

# Collaborating with VAMDC

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RADAM database workshop, Caen, October 2013

# Original use-case



Universität zu Köln  
Mathematisch-Naturwissenschaftliche Fakultät  
Fachgruppe Physik  
**I. Physikalisches Institut**

Teaching Research Instrumentation Modelling Jobs CDMS SFB 956

Home » Research » Services  
**The Cologne Database for Molecular Spectroscopy**

News  
Events  
Conferences

Research  
Methods  
Observatories  
Services



**BASECOL**

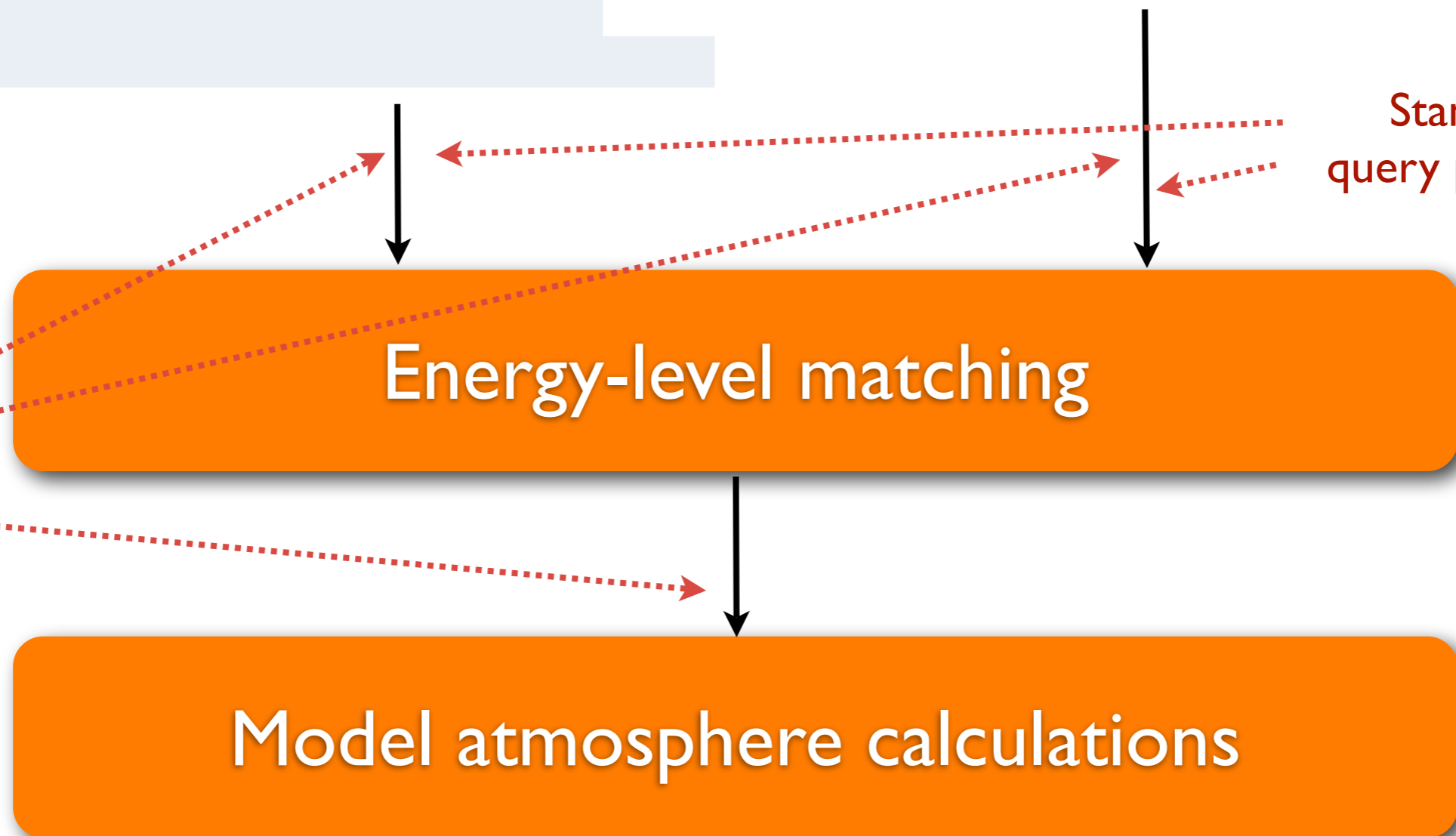
RO-VIBRATIONAL COLLISIONAL EXCITATION  
Database and Utilities

Standard  
query protocol

Energy-level matching

Standard  
data-format

Model atmosphere calculations



# More use cases...

- Composite spectrum for molecule
- Combine parameters for atomic lines
- Compare observation with theory
- Compare separate calculations of same levels
- Same modelling code uses multiple DBs
- New applications work with all DBs
- Self-describing format for data
- Bibliography of data sources
- etc...

# Synthesis of parts

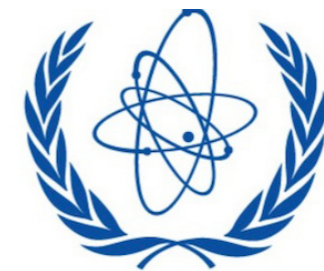
VALD CDMS  
HITRAN CHIANTI

BASECOL

Existing databases



Web-service protocols



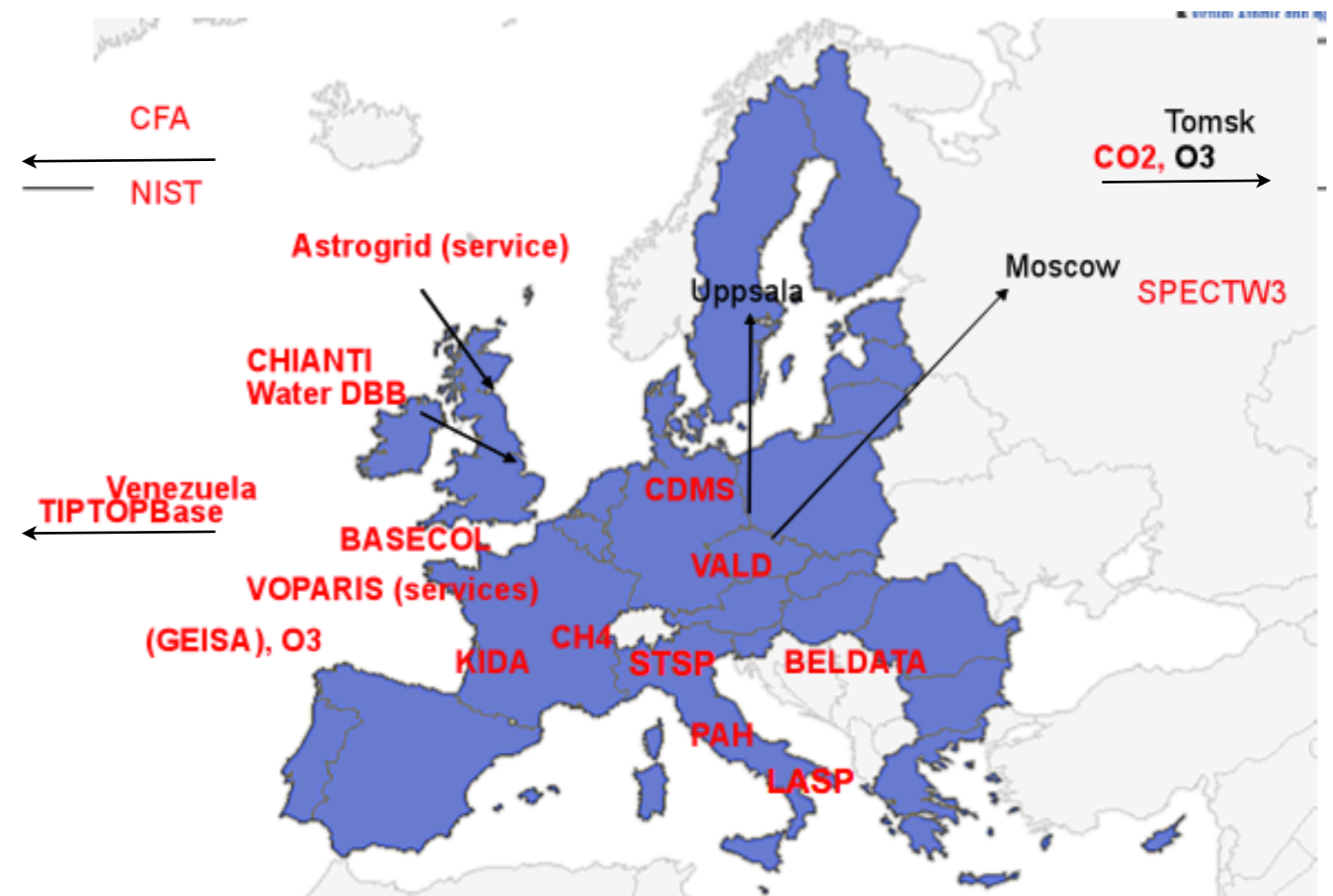
IAEA

XSAMS data-format

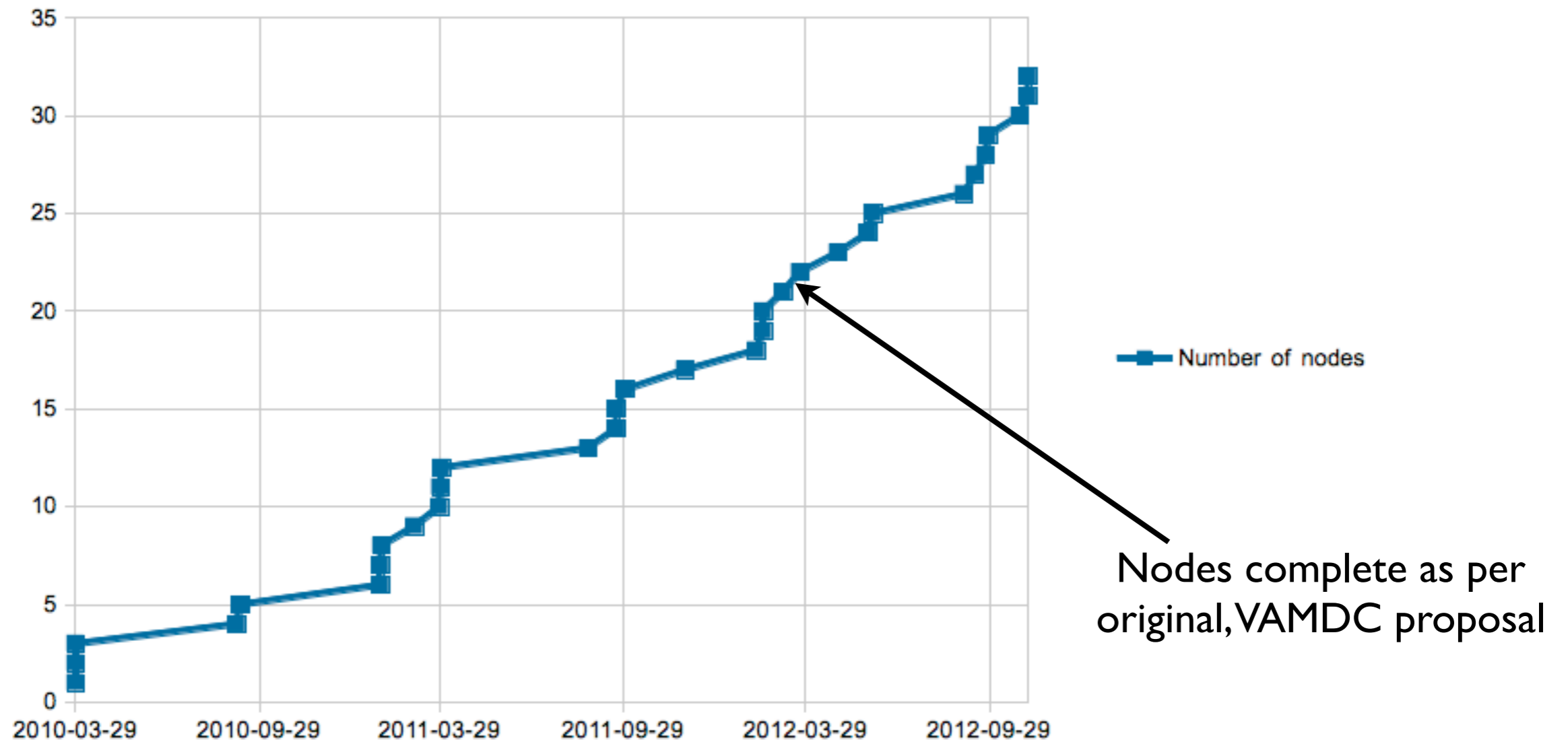


# Original VAMDC project

- EU FP7 funding, 2009-2012
- 15 partners, 21 institutions
- 7 EU countries
- + Russian Federation
- + Venezuela
- ~22 databases proposed initially



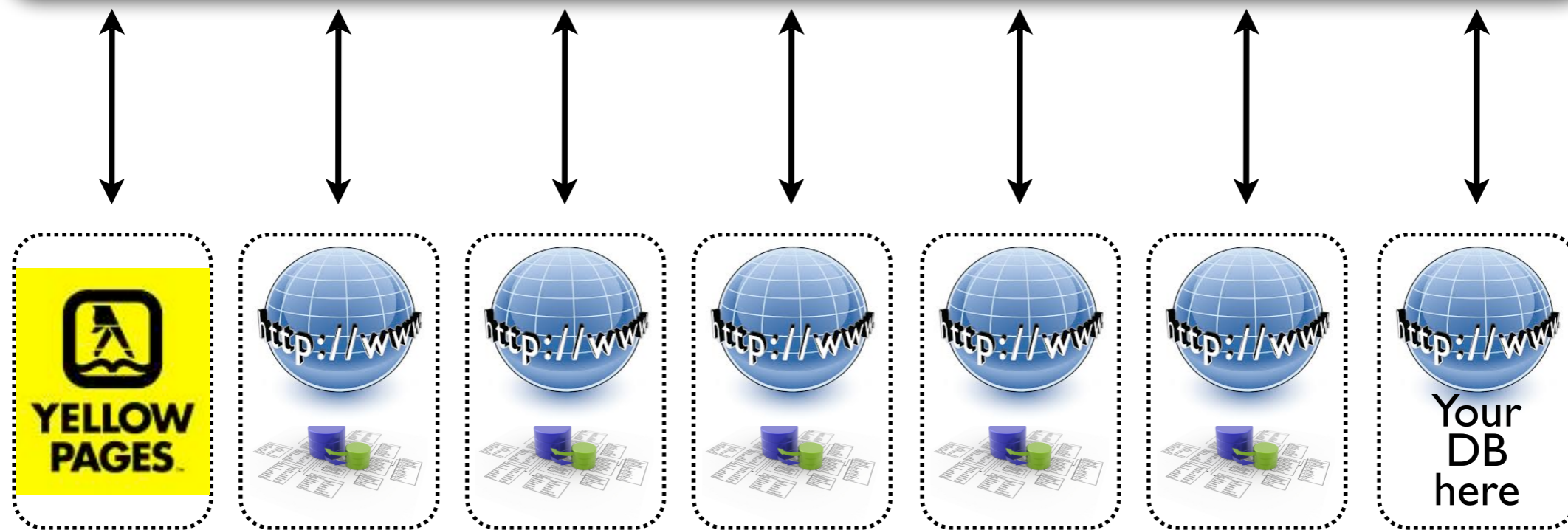
# Database growth



# A flock of databases



Science application



VAMDC  
data  
nodes

# For list of databases see:

[http://portal.vamdc.eu/vamdc\\_portal\\_test/nodes.seam](http://portal.vamdc.eu/vamdc_portal_test/nodes.seam)



Home VAMDC databases Query Saved queries | Info Known issues Login Register

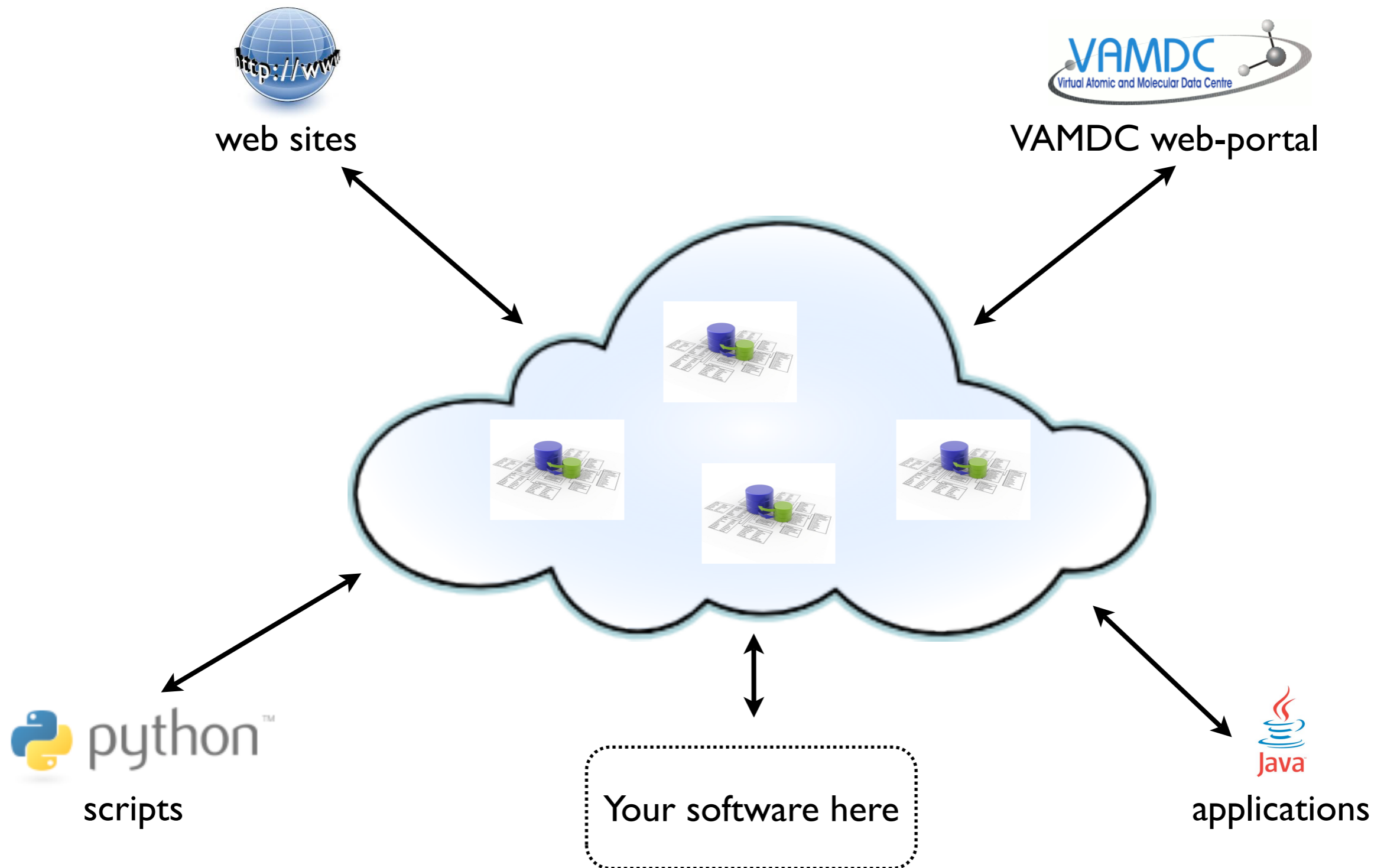
Name	Description	Maintainer	Status
<a href="#">Theoretical spectral database of polycyclic aromatic hydrocarbons</a>	The Cagliari/Toulouse PAH database is a collection of theoretical spectroscopic data about Polycyclic Aromatic Hydrocarbons and carbon clusters. It provides basic geometric characteristics, energetics, harmonic analyses and electronic photoabsorption data. It is maintained by the Astrochemistry group at INAF-Observatory of Cagliari and the Institut de Recherche en Astrophysique et Plan�tologie in Toulouse.	gmulas@oa-cagliari.inaf.it	OK
<a href="#">Chianti</a>	Chianti consists of a critically evaluated set of up-to-date atomic data, together with user-friendly programs written in Interactive Data Language (IDL), to analyse the spectra from astrophysical plasmas. The VAMDC interface presents just the data from the Chianti-v7 release.	gtr@ast.cam.ac.uk	OK
<a href="#">GSMA Reims S&amp;MPO</a>	Calculated line lists for ozone (16O3, 16O18O16O and 18O3). The data on methane contain the vibration-rotation energy levels, line positions and line strengths in the range from 0 to 8000 cm-1.	ylb@iao.ru, vladimir.tyuterev@univ-reims.fr	OK
<a href="#">ECaSDa - Ethene Calculated Spectroscopic Database</a>	Calculated data of ethylene (12C2H4). The data on ethylene contain the vibration-rotation energy levels, line positions and line intensities in the range from 500 to 7500 cm-1	ludovic.daumont@univ-reims.fr, maud.rotger@univ-reims.fr	OK
<a href="#">GhoSST</a>	The GhoSST database ("Grenoble Astrophysics and Planetology Solid Spectroscopy and Thermodynamics" database service) provides laboratory data on spectra (from UV to FIR) of natural and synthetic solids (ices, molecular solids, minerals, salts, inorganic materials, organic materials, meteorites, adsorbed molecules, hydrated solids,?) of space sciences, Earth sciences and astrophysical interest. It is completed with band list data (NIR to FIR) on molecular solids and adsorbed/hydratation molecules. The GhoSST data come from laboratory experiments performed since 1989 at IPAG (and formerly at LGGE and LPG) with different spectroscopy techniques (transmission, bidirectional reflection, micro-spectroscopy, ATR, Raman, Fluorescence, ...).	damien.albert@obs.ujf-grenoble.fr	OK
<a href="#">Lund laboratory spectroscopy</a>	Experimental data for transitions and lifetimes	hampus@astro.lu.se	OK



# DBs relevant to RADAM

- IDEADB
- RADAM template database, Caen
- BASECOL?
- Kinetic Database for Astrochemistry (KIDA)?
- ALADDIN-2 (IEAE)?
- UMIST Database for Astrochemistry (UDfA)?
- Various electron-molecule data to come from India, Korea, Japan?

# Many UIs



# VAMDC web portal: query

Atom symbol

Mass number  to

Nuclear charge  to

Ion charge  to

InChIKey

State energy  to  1/cm

Equivalent to  1/cm

Molecules (target) Clear Remove

Chemical name

Stoichiometric formula

Structural formula

Spin isomer

Standard InChIKey

[Select All](#) [None](#) Search by stoichiometric formula if no inchikey is selected.

Formula	InChIKey
<input checked="" type="checkbox"/> (12C)(16O)	UGFAIRIUMAVXCW-UHFFFAOYSA-N
<input checked="" type="checkbox"/> (13C)(16O)	UGFAIRIUMAVXCW-OUBTZVSYSA-N
<input checked="" type="checkbox"/> (12C)(18O)	UGFAIRIUMAVXCW-HQMMCQRPSA-N
<input checked="" type="checkbox"/> (12C)(17O)	UGFAIRIUMAVXCW-VQEHIDDOSA-N
<input checked="" type="checkbox"/> (13C)(18O)	UGFAIRIUMAVXCW-RGIGPVFXSA-N
<input checked="" type="checkbox"/> (13C)(17O)	UGFAIRIUMAVXCW-ZDOIHCCHA-N

Collisions Clear Remove

Process name

Process description

Process code

IAEA process code

Species	Role
Atoms	Role <input type="text" value="Collider"/>
Molecules	Role <input type="text" value="Target"/>

## Legend

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

- » Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
- » MeCaSDa - Methane Calculated Spectroscopic Database
- » VALD (atoms)
- » OACT - LASP Database
- » BASECOL: VAMDC-TAP interface
- » TOPbase : VAMDC-TAP interface
- » Theoretical spectral database of polycyclic aromatic hydrocarbons
- » IDEADB - Innsbruck Dissociative Electron Attachment Database
- » Chianti
- » TIPbase : VAMDC-TAP interface
- » GSMA Reims S&MPO
- » ECaSDa - Ethene Calculated Spectroscopic Database
- » Carbon Dioxide Spectroscopic Databank - 296K
- » GhoSST
- » Carbon Dioxide Spectroscopic Databank - 1000K
- » 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

# VAMDC web-portal: results

Done

select \* where (RadTransWavelength >= 5000.0 AND RadTransWavelength <= 5010.0)

**Comments**

**XSAMS processors**

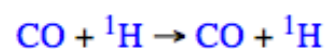
BibTeX from XSAMS
  Table views of XSAMS
  Xsams2SME

Name	Response	Download	Species	States	Processes	Radiative
<input type="checkbox"/> VALD sub-set in Moscow (obs)	OK	<a href="#">XSAMS</a>	81	1157	701	701
<input type="checkbox"/> Water internet Accessible Distributed Information System	OK	<a href="#">XSAMS</a>	1	591	601	601
<input type="checkbox"/> TOPbase : VAMDC-TAP interface	OK	<a href="#">XSAMS</a>	70	619	353	353
<input type="checkbox"/> HITRAN-UCL resource	OK	<a href="#">XSAMS</a>	8	64	149	149
<input type="checkbox"/> Chianti	OK	<a href="#">XSAMS</a>	18	81	43	43
<input type="checkbox"/> Spectr-W3	OK	<a href="#">XSAMS</a>	9	26	13	13
<input type="checkbox"/> GSMA Reims S&MPO	OK	<a href="#">XSAMS</a>	0	0	5	5
<input type="checkbox"/> Stark-b	OK	<a href="#">XSAMS</a>	4	6	3	3
<input type="checkbox"/> VALD (atoms)	TRUNCATED (9%)	<a href="#">XSAMS</a>	78	10076	65459	65459
Cologne Database for Molecular Spectroscopy: VAMDC-TAP service	EMPTY		0	0	0	0
Carbon Dioxide Spectroscopic Databank - 1000K	EMPTY		0	0	0	0
Carbon Dioxide Spectroscopic Databank - 296K	EMPTY		0	0	0	0
MeCaSDa - Methane Calculated Spectroscopic Database	EMPTY		0	0	0	0
Lund laboratory spectroscopy database	EMPTY		0	0	0	0
ECaSDa - Ethene Calculated Spectroscopic Database	EMPTY		0	0	0	0

# VAMDC web-portal: display



## Data for single collision



- M.-L. Dubernet, BASECOL database, , 2013
- N. Balakrishnan, M. Yan and A. Dalgarno, *Quantum-Mechanical Study of Rotational and Vibrational Transitions in CO Induced by H Atoms*, *apj*, **568**, 443-447, 2002

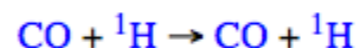
### rateCoefficient

(K)	(cm <sup>3</sup> /s)
5.0	1.78E-10
10.0	1.93E-10
20.0	2.02E-10
30.0	2.09E-10
40.0	2.15E-10
50.0	2.2E-10
60.0	2.25E-10
70.0	2.28E-10
80.0	2.32E-10
90.0	2.34E-10
100.0	2.37E-10



## Collisions with data sets

PBASC48t2T1c1C1

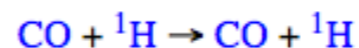


M.-L. Dubernet 2013; N. Balakrishnan et al. 2002

rateCoefficient

[Table \(CSV\): Rate coefficients](#)

PBASC48t3T1c1C1

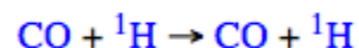


M.-L. Dubernet 2013; N. Balakrishnan et al. 2002

rateCoefficient

[Table \(CSV\): Rate coefficients](#)

PBASC48t3T2c1C1

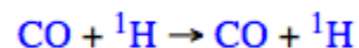


M.-L. Dubernet 2013; N. Balakrishnan et al. 2002

rateCoefficient

[Table \(CSV\): Rate coefficients](#)

PBASC48t4T1c1C1

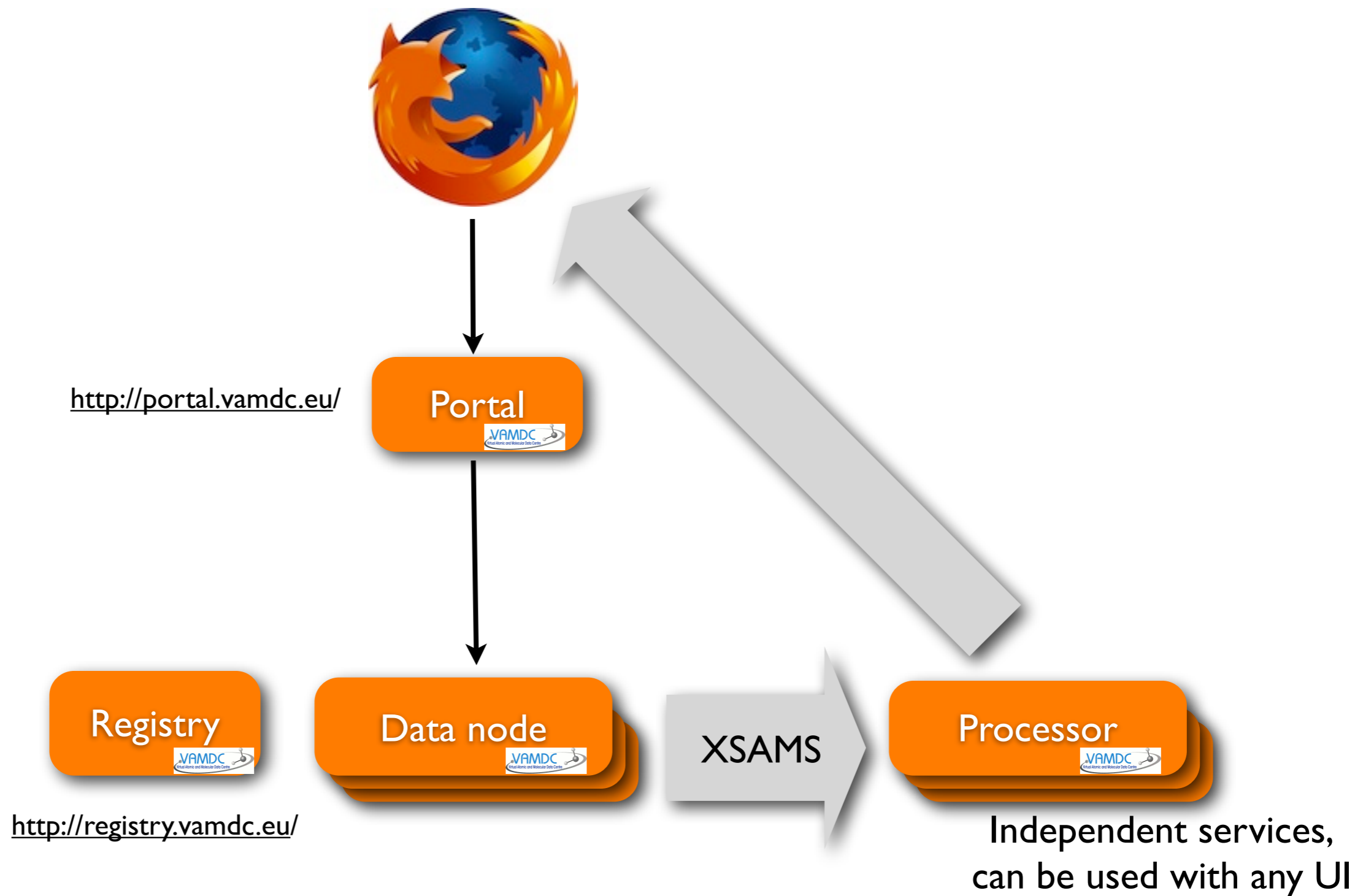


M.-L. Dubernet 2013; N. Balakrishnan et al. 2002

rateCoefficient

[Table \(CSV\): Rate coefficients](#)

# Portal, nodes & processors



# SpectCol application

The screenshot shows the SPECTCOL application window. At the top, there is a title bar with 'SPECTCOL' and window control buttons. Below the title bar, there are three main sections:

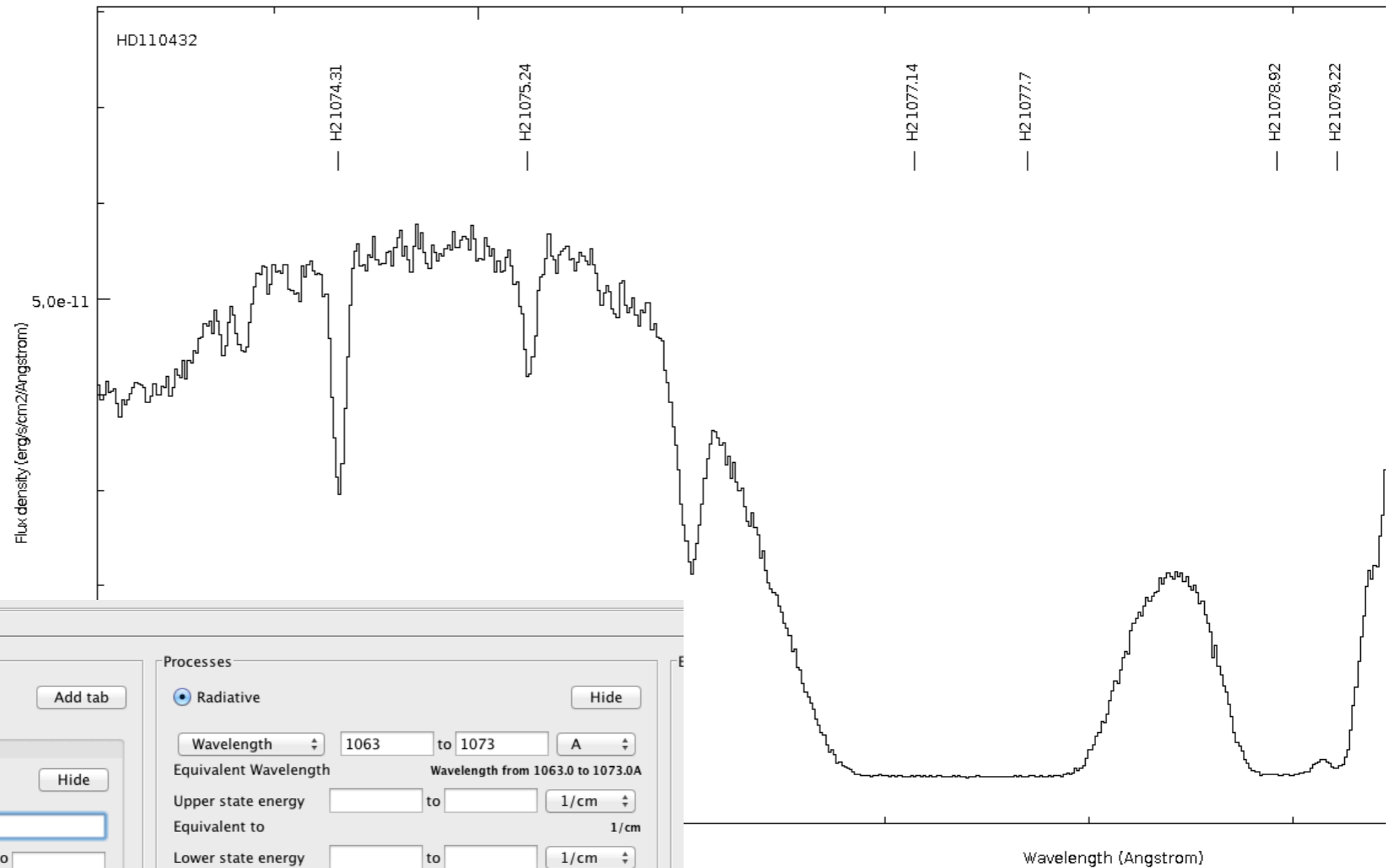
- Import data from file:** Includes a 'Browse...' button, a 'File path:' text input field, radio buttons for 'collisions' (selected) and 'transitions', and an 'Import' button.
- Search VAMDC databases:** Includes checkboxes for 'BASECOL', 'CDMS' (checked), 'HITRAN', and 'JPL'. Below this are three tabs: 'Species search', 'Transitions search' (selected), and 'Collision search'. The search fields include:
  - Nuclear spin: dropdown menu with '\_any\_' selected.
  - Molecular species inChiKey: text input field.
  - Molecular stoichiometric formula: text input field with 'CO' entered.
  - Ion charge: text input field.
  - Atomic symbol: text input field.
  - Particle name: text input field.Buttons for 'Submit query' and 'Cancel' are located at the bottom right of this section.
- Transitions:** A table displaying search results with columns for comment, source, structural formula, stoichiometric formula, spin, and InChI key. To the right of the table is a vertical stack of buttons: 'Clear', 'Sources', 'Energy table', 'Einstein coef.', 'Partition func.', 'Export', 'Group by hand', and 'Group by species'.

	comment	source	structural formula	stoichiometric formula	spin	InChI key
1	30502- v 1:CO-18; \$v=0\$	CDMS 2013-09-06 10:44...	CO-18	CO		UGFAIRIUMAVXCW-HQMMCQRPSA-N
2	28512- v1*:CO; \$v=1,2,3\$	CDMS 2013-09-06 10:44...	CO	CO		UGFAIRIUMAVXCW-UHFFFAOYSA-N
3	31502- v 1:C-13-O-18; \$v=0\$	CDMS 2013-09-06 10:44...	C-13-O-18	CO		UGFAIRIUMAVXCW-RGIGPVFXSA-N
4	28503- v 1:CO; \$v=0\$	CDMS 2013-09-06 10:44...	CO	CO		UGFAIRIUMAVXCW-UHFFFAOYSA-N
5	30503- v 1:C-13-O-17; \$v=0\$	CDMS 2013-09-06 10:44...	C-13-O-17	CO		UGFAIRIUMAVXCW-ZDOIHCISA-N
6	29501- v2*:C-13-O; \$v=0\$	CDMS 2013-09-06 10:44...	C-13-O	CO		UGFAIRIUMAVXCW-OUBTZVSYSA-N

Implements the original use case for matching spectroscopic and collisional data

# Specview application

Line IDs for astronomy:  
VAMDC data  
added to existing  
application



Use VAMDC

Species

Sp0

Atoms Hide

Atom symbol

Mass number  to

Nuclear charge  to

Ion charge  to

InChiKey

State energy  to  1/cm

Equivalent to  1/cm

Molecules Hide

Particles Hide

Add tab

Processes

Radiative Hide

Wavelength  to  A

Equivalent Wavelength  Wavelength from 1063.0 to 1073.0A

Upper state energy  to  1/cm

Equivalent to  1/cm

Lower state energy  to  1/cm

Equivalent to  1/cm

Probability, A  to

Collision Hide

This query UI available as a Java library



# SUP@VAMDC: successor project

- Further EU funding, 2012-2014
- 6 of 15 original VAMDC partners involved
- New partners in India, Korea, South Africa
- External partners in USA, Brazil, Australia, Japan, Austria
- Most nodes connected from outside the project
- Focused on **support** for users, data-providers

# Coding support

- Class libraries for Java
- Module and small-app collection for Python
- Open-source licensing

# Tutorials

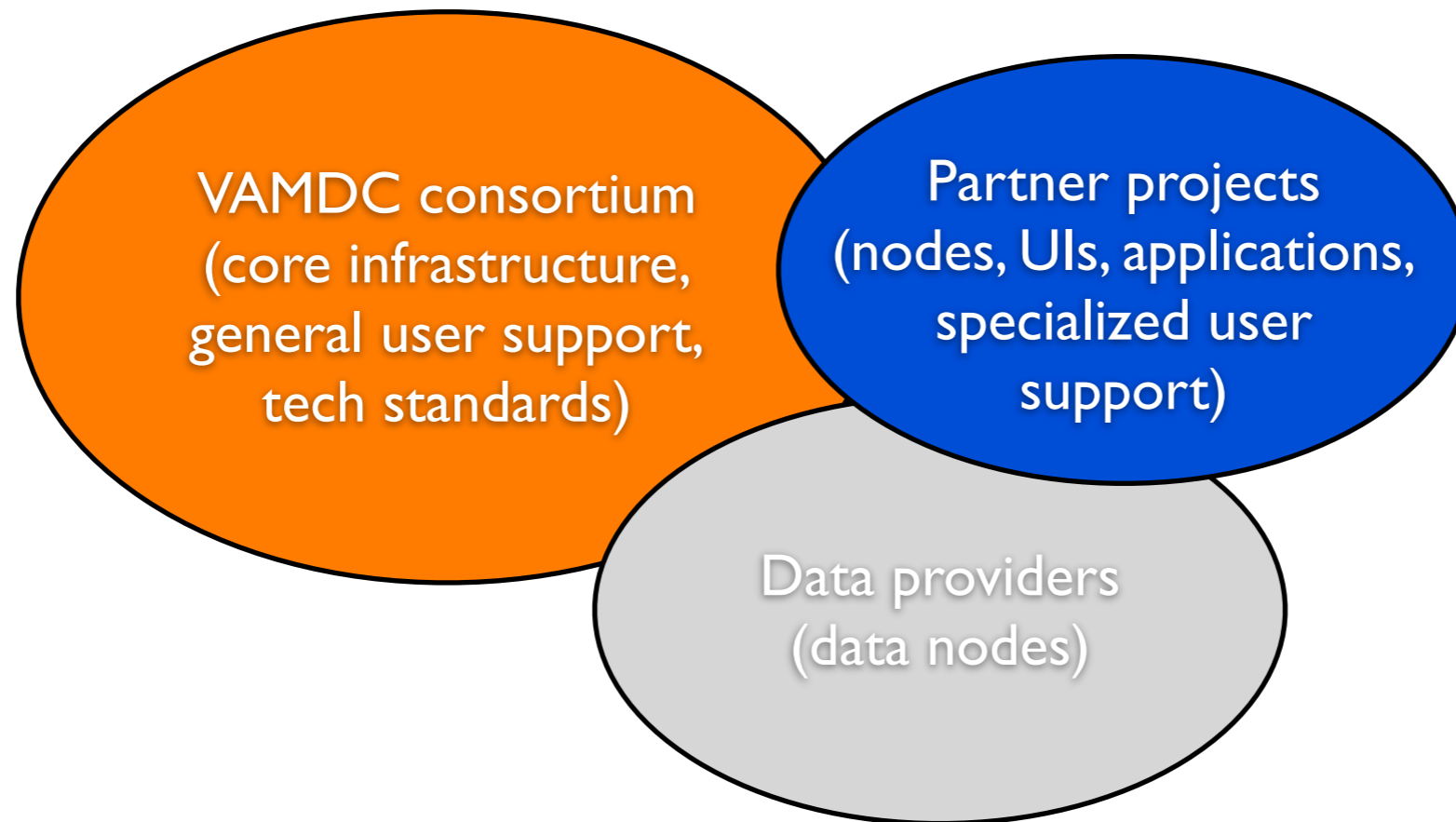
<http://www.vamdc.eu/usersupport/tutorials>

- Introductory papers
- Self-paced exercises
- Video guides
- Reference manuals

# Support after SUP@VAMDC

- VAMDC consortium continues support:
  - consortium of universities signatory to a MOU;
  - contains the active members of the SUP@VAMDC project, plus some others;
  - maintains the infrastructure for users and node-operators;
  - separate MOU between consortium and that node operators;
  - node operators do not need to join the consortium to get support;
  - consortium will seek grants to continue the work;
  - consortium → legal entity; EU recognition as a body rather than an ephemeral collaboration.

# Three-way cooperation



# Summary

- Collaborate with VAMDC to get:
  - standards for distributed databases;
  - established network of services for same;
  - technical support;
  - user training.
- Collaborate by:
  - making data nodes and XSAMS processors;
  - making UIs for VAMDC services;
  - acknowledging VAMDC.
- Collaborate with:
  - VAMDC consortium;
  - currently supported by SUP@VAMDC project;
  - later established as legal entity with grant/subscription support.