XSAMS: history, evolution, etc.

XSAMS

XML Schema for Atoms, Molecules, and Solids

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Why

- There is a need for a unified, standardized approach to A&M data exchange
  - Baltimore fire, 1904
    - 70 city blocks, >1500 buildings, 140 acres, 1231 firefighters
    - 600 hundred sizes and variations of hose couplings
  - GENIE search engine
    - Data retrieval from several databases
  - NLTE Code Comparison Workshop
    - GBytes of data to exchange

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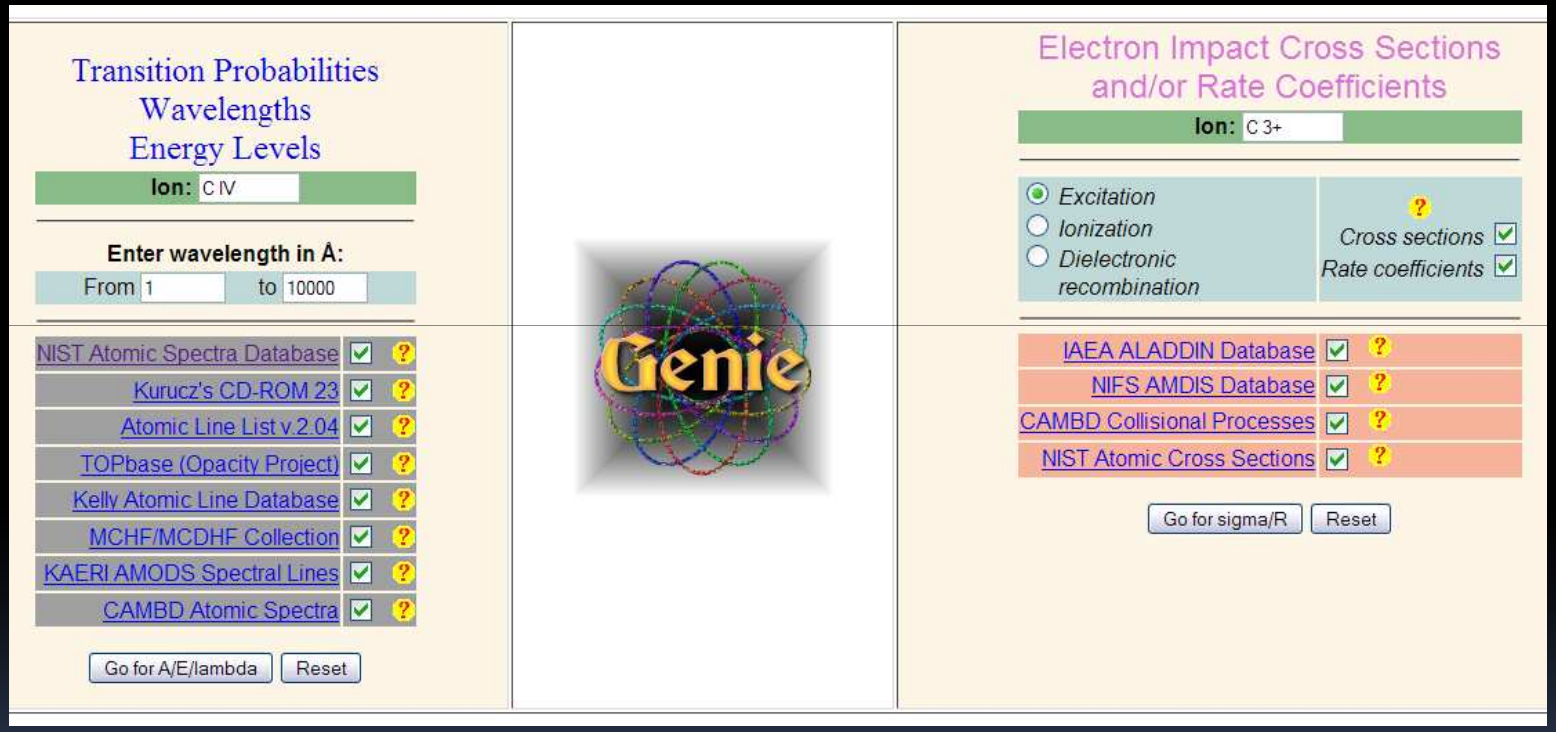
GENIE search engine



http://www-amdis.iaea.org/GENIE/

AMDML to XSAMS

- IAEA Data Center Network Meeting, Oct 2003
  - Atomic and Molecular Markup Language (AMDML), later became XSAMS
- IVOA: SLAP development
- ICAMDATA-2004, Toki, Japan
- Series of technical meetings at the IAEA, Austria and Paris, France (mainly supported by IAEA)
- Last meeting: March 2010, NIFS, Japan
  - Mar 26: first XSAMS file delivery

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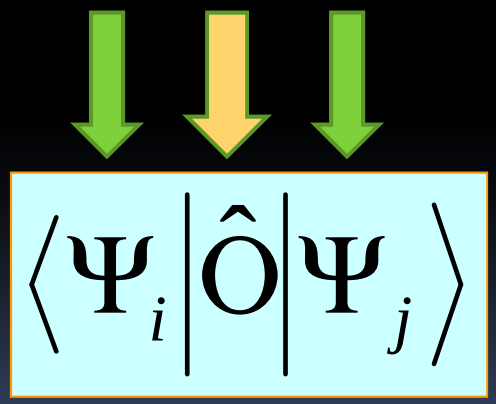
XSAMS Development Team

- IAEA, Austria
  - B.J. Braams
  - H.-K. Chung
- Obs. Paris-Meudon, France
  - M.-L. Dubernet (UPMC)
  - E. Roueff
- Oak Ridge Nat. Lab, USA
  - D.R. Schultz
- VNIITF, Russia
  - S. Gagarin
  - P.A. Loboda
- NIST, USA
  - Yu. Ralchenko
- Former participants
  - R.E.H. Clark
  - N. Moreau
  - D. Humbert

Atoms
Molecules
Programmers

Goal of XSAMS

- To develop a (rather) complete set of rules (tags, document structure, relations, etc.) for description of XML A&M data sets

A&M world: 

XSAMS

XML Schema for Atoms, Molecules, and Solids

http://www-amdis.iaea.org/xsams/

Current version 0.1

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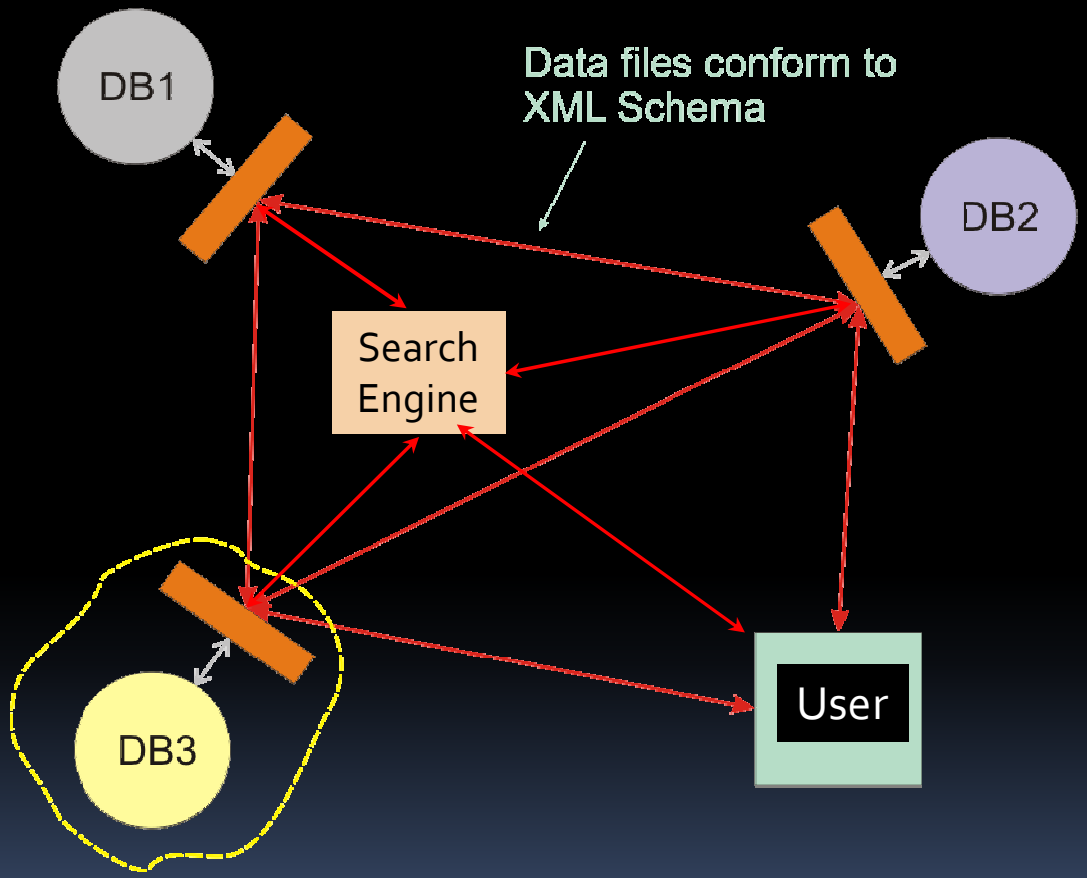
XSAMS: what it is and what it is not



XSAMS: what it is and what it is not

- Representation of AM physics through XML tagged structure
- Description of the format for the data file to be exchanged
- (*Partial*) Verification that whatever is exchanged is real physical data
- Verification that the exchanged data is exchanged correctly
- ***Draft*** schema
- Discussions, tests, new ideas are WELCOME

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SLAP (VOTable) from ASD NIST

- <TD>5.1020e-06</TD>
- <TD>O VII 51020 A</TD>
- <TD>O</TD>
- <TD>conf='1s.5d' term='3D' J='1'</TD>
- <TD>conf='1s.5p' term='3P*' J='1'</TD>
- <TD>1.14168974850248e-16</TD>
- <TD>1.14130040516339e-16</TD>

Table data entries are not verified

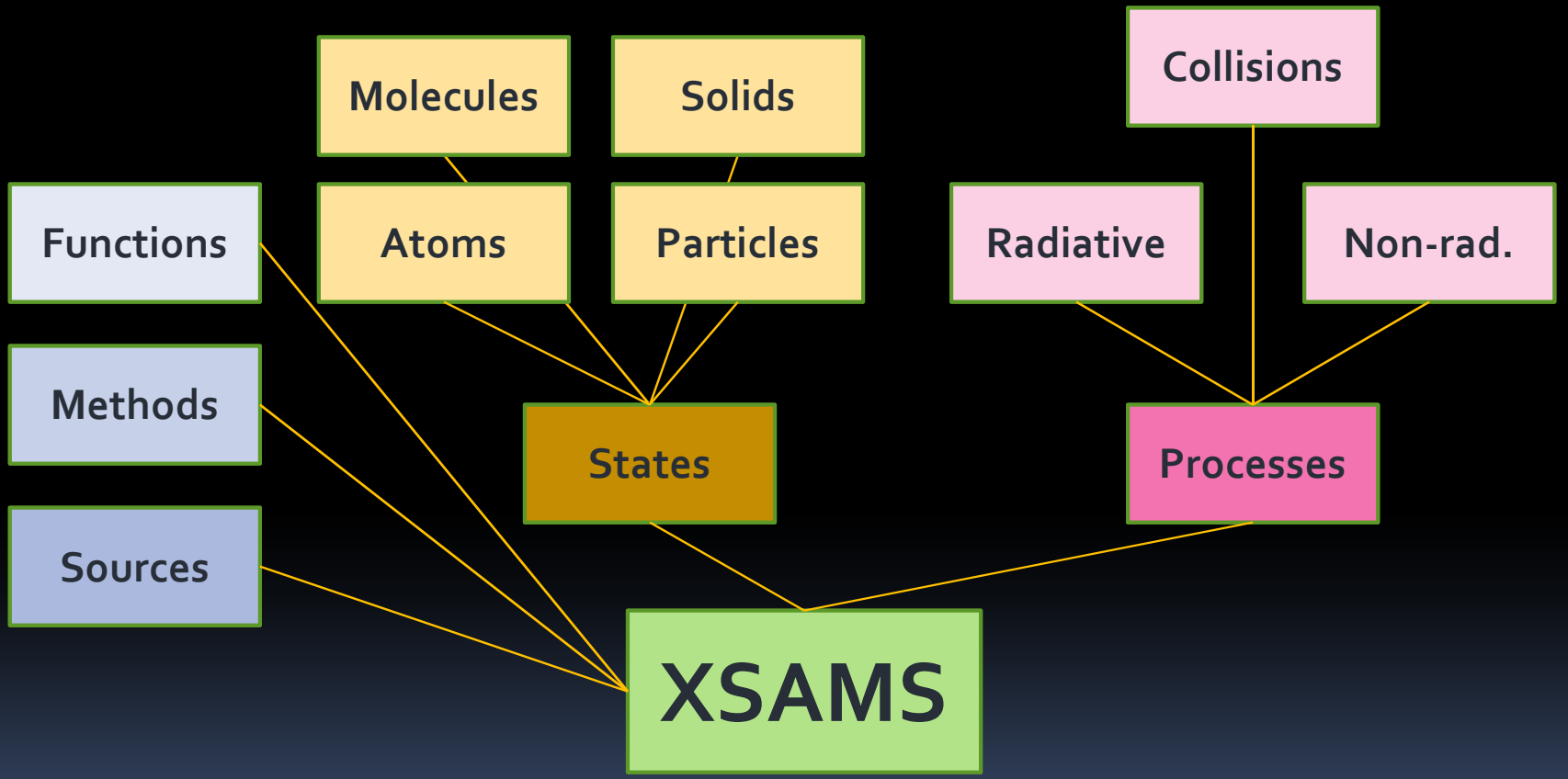
XSAMS: what it is and what it is not

- Not a format of a data file: it is a description of the format
- Not a format for data storage
  - DBMS better to be used
- Not an application or code
- Not good for tiny datasets
- XSAMS files are not created to be searched for data

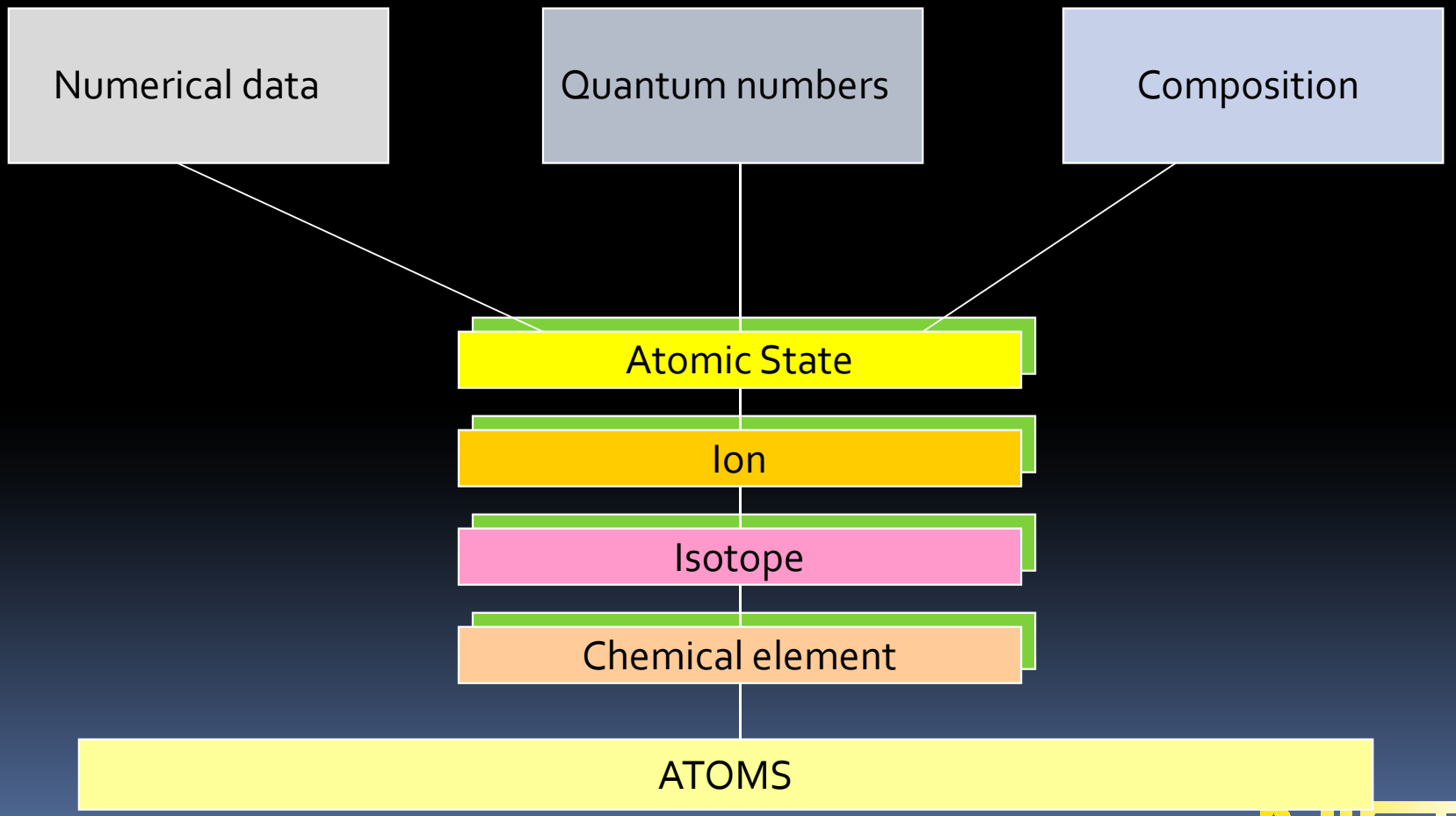
- Something mainly created by physicists, NOT programmers

XSAMS tree

$$\langle \Psi_i | \hat{O} | \Psi_j \rangle$$



XSAMS tree: atoms



XSAMS tree: atoms (cont'd)

- Numerical data
  - Energy (from g.s.)
  - Ionization energy
  - Lande factor
  - Quantum defect
  - Life time
  - Polarizability
  - Statistical weight
- Quantum numbers
  - Parity
  - Total angular momentum
  - Hyperfine momentum
  - Magnetic quantum number

…and composition

Where?

- Molecules
  - BASECOL
- Atoms
  - SPECTR-W^3
  - NIST (levels, testing phase)
- Collisions
  - IAEA

…and more and more

Current issues with XSAMS

- Tree vs. Case-by-case $\Psi = \Psi(\alpha, \beta, a, b, A, B, E, \ldots)$
- Speed
  - Usage frequency vs. file generation time
    - Is 20 seconds for a 10000 line query executed once in a while acceptable?
    - Programmatic issues: MySQL queries can be optimized…others?
- Units: use UnitsML in the future?
- Compactness vs. correctness?

New proposed modifications and extensions

- Atomic states
  - Seniority
- Environment
  - Species
  - Density
  - Temperature (or energy distribution function)
  - Pressure
  - Dimensions
- External fields
  - Electrical
  - Magnetic
  - Radiation
- Radiative transitions
  - Ritz, exp, theor -> attr
  - Dielectronic satellites
  - Extra label: K_{α}
  - Transition type (Raman etc)
- Line shapes and broadening
  - Doppler width
  - Natural width
  - Collisional width
  - Shifts
  - Broadening coefficients

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Discussions

- New ideas are **WELCOME**…
  - We should agree what is important:
    - Speed of file generation
    - File size
    - Data verification (although not validation)
- …but **prove is needed**

Who has the final word over XSAMS?

- IAEA sponsored all technical meetings but has never provided any additional funding (web site is there though)
- IAEA seems to be interested in supporting further development through meeting organization
- XSAMS group partially overlaps with VAMDC
- Currently VAMDC is leading the effort, at least for molecules
- Answer: right now it's the XSAMS development group but this may change in the future