IAEA
International Atomic Energy Agency

INDC International Nuclear Data Committee

Summary Report of Consultants' Meeting

XML Schema for Atomic and Molecular Data

IAEA Headquarters, Vienna, Austria
2–3 April 2007

Prepared by

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July 2007

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Abstract

Advanced developments in computer technologies offer exciting opportunities for new distributed 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 AMD Unit initiated within the collaborative efforts of the DCN (Data Centre Network) a new standard for atomic, molecular and particle surface interaction data exchange (AM/PSI) based on XML (eXtensible Markup Language). A working group composed of staff from the IAEA, NIST, ORNL and Observatoire Paris-Meudon, meets biannually to discuss progress made on the XML schema and to foresee new developments and actions to be taken to promote this standard for AM/PSI data exchange. This meeting is the first such gathering of these specialists in 2007.

July 2007

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IAEA Consultants' Meeting: XML Schema for Atomic and Molecular Data

2–3 April 2007, IAEA Headquarters, Vienna, Austria

<u>Present</u>

Mr. D. Humbert, IAEA *(Scientific Secretary)*

Attendees:

Mr. Yu. Ralchenko (United States of America)
Mr. D.R. Schultz (United States of America)
Ms. M-L. Dubernet (France)
Ms. E. Roueff (France)
Mr. R.E.H. Clark (IAEA)
Mr. V. Zerkin (IAEA (*part-time*))

ESA Workshop on "Astronomical Spectroscopy and Virtual Observatory" 21-23 March 2007

Evelyne Roueff presented a report on the workshop, and noted that the full agenda is accessible on the ESAC web site:
http://esavo.esac.esa.int/SpectroscopyAndVOWorkshopMarch2007/program.html
Presentations will be available later on the ESAC web site

XML Schema

Yuri Ralchenko explained that the schema is now split into different "containers" to improve maintenance. A single person is responsible for each container, with Yuri coordinating the *General schema*:

- general schema   *Yuri*
- biblio   *Dave Schultz*
- functions   *Denis Humbert*
- methods   *Denis Humbert*
- types and attributes   *Yuri Ralchenko*
- statesAtoms   *Yuri Ralchenko*
- statesMolecules   *M-L Dubernet*
- statesSolids   *Dave Schultz*
- singleReactanctProcess and multiReactantProcess   *Bob, Denis, Yuri*

This structure will be reviewed to check the possibility of merging two containers into one in order to simplify the structure and provide a better description of the physics. For example, absorption and emission are currently separated in *multiReactantProcess* and *singleReactantProcess*, but are essentially the same kinds of processes and therefore

should be described in the same way. Another issue is a consistent method to describe multiphoton absorption and emission. A new structure for all processes will be proposed by the end of April.

Action for each container:

- Check element name syntax.
- Check on structure consistency: *particles* → *particle* → *....*
- Check bounded and unbounded tags for consistency.

Action: new container: *Processes* by end of April.

Molecules

The method used to describe formula needs to be improved, perhaps through collaboration with NIST. The inChI (IUPAC International Chemical Identifier) method has been added.

Solids

Further discussions took place on the inclusion of temperature as a definition of a surface. Agreement was reached that temperature is a property of the surface. Most participants also agreed that data dependent on surface temperature should be described in a convenient way (e.g. reflection coefficient of a particle at fixed angle and fixed energy versus surface temperature). This approach would preclude entering a different surface for each temperature (which would be impossible in the case of a fitting function for temperature). This problem has some similarities to data that define the energy levels of H_2 vs. the vibrational excitation level. Can this last example be included in the schema with H_2 (no excitation level or ground state) and dataXY (X with n = 1,2,3,… and Y giving the energy)?

Actions:

- Dave to prepare a schema (or UML) to be presented later to a committee of experts (Eckstein, …).
- Next IAEA CRP on surface erosion (September 2007): first RCM should include a short presentation of AMDML in order to obtain comments from the PSI community.

Multi reactants process

If possible, *mutiReactantProcess* will be merged with s*ingleReactantProcess*. Processes can be "self-defined" or selected from the "Recommended Classification of Processes" compiled for DANSE and GENIE. The list of data types has to be improved: x-section, rate coefficient, differential x-section, and collision strength. The description of *dataXY* has not been solved.

Action: Denis to provide the list of processes.

Additional notes

- **BibMethRef**: mandatory as the left-hand entry; all others optional. If no meaningful information is available, can be set to "generic".
- **Units**: should include values with no units: (e.g. ratio).

- **Lifetime**: total lifetime is a property of an atom or molecule, and part of *stateAtoms* or *stateMolecules*. Lifetimes related to oscillator strength and transition probabilities are part of *singleReactantProcess*.
- **Z and isoelectronic series**: example of atomic data depending on Z arose from discussions on surface temperature. These data cannot be entered in the present version of the schema. Isoelectronic series are also not included in the schema.

Namespace, Registry, DAL

These topics should be brought up through a recognized international group. The problem is how to create and organized such an international body. Discussions resulted in some suggested actions:

- A+M Data Unit to check the history of INDC.
- Our project should maintain a web site. As this project is not fully related to fusion, such a web site cannot be hosted by the IAEA. NIST also cannot take responsibility, since the on-going study is not a NIST project. One solution might be to run the site with its own domain name.
- Find a logo and a proper name, since AMDML does not refer to PSI.

  Actions:

  Create home page: *Denis*
  Web site: *Yuri* to check the possibilities at NIST. *Denis and Marie-Lise* to check costs and procedure to adopt in creating a domain name (e.g. www.amdml.org)
  Everyone to make propositions for a domain name.

Communications/publicity concerning the existence of our project need to be improved. Information on our meetings will be posted on the AMD Unit web site. A first workshop on "A+M/PSI Data Exchange" will be held at NIST on 3, 4 May 2007. An annual Technical Meeting (TM) could be organized, may be at Meudon in 2008, with also the possibility of organizing meetings at ISSI and Lorentz Centre.

  Action: Information to be posted on the A+M Data Unit web site: *Denis*

Agreement was reached during the discussions that a first version of the XML schema (version 1.0) should be released by the end of 2007.

Collaboration

Yuri reported strong interest from the Republic of Korea and the Russian Federation to participate in this project. ROK (NFRC and KISTI) is developing databases for A+M/PSI with special focus on low temperature plasmas. Russia is interested through the SPECTR-W3 project. The workshop at NIST could also bring new collaborations.

Marie-Lise reported the possibility within the EU to develop a collaborating program (IUP FP7 Collaborating program).

Draft Document

No immediate need was expressed.

NIST Workshop on "A+M/PSI Data Exchange"

The first workshop will be held at National Institute of Standards and Technology (NIST), Gaithersburg, MD, USA from 3 to 4 May 2007.

Work Plan and Time Schedule

Monthly informal contacts will be made to monitor progress made on the XML schema. Following reviews of individual topics, different actions would be proposed and milestones formulated.

- Denis to send the list of processes "Recommended Classification of Processes".
- Yuri to send the new XML schema, with containers.
- By end of April:
    - html pages on AMDML meetings to be placed on the IAEA A+M Data Unit web site, beginning of April, *Denis.*
    - Home page proposition, end of April, *Denis.*
    - Review of each container (syntax, consistency), by end of April, *everyone.*
    - Reviewed schema for SingleReactantProcess and MultiReactantProcess, end of April, *Denis, Bob, (Yuri).*
    - Release of a new version of AMDML, *Yuri.*
- **NIST workshop on "A+M/PSI Data Exchange", 3-4 May 2007.**
- Presentation of the XML schema at 1st RCM of the IAEA CRP on "Surface Erosion", September 2007.
- **1-2 October: XML meeting in Vienna.**
- Presentation on progress to be made to the DCN (3-5 October 2007).
- *Nov-Dec 2007, XML meeting in Paris (to be decided 1-2 October 2007).*
- **Version 1.0 of the XML schema by end of 2007.**
- *March-April 20007: AMDML Meeting (to be decided 1-2 October 2007).*
- *First half 2007, TM in Paris (to be decided 1-2 October 2007).*

Next Meeting

Two days before the DCN meeting (1-2 October 2007).

IAEA Consultants' Meeting: XML Schema for Atomic and Molecular Data

2–3 April 2007, building-A, floor-23, room-11 (A23-11), IAEA Headquarters, Vienna, Austria

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MEETING AGENDA

<u>Monday, April 2</u>

09:15   Opening

Morning

1.   ESAC Workshop "Astronomical Spectroscopy and Virtual Observatory" 21-23 March
      2007.   *Evelyne*

2.   Review of present AMDML status
- Overview: *Yuri*
- Atomic data   *Yuri*
- Solid   *Dave*
- Molecular data   *Marie-Lise*
- Reactions   *Denis*
- Actions from last meetings (naming convention, frequency/energy/wavelength,…)

Afternoon

3.   Comments, corrections, new developments and unresolved issues from last meeting
- list of processes
- element "dataXY"
- list of data types: cross sections, reaction rates…
- structure consistency (see notes from last meeting, 6.)
- biblio
- units

Estimated end of first day 17h

<u>Tuesday, April 3</u>

09:00   Meeting Continued

Morning

4.   UML data model   *Denis*
5.   Data Access Layer
6.   AMDML web registry *(pending item)*
7.   Space name for "containers" *(pending item)*
8.   Draft document

Afternoon

9.   Collaboration
10. Call of the EU FP7 concerning building an infrastructure for exchange of atomic and molecular data   *Marie-Lise*
11. NIST Workshop on "AMD/PSI data Exchange", 3-4 May 2007
12. Work plan to next meeting and conclusions
13. Dates for next meetings

Estimated close 17h