



VAMDC

Virtual Atomic and Molecular Data Centre

D2.5

-

Final Science/Technical Report

Version 0.1

Grant agreement no: 239108

Combination of Collaborative Projects & Coordination and Support Actions



CAPACITIES

Final Technical Report 2



e-infrastructure

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Project Information

Project acronym: VAMDC
 Project full title: Virtual Atomic and Molecular Data Centre
 Grant agreement no.: 239108
 Funding scheme: Combination of Collaborative Projects & Coordination and Support Actions
 Project start date: 01/07/2009
 Project duration: 42 months
 Call topic: INFRA-2008-1.2.2 Scientific Data Infrastructure
 Project web sites: <http://www.vamdc.eu>

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

Consortium:

Beneficiary Number *	Beneficiary name	Beneficiary short name	Country	Date enter project**	Date exit project**
1(coordinator)	Centre National de la Recherche Scientifique	CNRS	France	Month 1	Month 42
2	The Chancellor, Masters and Scholars of the University of Cambridge	CMSUC	UK	Month 1	Month 42
3	University College London	UCL	UK	Month 1	Month 42
4	Open University	OU	UK	Month 1	Month 42
5	Universitaet Wien	UNIVIE	Austria	Month 1	Month 42
6	Uppsala Universitet	UU	Sweden	Month 1	Month 42
7	Universitaet zu Koeln	KOLN	Germany	Month 1	Month 42
8	Istituto Nazionale di Astrofisica	INAF	Italy	Month 1	Month 42
9	Queen's University Belfast	QUB	UK	Month 1	Month 42
10	Astronomska opservatorija	AOB	Serbia	Month 1	Month 42
11	Institute for Spectroscopy RAS	ISLAN	Russian Federation	Month 1	Month 42
12	Russian Federal Nuclear Centre All-Russian Institute of Technical Physics	RFNC-VNIITF	Russian Federation	Month 1	Month 42
13	Institute of Atmospheric Optics	IAO	Russian Federation	Month 1	Month 42
14	Corporacion Parque Tecnologico de Merida	CTPM	Venezuela	Month 1	Month 42
15	Institute of Astronomy of the Russian Academy of Sciences	INASAN	Russian Federation	Month 1	Month 42



This project is funded under “*Combination of Collaborative Projects and Coordination and Support Actions*” Funding Scheme of The Seventh Framework Program of the European Union

Document

Deliverable number: D2.5
Deliverable title: Final Science/Technical Report
Due date of deliverable: December 2012
Actual submission date: January 2013
Authors: N. Walton, M.L. Dubernet and WP2 team
Work Package no.: WP2-NA1
Work Package title: Scientific/Technical Coordination of the network
Work Package leader: CMSUC/CNRS
Lead beneficiary: CMSUC/CNRS
Dissemination level: PU
Nature: Report
No of pages (incl. cover):

Abstract	The objective of D2.5 is to describe VAMDC Science/Technical Activities . This report corresponds to Activities in WP2: NA1 “Scientific/Technical Coordination of the network”.
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Versioning and Contribution history

Version	Date	Reason for modification	Modified by
V0.1	December 2012	Preparation of Document	M.L Dubernet
V0.1	December 2012	WP2 Report P3	N. Walton
V1.0	January 2013	D2.5 document	ML Dubernet

Final Version (v0.1) released by		Circulated to	
Name	Date	Recipient	Date
M.L. Dubernet	12 th February 2012	Mr Bodo	12 th February 2012

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WP2 ACTIVITIES DESCRIPTION

Work package number	2		Start date or starting event:			1				
Work package title	NA1: Science/Technical Coordination of the network									
Activity Type	COORD									
Participant id	1	2	3	4	6	7	9	14	15	
Person-months per beneficiary: (Total = EU + Node Contributions)	12	9	9	2	6	6	6	6	6	

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1. WP2 Objectives

NA1 provides the scientific and technical work necessary for the operation of the VAMDC e-infrastructure developing its structures and integrating with other data services and placing the VAMDC in a more global context. NA1 will also provide effort for VAMDC to participate and interact with external infrastructure and standards groups such as EGEE, Euro-VO and the IVOA.

The organisation of WP2/NA1, and the technical coordination of the network, is overseen by the VAMDC Executive Project Team (EPT)

The EPT includes WPs leaders (WP2 to WP8). The EPT will have monthly teleconference meetings as well as bi-annual face-to-face meetings. It will collect reports from the SAs and JRAs and prepare the annual technical reports for the VPB. The EPT will be chaired by the VAMDC Deputy (Technical) Coordinator who is a member of the VAMDC Project Board and will advise the VPB on the technical validity and relevance of the project strategic plans.

WP2 leader is CMSUC (2), with co-leadership by CNRS(1)

2. WP2 Milestones and Deliverables

Milestones

M2.1	Approval of WP Plan	WP2	CMSUC/CNRS	Month 3	
M2.2	EPT meetings	WP2	CMSUC/CNRS	Months 3, 10, 16, 22, 28, 34, 38, 42	
M2.3	Approval of Revised WP WorkPlan	WP2	CMSUC/CNRS	Months 10, 22, 34	
M2.4	Approval of Final WP Reports	WP2	CMSUC/CNRS	Month 42	

Deliverables

D2.1 Science / Technical (S/T) Plan (PM 3)

Annual reports will provide publicly available summaries of the activity of the EPT for each project year.

D2.2 S/T Report to be included in report to EU– Year 1 (PM 10)

D2.3 S/T Report to be included in report to EU– Year 2 (PM 22)

D2.4 S/T Report to be included in report to EU – Year 3 (PM 34)

D2.5 Final S/T Report to be included in final report to the EU (PM41)

Annual S/T Plan revisions included in Revised Annual VAMDC Project Plans – Year 1,2,3

Internal deliverables for year 2 activities are listed below.

3. WP2 Tasks Description (see Annexe I)

WP2 Leader	N. Walton (CMSUC(2))	
Task Number	Leader	Other Partners
1	N. Walton (CMSUC)	All others
2	N. Walton (CMSUC)	All others
3	T. Ryabchikova (INASAN)	All others
4	E. Roueff (CNRS/LUTH)	All others
5	E. Roueff (CNRS/LUTH)	All others

Task 1: Internal Technical Activities (lead by CMSUC(2), all partners)

Task 1 deals with cross disciplinary technical coordination, identification and evaluation of proposed generic tools, preparation of plans for testing and benchmarking activities. This task also includes the organisation of the EPT meetings.

Task 2: Connection to External Technical Project (lead by CMSUC(2), partners 1,3,4,14)

Task 2 deals with coordination with IVOA (International Virtual Observatory Alliance), Euro-VO, the IDIS Data service of the Europlanet EU Research Infrastructure, EGEE (European Grid E-science Environment). The EPT will host annual small focussed meetings/workshops where relevant people from the external projects will be invited to present the status of their achievements. The EPT will assess the degree of interoperability with those projects, which will in turn influence the output of task 1.

Task 3: Collect the users and producers specifications (lead by INASAN(15), all partners)

The EPT will gather users/producers requirements by a number of techniques such as questionnaires, small face-to-face meetings and so forth.

Task 4: Policies concerning Standards (lead by CNRS(1), all partners)

Task 4 will define, review and update the way standards will be adopted and to that effect it will interact with organisations promoting standards, e.g. external projects cited in task 2, NIST project for defining units in XML schema. Other organisations will be identified during the project if they happen to be relevant to VAMDC.

Task 5: Policies concerning publication in VAMDC (lead by CNRS(1), all partners)

Other missions of the EPT are to define, update and maintain the policies concerning the publication of resources in VAMDC.

4. WP2 Final Tasks Report

Period: 01/07/2009 – 31/12/2012

WorkPackage: 2: NA1: Science/Technical Coordination of the network

WorkPackage Leader and co-Leader: Nicholas Walton, Nikolai Piskunov/ML Dubernet

Participants in the WorkPackage: CNRS (1), CMSUC (2), UCL (3), OU (4), UU (6), KOLN (7), QUB (9), CPTM (14), INASAN (15)

Part 1

A summary of progress towards objectives and details for each tasks

NA1 provides the scientific and technical work necessary for the operation of the VAMDC e-infrastructure developing its structures and integrating with other data services and placing the VAMDC in a more global context. NA1 also provides effort for VAMDC to participate and interact with external infrastructure and standards groups such as EGI, Euro-VO and the IVOA

The **Executive Project Team (EPT)** is responsible for technical activities. The EPT includes WPs leaders (WP2 to WP8) – with the full membership given at <http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/Na1Ept>

The EPT has had monthly or every other month face to face or teleconference meetings – namely EPT 18 (19 Jul 2012), EPT 19 (26 Sep 2012) and the final EPT 20 (08 Nov 2012) – with minutes of each meeting available from <http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/Na1Ept>

The agenda at each meeting allows for reviews of activities across each WP, notes actions against plan, and records decisions on activities for the upcoming period.

During the course of the final part of the VAMDC project (P4) there have been no significant deviations from the originally planned activities in WP2. The detailed NA1 plan is available at:

<http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/CycleFourWp2>

Task 1: Internal Technical Activities: (lead by (1))

This activity deals with the cross disciplinary technical coordination, identification and evaluation of proposed generic tools, preparation of plans for testing and benchmarking activities.

The main activity in Year 3/4 period 4 has been in the continued technical coordination of the project, in particular the EPT, and the definition VAMDC programme of work. Planning for the testing and benchmarking supporting the role out of the Level 3 service (details available at <http://voparis->

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twiki.obspsm.fr/twiki/bin/view/VAMDC/VamdcServiceLevelThree) was completed, followed by the release of the final VAMDC service – see http://portal.vamdc.eu/vamdc_portal.

Task 2: Connection to External Technical Project (lead by (2) with (1),(3),(4),(14))

Coordination and interaction continued to take place with a range of relevant external partners. The interaction with the International Virtual Observatory Alliance has been through participation in a number of the IVOA working groups and attendance at the twice yearly IVOA InterOp meetings (Oct 2012 at Sao Paolo, Brazil - <http://wiki.ivoa.net/twiki/bin/view/IVOA/InterOpOct2012> - where Le Petit and Le Sidaner attended).

IVOA interactions ensure that VAMDC is aware of developments in the standards underpinning the technologies adopted by VAMDC – primarily registry, data access and grid and web services. Additionally the experience from VAMDC in the development of AM specific standards such as XSAMS, is brought to the attention of the IVOA community. In this manner, for instance, the TAP interface has been developed by VAMDC for data presented through the XSMAS interface.

Presentations at the Oct 2011 IVOA Interop importantly focussed on deployment and use of the VAMDC service. In addition, through Le Petit's leadership of the IVOA VO Theory working group, aspects related to the interface of A+M data and theoretical simulations are considered.

The Cycle Four final project meeting – see <http://vamdcmeeting.sciencesconf.org/> – included presentations from a range of external science domains. These included presentations from the atmospheric physics domain, radiation, plasmas. In addition there was a session devoted to publishers.

Task 3: Collect the users and producers specifications (lead by (15))

The census of all VAMDC resources available was maintained (see <http://voparis-twiki.obspsm.fr/twiki/bin/view/VAMDC/DeploymentResourceCensus>). This includes a statement on how these resources are currently made available and used.

In year two – a census of high performance codes required by the A+M community, and accessed via the VAMDC grid, was carried out – see <http://voparis-twiki.obspsm.fr/twiki/bin/view/VAMDC/GridCodesCensus>. This was maintained in year 3.

Following on from the year one user requirement gathering process, a range of interactions have been held with users, to gauge their experience of the beta release of the Level Two service release, including a specific session at the Year 3 project meeting. This feedback led to refinements in the user interface – witnessed in the Level 3 release to the community November 2012. Evaluation of the VAMDC service release will be carried out during the next SUPP@VAMDC project activity in 2013.

Task 4: Policies concerning Standards (lead by (1))

WP2, T4 defined the VAMDC policy on the implementation of the standard infrastructure and interfaces. Full details can be found at

<http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/Na1T4>

Agreement was reached with NIST as to the ownership of the XSAMS schema, whereby NIST is the responsible body for this standard. See <http://www.xsams.org>. In year three it was agreed that VAMDC will continue with the definition of implementation of further enhancements to XSAMS – with support for this carrying into the SUP@VAMDC project (2013-2014).

Task 5: Policies concerning publication in VAMDC (lead by (1))

The publication policy for VAMDC was developed in WP2, T5. This covered the acknowledgement for the use of VAMDC services, principles for referencing VAMDC by referring to the initial refereed paper describing the system.

The initial meeting of the SAB ratified the VAMDC draft policy on publications (authorship and credits) and the open source license under which all VAMDC developed infrastructure software have been released to the community.

Full details can be found at:

<http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/Na1T5> and the publication policy at <http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/VamdcPolPub>

Significant results (Activities and Deliverables)

D2.1 S/T Plan – DONE –

See <http://www.vamdc-project.vamdc.eu/public-deliverables/13-deliverables-wp2>

D2.2 S/T Report to be included in report to the EU – Year 1 – Done –

See <http://www.vamdc-project.vamdc.eu/public-deliverables/13-deliverables-wp2>

D2.3 S/T Report to be included in report to the EU – Year 2 – Done –

See <http://www.vamdc-project.vamdc.eu/public-deliverables/13-deliverables-wp2>

D2.4 S/T Report to be included in report to the EU – Year 3 – Done–

See <http://www.vamdc-project.vamdc.eu/public-deliverables/13-deliverables-wp2>

Annual Interoperability Plan revisions included in Revised Annual VAMDC Project Plans – Year 1,2, 3

See D1.2, D1.5, D1.7 <http://www.vamdc-project.vamdc.eu/public-deliverables/12-deliverables-wp1>

Deviations from the contract (Annex I) and reasons for them (if applicable)

Not applicable

Failures to achieve critical objectives and/or not being on schedule and reasons for them (if applicable)

Not applicable

Proposed corrective actions (if applicable)

Not applicable