# VAMDC

# Virtual Atomic and Molecular Data Centre

## D4.1

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## Infrastructure Deployment Plan

Version 0.4

Grant agreement no: 239108

Combination of Collaborative Projects & Coordination and Support Actions

## Project Information

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|---|---|
| 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 |
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| 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 | ISRAN | 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 | IVIC | Venezuela | Month 1 | Month 42 |
| 15 | Institute of Astronomy of the Russian Academy of Sciences | INASAN | Russian Federation | Month 1 | Month 42 |

## Document

| | |
|---|---|
| Deliverable number: | D4.1 |
| Deliverable title: | Infrastructure Deployment  Plan |
| Due date of deliverable: | September 2009 |
| Actual submission date: | |
| Authors: | G. Rixon, M.L. Dubernet |
| Work Package no.: | WP4-SA1 |
| Work Package title: | |
| Work Package leader: | CMSUC |
| Lead beneficiary: | CMSUC |
| Dissemination level: | PU |
| Nature: | Report |
| No of pages (incl. cover): | |

| Abstract | The objective of D4.1 is to describe VAMDC Infrastructure Deployment Plan on PM3. This plan corresponds to Activities in WP4: SA1 "Infrastructure Deployment". This plan is included in the VAMDC Project Plan. |
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**Versioning and Contribution history**

| Version | Date | Reason for modification | Modified by |
|---------|------|------------------------|-------------|
| V0.1 | 21/10/2009 | WP4 Draft – no plan for period 1 – no name | M.L. Dubernet |
| V0.2 | 22/10/09 | Add plans for period 1 | G. T. Rixon |
| V0.3 | 18/11/09 | Priority changes after kick-off meeting. New task 3.3. | G. T. Rixon |
| V0.4 | 22/02/2010 | Plan Cycle 1 – Task 2. Change T1.1 with selection of databases | M.L. Dubernet |

| Final Version (v0.4) released by | | Circulated to | |
|----------|------|-----------|------|
| Name | Date | Recipient | Date |
| M.L. Dubernet | 04/03/2010 | Mrs Asero | 04/03/2010 |
| | | | |

# WP4 ACTIVITIES DESCRIPTION

| Work package number | 4 | | Start date or starting event: | | | | 3 | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Work package title | SA 1: Infrastructure Deployment | | | | | | | | | |
| Activity Type | OTHER | | | | | | | | | |
| Participant id | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 12 | 13 | 14 |
| Person-months per beneficiary: (Total = EU + Node Contributions) | 66 | 36 | 36 | 12 | 6 | 6 | 8 | 11 | 5 | 9 | 24 |

## Table of Content

## 1. WP4 Objectives

To provide Data Access via a homogeneous environment where the distributed user community can retrieve AM resources through a standard interfaces. This involves implementing standard outputs for the AM databases, finding the resources by interrogating registries, using querying and pipeline tools.

WP4 leader is CMSUC (2)

## 2. WP4 Milestones and Deliverables

### Milestones

| M4.1 | Deployment of Data Access | WP4 | CMSUC | Months 10, 22, 34, 42 | |
|---|---|---|---|---|---|
| M4.2 | Deployment of Infrastructure | WP4 | CMSUC | Months 10, 22, 34, 42 | |
| M4.3 | Evaluation of Available Software | WP4 | CMSUC | Months 10, 22, 34, 42 | Testing by Users Panels of prototype software |
| M4.4 | Open Call for New Resources | WP4 | CMSUC | Month 24 | Text of Call Available on Public Website |

### Deliverables

*D4.1 Infrastructure Deployment Plan (PM 3)*
*D4.2 Infrastructure Deployment Report to be included in report to the EU – Year 1 (PM 10)*
*D4.3 Infrastructure Deployment Report to be included in report to the EU – Year 2 (PM 22)*
*D4.4 Infrastructure Deployment Report to be included in report to the EU – Year 3 (PM 34)*

> *D4.5 Final Report of Service Deployment to be included in final report to the commission (PM41)*
>
> *Annual Infrastructure Deployment Plan revisions included in Revised Annual VAMDC Project Plans – Year 1,2,3*

## 3. WP4 Tasks Description

| WP4 Leader | G. Rixon (CMSUC) | |
|---|---|---|
| Task Number | Leader | Other Partners |
| 1 | G. Rixon (CMSUC) | All partners |
| 2 | L. Molina (CNRS) | CMSUC (2), IVIC (14), UU (6) + others TBD |
| 3 | K. Benson (UCL) | CNRS (1), UU (6), RFNC-VNIITF (12) |
| 4 | TBD (UCL) – not cycle 1 | TBD |
| 5 | TBD (CNRS) – not cycle 1 | TBD |
| 6 | TBD (CNRS) – not cycle 1 | TBD |

**Description of work** (possibly broken down into tasks)

The VAMDC infrastructure will be designed as an homogeneous environment where any AM producer or "community" users will be able respectively to publish their AM data or to retrieve and manipulate those data. The AM producers range from atomic physics to molecular physics handling complex molecules, solids and surfaces. The communities encompass astrophysics users from very different areas: stellar, galaxies, interstellar medium (those application areas are handled by the IVOA and Euro-VO projects), planetology and small bodies of the solar system (EuroPlanet Project), solar-earth system (EGSO and SPASE projects), atmospheric users (studies of earth atmosphere), environmental and combustion chemistry, fusion physics and industrial applications. The IVOA community is the most advanced project as far as building an interoperable infrastructure for astronomy and we will use some of their achievements, i.e. standards, tools, services when those are relevant to the project.

*Task 1: Standard access to AM data (lead by CMSUC(2), all SA1 partners)*
We will provide standard service interfaces to AM databases. JRA1 will define these interfaces and this task is to implement them on the existing databases held by each VAMDC node. Participants at all nodes will be involved.

*Task 2: Standard access to numerical codes (lead by CNRS(1), with partners (2), (6) )*
Where a VAMDC node has a useful numerical code for AM analysis or modeling, we will make it available as a service. These services will provide a uniform way of launching the codes and recovering their outputs. This task is complementary to the grid adaptation of code in SA2: the codes run on resources contributed by the node owners and need not be made portable to an external grid.

*Task 3: Implementing registries (lead by UCL(3) with partners (1), (6), (12))*
The registry facilities defined by JRA1, and implemented with the software produced by JRA2, must be populated with information. This task gathers the meta data for the services at each node and adds it to the registries.

## 4. WP4 Tasks Description for Period 1

### Task 1: Standard access to AM data

*Task 1.1 TAP access to A-M data*
Using existing software from the Virtual-Observatory movement, implement Table Access
Protocol (TAP) services for sample nodes with data in relational databases.

TAP is the IVOA standard for remote access to relational databases.  It is a low-level
protocol, applicable to A-M physics as well as astronomy, suitable for prototyping VAMDC
applications and workflows. Because complete, reusable, TAP software is available to us at
no cost, TAP is a cheap way to make data available in year 1 of VAMDC before the
VAMDC-specific web-services are defined.

Various databases will be selected for this trial according to schedule: CHIANTI, XSTAR,
VALD, BASECOL, CDMS.

*Task 1.2 Ingest data into databases*
Ensure that all data-publishing nodes in VAMDC have their data copied into database
systems suitable for supporting the VAMDC-standard web-services to be defined by WP6 and
WP7.

Some VAMDC partners already have their data-sets stored in relational databases; others
keep their data in flat files. The web services foreseen in the early planning require all data to
be loaded into some kind of database. The exact kind of database depends on the design of the
services.

*Task 1.3 Install early prototypes of VAMDC-standard data-access services*
Acquire an implementation of the VAMDC-standard data-access service, as defined by WP6
and implemented by WP7. Install this on all VAMDC node that have achieved a suitable
database (as per task 1.2). Register the data-access service in the VAMDC registry.

These VAMDC-standard services will probably be based on the XSAMS data-model,
possibly using the XQuery query-language. They operate at a higher semantic-level than the
TAP services.

This task presumes that WP6 and WP7 produce a design and implementation suitable for wide deployment. It is possible that the new software does not become sufficiently mature for full deployment by the end of period 1. To conserve resources, two sites should be chosen for test deployment and evaluation before the software is deployed on all sites.

### Task 2: Standard access to numerical codes
*Task 2.1:* Make a census in order to inventory numerical codes likely to be turned into public services
Task 2.2: Propose solutions to establish  services in order to launch  codes in VAMDC environment – Test solution on one or two codes

### Task 3: Implementing registries
*Task 3.1 Choose a host for the VAMDC registry*
Select a VAMDC partner to run the registry.

In period 1, we need only one registry on a single site. Towards the end of the VAMDC project we may set up a mirror of this registry on a separate site.

*Task 3.2 Install registry software*
Install the AstroGrid registry-service component at the chosen registry site. Establish registry access for all VAMDC partners who need to register resources.

The registry software for this task is a web service available ready-to-run from AstroGrid. The task does not include populating the registry with information; when the task is complete, the registry will be available to publishers but will not contain all the metadata needed by end users.

*Task 3.3 Register existing resources*
Register the existing, web-browser interfaces to data sets.

### Task 4: Augmenting VODesktop
*Task 4.1 Distribute TAP-capable copy of VODesktop*
Ensure that all VAMDC staff have access to a version of VODesktop that works with the early-access TAP services. Make this software available for download from the VAMDC site.

By the time that VAMDC needs it, the default version of VODesktop should be suitable.

*Task 4.2 Extend VODesktop to work with VAMDC-standard data services*
Add code to VODesktop such that it can query the new prototypes of the VAMDC data-services deployed in task 1.3.

This task is only possible once WP6 designs the service protocol. If that design is not stable during period 1, it is not worth altering VODesktop; instead, we should produce simpler, disposable clients to test the services.

**Internal deliverables**

- TAP services for selected sites – month 7
- VAMDC-standard data-access services – month 9
- Registry service, ready for publishing, not fully populated – month 6

- Registration of web-browser (pre-VAMDC) interfaces – month 7
- VODesktop version for TAP services – month 4