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XSAMS: XML Schema for Atomic and Molecular Data and Particle Solid Interactions

Summary Report of an IAEA Consultants' Meeting

IAEA Headquarters, Vienna, Austria

10–11 September 2009

Prepared by

D. Humbert and B.J. Braams

International Atomic Energy Agency, Vienna, Austria

January 2010

IAEA Nuclear Data Section, Vienna International Centre, 1400 Vienna, Austria

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Abstract

Developments in computer technology offer exciting new opportunities for the reliable and convenient exchange of data. Therefore, in 2003 the Atomic and Molecular Data Unit initiated within the collaborative efforts of the A+M Data Centres Network a new standard for exchange of atomic, molecular and particle-solid interaction (AM/PSI) data based on the Extended Markup Language (XML). The standard is named XSAMS, which stands for XML Schema for Atoms, Molecules, and Solids. A working group composed of staff from the IAEA, NIST, ORNL, Observatoire Paris-Meudon and other institutions meets approximately biannually to discuss progress made on XSAMS, and to foresee new developments and actions to be taken to promote this standard for AM/PSI data exchange. Such a meeting was held 10-11 September 2009 at IAEA Headquarters, Vienna, and the discussions and results of the meeting are presented here. The principal concern of the meeting was the preparation of the first public release, version 0.1, of XSAMS.

January 2010

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IAEA Consultants' Meeting: XSAMS: XML Schema for Atomic and Molecular Data and Particle Solid Interactions

10–11 September 2009, IAEA Headquarters, Vienna

Attendees:

Mr D. Humbert, IAEA (*Scientific Secretary*)
Mr R. Forrest, IAEA, (*Opening*)
Mr B.J. Braams (IAEA)
Ms M.-L. Dubernet (France)
Ms E. Roueff (France)
Mr S. Gagarin (Russian Federation)
Mr P. Loboda (Russian Federation)
Ms H.-K. Chung (United States of America)
Mr R.E.H. Clark (United States of America)
Mr Yu. Ralchenko (United States of America)
Mr D. Schultz (United States of America)

Welcome and Opening of the Meeting

Participants were welcomed by Dr Robin Forrest, Head of the Nuclear Data Section. He pointed out the importance of the development of an efficient tool for data exchange in atomic and molecular physics and wished success to the meeting, the main objective of which is the release of version 0.1 of XSAMS. Dr Bas Braams welcomed the participants and briefly introduced himself. Dr Braams is the new Head of the A+M Data Unit, replacing Dr Bob Clark who retired at the end of July 2009.

1. Introduction

XSAMS has been tested successfully on the IAEA ALADDIN database and the NIST Atomic Spectra database; exploratory tests were also carried out on the Spectr-W3 spectroscopic database in Russia and the BASECOL collision database in France. The schema has been stable over the past year, although the documentation and web site have been revised over that time. The main objective of the present meeting is to define the procedure and set the launch date for the first public release of XSAMS (version 0.1).

The previous meeting report and the agenda were adopted without modifications.

2. Presentation of the Schema at Various Technical Meetings

ICAMDATA, Beijing, China, 28-31 October 2008

One oral paper (Yu. Ralchenko et al.) and one poster (D. Humbert et al.) with focus on XSAMS were presented at the conference. The project received a warm welcome from data users as well as data producers, who agree on the need for a reliable tool for data exchange. Many participants are ready to test XSAMS as soon as a stable release is available.

F-VAMDC meeting, Meudon, France, 11-12 December 2008.

XSAMS is foreseen as the tool for data exchange within the VAMDC project. XSAMS was presented and discussed in multiple contributions at the first French National VAMDC meeting.

XVI Symposium on High-Resolution Molecular Spectroscopy, Lake Baikal, Russia, 5-10 July 2009
Marie-Lise Dubernet presented XSAMS in her talk on VAMDC at HighRus-2009, and then in more detail in a discussion session with VAMDC collaborators.

IAEA Data Centre Network Meeting, Vienna, Austria, 7-9 September 2009
Yuri Ralchenko presented progress on XSAMS at the IAEA Data Centre Network meeting. Members of the DCN are very involved in the XSAMS projects as developers and as users.

3. XSAMS in the VAMDC Project

Marie-Lise described the status of the VAMDC project, <http://www-vamdc.eu/>. There are 21 partners in the project, and it has received EU funding for a period of 42 months starting 1 July 2009. An intended outcome is to have a laboratory without walls concerned with molecular spectroscopy microwaves and ultrawaves. The group has a very strong database focus. The virtual laboratory is built on existing structures including XSAMS, which is a major standard for VAMDC. The virtual laboratory looks forward to the 1st release of XSAMS.

There will probably be an IAEA representative on the VAMDC advisory group, and it is intended to invite an IAEA representative at each VAMDC meeting.

4. Review of the XSAMS Status

As some participants were new to XSAMS Yuri Ralchenko provided a review of the schema. He explained the tree structure and demonstrated the flexibility of XSAMS. Only a few changes were implemented since the last meeting. It was nevertheless proposed:

- To introduce a list of elements for the “ElementSymbol” element
- To set a rule to associate the element “Z” and the element “ElementSymbol”

At the end of the meeting some proposals of Peter Loboda for improvements in the schema were discussed. Proposal elements include:

- Ritz, Observed, Theory
- Name of the line
- Single electron transition
- Uc and Ud as new parameters
- New radiative transition types
- Branching ratio
- Total life time, radiative and non-radiative
- Q_D, Q_C
- Total radiation prob and total radiation with
- EnergWaveLength mandatory?

Action on these issues was deferred to the next XSAMS technical meeting, after the release of version 0.1.

5. Action from Last Meeting

Actions from last meetings were reviewed.

- Namespace and location of web pages: one site at IAEA.

- The function block has been revised and tested successfully on a few examples on ALADDIN.
- For missing values (in case of multidimensional tables) in the “Datalist” element, the problem is solved.
- The problem to create an automatic LaTeX index for all types and attributes in the documentation is not solved. This topic is considered as minor for the time present. It may be of interest to transcribe the LaTeX documentation into html.
- The 3 types (User, IAEA Code and XSAMS codes) to describe a process are kept.

6. XSAMS Website

The IAEA will be the official and unique web site for XSAMS (<http://www-amdis.iaea.org/xsams/>). The IAEA will host the schema and the documentation. It was not considered of interest to have a mirror site.

The namespace for XSAMS will be at the IAEA at <http://www-amdis.iaea.org/xsams/schema/xsams-0.1.xsd>. It was agreed to have the version of the schema in the name space location. A domain name will be bought for XSAMS as “xsams.org”; the IAEA (Bas Braams) will be responsible of the custody and the maintenance. The fact that the IAEA website could be out of service was brought up, raising again the utility to have a mirror site. With a domain name for XSAMS, in case of a failure of service at the IAEA, the domain name can be automatically switched to a second server (at NIST for example). Nevertheless the server at the A+M Data Unit showed a very stable operation, with rare cuts, over the last years. It was decided not to consider the case for the moment.

The web site was thoroughly reviewed. Modifications were done during coffee breaks. The website was approved by everyone at the end of the session. Some future improvements were proposed:

- XSAMS logo was approved.
- The possibility was discussed to post on the web site the XMLSPY generated documentation. This can be done in the near future.
- A history page should be developed to keep track of updates.
- As contact the AMD Unit will check the possibility to have a generic email for XSAMS as xsams@iaea.org
- All publications on XSAMS will be posted on the website.

The traffic to the schema page may be an issue once NIST will make available its data in XML, using XSAMS. It was decided to merge all containers (sub-files) into one file. The schema version will then appear in the name. The name space schema location is <http://www-amdis.iaea.org/xsams/schema/xsams-0.1.xsd>. All sub files will also be accessible.

7. Documentation

The first version of the XSAMS documentation is ready. The first page was reviewed. A version in html should be developed. The creation of an index for types and attributes was postponed.

As a reminder, the inside structure of a chapter uses the following rules:

- Section and sub-sections should always refer to a type
- All diagrams are a type representation
- All types have a tag to be referenced in the index table
- All paragraphs are separated by a blank line with no indentation

Action: to provide Yuri with materials to produce the complete document by 15 November 2009.

8. Working Methods and Web Maintenance

Committee to evaluate proposed changes. Bug reports and suggestions will be sent to the XSAMS Google Group as the forum for developers and users involved in the project.

The XSAMS googlecode is not used. Most of the participants are not familiar with the functioning of googlecode. The AMD Unit mentioned the difficulty to access the web site as the vsn protocol is not permitted at the IAEA. It was decided not to use XSAMS googlecode for now. It is recommended to everyone to make nevertheless an evaluation on the interest of googlecode.

Pending items:

1. Units, link with UNITSML.
2. Isoelectronic series, isonuclear sequences, branching ratio, line shift.
3. Band properties: system, type, origin, transition energy, oscillator strength, head.
4. Raman transitions.

9. Working Plan and Time Schedule

Launch of XSAMS 0.1 to take place in September still. The release will be announced on the Daff email list (Denis), and to IVOA and VAMDC (Marie-Lise).

The meeting was adjourned at 15:00 as the room was reserved for the ICAMDATA board meeting. The following milestones and working plan is summarized:

- 16 Sep 2009 Release of XSAMS 0.1
- 23 Oct 2009 VAMDC kick-off meeting
- Sep 2010 ICAMDATA, Vilnius

A date and a location for the next XSAMS meeting will be discussed on the XSAMS Google forum. Besides having it in Vienna also the option to meet in conjunction with a VAMDC meeting will be considered.

10. Miscellaneous

Peter Loboda drew attention to the 10th International Conference “Zababakhin Scientific Talks”, 15-19 March 2010, at the All Russia Research Institute of Technical Physics, Chelyabinsk region. The conference is concerned with high energy density physics.

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AGENDA

Thursday 10 September

09:30-11:00

1. Opening, *Robin Forrest, NDS Head*
2. Last meeting minutes review and adoption of the agenda
3. Reports on presentation of the schema to various technical meetings if any
4. I3-FP7 VAMDC, *Marie-Lise*
5. Review of present "XSAMS" status
 - Overview *Yuri*
 - Atomic data *Yuri*
 - Solid *Dave*
 - Molecular data *Marie-Lise*
 - Processes
 - 1. Radiative transitions *Evelyne*
 - 2. Non-Radiative transitions *Denis, Bob*
 - 3. Collisions *Denis, Bob*
 - Biblio *Dave*
 - Functions, methods *Denis*
 - Types and attributes *Yuri*
 - Review of present "XSAMS" status

11:00-11:30 *Coffee break*

11:30-13:00 **Actions from last meeting**

6. sourceRef of type IDREFS
7. NonRadiative replaces Ionization
8. Choice of value 0 or -1 in case of missing data in the "Datalist" element
9. Fit Functions
10. Check Latex possibilities to create an automatic index for all types

13:00-14:00 *Lunch*

14:00:15:00 **Web site**

11. XSAMS web site (<http://www-amdis.iaea.org/xsams/index.html>)
 - Namespace: NIST or IAEA
 - Review of the web pages
 - Web pages at NIST?
 - Logo approval
 - Miscellaneous

15:00-15:30 *Coffee break*

15:30:17:00 **Documentation**

12. Documentation (<http://www-amdis.iaea.org/xsams/documents/>)
 - Classification of Processes (Annex D, XSAMS List of Processes)
 - Logo without trailer
 - Missing chapters

Friday 11 September

09:00

Morning

13. Forum to report suggestions or problems: XSAMS googlegroup?
14. Status on the XSAMS googlecode site
15. DAL and Registry
16. Comments, corrections, new developments and unresolved issues from last meeting:
 - units, link with UNITSML
 - isoelectronic series, isonuclear sequences, quantum defects, average atom
 - isotopes

Afternoon

17. Collaboration, links with VAMDC
18. Working plan and milestones
19. Launch of version 0.1

Estimated end of day 2: 16h

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