VAMDC

Virtual Atomic and Molecular Data Centre

T. Lueftinger¹ and the VAMDC Collaboration** (P.I. M.-L. Dubernet^{2,3})

¹Institute of Astronomy, Faculty of Earth Sciences, Geography and Astronomy, University of Vienna, Austria ²LPMAA, Université Pierre et Marie Curie, France, ³LUTH, Observatoire de Paris, France

An e-science Platform for the Exchange of AM Data and Services

Objectives

The Virtual Atomic and Molecular Data Centre (VAMDC) aims The Virtual Atomic and Molecular Data Centre (VAMDC) aims at building a secure, documented, flexible, easily accessible and interoperable e-infrastructure for AM data. The VAMDC will be built upon the expertise of existing AM databases, data producers and service providers with the specific aim of creating an infrastructure that on one hand can directly extract data from the existing depositories while one the other hand is sufficiently flexible to be tuned to the needs of a wide variety of users from academic, governmental, industrial communities or from general public both within and outside the ERA. The project will address the building of the core consortium, the deployment of the infrastructure and the development of specific software as well as providing a forum for training of potential users and providing a forum for training of potential users and dissemination across the ERA. It is expected that VAMDC becomes a European legal entity during the course of the project.

Service Activities

The key objective of the Service Activities is to provide access to In every objective of the Service Activities is to provide access to an inclusive range of high quality data and applications services to the research community. The VAMDC partners represent major data producers. By integrating their existing and, importantly, future resources through the standard VAMDC infrastructure the wider community of diverse end users will gain enhanced access to this eco-system of fundamental scientific data. The SA to this eco-system of fundamental scientific data. The SA activities will ensure the availability of these major data resources in interoperable formats, the maintenance of services allowing publications of small datasets by producer's teams, the maintenance of registries and dictionaries, the maintenance of nodes listing the needs for the various communities (in relation with other ELL initiation). These consider will be defined the with other EU initiatives). These services will be delivered by use of the latest virtual observatory and grid e-science infrastructures

Networking Activities

The ensemble of Networking Activities (NAs) aims to foster a culture of cooperation between A&M scientists, database providers and data users throughout Europe.

The objectives of Nas are: to coordinate the infrastructure's activities among all trans-disciplinary fields (atomic and molecular physics, users such as the astrophysics, atmospheric, fusion, ICT communities); to develop a coherent research community within the EU and to create a direct partnership to key external communities in both the Russian Federation and central and southern America via Venezuela: to link VAMDC to other international projects relevant to VAMDC; to interact with nonpartner teams from other EU and non-EU countries in order to take the largest possible approach to the development of the infrastructure: to disseminate VAMDC achievements and to get feedback from data provider and users on the content and operation of VAMDC. The NAs will therefore have both a practical and a political role in defining the policies and evolution of the infrastructure

Present Status

VAMDC is funded under the "Combination of Collaborative Projects and Coordination and Support Actions" Funding Scheme of The Seventh Framework Program. Call topic: INFRA-2008-1.2.2 Scientific Data Infrastructure. Grant Agreement number: 239108

The Project has been funded for 42 months starting on the 1rst of July 2009 for 2.9 Meuros.

To be kept informed about the VAMDC project, send a mail to and visit our website (and wiki)

Participants (Contact persons)

CNRS (France): ML Dubernet, E. Roueff, V. Boudon, C. Joblin, P. Le Sidaner, B. Schmitt, V. Tyuterev, V. Wakelam, S. Sahal-Bréchot/C. Zeippen [LPMAA, LUTH, ICB, CESR, VOPARIS Data Centre, LPG, GSMA, L3AB, LERMAI

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, T. Lueftinger, 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)



VAMDC RESOURCES AND APPLICATION FIELDS

- Astrogrid, CHIANTI, Water DBB, UMIST - Fusion, Atmospheric, Solar, ISM, Planeto •Austria, Sweden, Russia = VALD

•Serbia = BELDATA – Stellar, Solar – •Germany = CDMS - ISM, Atmospheric .Italy = PAH, LASP, ISM, Planetology •Russia, Tomsk = - Atmospheric Databases

Venezuela, Caracas = TIPTOPBase, Stellar - GRID

- France (CNRS) LPMAA/LUTH: Coordination, ISM – BASECOL, Standards, GRID
 - VOPARIS Data Center: Technical Node, GRID, Archiving, Registries -
 - LERMA: TIPTOPBase Stellar, Fusion. BELDATA -
 - GSMA: O3 Coll. Tomsk Atmospheric - ICB: CH4 - Planetology - ISM -
 - LPG: Spectroscopy of Solids Planeto -
 - L3AB: KIDA (Reactions) ISM Planeto
 - CESR: PAH Database ISM Coll. INAF

** Reference: M.L. Dubernet et al, 2010, JQSRT, Volume 111, Issue 15, p 2151

Design of the Infrastructure

•Data Models and XML Schema: Extension of current Schemas for example with

- inclusion of solid, surface spectroscopy for interstellar medium and planetology
- inclusion of larger molecules such as PAH
- description of atomic and molecular line shapes arising from different sources

•Dictionnaries: In order to uniquely identify resources we will need to define and build dictionaries both general and specific to applications

- Access Protocols and Query/Retrieval Language: We will define protocols retrieving different types of resources: numerical data, libraries, documentation, references. In a second step we will design a general query language 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

•Task5: 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.



•UK: Cambridge + UCL + Open University + Belfast

- Stellar, Fusion