Atomic, molecular and particle-surface interaction web databases and data exchange

Lecture 4
New Trends in Data Exchange

ICTP Workshop on Atomic and Molecular Data for Fusion Energy Research
Trieste, 20-30 April 2009

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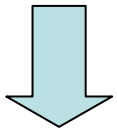
Content

1. **Atomic and Molecular Data Unit of the IAEA**
2. **Bibliographic data**
3. **Numerical data**
4. **New Trends in Data exchange**
   - History
   - XML
   - AM/PSI XML applications
   - XSAMS a XML Schema for Atoms, Molecules and Solids
   - Future

Why we need **NEW METHODS**

- Old methods (e.g., ALADDIN) are clearly outdated
- Data exchange is presently determined by internet technologies (IT)
- New techniques are permanently developed
- Structured data, consistency, relationships



To teach different *databases* and *applications*
to speak the same language

Old Standards for Data Exchange

- Mid-1980: ALADDIN (A Labeled Atomic Data INterface)
- What delivered
  - ASCII files of a fixed format
  - Included set of fit functions
- Set of FORTRAN-77 subroutines for reading and processing the files
- Major problems:
  - limited amount of data
  - not flexible
  - very restricted usage
  - too old!

ALADIN Format

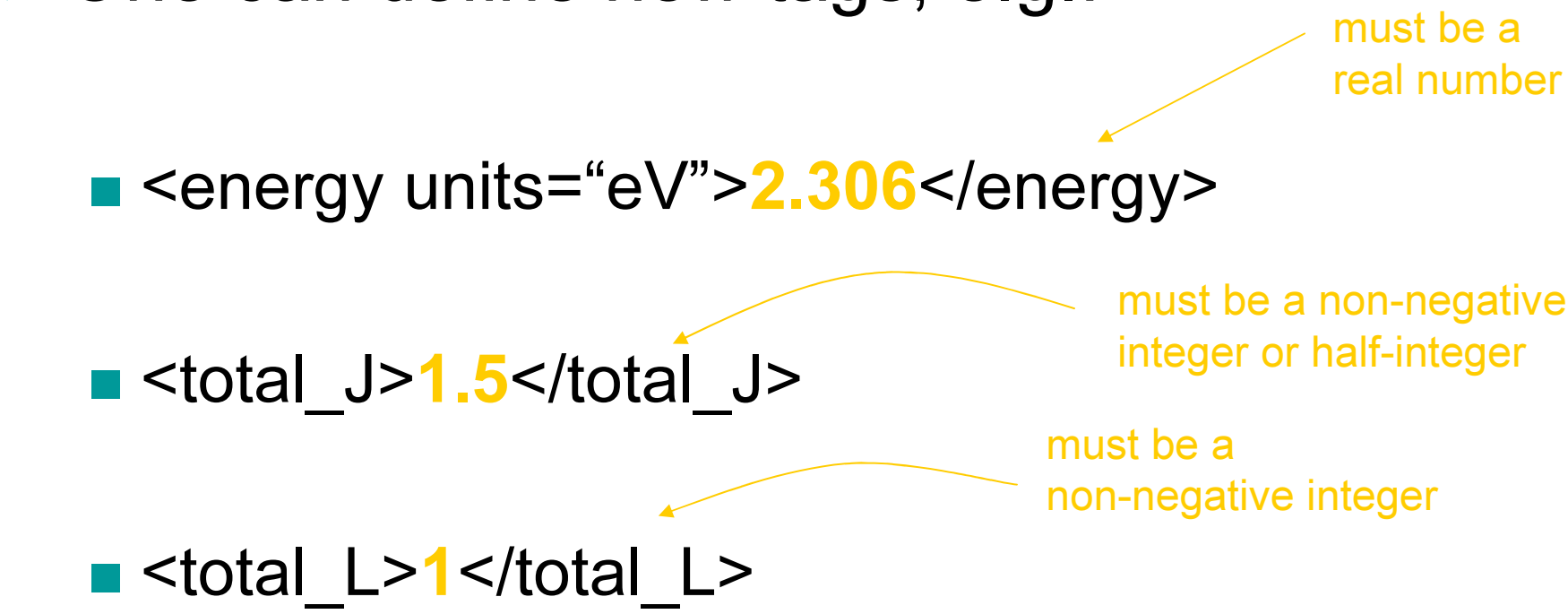
```
$ CX C [+1] H [+0]
& XS EVAL ACC=C ORNL-CFADC DOC=ORNL-6090 20/06/89 #CHEB
! This is a typical data entry from the ORNL "Redbook" series of
! recommended atomic collision data
-74.279300000 -1.752060000 -2.426830000 -0.689407000 0.025926900
-0.091239700 0.005814900 0.095765200 -0.042658600 50.000 330000.0
```

Tools for development of data exchange standards

- **XML**: e**X**tensible **M**arkup **L**anguage
- Metalanguage: tool for development of new languages
- XML facilitates the sharing of data across different systems, particularly systems connected to the internet
- XML is an important medium for exchanging, integrating, and storing data from diverse sources
- XML separates content from presentation

Example: **atomic energy level**

- HTML:
- One can define new tags, e.g.:

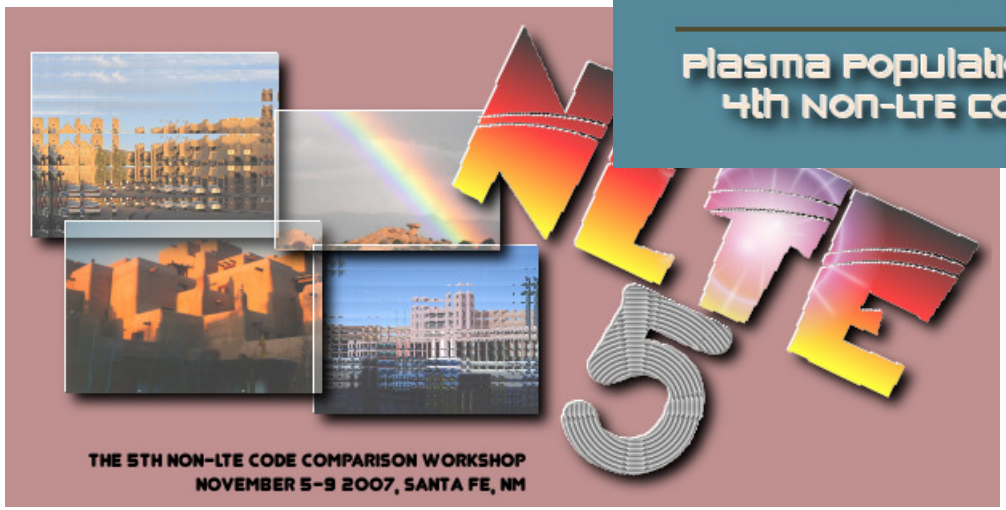


Applications in AM/PSI Physics

- NLTE Workshops
- IVOA
  - Spectral Line Data Model
  - SLAP
- XSAMS

NLTE Code Comparison Workshops

http://nlte.nist.gov/SAHA



http://nlte.nist.gov/NLTE4

International Virtual Observatory Alliance

- IVOA: 16 national VO's
- Mission: to *facilitate the international coordination and collaboration necessary for the development and deployment of the tools, systems and organizational structures necessary to enable the international utilization of astronomical archives as an integrated and interoperating virtual observatory*
- Develop various (XML-based) standards for data querying and exchange (Simple Line Access Protocol etc.)

IVOA Spectral Line Data Model

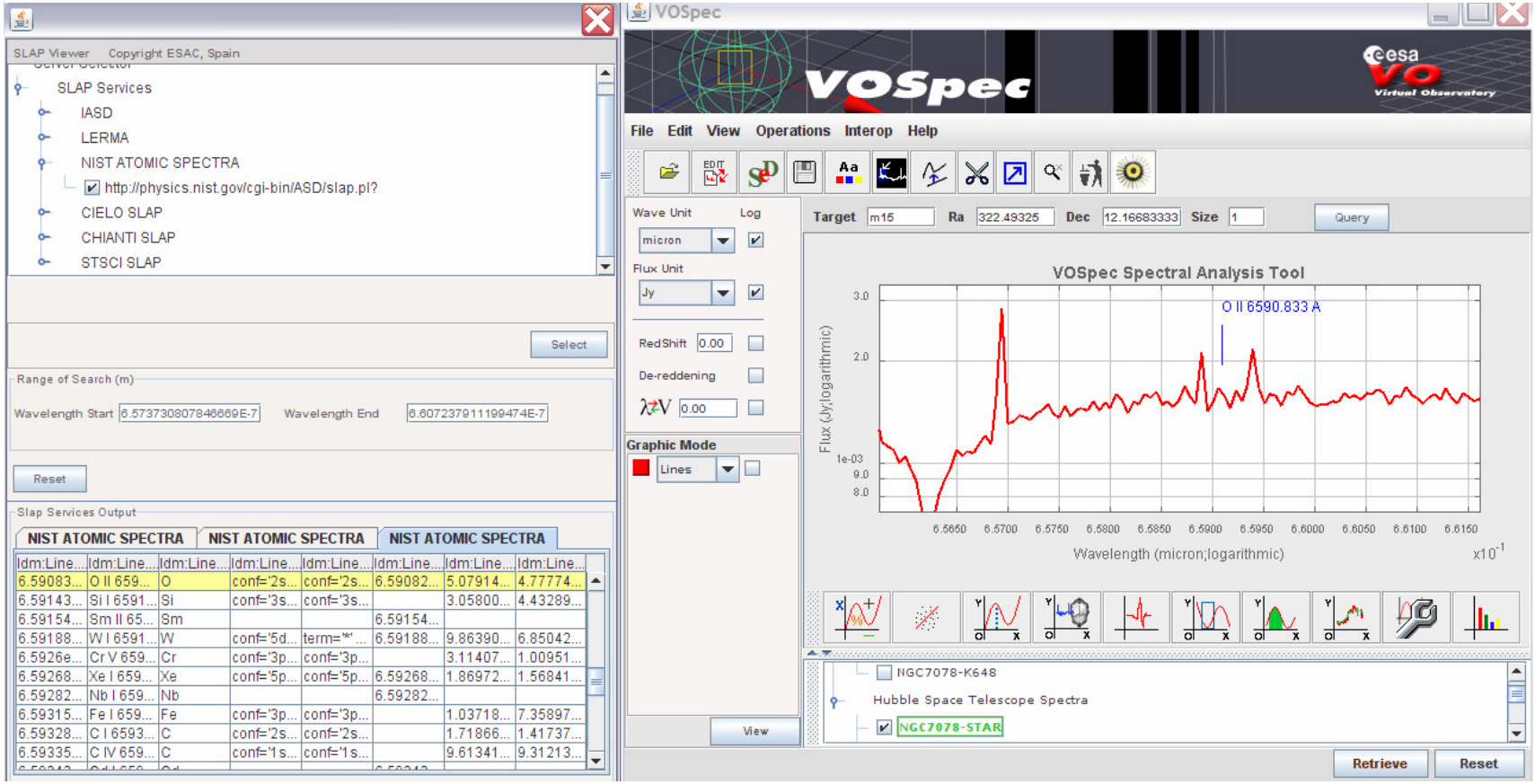
- Main feature: **line oriented!**
- Line Data Model
  - Level
    - Quantum state
      - Quantum number
  - Process
  - Environment
- Spectral Line Access Protocol (SLAP)
- Main data carrier: VOTable

http://physics.nist.gov/cgi-bin/ASD/slap.pl?WAVELENGTH=5.1E-6/5.6E-6

VOSpec: http://esavo.esa.int/vospec/

IVOA VOSpec example

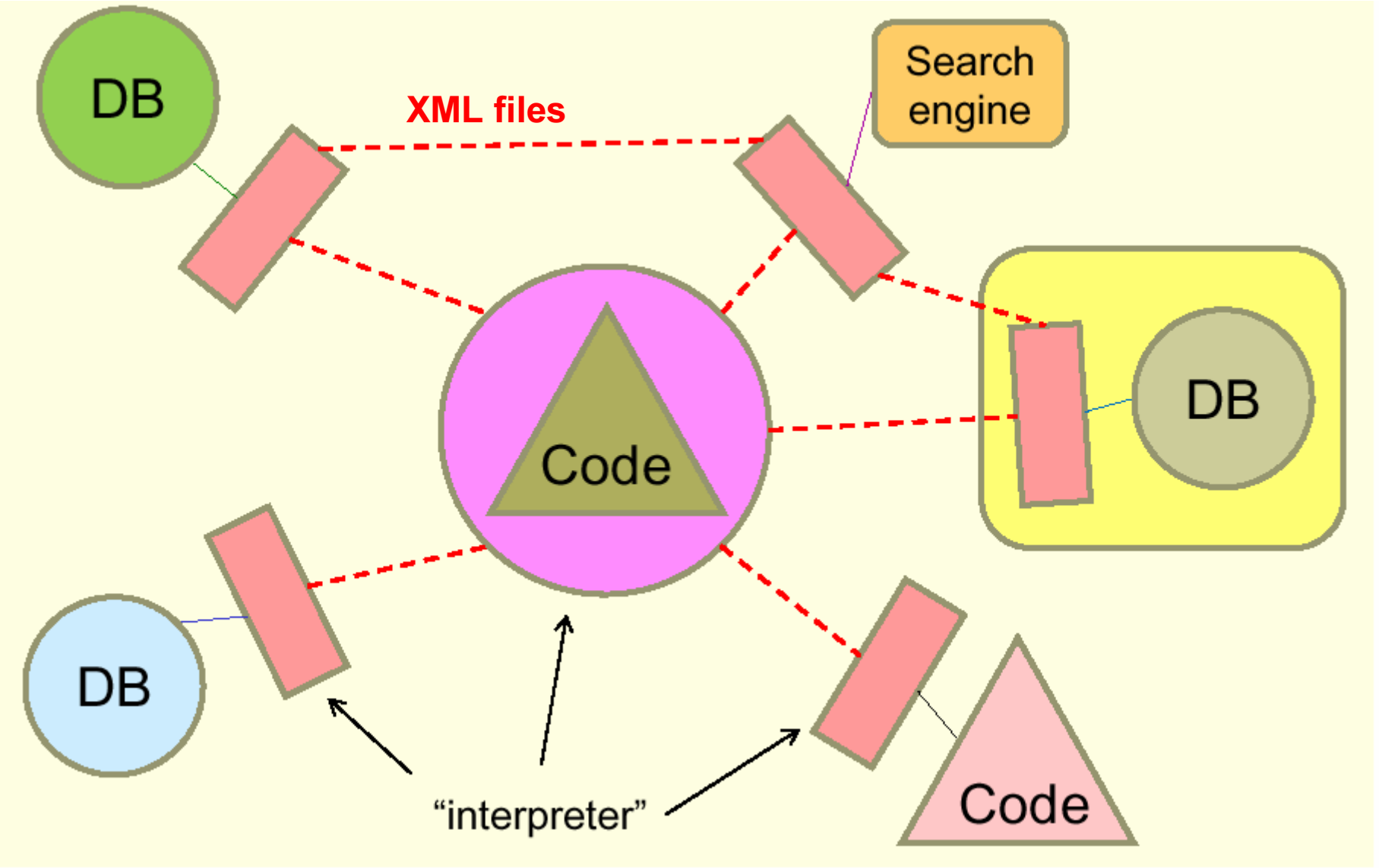
http://esavo.esac.esa.int/vospec/



VOtable output

```
<?xml version="1.0"?>
<VOTABLE version="1.1" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instan
 xsi:noNamespaceSchemaLocation="http://www.ivoa.net/xml/VOTable/v1.1">
  <RESOURCE name="results">
    <INFO name="QUERY_STATUS" value="OK" />
    <TABLE>
      <DESCRIPTION>Output from the NIST Atomic Spectra Database</DESCRIPT
      <FIELD name="Wavelength" ID="wl" utype="ldm:Line.wavelength" ucd="e
      <FIELD name="Title" ID="title" utype="ldm:Line.title" ucd="em.line"
      <FIELD name="Element" ID="element" utype="ldm:Line.species.name" uc
      <FIELD name="IniLev" ID="inilev" utype="ldm:Line.initialLevel.name"
      <FIELD name="FinLev" ID="finlev" utype="ldm:Line.finalLevel.name" u
      <FIELD name="ObsWl" ID="obswl" utype="ldm:Line.observedWavelength"
      <FIELD name="IniLevEn" ID="inien" utype="ldm:Line.initialLevel.ener
      <FIELD name="FinLevEn" ID="finen" utype="ldm:Line.finalLevel.energy
      <DATA>
        <TABLEDATA>
          <TR>
            <TD>5.000509e-07</TD><TD>Fe I 5000.509 A</TD><TD>Fe</TD><TD>c
          </TR>
          <TR>
            <TD>5.00086e-07</TD><TD>La II 5000.86 A</TD><TD>La</TD><TD></
          </TR>
          <TR>
            <TD>5.0009e-07</TD><TD>Ti I 5000.9 A</TD><TD>Ti</TD><TD>conf=
          </TR>
```

AM/PSI Data Exchange Strategy



XSAMS

- XML Schema for Atoms, Molecules and Solids
- Development suggested at the 2003 IAEA DCN meeting
- Start up at 2004, Toki, Japan
- Attempt to structure the whole field of AM/PSI physics

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

XSAMS Development Team

- IAEA, Austria
  - *R.E.H. Clark*
  - *D. Humbert*
- Obs. Paris-Meudon, France
  - *M.-L. Dubernet*
  - *E. Roueff*
- ORNL, USA
  - *D.R. Schultz*
- VNIITF, Russia
  - *S. Gagarin*
  - *P.A. Loboda*
- NIST, USA
  - *Yu. Ralchenko*

IAEA
International Atomic Energy Agency
Atoms for Peace

ВНИИТФ

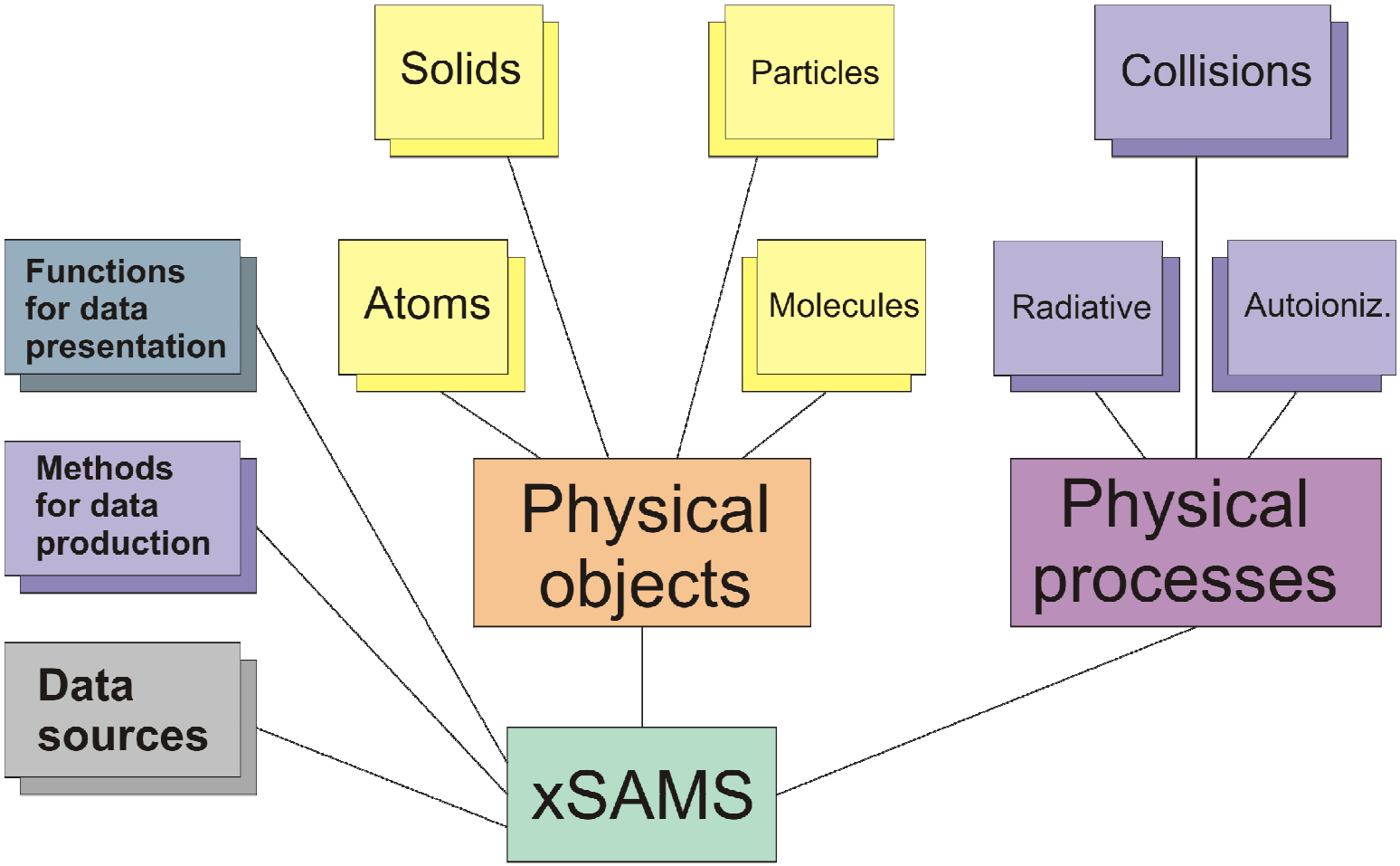
NIST
National Institute of Standards and Technology
U.S. Department of Commerce

l'Observatoire de Paris

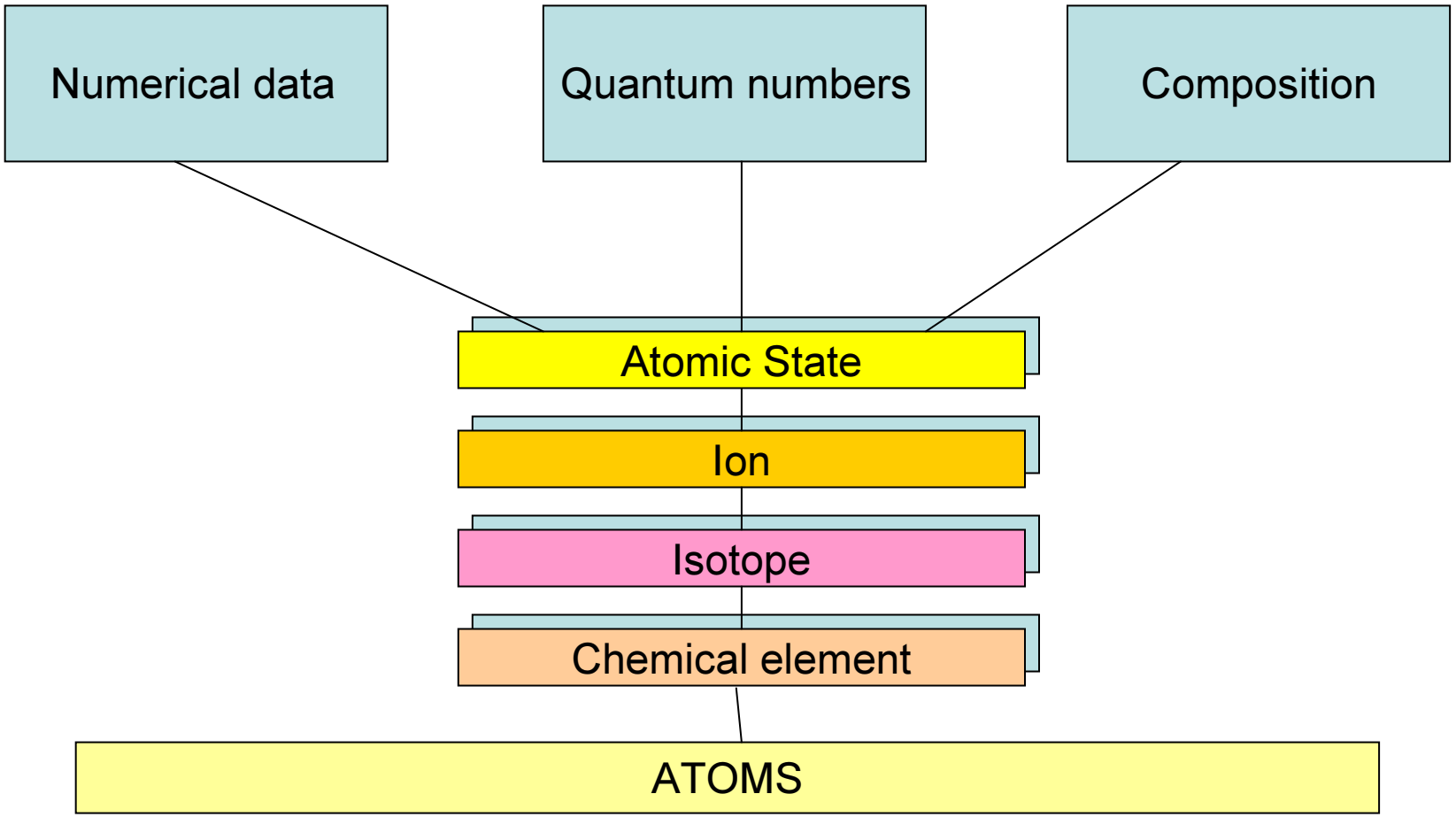
Development Issues

- Project initiated within the DCN in October 2003
- Technical meetings twice a year in Paris or Vienna
- Collaboration with CRAAMD (China) and NIFS (Japan)
- Development of DB interfaces
  - NIST ASD
  - IAEA ALADDIN
  - BASECOL, Observatoire de Paris
  - SPECTR-W3, VNIITF, Russia
- Presentation and panel discussion at ICAMDATA, 28-31 October 2008, Beijing, China

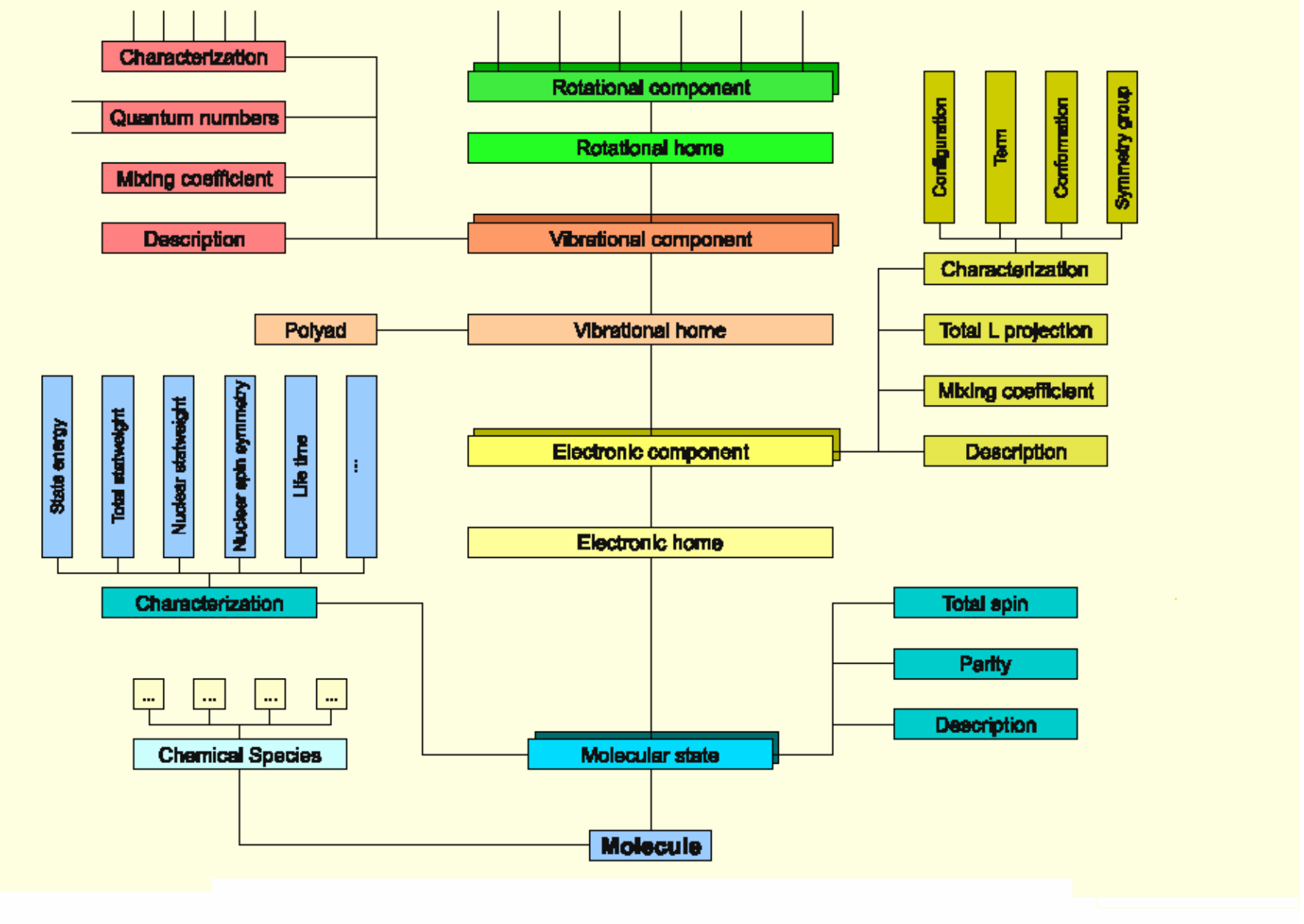
xSAMS tree


Solids
Particles
Collisions
Functions for data presentation
Atoms
Molecules
Radiative
Autoioniz.
Methods for data production
Physical objects
Physical processes
Data sources
xSAMS

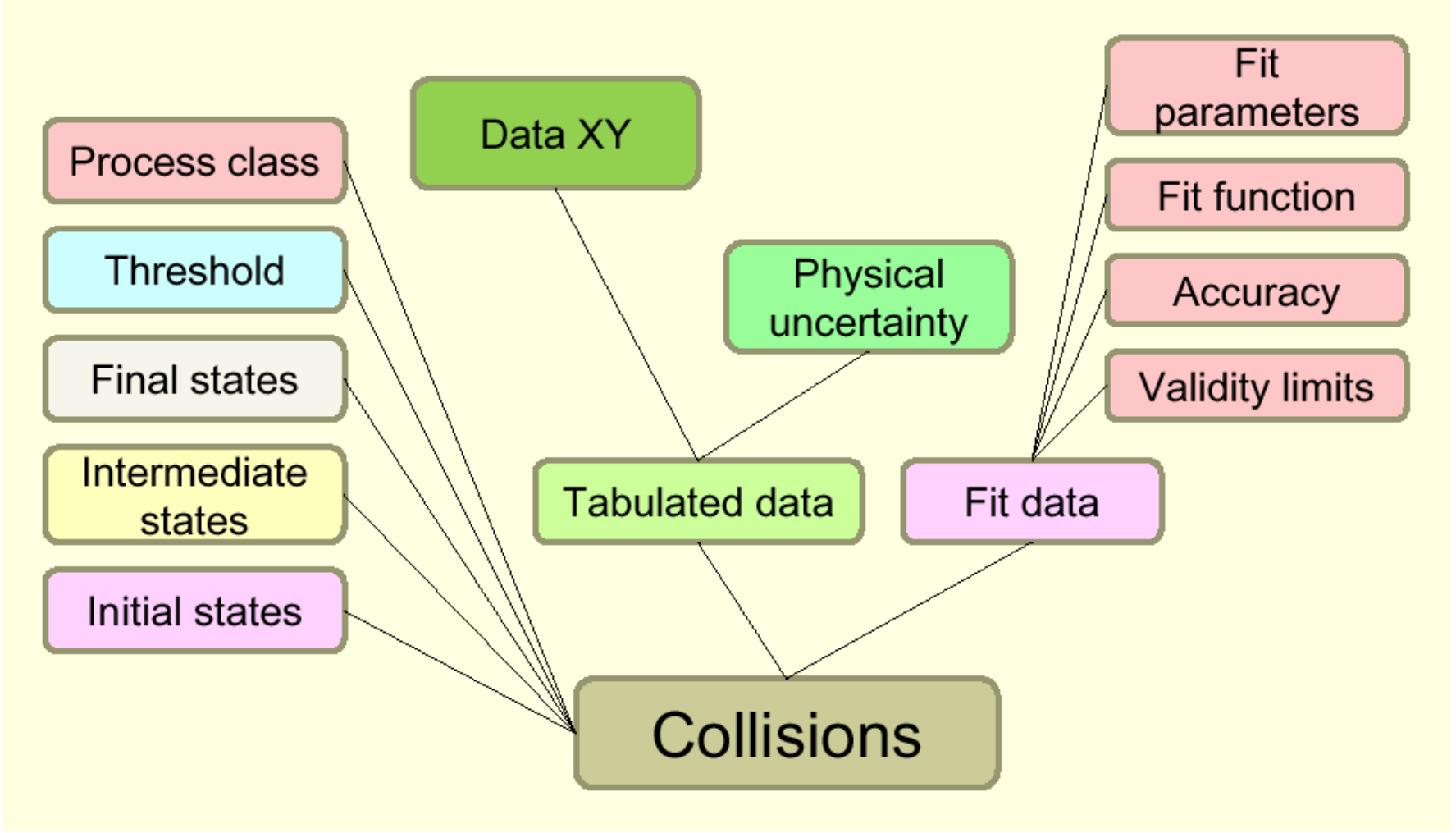
XSAMS tree : atoms



XSAMS tree: molecules



XSAMS tree: collisions



XSAMS Applications

Databases

- IAEA ALADDIN
- NIST ASD
- BASECOL, Observatoire de Paris
- SPETR-W3, VNIITF, Russia

Search Engine

- GENIE

NIST Atomic Spectra Database Levels Data

Example of how to reference these results:
Ralchenko, Yu., Jou, F.-C., Kelleher, D.E., Kramida, A.E., Musgrove, A., Reader, J., Wiese, W.L., and Olsen, K. (2007). *NIST Atomic Spectra Database* (version 3.1.3), [Online]. Available: http://physics.nist.gov/asd3 [2008, October 7]. National Institute of Standards and Technology, Gaithersburg, MD.

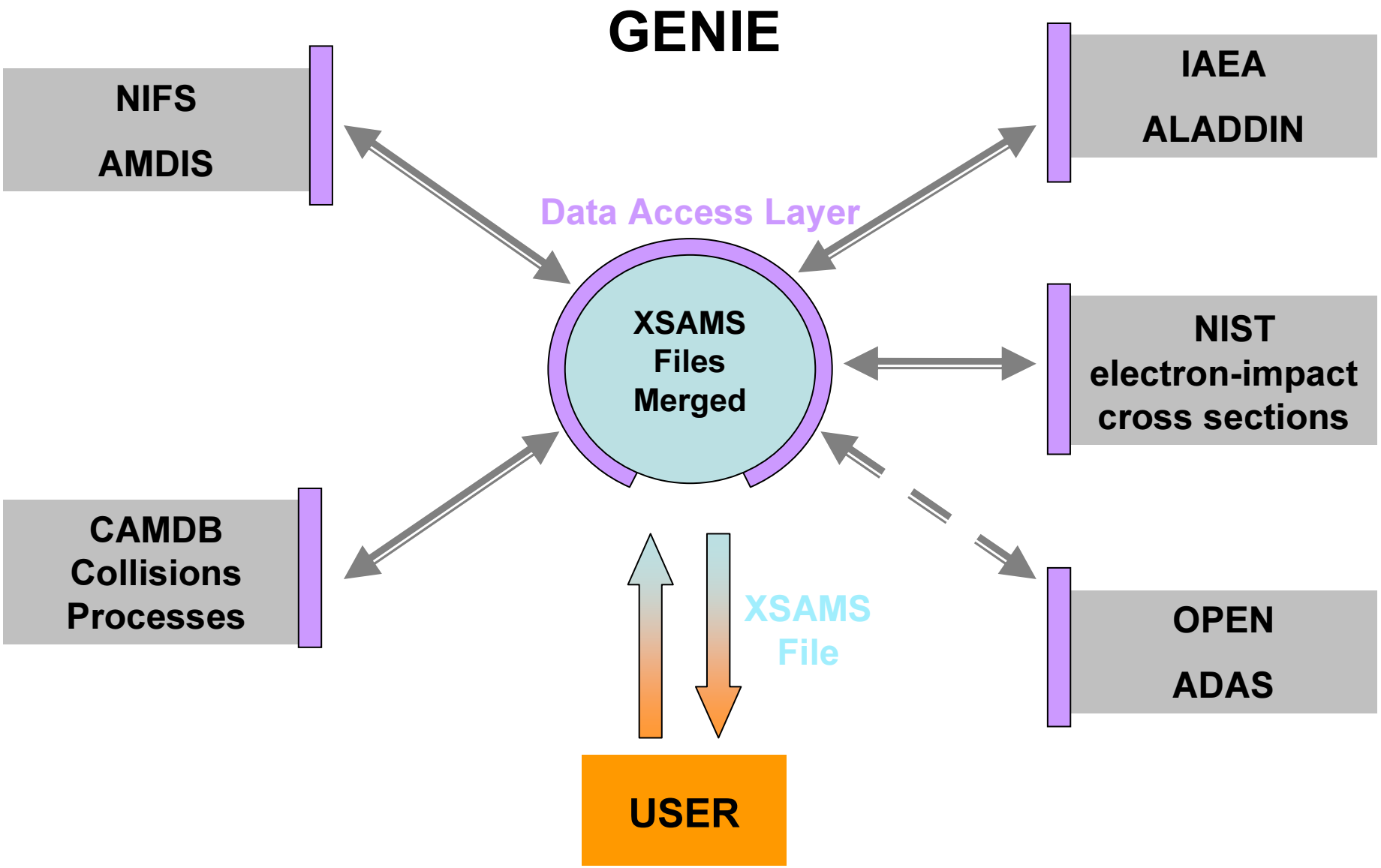
Some data for neutral and singly-charged ions are available in the Handbook of Basic Atomic Spectroscopic Data

Query the NIST Atomic Energy Levels Bibliographic Database for Fe I (new window)

Fe I 493 Levels Found

Configuration	Term	J	Level (cm^{-1})	Lande-g	Leading percentages
$3p^6 3d^6 4s^2$	a ^{5}D	4	0	1.50020	100
		3	415.932	1.50034	100
		2	704.004	1.50041	100
		1	888.129	1.50022	100
		0	978.072		100
$3p^6 3d^7(^4F)4s$	a ^{5}F	5	6 928.266	1.40021	100
		4	7 376.760	1.35004	100
		3	7 728.056	1.24988	100
		2	7 985.780	0.99953	100
		1	8 154.710	-0.014	100
$3p^6 3d^7(^4F)4s$	a ^{3}F	4	11 976.234	1.254	98 1 $3d^6 4s^2$ ^{3}F2
		3	12 560.930	1.086	98 1 $3d^6 4s^2$ ^{3}F2
		2	12 968.549	0.670	98 1 $3d^6 4s^2$ ^{3}F2

```
- <AtomicState sourceRef="B1" stateID="S026001.000011">
    <Description>Conf: 3p6.3d7.(4F).4s; Term: a 3F</Description>
  - <AtomicNumericalData>
    - <StateEnergy sourceRef="B1">
        <Value units="cm-1">11976.234</Value>
      </StateEnergy>
    + <LandeFactor sourceRef="B1">
    + <StatisticalWeight sourceRef="B1">
    </AtomicNumericalData>
  - <AtomicQuantumNumbers>
      <Parity>even</Parity>
      <TotalAngularMomentum>4</TotalAngularMomentum>
    </AtomicQuantumNumbers>
  - <AtomicComposition>
    - <Component>
      - <Configuration>
          <ConfigurationLabel>3p6.3d7.(4F).4s</ConfigurationLabel>
        </Configuration>
      - <Term>
        - <LS>
          - <L>
              <Value>3</Value>
              <Symbol>F</Symbol>
            </L>
            <S>1.0</S>
            <Multiplicity>3</Multiplicity>
          </LS>
          <TermLabel>a 3F</TermLabel>
        </Term>
        <MixingCoefficient mixingClass="squared">98</MixingCoefficient>
      </Component>
    + <Component>
    </AtomicComposition>
  </AtomicState>
```



Each database:

- accessed using the same protocol
- returns a XSAMS file

What's next?

- Schema v.0.1: 2009
  - Schema and documentation
  - Website: NIST and IAEA
  - PSI data for a future release
- Data Access Language (DAL)? Data registry?
- Development of DB interfaces and XSAMS Applications

Exercises

Using VOspec web site, http://esavo.esa.int/vospec/ , find the major oxygen atomic lines for the LLNL O Spectra (LLNL_O_spectra.xml)

Exercises on line at:

1. ICTP web site
2. IAEA: http://www-amdis.iaea.org/ICTP/exercises.html