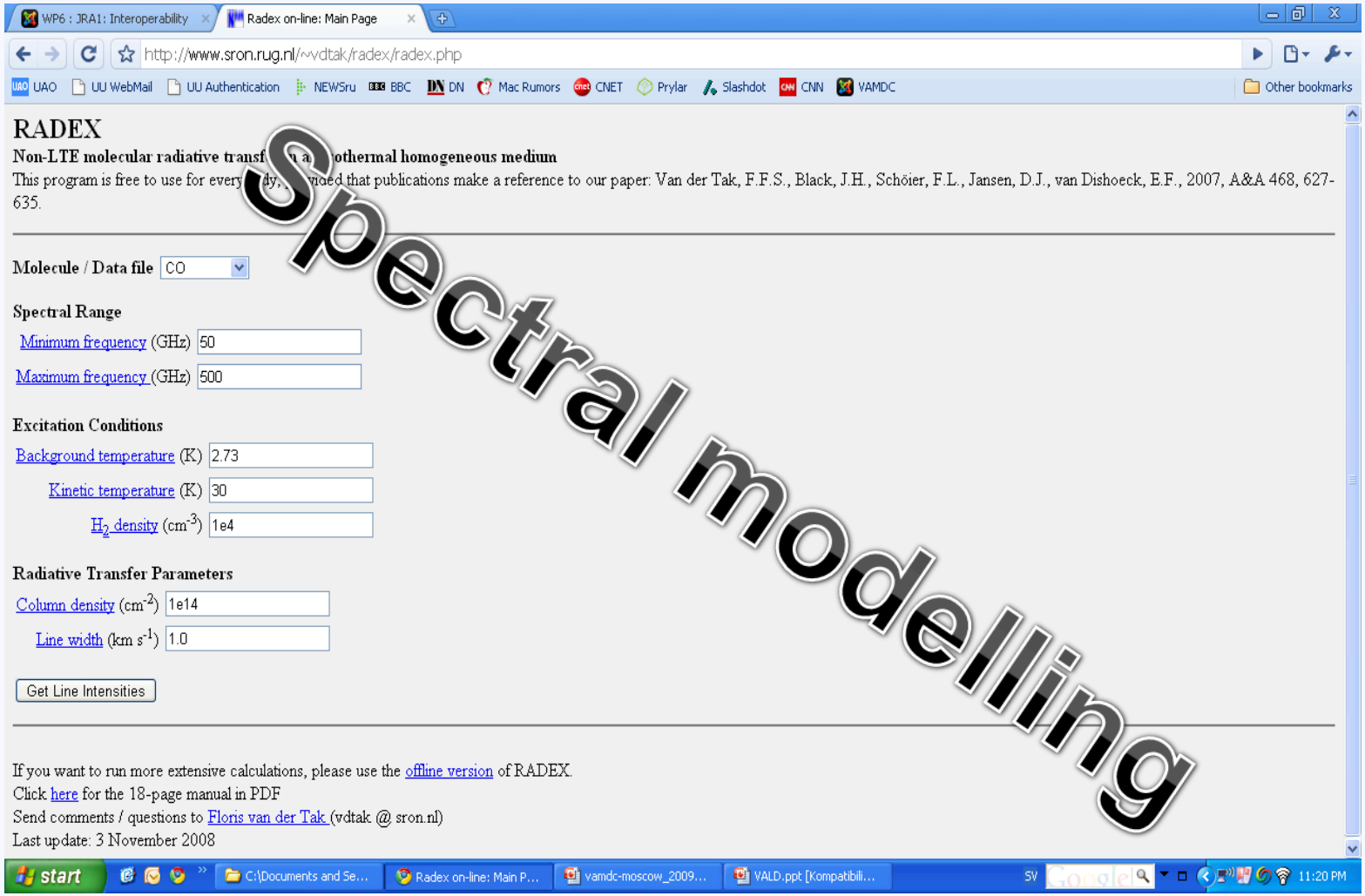
Chianti atomic line database (example courtesy of N. Piskunov)



Astronomical Examples II

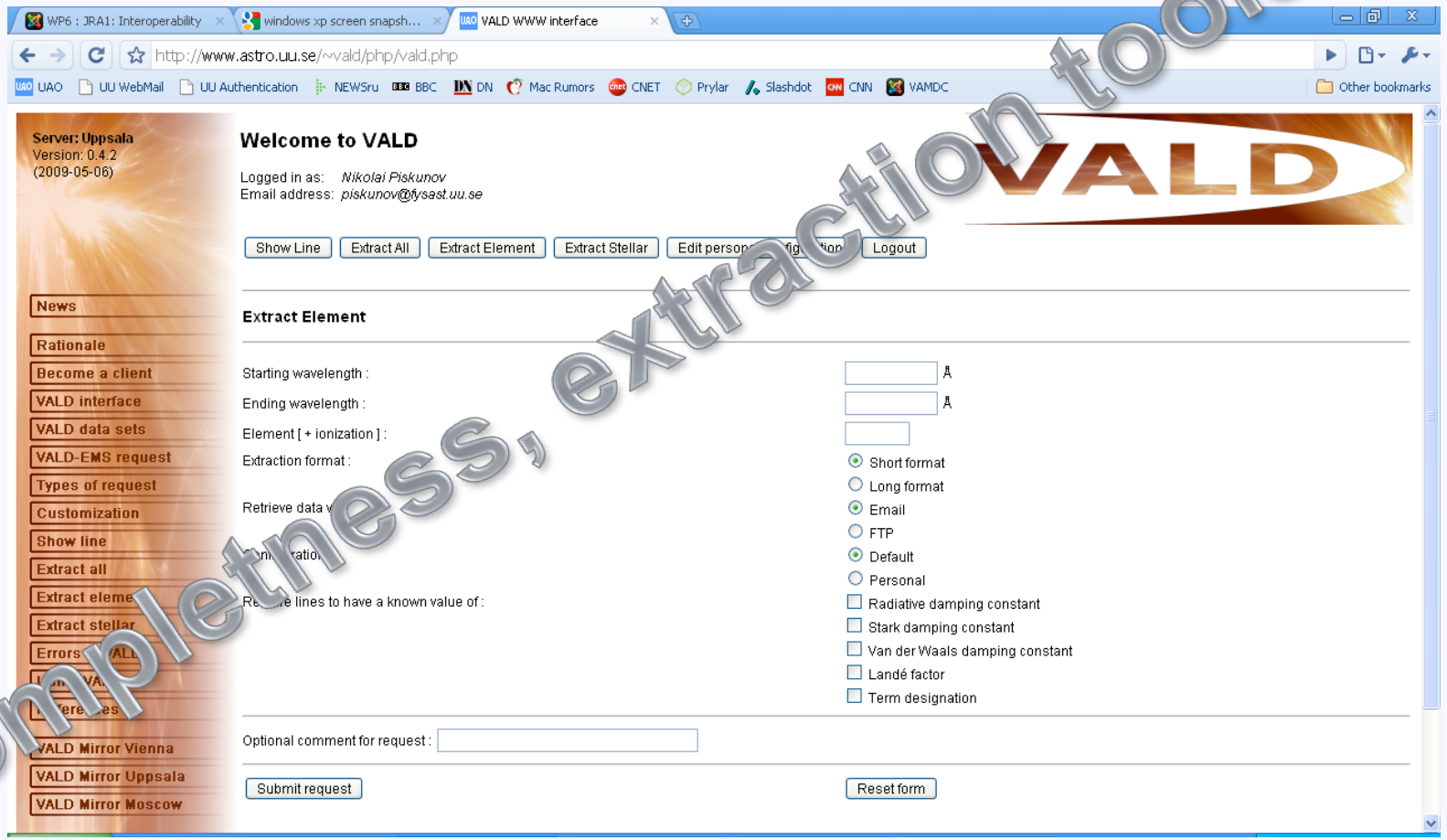
Leiden Atomic and Molecular Database

(example courtesy of N. Piskunov)



Astronomical Examples III

Vienna Atomic Line Database



(example courtesy of N. Piskunov)

Technology I: VAMDC Components

"Grand Central" in Paris

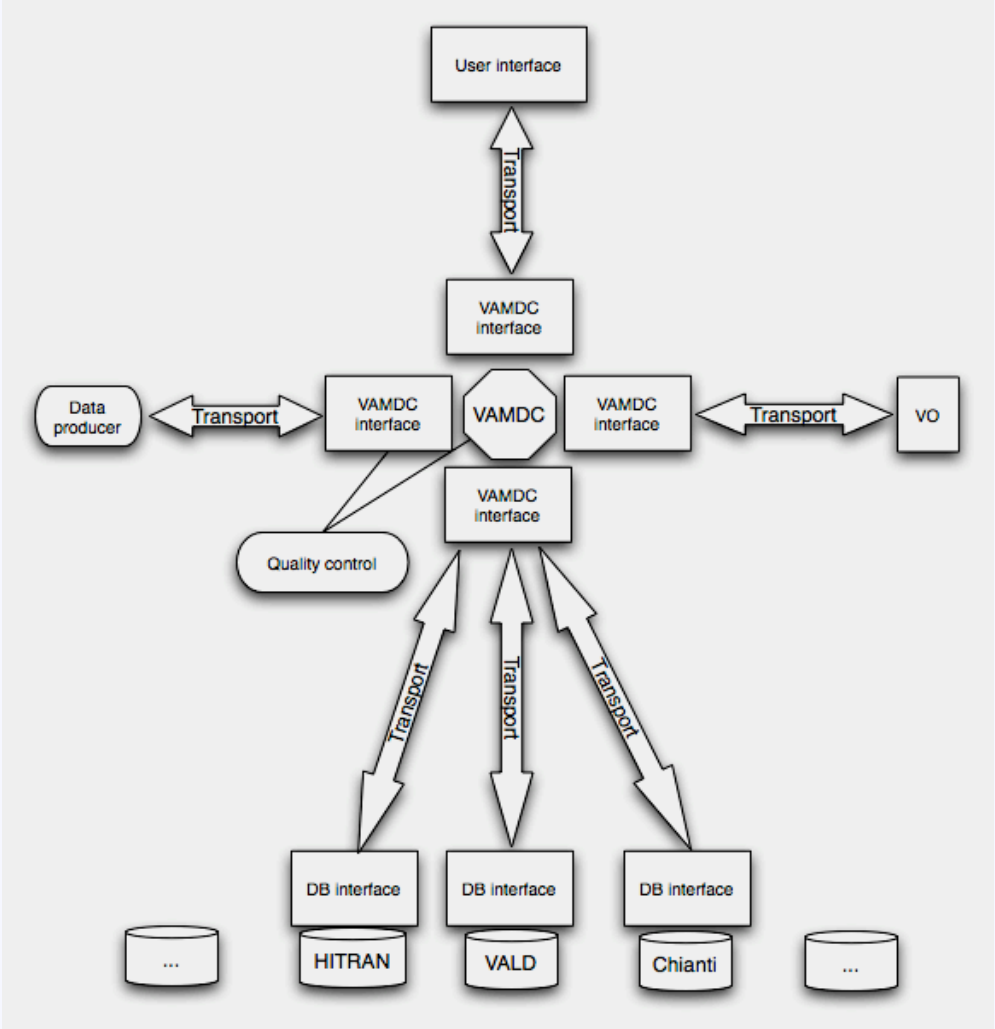
Web-based transport protocol

Interface(s) to DBs

User interface

Automatic interface (e.g. to VO)

Data publishing tools



Technology II: Web-Based Transport Protocol

- The transport protocol handles:
  - database (DB) queries for status and data content (registry update)
  - query / data transfer between user and Grand Central
  - query / data transfer between a DB and Grand Central
- The transport protocol is:
  - self-descriptive (XML description of what is sent including units, formats etc., use of XSAMS data format)
  - efficient for large data sets (compressed binary tables)

Technology III: Interface to Databases

- Fully compatible with the VAMDC transport on the outside
- Tuned to the specific DB on the inside:
  - converting incoming queries to the internal query format
  - converting the DB extraction to the transport-compatible format
- Capable of responding to VAMDC-specific queries (registry update)
- Capable of collecting the accounting information

Technology IV: Registry Browser

snapshot of webpage of test version as of 3 June 2011

Databases for Cycle 2 Service Release I

Database	Node	Included?
KIDA	Bordeaux	Yes
Methane lines	Dijon	Yes
VALD	Uppsala	Yes
BASECOL	LPMAA	Yes
S&MPO	Reims	Yes
Ethelyne	Reims	Yes
GhoSST	Grenoble	Yes
CDSD	IAO	Yes
eMOL	OU	Maybe
Line lists	UCL	No
Energy levels	UCL	No
Electron collisions	UCL	No

Status according to Guy Rixon at 2nd VAMDC annual conference in March 2011

Databases for Cycle 2 Service Release II

Database	Node	Included?
PAH	OAC	Probably
Mols./Mixtures/Solids	OAC	Probably
UDMA	QUB	Maybe
CDMS	Koln	Yes
Stark-B	OPM	Yes
Stark-B	AOB	Maybe (mirror)
Stark-C	OPM	No
TipTopBase	IVIC/Cambridge	Yes
uADB	IVIC/Cambridge	Probably
CHIANTI	Cambridge/MSSL	Yes
HITRAN	UCL	Yes
Spectr-W	RFNC-VNIITF	Yes
Lund data	Uppsala	Yes

Status according to Guy Rixon at 2nd VAMDC annual conference in March 2011

The VALD Team I

- **VALD Team and Server Locations**
  - Vienna: Inst. for Astronomy (founding site, server main site)
  - Uppsala: Observatory (mirror site, now main developer site)
  - Moscow: Institute of Astronomy RAS (mirror site, now main data collection site)
  - non-public mirror sites: GSFC, STSI Baltimore, AIP Potsdam (VALD-2, US sites no longer maintained for practical reasons)
- **Team Members of VALD-2**

  P. Barklem, F. Kupka, N.E. Piskunov, T.A. Ryabchikova, H.C. Stempels, W.W. Weiss
- **Collaborators & Data providers of VALD-2**

  CCP7, NIST, R.L. Kurucz, C.R. Cowley (initially, followed by many more in the mean time → VALD-3)

The VALD Team II

- **Team Members of VALD-3 (Software, Core Team)**
  - Vienna: F. Kupka, T. Rank-Lüftinger, W.W. Weiss
    (previous members: N. Nesvacil, M. Obbrugger, Ch. Stütz)
  - Uppsala: U. Heiter, N. Piskunov, H.C. Stempels
    as well as P. Barklem and O. Kochukhov (+ VAMDC team)
  - Moscow: T. Ryabchikova, Yu. Pakhomov (+ data providers)
- **Members of the VALD-3 data providing teams**
  - Univ. of Wisconsin: J.E. Lawler, E.A. Den Hartog, et al. (REE)
  - Lund University: Lund team (Fe peak, Th+U)
  - DREAM Database: E. Biemont, et al. (REE)
  - Univ. of Montpellier: B. Plez (molecules)

VALD Concepts and Facilities I

Main publications on VALD-1 and VALD-2

- VALD-1: Piskunov N.E., Kupka F., Ryabchikova T.A., Weiss W.W., Jeffery C.S., A&AS 112, 525 (1995)
- VALD-2: Kupka F., Piskunov N.E., Ryabchikova T.A., Stempels H.C., Weiss W.W., A&AS 138, 119 (1999)
- VALD-2/Overview: Ryabchikova T.A., Piskunov N.E., Stempels H.C., Kupka F., Weiss W.W., Physica Scripta T83, 162 (1999)
- **VALD-3: in preparation**

VALD Concepts and Facilities II

Goal of the VALD project

- compile accurate and complete line lists
  → for stellar atmospheres & spectroscopy
- evaluate line lists → provide a ranking
- provide a database which features
  - expandability with respect to data and contents
  - simple access through “customized” extraction software
  - fast access to individual data entries
  - an overview of parameters from different sources
  - compilation of data references and provision of quality criteria
  - to extract sets of best data according to data ranking lists

VALD Concepts and Facilities III

General architecture

- Standard data format
  - units which are common in astrophysics
  - one record with fixed length per spectral line
- Semi-direct access (compressed binary line lists)
- Ranking (for merging data)
- Multiple extraction layers within VALD-2:
  - access files / merge VALD data
  - prepare output for applications
  - remote access (EMS)
  - Web interface for EMS

VALD Concepts and Facilities IV

File format of VALD-2 data

- each line of each list: 1 record, fixed length
- junks of 1024 lines: compressed, index file (λ sorted), compression factor ~ 25...40

One VALD-2 Data record is one VALD line

- Mandatory entries (no defaults)
  - central λ, species identifier, log(*gf*), E_i, J_i, E_k, J_k
- Optional entries (defaults exist)
  - g_i, g_k, log(Γ_r), log(Γ_s), log(Γ_w), terms (i,k), accuracy, comments (multiplets, e.g.)
  - flags (links to specific data for a line & to other data bases)

VALD Concepts and Facilities V

Ranking Lists

- generic extraction constraints
  - wavelength window: species + J values + $\Delta E_k < 0.1\% \rightarrow \Delta \lambda$
  - max. spectrum number
  - max. excitation potential
- extraction constraints for merging line data
  - VALD internal index number (switch list status to on / off)
  - element range of list
  - ranking for λ, *gf,* E_i, E_k, $\langle g_{eff} \rangle$, Γ_r, Γ_s, Γ_w, level classification
- VALD default ranking or user defined ranking

VALD Concepts and Facilities VI

Extraction constraints & ranking

- Line found in different source lists ?

  → choose for each atomic parameter the value from the list with the highest ranking

- Line lists
  - homogeneous, high quality → high ranking
  - inhomogeneous or low quality → low ranking
  - VALD made lists for homogenization → usually high ranking
  - separate line lists usually correspond to separate data files

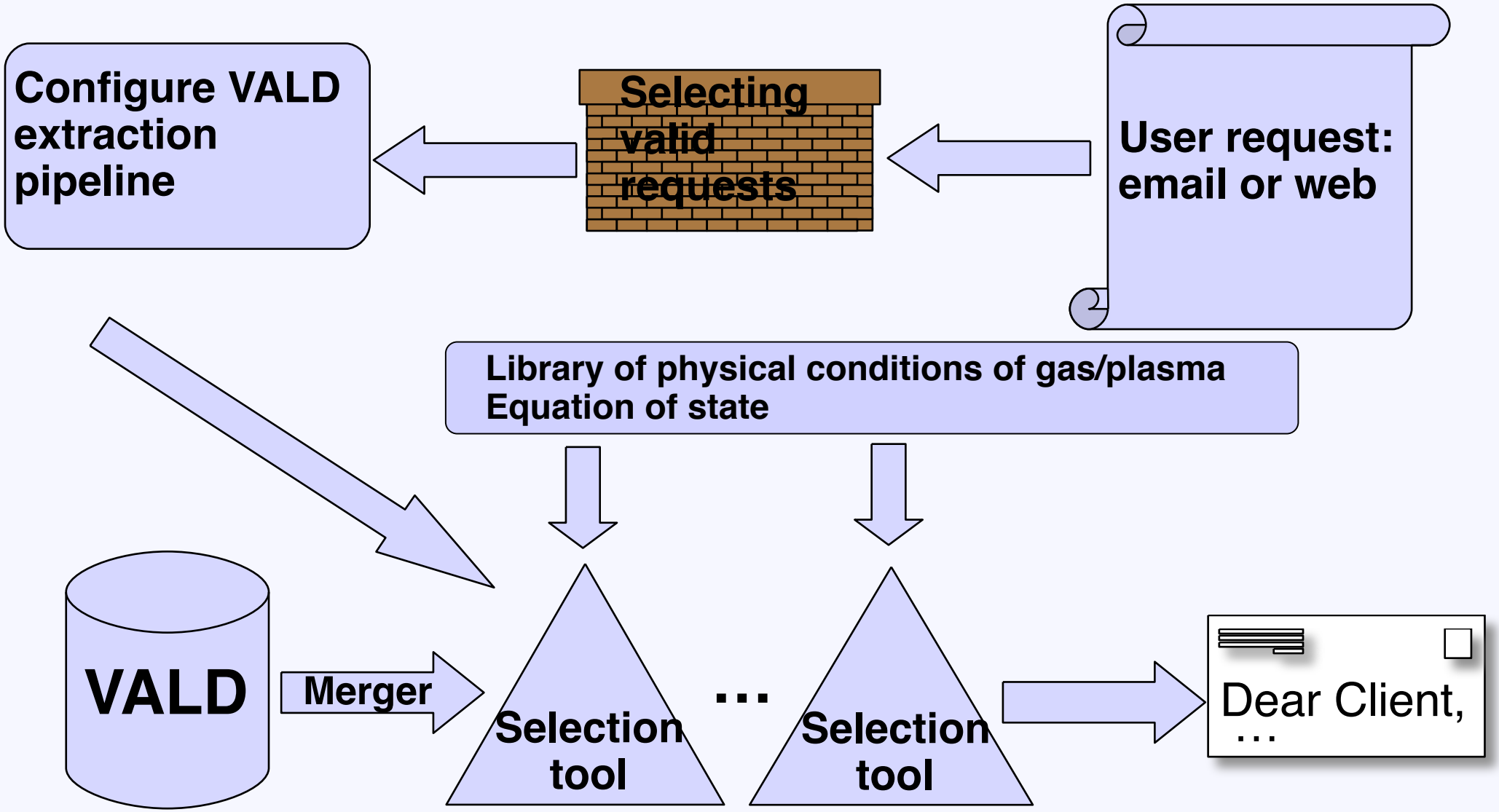
VALD Concepts and Facilities VII

Quality determination based on

- Error estimates from original sources
- Intercomparison of existing, alternative sources
- Applications in astrophysics (user feedback)
- Reranking possible
- General guidelines
  - prefer experimental data over calculations
    (with few exceptions such as the work of Uyling & Raassen)
  - prefer data with individual error estimates

VALD Structure

VALD from outside...



In Preparation of VALD-3: The Current Status of VALD

- Over 150 line lists, over 66 million atomic lines provided by all major spectroscopy centers across the world
- Mirror sites in Vienna, Uppsala and Moscow
- Close to 1500 users from more than 50 countries, in average 30 requests processed per day

VALD-3 – The new VALD, Part I

- data is still sorted as a function of wavelength and
- still stored in a special compressed format with semi-direct access
- stored data (changes & additions indicated) contains:
  - species, wavelengths (Å, vac), level energies (now cm^{-1}), total angular momentum quantum number, log *gf,* Landé-factors, damping constants, accuracy in log *gf,* data reference, full level designation and term name
- publishing a new dataset in VALD means adding a new data file
- data description stored in various support files (list of species, configuration file)
- configuration file stores ranks for every field in each file
- reference data of each data set provided in BibTeX format

VALD-3 – The new VALD, Part II

- in addition to many smaller new lists from data providers previously mentioned VALD-3 containts the
- New Kurucz Calculations (2006-2010) for Fe-peak elements
- Model-based selection improved:
  - for a set P-T-[abundance] VALD-3 solves the equation of state and estimates the contribution to opacities,
  - if a sequence of P-T is available (e.g. model atmosphere), VALD-3 will solve the radiative transfer to predict the line strength.

VALD-3 – The new VALD, Part III

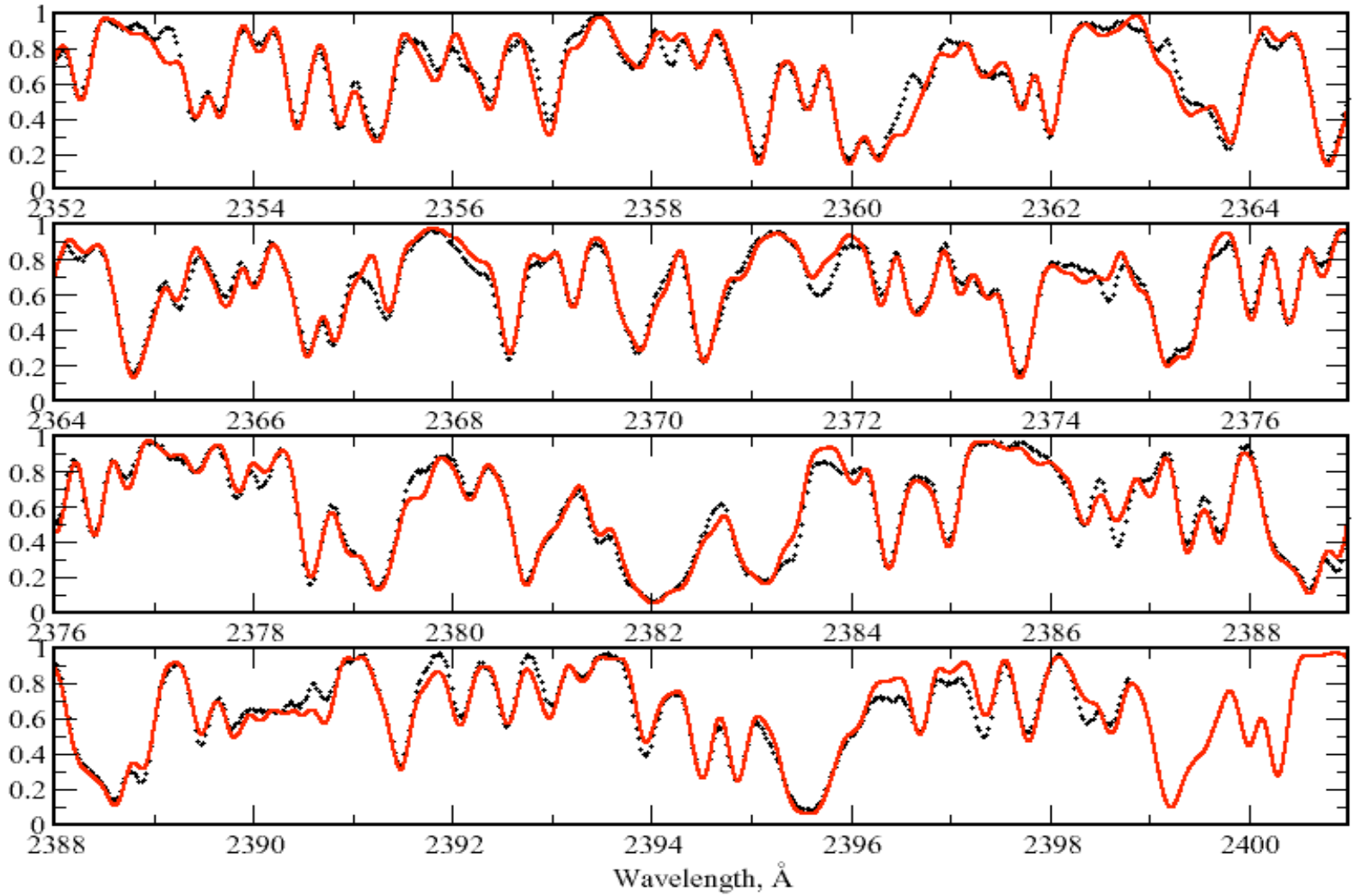
Number of lines in new (experimental and predicted) and old (total) Kurucz data:

	new		old
	exp	pred	
Sc I	15546	737992	191253
Sc II	3436	116491	49811
Sc V	2180	645368	130563
Ti I	33815	4758992	867399
Ti II	8188	835027	264867
Ti III	4090	499739	23742
V I	23342	7043556	1156790
V II	18389	3932853	925330
V III	9892	966528	284003
Cr I	35315	2582957	434773
Cr II	58996	6970052	1304043
Cr III	23150	5535931	990951
Mn I	16798	1481464	327741
Mn II	31437	4523390	878996
Mn III	17294	10525088	1589314

	new		old	
	exp	pred		
Fe I	93508	6029023	789176	
Fe II	103357	7615097	1264969	
Fe III	37199	9548787	1604934	
Co I	15441	3771900	546130	
Co II	23355	10050728	1361114	
Co III	9356	11515139	2198940	
Ni I	9663	732160	149925	
Ni II	55590	3645991	404556	
Ni III	21251	11120833	1309729	
Total	623360	115185086	21778816	5.3/1

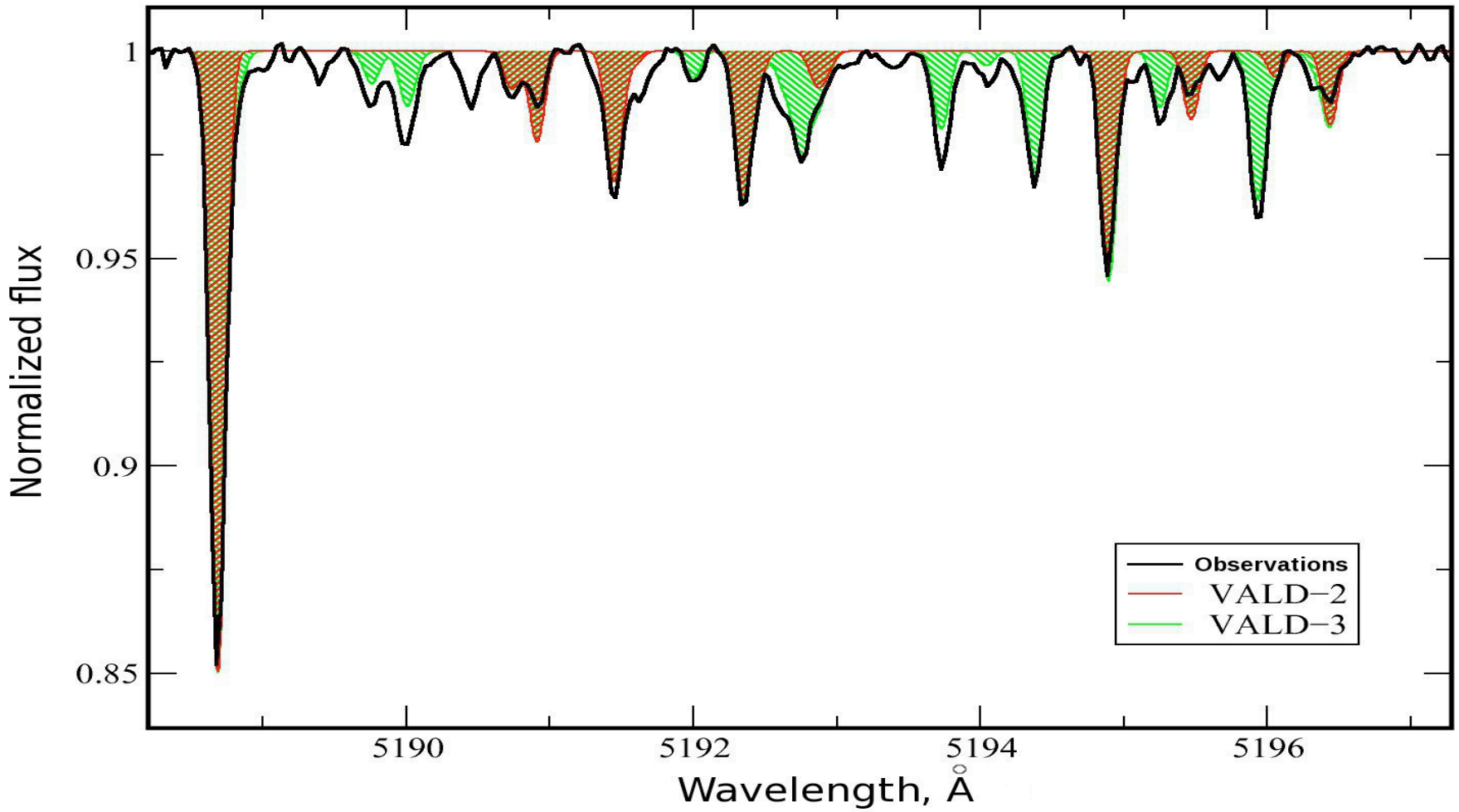
(example by courtesy of T. Ryabchikova)

VALD-3 in Action I



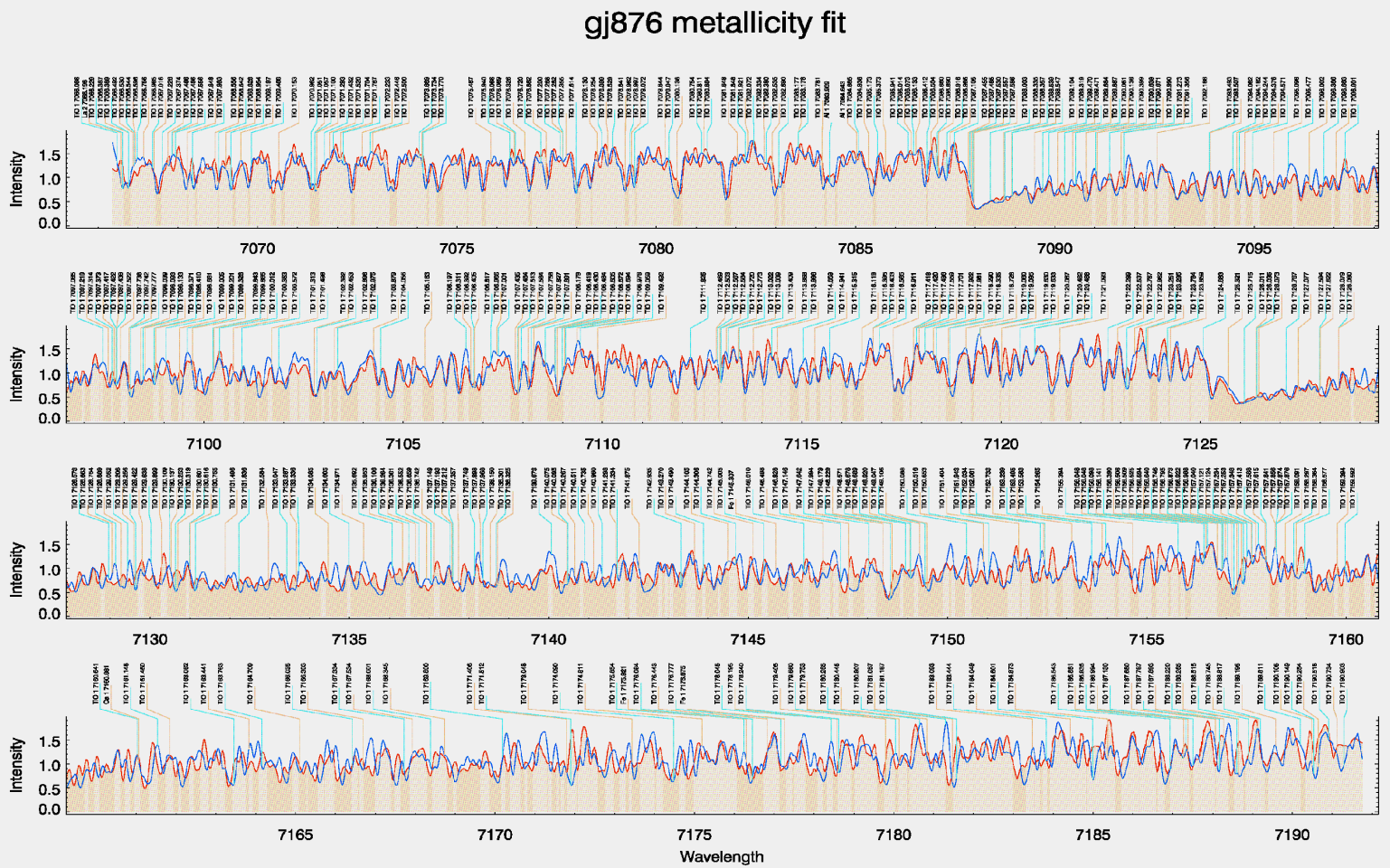
Sirius A (GHRS@HST): fit to UV region observations (courtesy John Landstreet), example courtesy of T. Ryabchikova

VALD-3 in Action II



Solar composition star 21 Peg (T_{eff}=10400 K): fit to optical region observations, example courtesy of T. Ryabchikova

VALD-3 in Action III



Molecular lines in the near infrared spectrum of an M dwarf (low mass star), (example courtesy of N. Piskunov & the VALD team)

VALD-3 Shortcomings

- Limited range of ionization stages (neutral up to 8 times).
- Only simple molecules will be included in VALD-3 (basically diatomics: TiO, CO, CN, CH, FeH).
- Generally missing data include collisional transition probabilities, advanced broadening approximations.
- VALD consortium has no manpower or expertise to fix these deficiencies !

➔ possible solution: access VAMDC data resources !

Upcoming Conferences which will provide training on using VAMDC

3rd annual VAMDC Conference, Vienna, Austria, 21-24 February 2012

(see http://www.vamdc.eu/)

VAMDC Regional Workshop and School in Atomic and Molecular Data, Belgrade, Serbia, 7-9 June 2012

(see http://poincare.matf.bg.ac.rs/~andjelka/VAMDC/)

...THANK YOU FOR YOUR TIME !