

VAMDC Portal

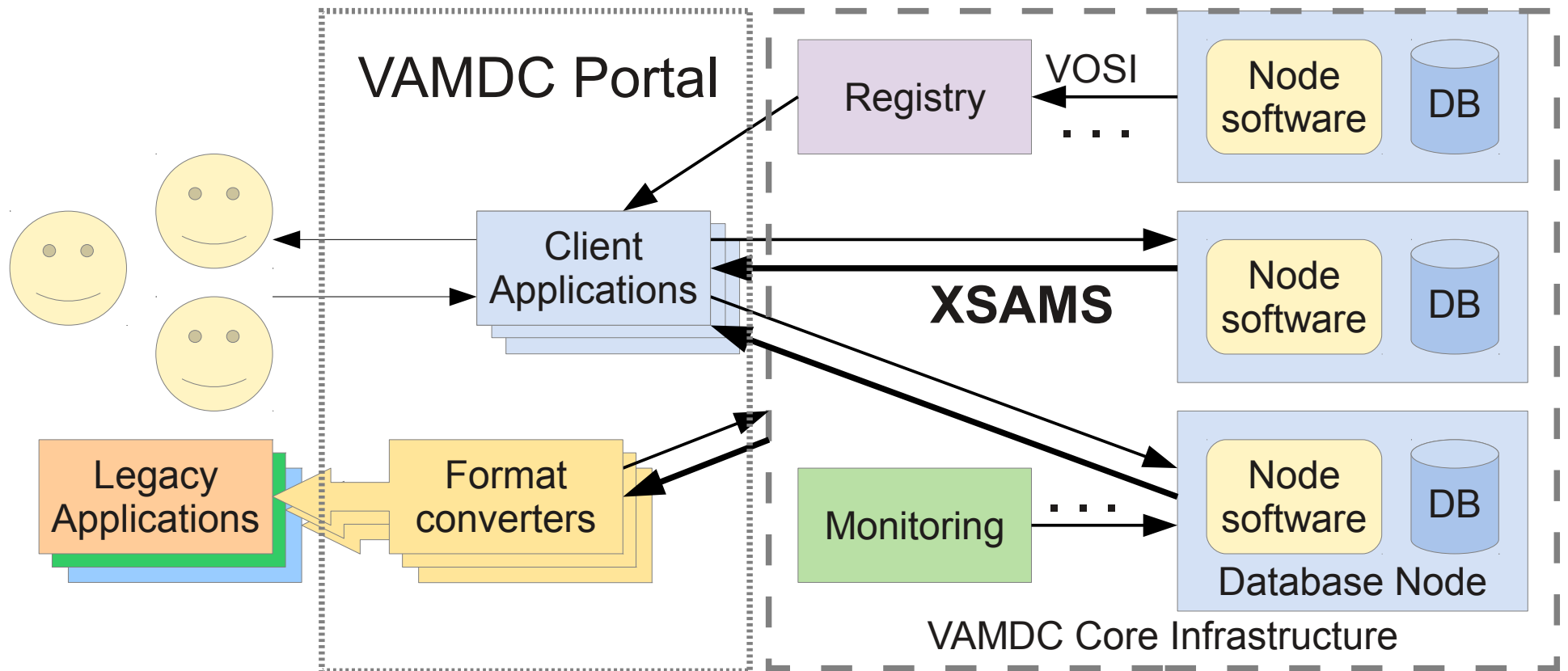
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VAMDC final project meeting, Meudon, 14-16 Nov. 2012

VAMDC portal

- Entry point for new-coming user to VAMDC
- Should:
 - Be easy and straight-forward to use
 - Give a view on the complete functionality of VAMDC
 - Allow to query all kinds of member databases
- Portal is:
 - A query interface
 - A list of VAMDC databases
 - Access point to XSAMS Processors

VAMDC infrastructure



Development History

- First concepts during P1 and P2
- Redesign in the beginning of P3
 - Revised user interface
 - Concept of preview
 - Concept of modular XSAMS processor webservice
- New in 12.07 version
 - Node and registry mirrors support
 - Updated species database for molecules form
 - Data extract last modification date

User interface design

Think and design first, write code later:

<http://bit.ly/xzzOMH>

VAMDC Portal

[Home](#) | [Query builder](#) | [Saved queries](#)

Select All where Blah >0 and foo !='Some'

User notes

Status: waiting, response from 4 nodes, 2 with data, 10 seconds left

Consumers

- XSAMS display
- XSAMS merge tool
- SLAP broker
- FITS converter

Node	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
V BASECOL	OK	_XSAMS_	10	200	1	0	1	0
V VALD	OK	_XSAMS_	5	1000	900	900	0	0
X EMPTY	NONE		0	0	0	0	0	0
X FAULTY	FAIL		0	0	0	0	0	0

'Refine' button returns to the query builder,
'Stop waiting' button allows to select and query
without waiting for all nodes to respond

Pressing the query button sends the query to
the checked nodes, opens QueryLog page

'Query' becomes active after all nodes
responded or 'Stop waiting' was pressed.

Query generator

Molecules Clear Remove «

Chemical name

Stoichiometric formula

Structural formula

Spin isomer

Standard InChIKey

[Select All](#) [None](#) Search by stoichiometric formula i

Isotopologues

Carbonyl Sulfide OCS

Carbonyl sulphide $^{16}\text{O}^{12}\text{C}^{34}\text{S}$

Carbonyl sulphide O^{13}CS

Carbonyl Sulfide $^{16}\text{O}^{12}\text{C}^{33}\text{S}$

Carbonyl sulphide $^{18}\text{O}^{12}\text{C}^{32}\text{S}$

Radiative Clear Remove «

Frequency to GHz

Equivalent Wavelength to Wavelength from 3.33102731111111112E7 to 4.2827494E7A

Upper state energy to $1/\text{cm}$

Equivalent to $1/\text{cm}$

Lower state energy to $1/\text{cm}$

Equivalent to $1/\text{cm}$

Probability, A to $1/\text{s}$

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 \(VAMDC-TAP\)](#)
- » [OACT - LASP Database](#)
- » [TOPbase : VAMDC-TAP interface](#)
- » [Theoretical spectral database of polycyclic aromatic hydrocarbons](#)
- » [BASECOL: VAMDC-TAP interface](#)
- » [VALD: Vienna Atomic Line Database](#)
- » [Chianti](#)
- » [Cologne Database for Molecular Spectroscopy: VAMDC-TAP service](#)
- » [TIPbase : VAMDC-TAP interface](#)
- » [GSMA Reims S&MPO](#)
- » [GSMA Reims Ethylene](#)
- » [GhoSST](#)
- » [Lund laboratory spectroscopy database](#)
- » [Stark-b](#)
- » [Spectr-W3](#)
- » [Water internet Accessible Distributed Information System](#)
- » [HITRAN-UCL resource](#)
- » [VALD sub-set in Moscow \(obs\)](#)
- » [KIDA: VAMDC-TAP interface](#)

Query by...

Species

Processes

Environment

Advanced

Query preview

Done

select * where (RadTransWavelength >= 99999.0 AND RadTransWavelength <= 100000.0)

Comments

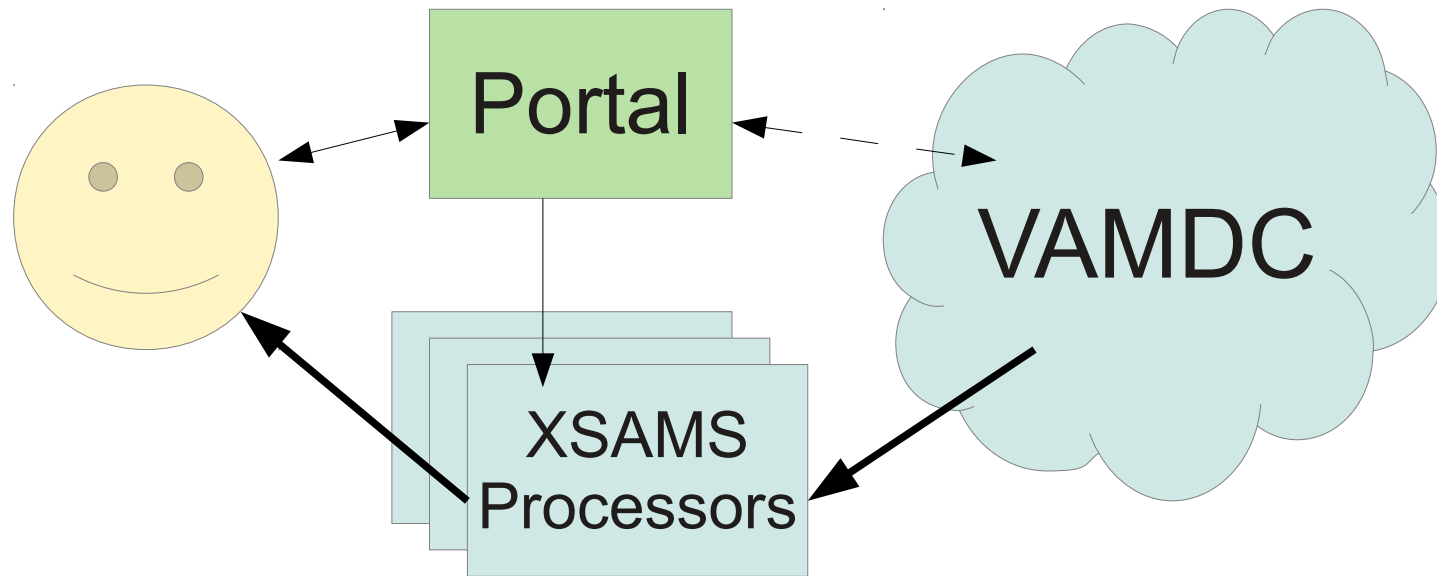
XSAMS processors

BibTeX from XSAMS
 Table views of XSAMS
 Xsams2SME

General views of data in XSAMS format. The display is tabular and textual. Initial display is a list of states, with links to details of each state. An alternate display of radiative transitions is available.

Name	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
<input type="checkbox"/> HITRAN-UCL resource	OK	XSAMS	5	3	8	8	0	0
<input checked="" type="checkbox"/> Carbon Dioxide Spectroscopic Databank - 1000K	OK	XSAMS	3	12	6	6	0	0
<input type="checkbox"/> Chianti	OK	XSAMS	4	10	5	5	0	0
<input type="checkbox"/> GSMA Reims S&MPO	OK	XSAMS	2	8	4	4	0	0
<input type="checkbox"/> Lund laboratory spectroscopy database	OK	XSAMS	0	0	0	0	0	0
<input type="checkbox"/> Water internet Accessible Distributed Information System	OK	XSAMS	0	0	0	0	0	0
Cologne Database for Molecular Spectroscopy: VAMDC-TAP service	EMPTY		0	0	0	0	0	0
TOPbase : VAMDC-TAP interface	EMPTY		0	0	0	0	0	0

XSAMS processors



- Stand-alone web-service
- Can be used on its own using scriptable interface or web GUI
- Multiple processors can be quickly implemented using XSLT stylesheets

Query history

- Permanent history for registered users
- Edit/clone queries
- Process results

XSAMS processors

BibTeX from XSAMS

Table views of XSAMS

Xsams2SME

Process

General views of data in XSAMS format. The display is tabular and textual. Initial display is a list of states, with links to details of each state. An alternate display of radiative transitions is available.

Query	Comments	Date	Database	Results	Download
<p>Edit</p> <p>Clone</p> <p>Delete</p> <p>select * where (RadTransWavelength >= 5007.0 AND RadTransWavelength <= 5008.0) AND ((AtomSymbol = 'Fe' AND IonCharge >= 1 AND IonCharge <= 4))</p>	iron ionized	Apr 18, 2012	<input type="checkbox"/> VALD (atoms) <input type="checkbox"/> TOPbase : VAMDC-TAP interface <input type="checkbox"/> VALD sub-set in Moscow (obs)	Sp: 4 -st:1497 - Pr:885 Sp: 3 -st:43 - Pr:22 Sp: 2 -st:23 - Pr:12	XSAMS XSAMS XSAMS
<p>Edit</p> <p>Clone</p> <p>Delete</p> <p>select * where (RadTransWavelength >= 1.9986163866666667E7 AND RadTransWavelength <= 2.99792458E7) AND ((InchiKey = 'JJWKPURADFRFRB-UHFFFAOYSA-N'))</p>	OCS query	Nov 13, 2012	<input checked="" type="checkbox"/> Cologne Database for Molecular Spectroscopy: VAMDC-TAP service <input type="checkbox"/> Water internet Accessible Distributed Information System <input type="checkbox"/> HITRAN-UCL resource	Sp: 2 -st:15 - Pr:12 Sp: 1 -st:5 - Pr:8 Sp: 1 -st:1 - Pr:4	XSAMS XSAMS XSAMS

Technologies

- Written in Java (JBOSS Seam)
- Re-use of VAMDC Java libraries
- Use of apache maven for dependency management
- Source code on GitHub, automatic builds of development version

Future

- Code base is stable, design seems to work fine
- Further development:
 - More XSAMS Processors (Developers, welcome!)
 - User interface and user experience improvements, based on feedback
 - Implementation of new versions of standards (12.07 version is ready)
- Standards are open, don't hesitate to implement other application-specific clients

Welcome!

<http://portal.vamdc.org/>