SUP@VAMDC—
Uniting the international atomic and molecular community
N J Mason, Open University, UK
There many A&M related DATABASES have been developed but such databases are....

• Often in different formats
• Access maybe restricted or ‘regional’
• Often fragmentary providing ‘partial resource’
So ……VAMDC

- A database of Atomic and molecular data for applications including astronomy.
- Http://www.vamdc.org/
Guide to this presentation

Who are VAMDC
What are aims of VAMDC?
VAMDC -- the product

VAMDC -- the culture

SUP@VAMDC the project - and getting involved
Who are VAMDC?

**CNRS (France):** ML Dubernet, V. Boudon, C. Joblin, P. Le Sidaner, B. Schmitt, V. Tyuterev, V. Wakelam, C. Zeippen [LPMAA, ICB, CESR, VOPARIS Data Centre, LPG, GSMA, L3AB, LERMA]

**UK:** N. Mason (Open University), J. Tennyson, L. Culhane (UCL), T. Millar (Belfast University), H. Mason, G. Del Zanna, N. Walton, (Cambridge University)

**VALD Consortium:** U. Heiter, N. Piskunov (Uppsalla University, Sweden), T. Ryabchikova (INASAN, Russian Federation), A. Ryabtsev (ISAN, Russian Federation), F. Kupka, W. Weiss, C. Stuetz (Vienna University)

**Germany (Cologne Univ):** S. Schlemmer

**Belgrade (Astronomical Observatory):** M. Dimitrijevic

**INAF (Italy):** G. Mulas, G. Malloci (Observatory of Catania, of Cagliori)

**Russian Federation:** V. Perevalov, A. Fazliev (IAO, Tomsk),

**Russian Federation:** P. Loboda (RFNC-VNIITF, Moscow)

**Venezuela:** C. Mendoza, L. Nunez IVIC, Caracas)

**USA:** Y. Ralchenko (NIST), L Rothman (CFA)
What is VAMDC?

Funded under the “Combination of Collaborative Projects and Coordination and Support Actions” Funding Scheme of The Seventh Framework Program.

42 months from July 2009 with 3,2 million Euros end December 2012

Grant Agreement number: 239108
Followed by SUP@VAMDC?

24 months from November 2012

To extend concept, teams and culture outside EU
What is VAMDC?

VAMDC will provide a scientific data e-infrastructure enabling easy access to A+M resources

Http://www.vamdc.eu/
Why VAMDC?

Databases are dispersed
Often in different formats
Access maybe restricted or ‘regional’

So need a common portal ‘single point entry’
KEY VAMDC OUTCOMES

- Develop or/and extend standards for interoperability of AM resources
- Implementation of selected databases / Compatibility with existing extraction tools
- Find resources easily
  - Registries at a fine granularity
- Query those resources
  - Query protocols or/and languages
- Transfer large quantities of data, Asynchronous Queries
- Create a safe environment where latest AM data can be easily published (even small sets)
- Linking producers and users

KEY BENEFITS

- Find any type of AM with a “click”
- Uniform access, i.e. saving time with format of data, tools development
- Increase level of scientific analysis of ground/space missions or experiments
  - good standardisation implies Documentation
  - allows cross-matching of different sets of AM data
  - allows wide access to the latest published AM data
- At present all the above items are not fulfilled
What is VAMDC?

VAMDC does not collect or commission data but...

Will be a ‘one stop shop’ access to databases (currently 21 are included)
What is VAMDC?

Current databases include:

- Vienna Atomic Line Database (VALD)
- CHIANTI
- Cologne Database for Molecular Spectroscopy (CDMS) and Jet Propulsion Laboratory Submillimeter Catalogue
- BASECOL
- GhoSST
- UMIST database for astrochemistry
- KInetic Database for Astrochemistry (KIDA)
- Polycyclic Aromatic Hydrocarbon spectral database
- LASP Database
- Stark-B
- Spectr-W3
- TIPTOPbase
- HITRAN
- NIST atomic database
How does VAMDC operate?

- Building an e-science Network built on the existing Euro-VO and Grid infrastructures:
  - connection to Euro-VO, EuroPlanet IDIS, IVOA, other EU initiatives, e.g. solar, fusion (ITER/Euratom – we hope !!).

  - connection to projects outside the EU
    - Russia, South America (direct partners)
    - USA (external partners)
The network MUST be built in collaboration with many A&M specialists

- long term maintenance with high quality expertise
- cover the widest community using uniform approach

The network MUST meet the users requirements but also the producers requirements
End User Communities

- Astrophysical, atmospheric, plasma, combustion media
- Industrial Applications, e.g. lighting, plasma etching -- Ex: PLASIMO
- Radiation Damage (New RADAM DATABASE)
- Range of Complexity of user requirements

End User: Comparison Models/Observations for Interstellar Medium

Courtesy of F. Le Petit (LUTH, Obs. Paris)
Where are we now?
VAMDC: a working infrastructure

VAMDC UI: based on VOExplorer

User Interface

Astro Runtime [AR]

Community

Registry

VOSpace

Workflow

VO Desktop Tools scripting and workflow interface

VO middleware

Taverna workflow

VO compliant registry

Applications environment

CEA [UWS]

DSA

Common data interfaces

VAMDC applications

VAMDC data resources

Applications environment

DSA: Data Set Access; UWS Uniform Worker Service
EuroVO infrastructure connects to VO compute and data grid.

Data grid can connect to Grid storage (e.g. iRODS).

EuroVO user interface allows submission of jobs to Grid (e.g. EGEE).

Therefore, multiple, compatible implementations are encouraged. E.g.:

- Euro-VO
- SDSC, CDS, INAF
- EuroVO

Flexible infrastructure to connect to VAMDC resources.
SA / JRA dependencies

JRA1: Standards
    12–24–36-42
T1: DM & XML
T2: Dictionaries
T3: Query
T4: Registries

JRA2: Publishing
    Tools
15, 27, 39

JRA3: Mining Tools
    T1: Registries Queries (24)
    T2: Manipulation of Data (24-36)
    T3: Advanced Data Mining (36-41)

SA1: Deployment
    T1: Access to data (15 to 42)
    T2: Access to codes (15 to 42)
    T3: Implement Registries (18)
    T4: Augmenting VODesktop (33)
    T5: Desktop Software (21 + n6)
    T6: Expansion Infrastructure (39)

SA2: Support (12, 24, 36,42)
    T1: Monitoring
    T2: Grid Operations
    T3: Support to users
    T4: Preservation
    T5: QA
Data Models and XML Schema:

Dictionaries:

In order to uniquely identify resources we have defined and built dictionaries both general and specific to applications.
Access Protocols and Query/Retrieval Language:

We are defining protocols retrieving different types of resources: numerical data, libraries, documentation, references. In a second step we will use a general query language (Xquery) allowing to access and retrieve any atomic and molecular data.
Registries:

Registries provide a mechanism with which applications can discover and select resources—e.g. data and services—that are relevant for a particular scientific problem. We wish to implement ways of finding resources at various levels of granularity.
Design of Publishing and Mining Tools

The following software are aimed at enhancing scientific research through allowing easy and secure publication and mining of A&M resources within the VAMDC infrastructure:

**Task 1:** Create/adapt tools to go from an DM/XML schema to a full database deployment with generation of automatic administrative interface.

**Task 2:** Create/adapt tools to build registries from the content of databases

**Task 3:** Create/adapt interfaces to easily update dictionaries

**Task 4:** Develop software libraries using various languages allowing to easily generate output of already existing resources in standardized format

**Task 5:** **Tools for Manipulation of Data** Our queries will return data organised according to schemas defined in JRA1. Those schemas will be quite complex because they will reproduce all the scientific concept attached to the data. Therefore the handling of the XML files will be complex and will require specific tools. For now we identify too main generic tools: one performing cross-matching of data and one performing cross-federation of data.
Where are we now?

VAMDC level-2 release
Open to beta testers

Evaluation period – ended July 2012
Now ‘final’ version for release November 2012
Now look on line
For latest news see

www.vamdc.eu

Public/user webpages in October 2012)

and for published review see

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SUP@VAMDC
Support at the Virtual Atomic and Molecular Data Centre

INFRA-2012-3.3  24 months
Coordination and Support Actions - Supporting Action (CSA-SA)  Coordinating person: Dr M.L. Dubernet
SUP@VAMDC

2 year follow on from VAMDC that outlines next step in VAMDC development

International partners

Wider adoption

Requires further technical development
PARTNERS

• Observatoire de Paris, France – Coordinator
• The University of Cambridge, UK
• Uppsala Universitet, Sweden
• Open University, UK
• Universitaet zu Koeln, Germany
• University College London, UK
• Korea Atomic Energy Research Institute, South Korea
• University of South Africa, South Africa
• Tata Institute of Fundamental Research, India
EXTERNAL AND ASSOCIATED PARTNERS:

- Yuri Ralchenko, Atomic Spectroscopy Group, NIST, USA
- Laurence S. Rothman, The Harvard-Smithsonian Center for Astrophysics, Cambridge, USA
- Brian Drouin, JPL, California Institute of Technology, USA
- Carlos Gonzales, The Chemical and Biochemical Reference Data Division, NIST, USA
- Milton M. Fujimoto, Universidade Federal do Paraná, Brazil
- Stephen Buckman, Atomic and Molecular Physics Laboratory, Australian National University, Australia
- Michael Brunger, The Electron Scattering and Modelling Group, Flinders University, Australia
- Izumi Murakami, National Institute for Fusion Science, Japan
- Bas Braams, Atomic and Molecular Data Unit, IAEA, Austria
• **SUP@VAMDC (Support at VAMDC)** aims at building upon the VAMDC e-infrastructure portal, supporting different studies and actions linked to the VAMDC e-infrastructure.

• **SUP@VAMDC** will establish the necessary coordination methodology by formulating the **roadmap** that will ultimately combine VAMDC with complimentary (e)-infrastructures organised by existing international bodies/committees/networks dealing with the production, evaluation and dissemination of A+M data.
• Provides the support and medium for including authentication, authorization and accounting and licensing tools within the VAMDC brand

• Promote and fashion future interoperability (technical, semantic, reference architecture, etc) across the A&M data community through the promotion, monitoring and adoption of common standards.
Provides support for dissemination actions aimed at raising the visibility of VAMDC towards wider audiences.

Includes EDUCATION audience;
Students and Citizen Scientists
Dissemination programme

Develop a global VAMDC e-infrastructure between the EU and the rest of the world, including Brazil, South Africa, Asia, Australia, India, through hosting workshops and supporting dialogue.
• Explore business models for supporting an Open Science model (OPEN VAMDC) whilst assessing the impact of such a modeling in achieving financial sustainability of VAMDC itself
• WP1 Management
• WP2 Policies/Strategy
• WP3 Connection to wider audience
• WP4 Extension towards other e-infrastructure and EU schemes
• WP5 Operational Support
Workshops begin in 2013

Roadmap by Summer 2014

Similar aims to discussions of IAEA meetings
So lets unite!