

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



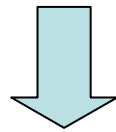
*Denis Humbert*

# 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- Old methods (e.g., ALADDIN) are clearly outdated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: eXtensible Markup Language**
- 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: `<b>` `</b>`
- One can define new tags, e.g.:

- `<energy units="eV">2.306</energy>`

must be a  
real number

- `<total_J>1.5</total_J>`

must be a non-negative  
integer or half-integer

- `<total_L>1</total_L>`

must be a  
non-negative integer

# Applications in AM/PSI Physics

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



# NLTE Code Comparison Workshops

**SAHA**

Plasma Population Kinetics Modeling Database



<http://nlte.nist.gov/SAHA>

**NLTE 4**

Plasma Population kinetics database of the  
4th Non-LTE code comparison workshop



<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/>

The screenshot displays the VOSpec web interface, which is used for spectral analysis. The interface is divided into several sections:

- SLAP Viewer (Left Panel):** Shows a tree view of SLAP Services, including IASD, LERMA, NIST ATOMIC SPECTRA, CIELO SLAP, CHIANTI SLAP, and STSCI SLAP. The NIST ATOMIC SPECTRA service is selected, and its URL is shown as `http://physics.nist.gov/cgi-bin/ASD/slap.pl?`.
- Search Parameters (Middle-Left):** Includes a "Range of Search (m)" section with "Wavelength Start" set to `6.573730807846669E-7` and "Wavelength End" set to `6.607237911199474E-7`. A "Reset" button is also present.
- SLAP Services Output (Bottom-Left):** A table displaying NIST Atomic Spectra data. The table has three columns for "NIST ATOMIC SPECTRA" and contains the following data:

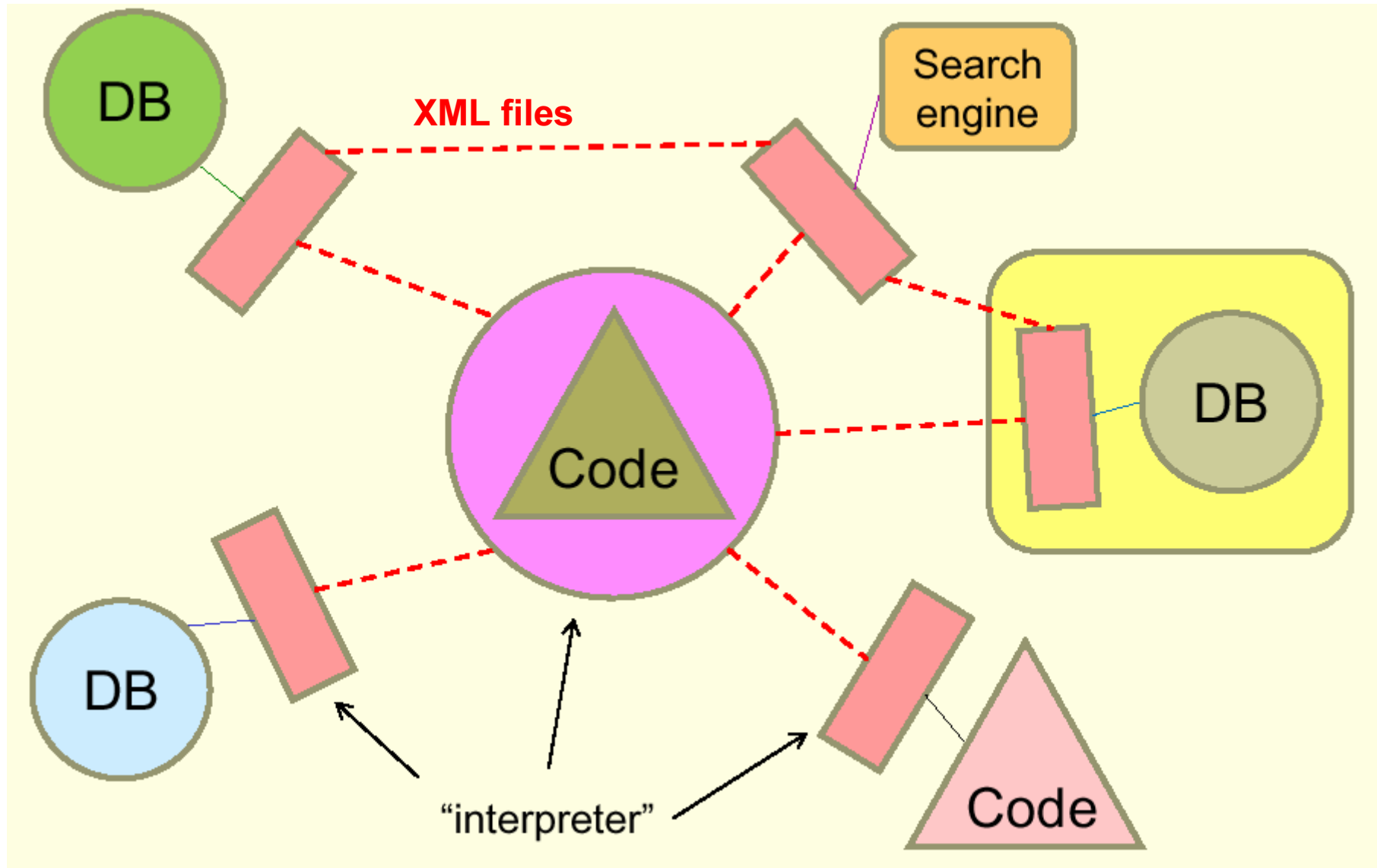
Idm:Line...	Idm:Line...	Idm:Line...	Idm:Line...	Idm:Line...	Idm:Line...	Idm:Line...	Idm:Line...
6.59083...	O II 659...	O	conf=2s...	conf=2s...	6.59082...	5.07914...	4.77774...
6.59143...	Si I 6591...	Si	conf=3s...	conf=3s...	6.59154...	3.05800...	4.43289...
6.59154...	Sm II 65...	Sm			6.59188...	9.86390...	6.85042...
6.59188...	W I 6591...	W	conf=5d...	term="*"	6.59188...	3.11407...	1.00951...
6.5926e...	Cr V 659...	Cr	conf=3p...	conf=3p...	6.59268...	1.86972...	1.56841...
6.59268...	Xe I 659...	Xe	conf=5p...	conf=5p...	6.59282...	1.03718...	7.35897...
6.59282...	Nb I 659...	Nb			6.59328...	1.71866...	1.41737...
6.59315...	Fe I 659...	Fe	conf=3p...	conf=3p...	6.59335...	9.61341...	9.31213...
6.59328...	C I 6593...	C	conf=2s...	conf=2s...			
6.59335...	C IV 659...	C	conf=1s...	conf=1s...			

- Wave Unit and Flux Unit (Middle-Left):** "Wave Unit" is set to "micron" and "Flux Unit" is set to "Jy".
- Redshift and De-reddening (Middle-Left):** "RedShift" is set to 0.00 and "De-reddening" is unchecked.
- Graphic Mode (Middle-Left):** "Graphic Mode" is set to "Lines".
- Target Information (Middle-Right):** "Target" is "m15", "Ra" is "322.49325", "Dec" is "12.16683333", and "Size" is "1". A "Query" button is present.
- VOSpec Spectral Analysis Tool (Middle-Right):** A plot showing "Flux (Jy, logarithmic)" on the y-axis (ranging from 8.0 to 3.0) versus "Wavelength (micron, logarithmic)" on the x-axis (ranging from 6.5650 to 6.6150). A prominent peak is labeled "O II 6590.833 A".
- Bottom Panel (Bottom-Right):** Shows a list of Hubble Space Telescope Spectra, with "NGC7078-STAR" selected. "Retrieve" and "Reset" buttons are at the bottom.

# VOTable output

```
<?xml version="1.0"?>
<VOTABLE version="1.1" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instanc
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

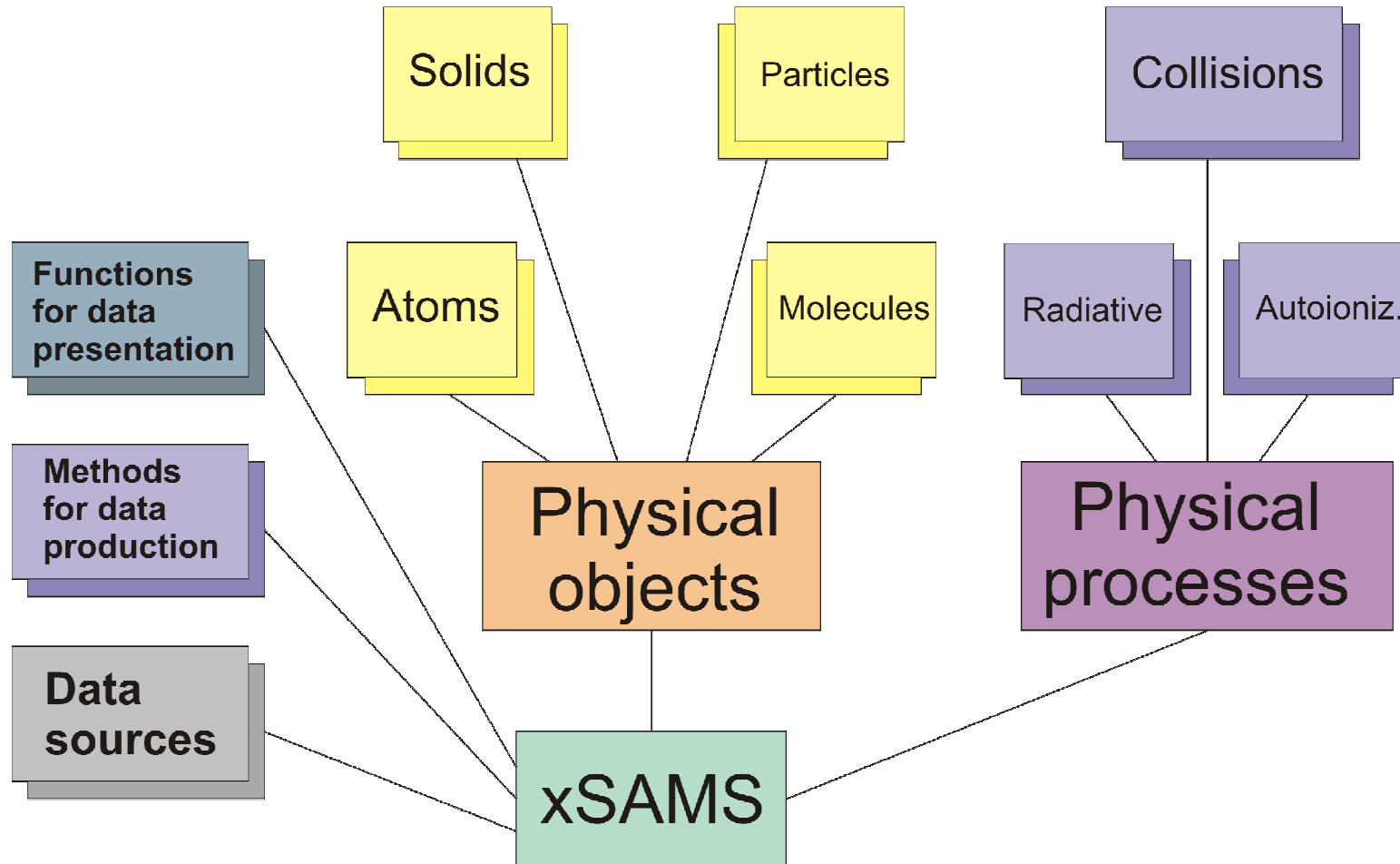




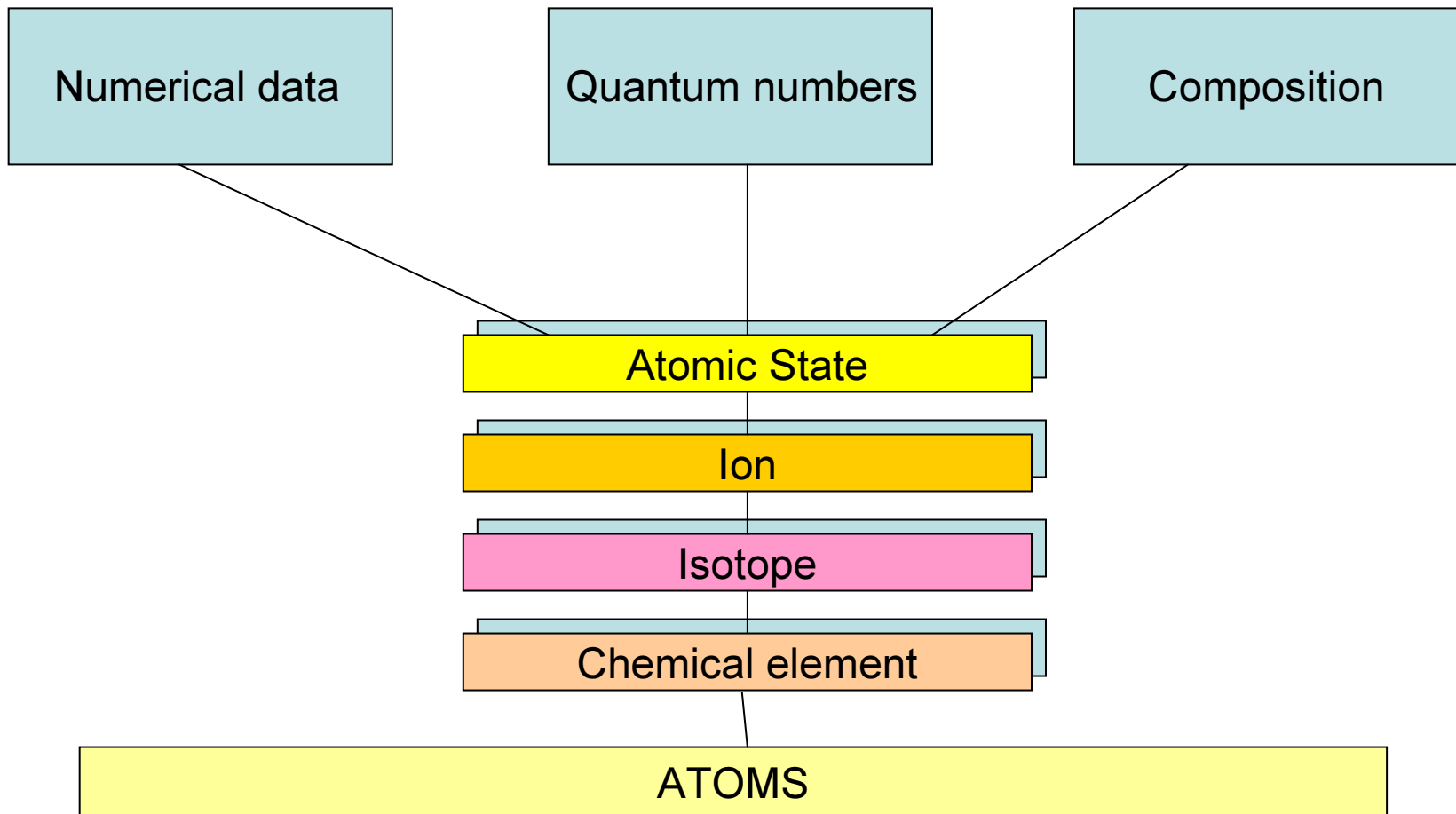
# Development Issues

- 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

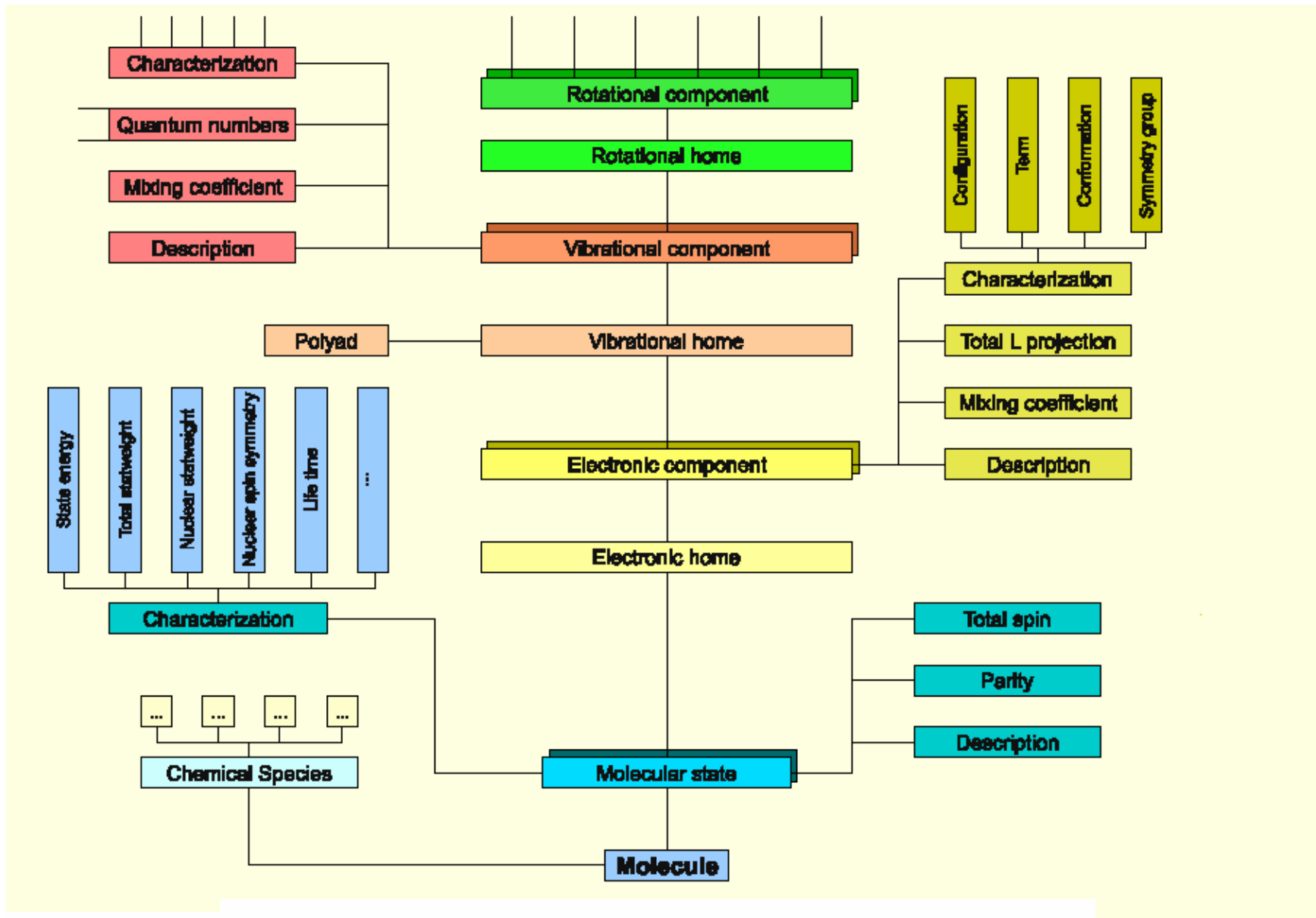
# xSAMS tree



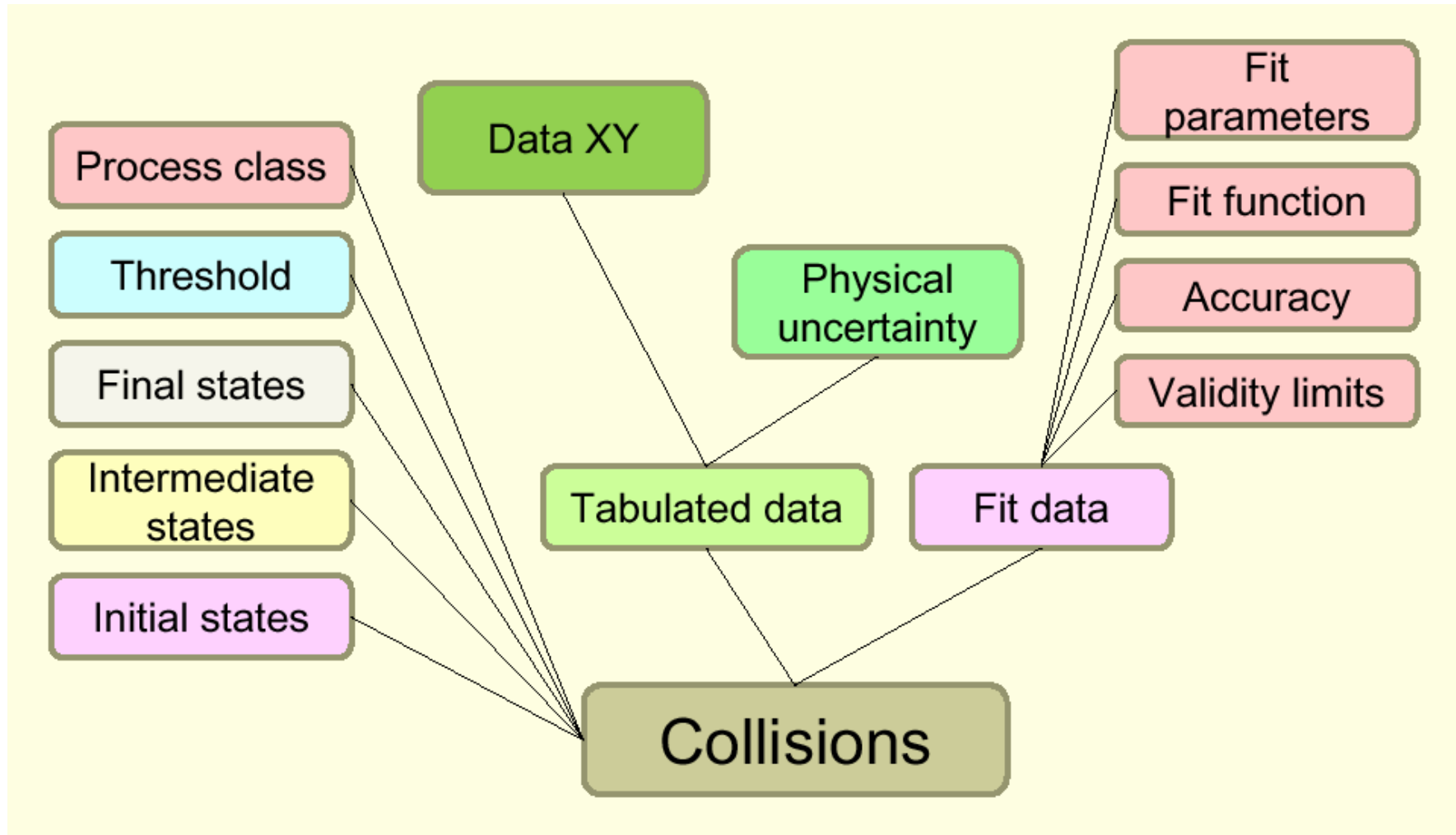
# XSAMS tree : atoms



# 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

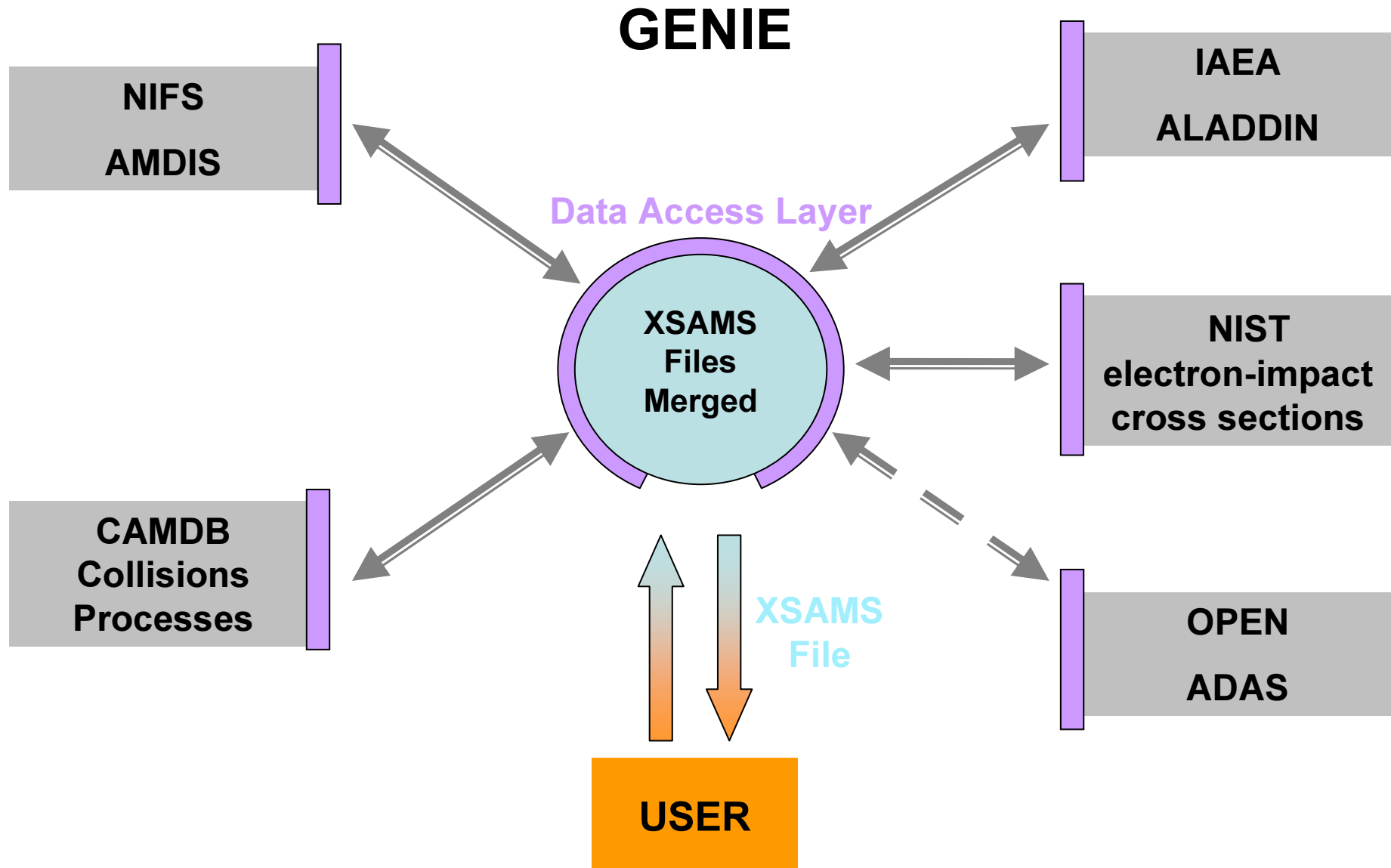
Configuration	Term	J	Level (cm <sup>-1</sup> )	Lande-g	Leading percentages
3p <sup>6</sup> 3d <sup>6</sup> 4s <sup>2</sup>	a <sup>5</sup> D	4	0	1.50020	<b>100</b>
		3	415.932	1.50034	<b>100</b>
		2	704.004	1.50041	<b>100</b>
		1	888.129	1.50022	<b>100</b>
		0	978.072		<b>100</b>
3p <sup>6</sup> 3d <sup>7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