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Summary Report of an IAEA Consultants' Meeting

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

Congress Room No. 5, Beijing Friendship Hotel, China
27 October 2008

Prepared by

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International Atomic Energy Agency, Vienna, Austria

February 2009

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Abstract

Advanced developments in computer technologies offer exciting opportunities for new distribution tools and applications in various fields of physics. The convenient and reliable exchange of data is clearly an important component of such applications. Therefore, in 2003, the A+M Data Unit initiated within the collaborative efforts of the DCN (Data Centres Network) a new standard for atomic, molecular and particle surface interaction data exchange (AM/PSI) based on XML (eXtensible Markup Language). The schema is named XSAMS which stands for "XML Schema for Atoms Molecules and Solids". A working group composed of staff from the IAEA, NIST, ORNL and Observatoire Paris-Meudon meets 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 on 27 October 2008, and the discussions and progress made in the schema are considered within this report.

February 2009

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

27 October 2008, Friendship Hotel, Beijing, China

Present

Mr D. Humbert, IAEA *(Scientific Secretary)*
Mr Yan Jun *(Opening of the meeting)*

Attendees:

Mr R.E.H. Clark (IAEA)
Ms M-L. Dubernet (France)
Ms E. Roueff (France)
Mr Yu. Ralchenko (United States of America)

Welcome and Opening of the Meeting

The ICAMDATA conference in Beijing provided the meeting facility for this one day CM on XML. Participants were welcomed by Dr Yan Jun, chairman of the local ICAMDATA organizing committee. He pointed out the importance of the development of an efficient tool for data exchange in atomic and molecular physics. The ICAMDATA conference has the goal to gathering data producers, developers and data users in the fields of atomic and molecular physics as well as plasma-surface interactions. One session is dedicated to data exchange, and the results of our work were of very high interest to attendees. An oral paper and one poster on XSAMS will be presented during the conference.

1. Introduction

Due to time constraints, the CM focused on the release of the first version of XSAMS. The main topics discussed are the problems encountered by developers to implement the schema on different databases and the release of the documentation.

Minutes from the previous meeting and the agenda were adopted with no further modifications.

2. XSAMS

Participants agreed that XSAMS is preferred to xSAMS, and stands for **X**ML **S**chema for **A**toms, **M**olecules and **S**olids.

3. Presentation of the Schema at Various Technical Meetings

Progress on XSAMS was presented at the ADAS meeting in September. ADAS is joining the IAEA Data Centre Network and will bring valuable contributions to the development of XSAMS.

4. Namespace

NIST confirmed that they will host all schema files and documentation, as the official XSAMS web site. Nevertheless, the important role of the IAEA in the development of the schema was underlined. The IAEA should therefore act as mirror site for XSAMS, also hosting all schema files and documentation – only available web site for XSAMS at the present time is at the IAEA (http://www-amdis.iaea.org/xsams/).

5. Review of Status of XML Schema

The physics part of the schema is now very stable, with some improvement needed in only the physics of 'Solids'. The main points addressed by developers were as follows:

- **sourceRef of type IDREFS**: some source databases require different sources for the numerical data – essential to keep not only the traceability on the production of the data, but also the history of the xml file generation. Traceability is therefore of two types:
    - origin of the data production,
    - history of the xml file.

  The last bibliography reference is sufficient for data production, and the user should refer to this publication to define the further history of the data. File generation is a little more difficult; the file may have been manipulated by different tools or users, as for example, a file generated by GENIE which will merge together xml files from different databases. As no satisfactory solution was proposed, the decision was taken to make the 'sourceRef' an attribute of type 'IDREFS'.
  Action: find a better solution (*everyone*).
- Noted that a 'sequence of unbounded elements' rather than an 'unbounded sequence of one element' is preferred in XSAMS.
- **Units**: Unless there is a major conflict, XSAMS will adopt "Unitsml" as the standard once "Unitsml" is released. Meanwhile, a short list of values according to defined rules was set at the last meeting in August 2008. Minor new accepted propositions are:
    - actual definition of powers apply only to positive powers,
    - negative powers are considered as division using positive powers,
    - arbitrary units are coded 'ArbitraryUnits'.
- '**AutoIonization**' is replaced by '**NonRadiative'**. This will encompass all one single element transitions: radiative and non-radiative. Non-radiative transitions include for example autoionisation, autodissociation and any other single-reactant non-radiative processes.
  Action: Review the ICAMDATA presentation (*Yuri*).
- **Reference Frame**: for some collision data it is essential to know in which reference frame the energy is calculated. A new element named 'ReferenceFrame' of type 'ReferenceFrameType' is introduced with the following enumeration: CenterOfMass, LaboratoryFrame, TargetFrame.
- **Enumerations** have a standard format: UpperCamelCase.
- If data in enumeration are missing, or the schema does not fulfill the description of some A+M/PSI data, problem should be reported on the XSAMS forum for a quick solution. If some problems can be solved quickly such as a missing value in an enumeration, others may prove more problematic and result in some delay. For the case of undefined quantum numbers representation for molecules, the schema is flexible enough to provide a temporarily solution.
- **Methods**: Methods has as attribute 'functionRef'. This reference indicates that the tabulated numerical data are issued from the fit function referenced by the 'functionRef' attributes. No parameter values and fit validity limits are provided in this case.
- **sourceRef, methodRef and functionRef** have no specific type because they are only used as attributes. **StateRef** has its own specific type 'StateRef'.
- **DataXY:** all 'Datalist' elements must have the same number of values. This could be a problem as one value in a data list may have no defined uncertainty – recommended to use the

value 0 or -1. This case only applies to the error data list; X or Y data lists cannot mathematically have any gap.
Action: choice of the best value: 0 or -1 (*everyone*).

- **Functions:** ALADDIN is the only database at present using fit functions to provide numerical data and the actual schema can not accommodate a usable description of the fit data. Therefore, the schema needs some improvement. Agreed that the 'Function' element will not only describe the mathematical expression of the function, but will also explain the physics. The collisions part will only give the numerical values of the parameters and the validity limits of the fit function.
  Action: *Denis* to propose a better solution.

Action: review the schema according to the above remarks (*everyone*).
New xsd files will be sent to Yuri or posted on the xsams google site for version 0.1. The schema, in version 0.1, should be ready by Friday, 7 November 2008.

6. Documentation

Good progress has been made in the formulation of appropriate XSAMS documentation. All contributions must be merged in a consistent way. The overall structure and presentation of the documentation were discussed. From the previous meeting and from new decisions, the overall structure was established:

- Introduction and overall document *Yuri Ralchenko*
  - Motivation
  - Requirement (domain covered by the schema)
  - Limitations
  - Overall XSAMS structure
- sources *Dave Schultz*
- statesAtoms *Yuri Ralchenko*
- statesMolecules *M-L Dubernet*
- statesSolids *Dave Schultz*
- processes
  - radiative *Evelyne Roueff*
  - non-radiative *Evelyne Roueff*
  - collisions *Denis Humbert*
- functions *Denis Humbert*
- methods *Denis Humbert*
- types and attributes *Yuri Ralchenko*
- rules and convention adopted to build XSAMS: naming convention….

This layout represents approximately 13 chapters, although they may not appear in this order in the final release. The radiative, nonRadiative and Collisions sections are separate chapters.

An index will be established for all types.
Action: check the LATEX possibilities *Denis and Marie-Lise.*

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 2008.

7. Collaboration

A proposal for a I3-FP7 project in support of XSAMS development and applications. I3-FP7 (see INDC-(NDS)-0537 with weblink) passed through the first phase of approval. France, with M-L. Dubernet as coordinator, is the leading country of the project. EU partners are UK, Germany, Austria, Sweden and Italy. External partners are Russian Federation, Venezuela and USA. China, Japan, Belgium and Netherlands are expected to join the project if funded. Unfortunately, the IAEA as an international organization cannot join this project.

If the project is not accepted this year, the next I3-FP7 call for applications is planned in spring 2010.

8. Working Plan and Time Schedule

The following milestones and working plan are summarized:

- **28-31 Oct** **ICAMDATA, Beijing, China**
- 7 Nov 2008 Version 0.1 posted on the xsams google site
- 15 Nov 2008 Draft document posted on XSAMS Google group or given to Yuri *(everyone)*
- tbd *NIST web site*
- tbd Next meeting in Paris or Vienna

9. Future Meeting

A date and a location for the next meeting will be agreed later.

Appendix A

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

27 October 2008, Congress Room No. 5, Beijing Friendship Hotel, China

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Appendix B

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

27 October 2008, Congress Room No. 5, Beijing Friendship Hotel, China

AGENDA

Monday, 27 October

09:00 Opening, Dr. Jun Yan

1. Last meeting minutes review and adoption of the agenda
2. Reports on presentation of the schema to various technical meetings
    a. ADAS workshop, 30 Sept-1 Oct 2008
    b. Other
3. ICAMDATA: talk, posters, demo
4. Schema review
    - Update from last meeting (*Yuri + Denis*)
    - Questions and unresolved issues (*attached document XSAMSreview*)
5. Classification of processes
   Attached Dave document, version 0.2: Reactant-Process-Codes-v0.2
    a. Atomic and molecular collisions
    b. Particle surface interactions
6. Comments, corrections, new developments and unresolved issues from last meeting:
    - structure consistency, rules: draft document *(Denis)*
    - units, link with UNITSML
    - isoelectronic series, isonuclear sequences, clusters, branching ratio, air and Stark broadening

12:30 – 13:30 *Lunch break*

13:30

7. XSAMS applications
    - ASD, *Yuri*
    - ALADDIN, *Denis*
    - BASECOL, *Marie-Lise*
8. Web site and Space Name: IAEA *(Denis)*, NIST *(Yuri)*
9. XSAMS Logo
10. Documentation, *All*
11. Data Access Layer *(pending item)*
12. XSAMS web registry (*pending item)*
13. Collaboration, XSAMS googlegroup and googlecode
14. Work plan, milestones and next meeting

15:00 ***Adjournment of meeting***

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