VAMDC 3rd Annual Meeting

Vienna University

21rst-24th February 2012

Thank you to Werner, Friedrich, Theresa

WP1 – MANAGEMENT
VAMDC Status and Update

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And
Observatoire de Paris

VAMDC in a nutshell

- International collaboration between groups involved in the generation, evaluation, and use of atomic and molecular data (A&M data).
- Aims: creating a well-documented interoperable interface to existing A&M data resources.
- Funded by EU-FP7 E-Science Infrastructures programme, started July 2009, until end 2012.

User Communities

- Atmospheric Science
  - input for complex terrestrial atmosphere/climate models, determination of concentrations and radiative transport of about 100 species, e.g. water
- Astrophysics, Astrochemistry and Planetary Science
  - great need for reliable A&M data because of extraordinary range of physical conditions
- Plasma Technologies
  - plasma-assisted materials processing or surface modification, e.g. manufacture of semi-conductor chips. A&M data needed for modeling chemically active plasmas.

User Communities cont'd

- Lighting
  - A&M databases needed for development of future light sources – new working gas species, e.g. Xe, and metal alloys such as InSb (Indium antimonide)
- Fusion Energy Research
  - design and operation of vital fusion device systems require large amounts of A&M collisional and spectroscopic data
- Radiation Science
  - radiotherapy models exploring damage of DNA by radiation need A&M data, e.g. electron collisions with DNA components and other biomolecules

VAMDC Consortium

- 21 Partners= 5 French Universities, 10 EU Universities, 4 Russian Institutes, 1 Venezuela
- 3 External partners: Harvard University, JPL/NASA, NIST
- 1 Associated partner : IAEA

→ Aim at worldwide connection (Interest from Korea, Japan, Australia, Brezil, South Africa)

- Connecting Different Fields of Producers of Atomic and Molecular Physics and Chemistry
- Connecting A.& M. Producers to A. & M. Users
- Connecting to Research/E-Infrastructures: Euro-VO (IVOA), Europlanet, HELIO

Core databases

- 19 Databases developed and maintained at partner institutes
  - 8 Atomic DB for astrophysics, lighting, etc..
    - Linelists, Broadening, Shifting Coefficients, Collision Xs, etc..
  - 9 Molecular DB for astrophysics, planeto, atmosphere
    - Linelists, Broadening, Shifting Coefficients, Collision, Reaction Rate Coefficients, etc..
  - 2 Solid Spectroscopy DB for planeto & astro

+ Technological Nodes

  - Cambridge University, UCL –
  - Uppsala University –
  - VO-Paris Data Center -

Project Organisation

- P1 = July 2009-June 2010 (Real Start in January 2010)
- P2 = July 2010-June 2011 → First official Standards release r11.05, Softwares and first Nodes implementation
- P3 = July 2011-June 2012 → Current Period (Release 11.12, Portal, All Nodes implemented + Final Release in June 2012)
- P4 = July 2012-December 2012 → Wrap-Up Period with Final Meeting in Paris (November 2012 ?), Sustainability solution worked out and Final Reports.

Work packages – Management and Networking Activities

1. Project Management
   - financial control, reporting to EU, web site, wiki
   - appointing Strategic Advisory Board (external experts) and interacting with it
2. Scientific/Technical Coordination
   - project planning and progress monitoring
   - work package leader meetings
   - interaction with external projects, e.g. IVOA, EuroPlanet, HELIO
3. Dissemination and Training
   - interface of VAMDC to wider community of producers and users of data
   - organization of one annual “VAMDC meeting” and 2−3 scientific workshops per year, development of tutorials

Work packages – Service Activities

4. Infrastructure Deployment
   - Implementation of standards into data access protocols for core databases, implementation of registries
   - Development of web portal and desktop access software
   - Expansion of VAMDC with new resources
5. Support to the Infrastructure
   - Maintainance and monitoring of the infrastructure
   - Technical support to users
   - Data preservation – backup and mirroring
   - Quality assurance and testing

Work packages – Joint Research Activities

6. Interoperability
   - extension of data model and XML schema (XSAMS), e.g. different description of molecular states, description of line shapes, Solid Spectroscopy
   - creation of dictionaries, definition of access protocols and query languages, definition of registry structure
7. Publishing Tools
   - developing tools and formulating procedures to include new atomic and molecular data into VAMDC

Work packages – Joint Research Activities

8. New mining and Integration Tools
   - tools for manipulation of data, e.g. cross-matching data from different databases
   - advanced data mining services: data access work flows targeted at specific user groups, e.g. solar physics, astrochemistry

MGT Tasks

- Task 1: Initial Establishment of Mgt Structure
  - T1.1 : VAMDC Website + Mailing Lists + WIKI with Public and Private Sections

http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/WebHome

  - T1.2 : VPB, SAB, VEB
  - T1.3 : Provide Administrative Informations

http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/MgtT1

    - Templates for letters, presentation, logos, documents
    - Consortium Agreement
    - Grant Agreement Annexes on WIKI

MGT Task 2

http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/MgtT2

- T2.2 : VAMDC Board and SAB Meetings
- T2.3 :Dissemination of Templates for Plans, Reports, Financial Guidance
- T2.4 : Risk Registry
- T2.5 : Self-evaluation Matrix
- T2.6 Plans, Reports, Budget Review to EU
  - Organisation of WIKI for all these reports

BUDGET Issues

- Received P1 payment start of July 2011
  - Transfered to partners end of July 2011 with payment by Bank of France start of August
- Reporting P2 from June 2011 to 25th August 2011
- Received P2 payments in December 2011
  - For Transfer of P2: Vote of VPB for maximum of 90% per node
  - Transfer P2 to partners February 2012

Comparison % PM and % Budget Period 1 and 2

	RTD	COORD	MGT	OTHER	TOTAL
% MP	78	64	47	65	68
% Budget	76	49	36	50	55

Apart from RTD, %PM always higher than % BUDGET → significant PM and not much claim from senior scientists (in particular French have been forbidden to claim senior time in P2) – though quite a lot of meetings/dissemination

RTD = Low activity in P3 → this is planned

COORD = Normal status at the end of P2 – More training in P3

MGT = MGT from Coordinator accounting for 60% FTE at a high rate has not been claimed → this will change in P3 and P4

OTHER = Normal status at the end of P2 – A lot of work on testing, support, implementation training, upgrading portal in P3

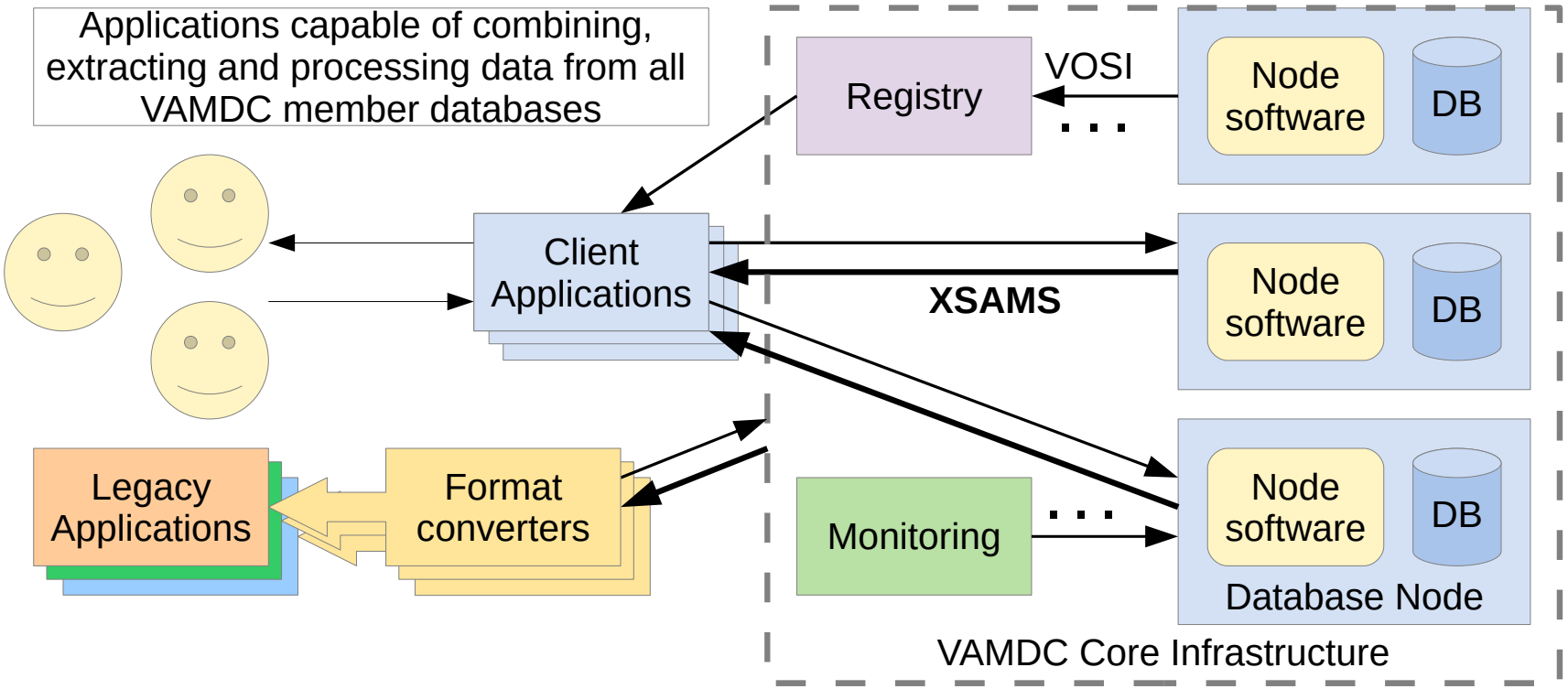
WP2 – WP3

- WP2 = Policies → Please go to WIKI to apply « Publishing Policies »
- WP3 = Dissemination by many groups
  - Conferences Leading to Proceedings
  - Send references to Yaye Awa Ba (LPMAA) - yaye.awa.ba@gmail.com in order to complete www.vamdc.eu website for publication
  - Importance of CORRECT COMMUNICATION → necessity to have/use a standard description of VAMDC.
    - In particular for technological aspects
    - In the future for description of Consortium

WP2-WP3: List of Project Meeting

Name	Dates	Type	WP	Place
Annual Meeting	March 2011	VAMDC	3	Cambridge (CMSUC) http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PmCycleTwo
VEB, VPB	March 2011	Boards	1	Paris (CNRS) & OU http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/MgtVpb http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/MgtVeb
EPT Teleconfs	09/07/10; 06/09/10; 24/11/10; 13/01/11; 16/03/11; 16/03/11; 23/05/11	Board	2	http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/Na1Ept
CTC Meeting	March 2011	CTC	3	

WP4 – WP5 - Infrastructure



WP4

Home | VAMDC databases | Query | Saved queries | Help

Query by...

- Species
- Processes
- Environment
- Advanced

Molecules Clear Remove

Chemical name	
Stoichiometric formula	
Ion charge	to
InChIKey	

Transitions Clear Remove

Wavelength	to A
Upper state energy	to 1/cm
Equivalent to	null to null1/cm
Lower state energy	to 1/cm
Equivalent to	null to null1/cm
Probability, A	to 1/s

Find data | Save query

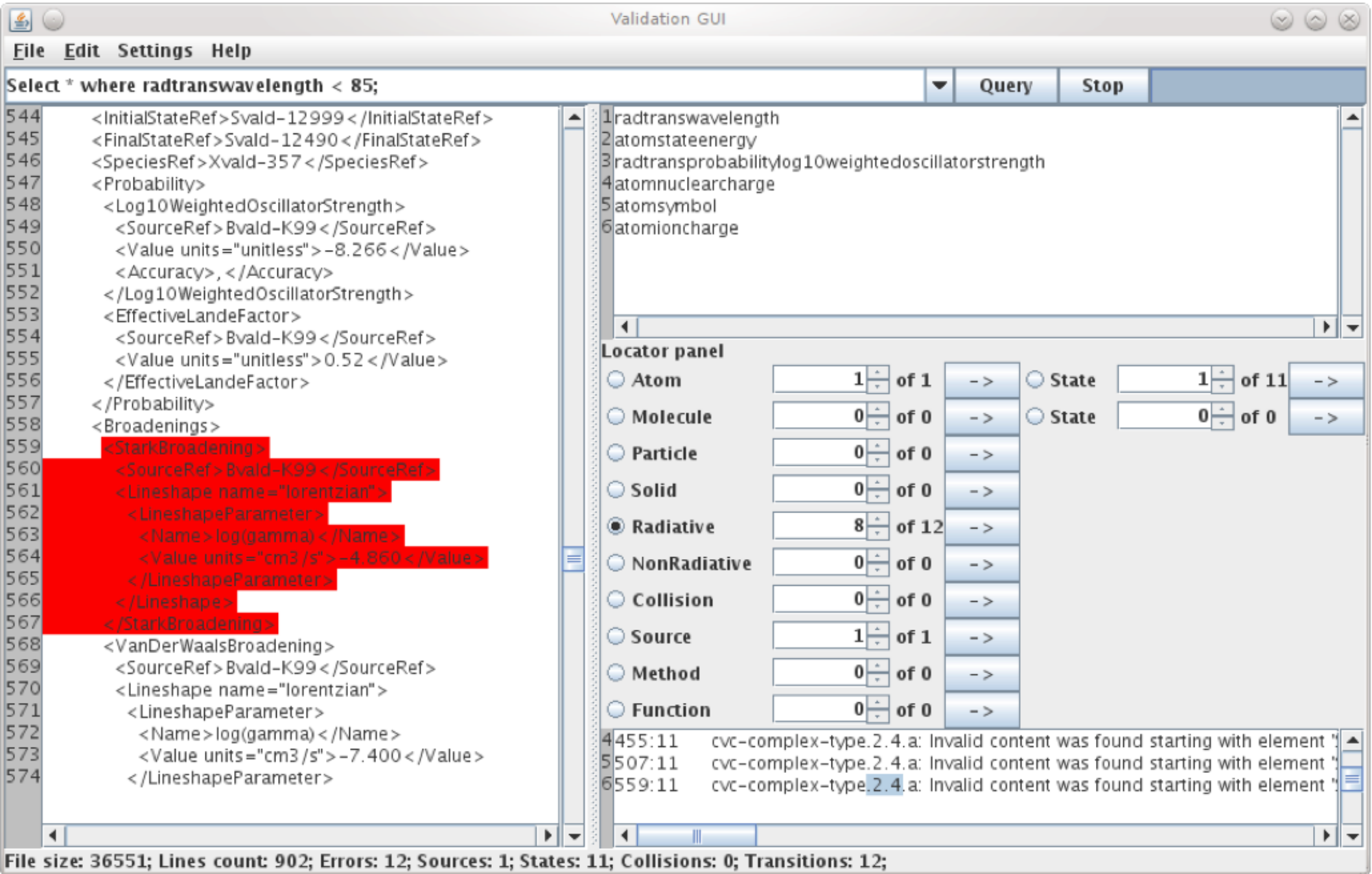
Legend

available, can answer
available, don't support query
unsupported keyword

- Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
- ICB Dijon Methane
- VALD (atoms)
- Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)
- BASECOL: VAMDC-TAP interface
- TOPbase : VAMDC-TAP interface
- Theoretical spectral database of polycyclic aromatic hydrocarbons
- Chianti
- TIPbase : VAMDC-TAP interface
- GSMA Reims S&MPO
- GSMA Reims Ethylene
- TAP-XSAMS for GhoSST database
- BASECOL: development VAMDC-TAP interface
- Stark-b
- Spectr-W3
- HITRAN-UCL resource
- KIDA: VAMDC-TAP interface

LPMAA UPMC PARIS UNIVERSITAS cnrs l'Observatoire de Paris
SEVENTH FRAMEWORK PROGRAMME e-infrastructure

TAPValidator WP5



→ To be done in P3

- Tests of Databases → responsability of each node
  - via TAPValidator
  - Via individual tests
  - Feedbacks to standards group
- Test of Portal to be started including users
  - Feedback via support@vamdc.eu

→ WP5 = Support

- Use mailing lists such as developer
- Contact wp4, wp7 for node implementation
- Contact wp6 for standards
- Use **RT system** to report bug (see WP5 talk)
- DO NOT USE PRIVATE WEBPAGES
- vamdc.eu webpages (and links from there) are the ONLY reference pages for standards and softwares in VAMDC

WP6-WP7-WP8 = How does VAMDC work ?

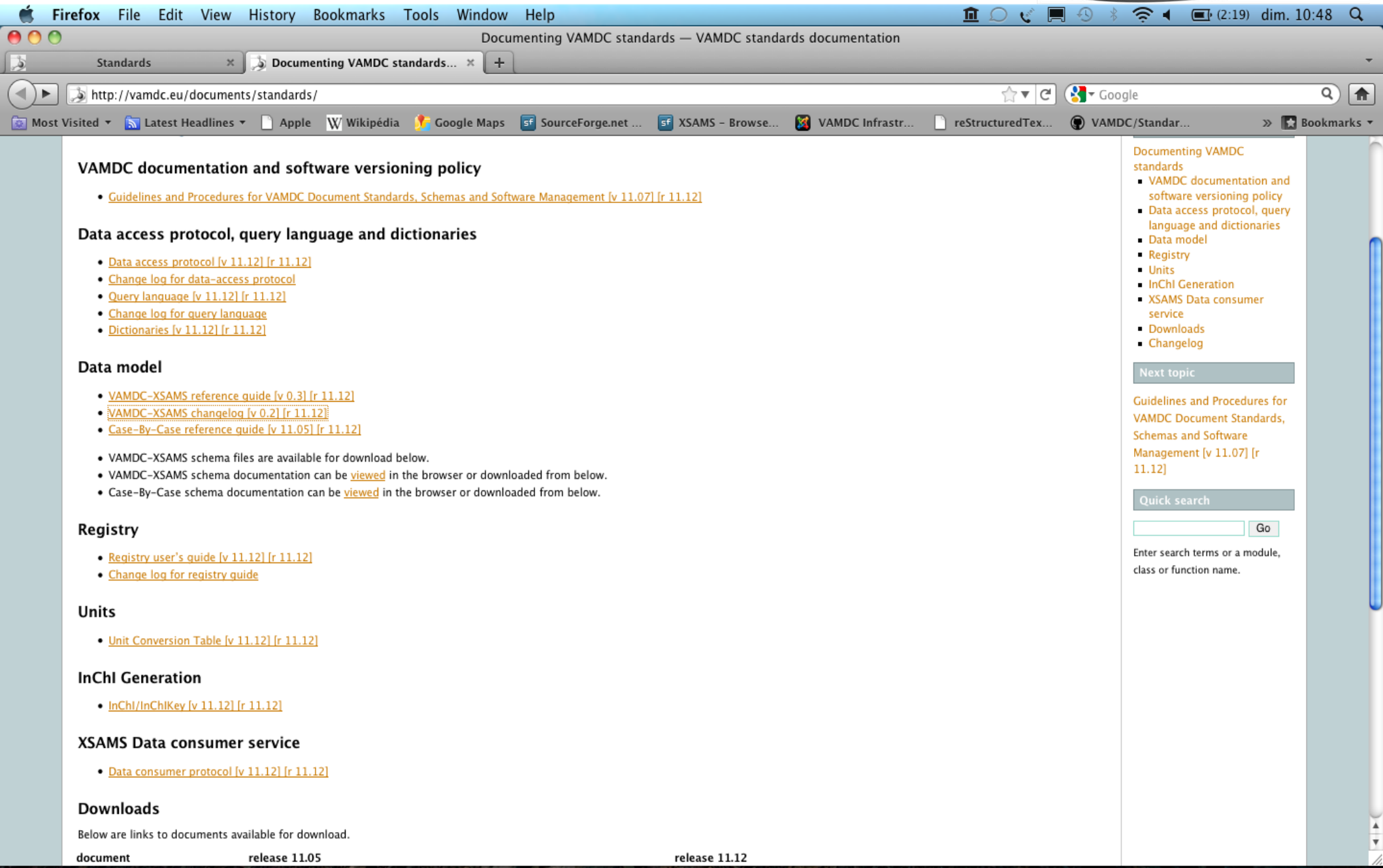
- Requirements from Databases, from Clients included in Standards
- Regular « Tiger Team Meetings »
- Release of standards every 4 months
  - 11.05, then 11.12 – Next : June 2012 – Final: End 2012
- Followed by release of Upgraded Node Software + Portal + Tool

List of Project Meetings « Tiger Team Meetings »

- JRA1-2-3 - XSAMS:Meeting1 23-24th July 2010, Paris (Invitation of NIST)
- JRA+SA Workshop 3 28-30th September 2010, Paris
- JRA3UserWorkshop1 2-4th November 2010, Paris (CASSIS TEAM)
- WP4-5 CNRS Meeting 4 Nov 2010 Paris
  - GRID tutorial, Paris, December 2010
- JRA2 Coordination meeting, Cycle 2 26th November 2010, Moscow
  - Implementation Tutorial, Paris, January 2011
- JRA+SA Workshop 4 16-18th February 2011, Vienna
  - Annual Meeting, Cambridge, March 2011
- JRA1-2-WP5-Workshop:VALD3-XSAMS 24-27 May 2011, Moscow
- JRA+SA Workshop 5 7-10th June 2011, Belfast
- JRA+SA Workshop 6 12-15 September 2011, Paris
  - Implementation Tutorial for some databases, Reims, October 2011
- JRA+SA Workshop 7 December 2011, KOELN
- 2 Other workshops in 2012

WP6 : Standards Release:

http://www.vamdc.eu/documents/standards/



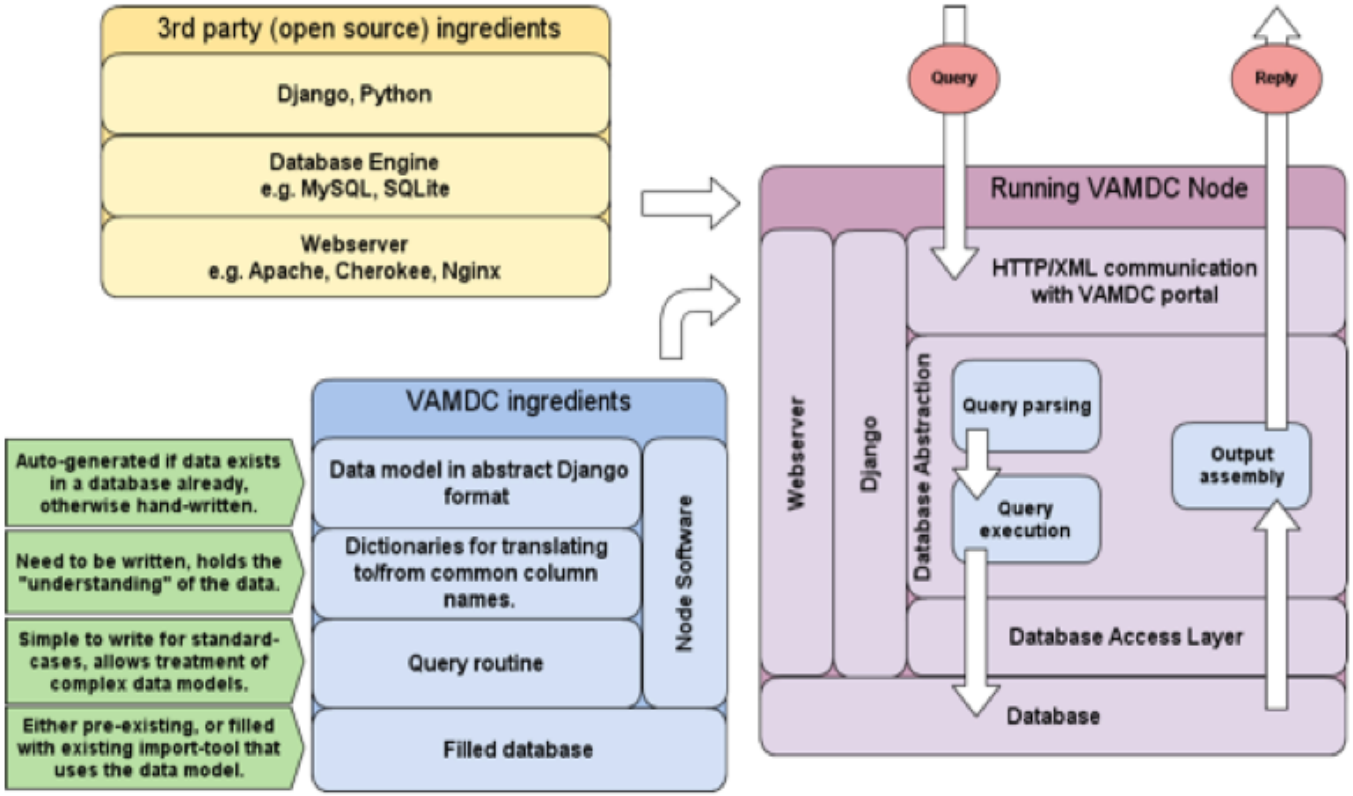
Data Models and XML schema

- VAMDC has decided to split from IAEA during the course of the project and most improvements have been made within VAMDC consortium. New version of XSAMS is called VAMDC-XSAMS.
- Official Releases of VAMDC-XSAMS standards are on http://www.vamdc.eu/documents/standards/
- At a slower pace XSAMS is updated with latest VAMDC-XSAMS after discussion within the XSAMS steering group.
- VAMDC-XSAMS v. 0.3 is current version → XSAMS version 1.0 very likely this week

WP7 update

Step by step guide to a new VAMDC node

Let's have a look at the structural diagram from the *Introduction* once more:



If you have followed the instructions of the page on *Software prerequisits and installation*, you are done with the yellow box in the figure. This page will tell you first how to configure and write the few code bits that your node needs before running (blue box), and then how to deploy the node and make it run as shown in the violet box.

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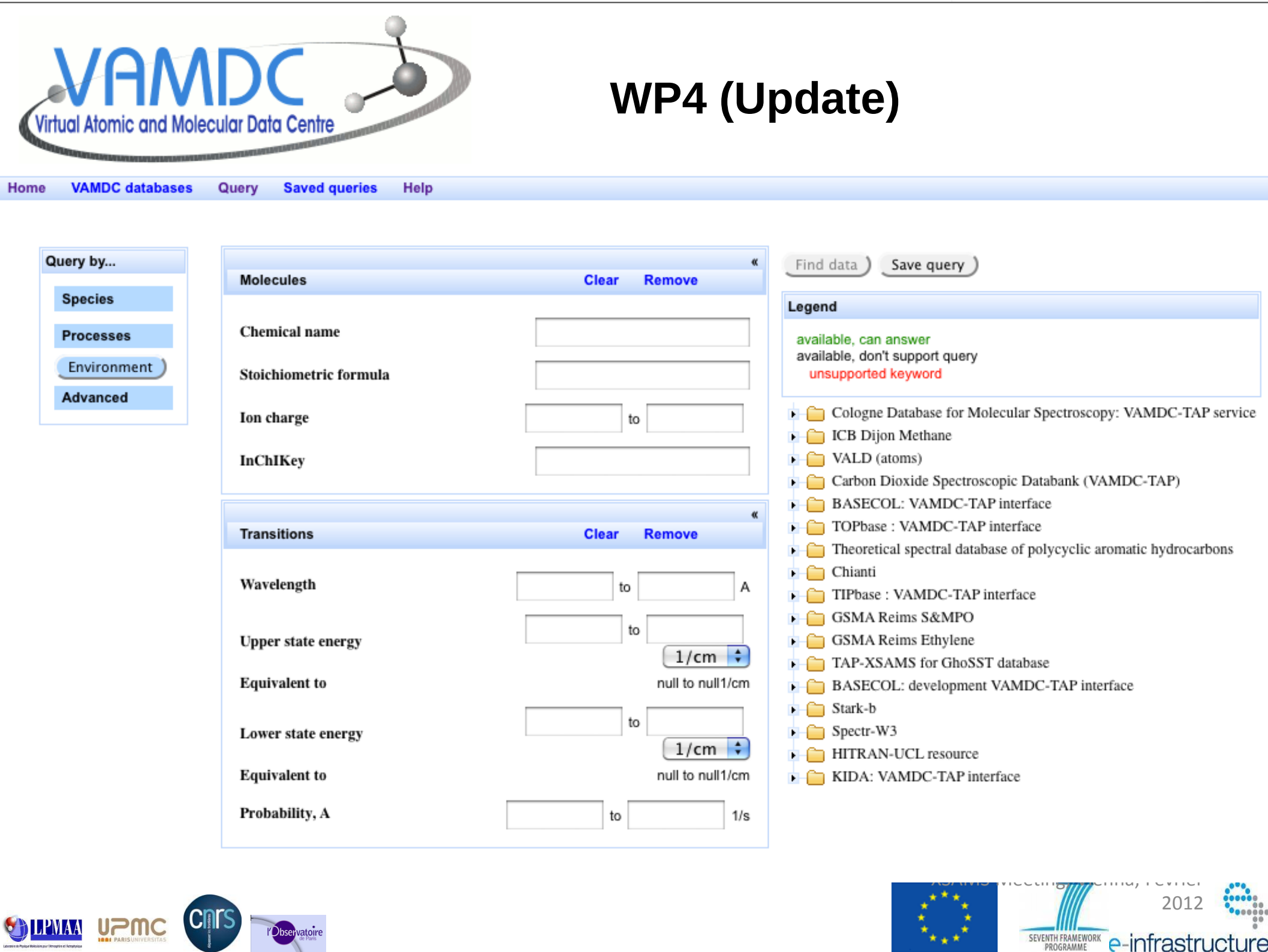
Previous topic

Software prerequisits and installation

Next topic

How to get your data into the database

WP4 (Update)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Equivalent to
null to null1/cm
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Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
ICB Dijon Methane
VALD (atoms)
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)
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TOPbase : VAMDC-TAP interface
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BASECOL: development VAMDC-TAP interface
Stark-b
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HITRAN-UCL resource
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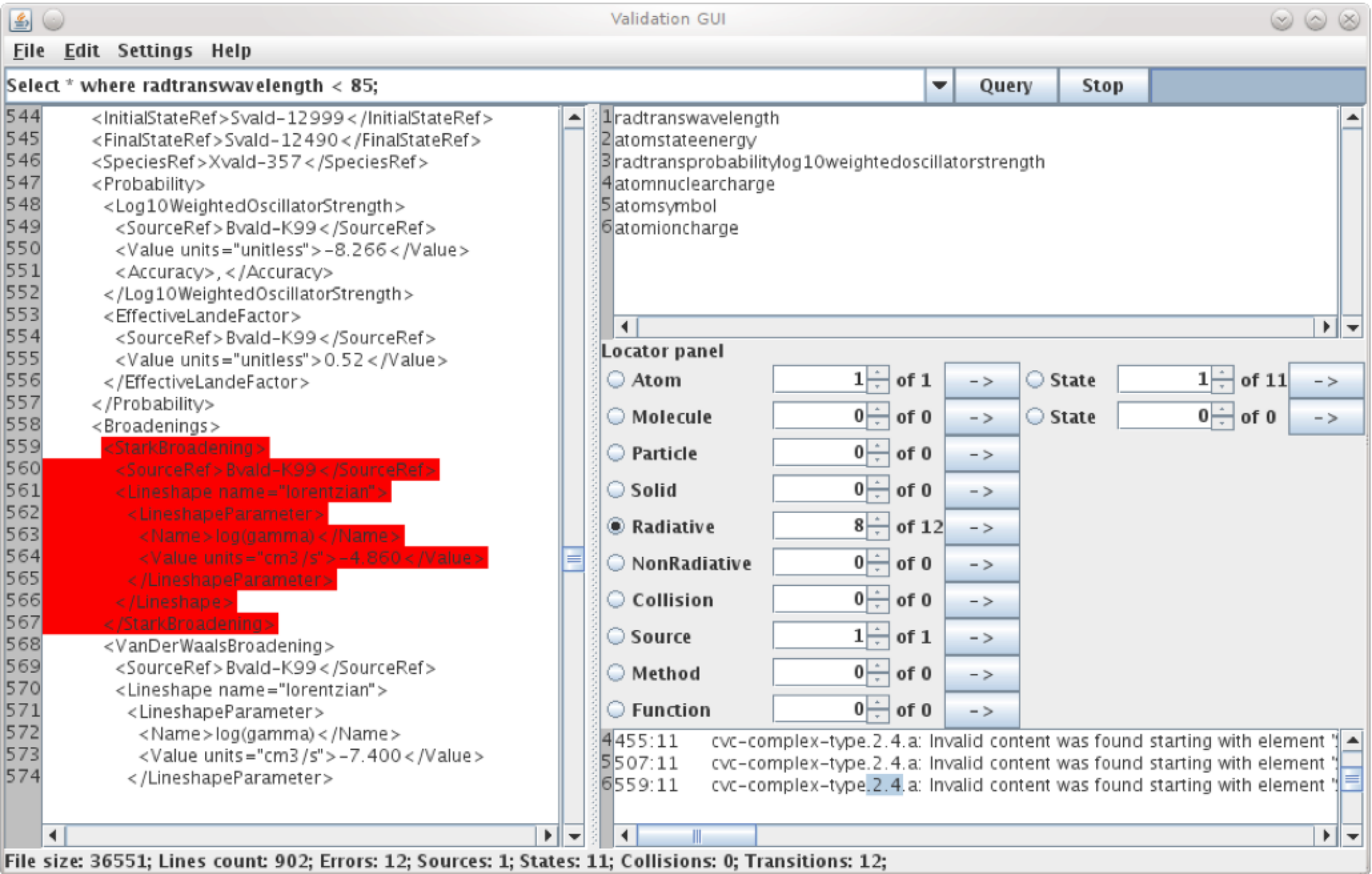
TAPValidator WP5 (Update)



WP8 = exemple -Update = SPECTCOL Tool

- Handles
  - VAMDC-XSAMS files from different databases
  - Matching and Cross-Federation of Spectroscopic data and Collisional Data From Different Databases
- Spectroscopic Data
  - Species, Energy Tables, Frequencies, Einstein Coefficients (CDMS for now), Sources
- Collisional Data
  - Species, Energy Tables (not the same), Rate Coefficients

→ Sustainability of VAMDC

Is about Maintenance and Upgrade of :

- Standards
- Node Softwares and librairies
- Portal
- Tools
- Nodes Implementation

VAMDC Meeting (I)

- Today = WP and Node Reports
- In the evening Board Meeting → sustainability
- Wednesday =
  - Morning = Presentation of Technical Achievements and some short discussion
  - Afternoon = ROADMAPS for 2012
    - Some key points will be presented by the speaker
    - Then DISCUSSIONS with all participants in order to draw the roadmaps for 2012
    - Notes to be taken during each session

VAMDC Meeting (II)

- Thursday Morning
  - Different scenarios for sustainability
  - Expected active participation from the audience
- Thursday Afternoon
  - User Meeting
  - Parallel technical session = mostly for developers
    - Program to be decided between today and Thursday morning → coordination G. Rixon
- Conference Dinner

VAMDC Meeting (III)

- Friday Morning
  - Some Demos
  - Organisation of Next Releases
  - Additional Technical Issues
- Friday afternoon
  - VAMDC Future Roadmap
- Official End of Meeting at 3 pm