The Abdus Salam
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IAEA
International Atomic Energy Agency

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# Joint ICTP/IAEA Workshop on Atomic and Molecular Data for Fusion

***20 - 30 April 2009***

## Atomic Molecular and Particle-Surface Interaction Web Databases and Data Exchange Lecture 4 - New Trends in Data Exchange

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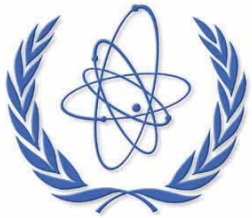
# Atomic, molecular and particle-surface interaction web databases and data exchange

## Lecture 4
## New Trends in Data Exchange

**ICTP Workshop on Atomic and Molecular Data for Fusion Energy Research**

Trieste, 20-30 April 2009

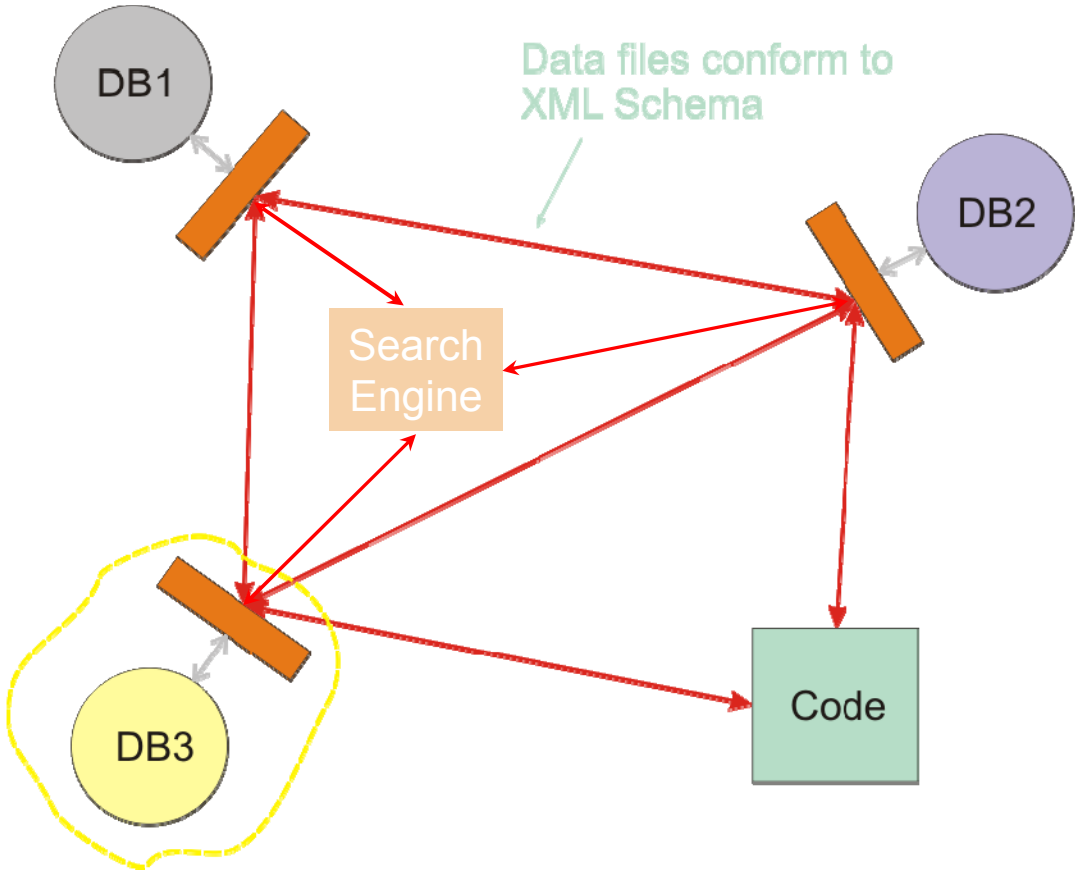
*Denis Humbert*



IAEA

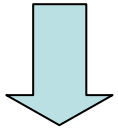
# Content

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


DB1
Data files conform to
XML Schema
DB2
Search
Engine
DB3
Code

# 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- Old methods (e.g., ALADDIN) are clearly outdated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.:

  - <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

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

# 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.)

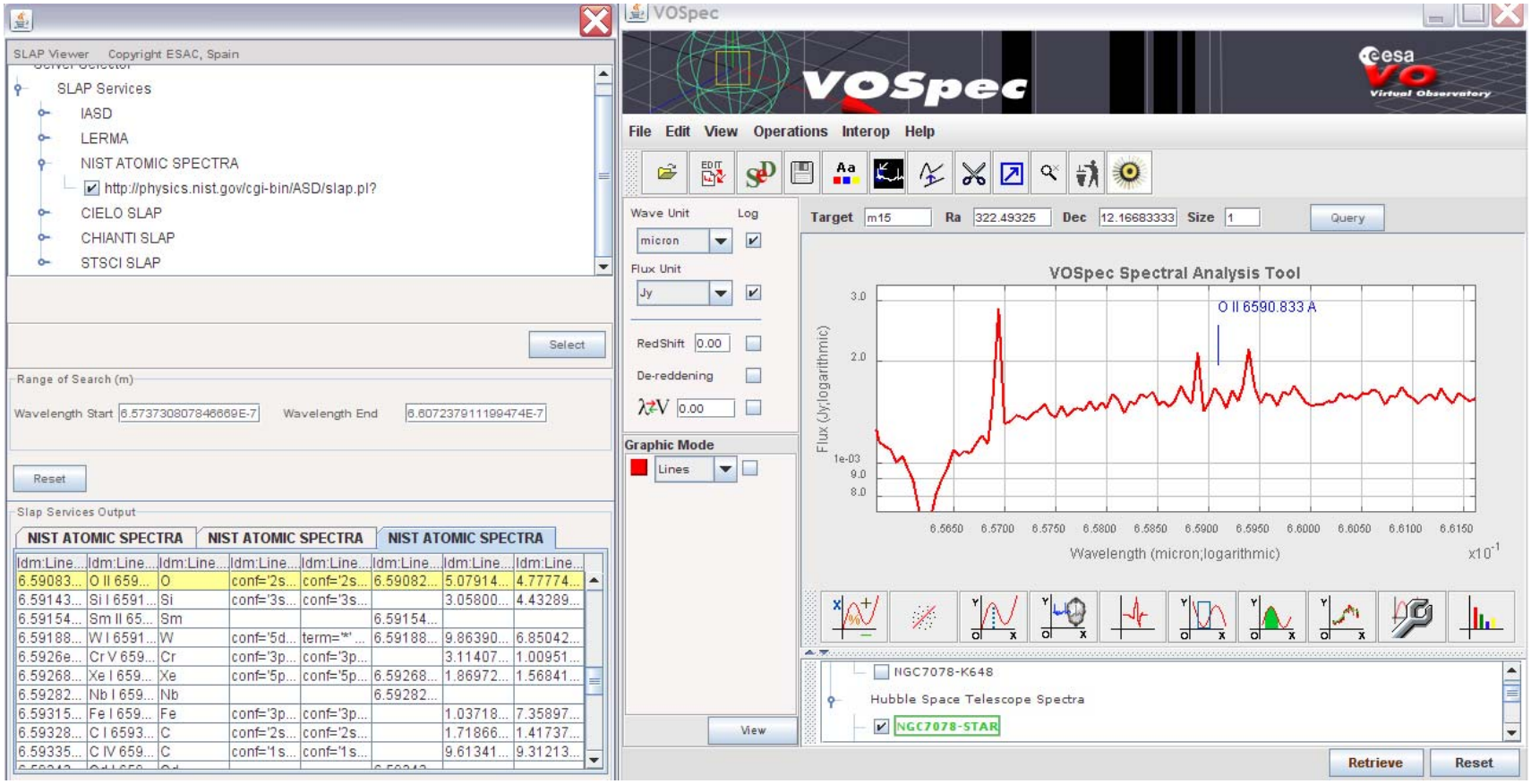
# IVOA Spectral Line Data Model

- 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

# IVOA VOSpec example

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



# NLTE Code Comparison Workshops


http://nlte.nist.gov/SAHA



http://nlte.nist.gov/NLTE4

# XSAMS

- XML Schema for Atoms, Molecules and Solids
- Attempt to structure the whole field of AM/PSI physics

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

# XSAMS Development Team

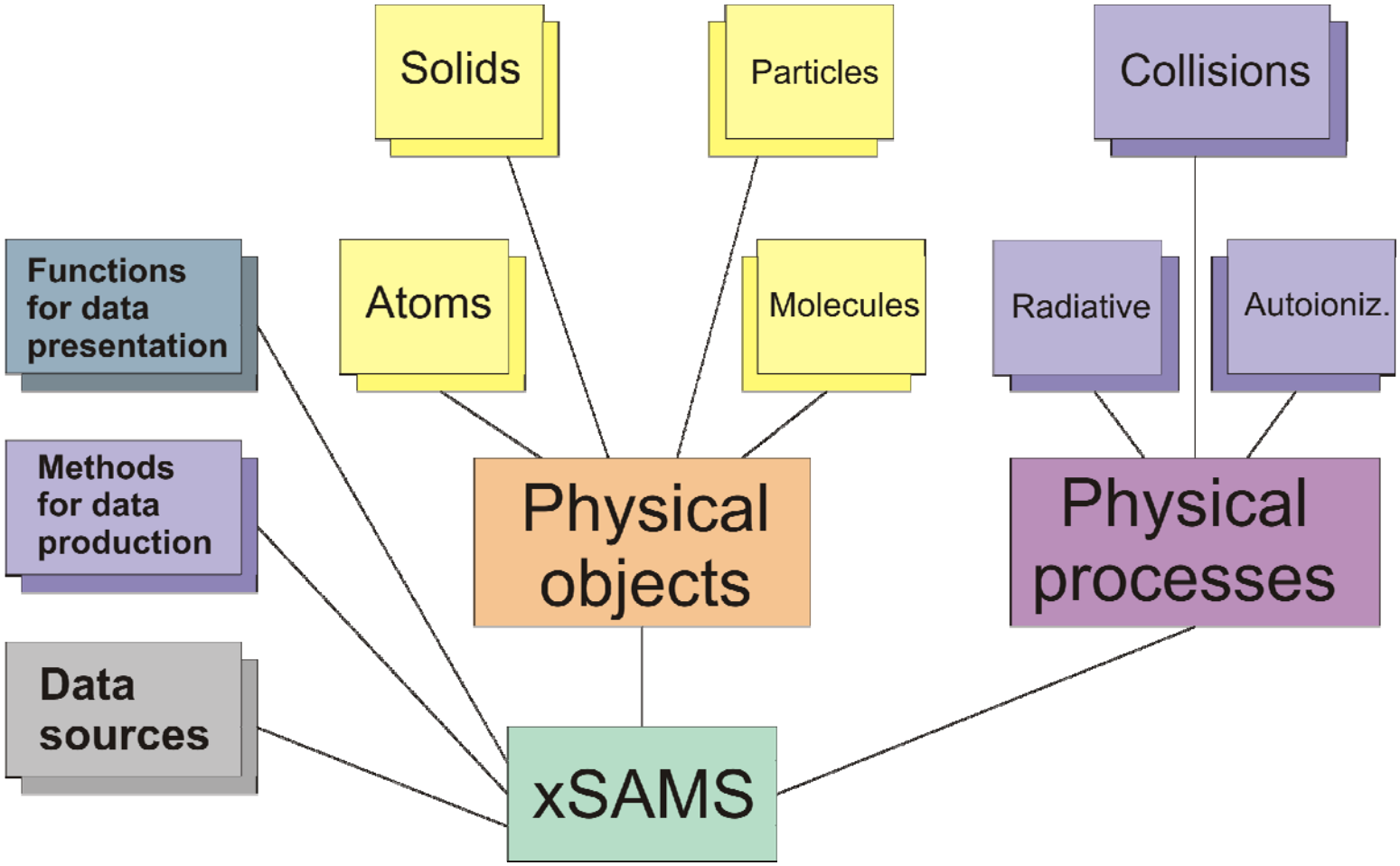
- IAEA, Austria
  - *R.E.H. Clark*
  - *D. Humbert*
- Obs. Paris-Meudon, France
  - *M.-L. Dubernet*
  - *N. Moreau*
  - *E. Roueff*
- ORNL, USA
  - *D.R. Schultz*
- VNIITF, Russia
  - *S. Gagarin*
  - *P.A. Loboda*
- NIST, USA
  - *Yu. Ralchenko*



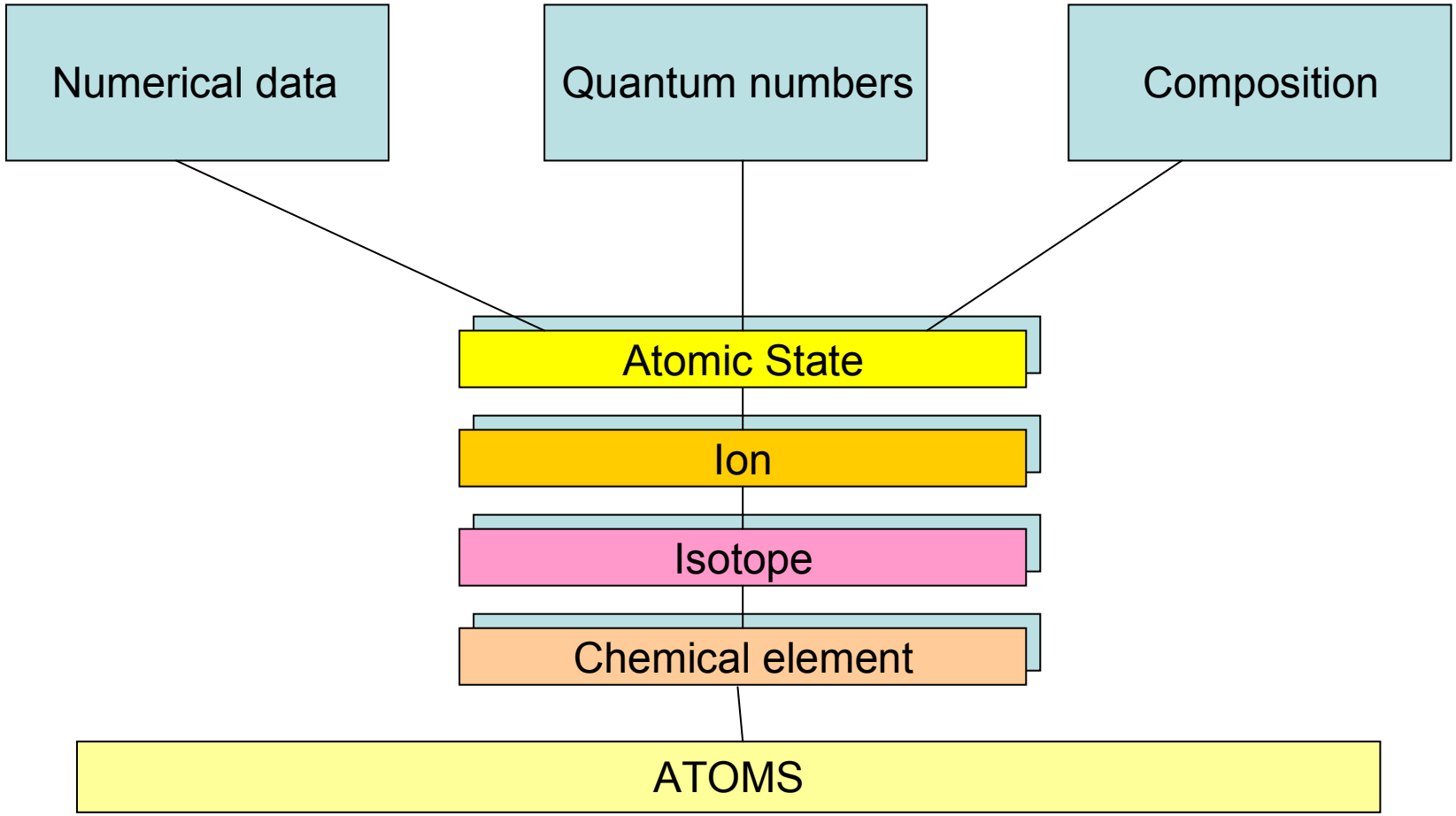

# Development Issues

- Project initiated within the DCN in October 2003
- Technical meetings twice a year in Paris or Vienna
- Collaboration with VNIITF (Russia), 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 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

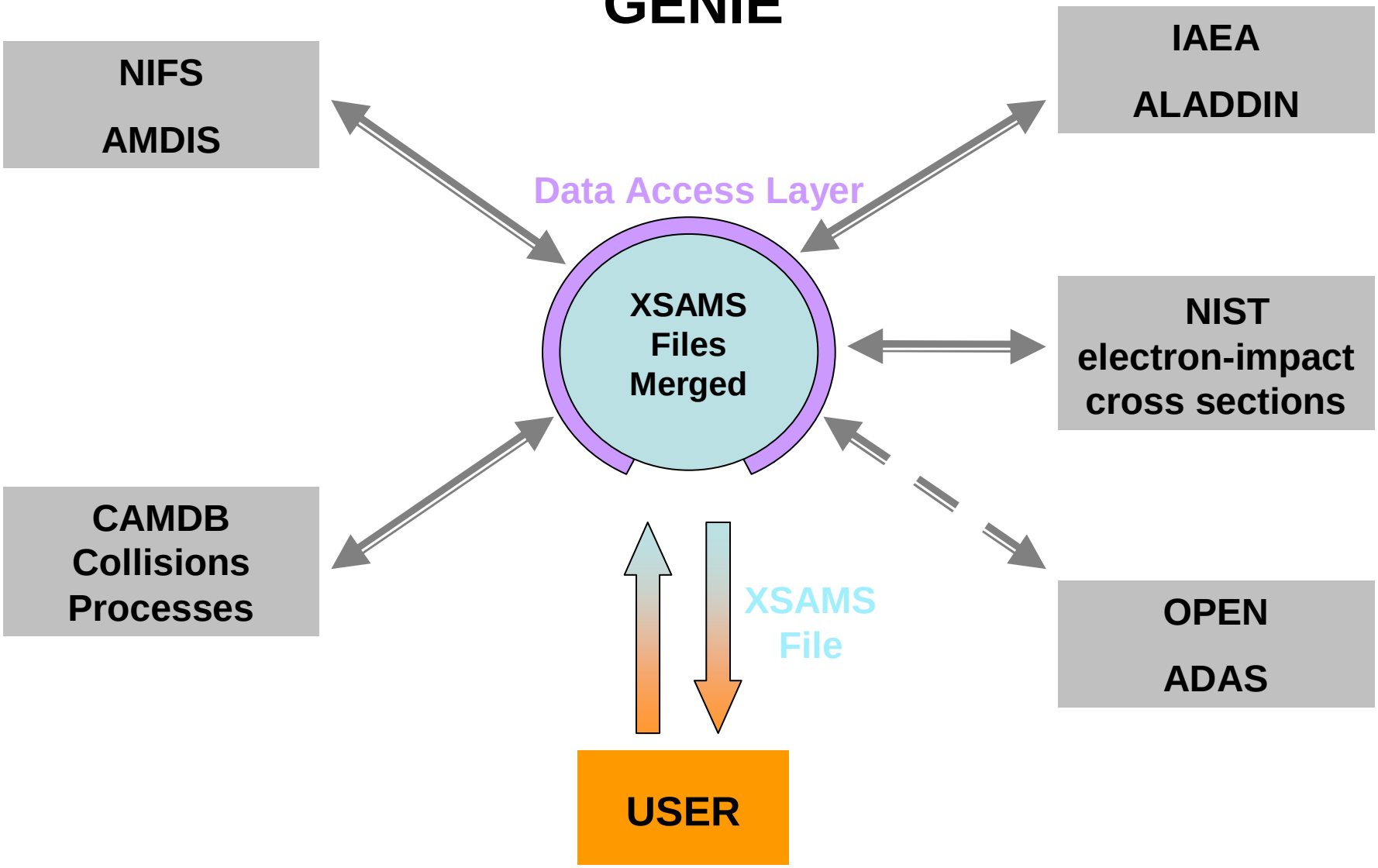
Query the NIST Atomic Energy Levels Bibliographic Database for Fe I (new window)

## 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>
```

# GENIE




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