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Atomic Molecular and Particle-Surface Interaction Web Databases and Data Exchange

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

ICTP Workshop on Atomic and Molecular Data for Fusion Energy Research

Trieste, 20-30 April 2009

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Where and how to find AM/PSI data

- Internet: major support for information
- Data Centres major actors on Internet
- Data Quality
  - Traceability, reference sources
  - Methods
  - Accuracy
- Data exchange
  - Huge amount of available data
  - How to store, to retrieve and exchange the data
  - Data structure and data integrity

Content

1. **Atomic and Molecular Data Unit of the IAEA**
   - Objective
   - Tools, The Data Centre Network (DCN), the Coordinated Research Projects (CRP)
   - Achievements: databases ALADDIN and AMBDAS, search engine GENIE, web calculations tools

2. **Bibliographic data**
   - Databases
   - AMBDAS
   - Web search engines
   - Electronic publishers
   - Web libraries

3. **Numerical data**
   - Data quality
   - Data centres
   - Web numerical databases
   - ALADDIN
   - A search engine: GENIE

4. **Data exchange**
   - New trends in data exchange
   - XSAMS a XML Schema for Atoms, Molecules and Solids

Atomic and Molecular Data Unit

http://www-amdis.iaea.org

- Objective: establishment of recommended numerical databases for use in fusion energy research:
  - atomic and molecular collisions
  - radiative processes
  - atomic and molecular structure characteristics
  - particle surface interactions
  - (physico-chemical and thermo-mechanical material properties)

- WWW, main support to provide the information
  - AMBDAS, a bibliographic database
  - ALADDIN, a numerical database
  - GENIE, a web search engine
  - Web calculation tools

Atomic and Molecular Data Unit

- CRP: Coordinated Research project
  - Numerical data (experimental and theoretical): data collection, data production, data evaluation
- DCN: Atomic and Molecular Data Centre Network
  - Bibliographic data for AMBDAS
  - Priorities in data generation, compilation and evaluation
  - Development of web search engines
  - Data exchange
- CCN: Code Centre Network
- Consultancies
  - Web calculation tools
  - XSAMS, XML format for atoms, molecules and solids
  - Numerical data inputs

DCN

- The A+M/PMI Data Centre Network (DCN) includes 12 national data centres
- Activities in collection, assessment (evaluation) and generation of atomic and molecular (A+M), particle surface interaction (PSI) and bulk material properties (plasma-material interaction - PMI) data for fusion and other applications.
- The activities of this DCN related to fusion research are coordinated by the IAEA A+M Data Unit
- The DCN represents one of the main instruments by which the international fusion related A+M/PMI data collection and evaluation programmes are implemented. The heads of the national A+M/PMI data centres, members of the A+M/PMI DCN, constitute a standing Advisory Group for advising the Agency on the technical aspects of A+M/PMI data exchange and processing.
- Advisory Group meets every 2 years

DCN Members

- IAEA AMD Unit, Austria
- NIST, USA
- CRAAMD, China
- NIFS, Japan
- KAERI, South Korea
- ADAS, UK

- ORNL, USA
- JAERI, Japan
- GAPHYOR, LPGP, France
- Kurchatov Institute, Russia
- ENEA, Italy
- Max-Planck-Institut fur Plasmaphysik, Germany

CRP: Co-ordinated Research Project

Joint Project with research effort on topic of interest to fusion:

- Representatives from approximately 12 research institutions
- Duration of 3-5 years
- Research Coordination Meeting (RCM): periodic meeting at IAEA Headquarters

Goals:

- Data generation
- Compilation and assessment of data
- Data evaluation
- Establishment of databases

Data and results:

- Final results published in "**Atomic and Plasma-Material Interaction Data for Fusion" (APID)**
- Data included in the IAEA ALADDIN database: http://www-amdis.iaea.org/ALADDIN/

Active and Planned CRPs

Title	Duration
Core Concentrations of Hydrogen Isotopes and Light Elements in Burning Plasmas	*2009*
Characterization of size, composition and origins of dust in fusion devices	2008-2012
Data for surface composition dynamics relevant to erosion processes	2007-2011
Atomic data for high Z element impurities in fusion reactors	2005-2009
Atomic and molecular data for plasma modelling	2005-2009

CRP on Characterization of Size, Composition and Origins of Dust in Fusion Devices

Tritium is a main issue for future fusion reactors

- **Safety hazard**: dust can be flammable and toxic, it can bring potential respiratory problems and radiation concerns with tritium.
- **Tritium inventory**: a significant uptake of hydrogen isotopes occurs in dust, making the transport behaviour of this material a significant factor in tritium inventory studies of next generation machines such as ITER and DEMO

Plasma behaviour

- Dust can become electrically charged from radioactivity, leading to the interaction of the dust with the plasma and electric fields

Objective

Dust and tritium issues are not of high importance for operational machines, but will become significant for ITER and later production machines.

Data needs to addressed

- particle size and distribution
  physical and aerodynamic mass median diameter
- composition (elemental and chemical)
- origins of dust in fusion machines

Period 2008-2012, first RCM in December 2008

CRP on Data for Surface Composition Dynamics Relevant to Erosion Processes

Objectives

- Increase understanding of erosion processes in fusion devices, such as ITER
- Better knowledge of pathways of eroded materials
- Propose possible methods to mitigate erosion effects in future fusion devices

Outputs

- New data on physical sputtering, reflection, radiation enhanced sublimation…

Period 2007-2011, second RCM in March 2009

CRP on A + M Data for Plasma Modeling

Objective

Gathering and generating new data relevant to modeling the edge region of plasmas relevant to nuclear fusion energy devices

Outputs

- Cross sections, rate coefficients, branching ratios, and kinetic energies from various sources for hydrides (with isotopes) and hydrocarbons
- Surface interactions, such as sticking and generation of hydride species

Ending 2009

CRP on Atomic Data for High Z elements impurities in Fusion Reactors

Overall objective

Heavy elements from erosion of plasma facing components, introduction for diagnostics purpose, unavoidable contamination

- $Z \geq 13$, priority to noble gases (Ar, Kr, Xe) and Si, Cl, Cr, Fe Ni, Cu, Mo, W
- Ion stage considered: ion stages giving rise to the most distinct spectral line

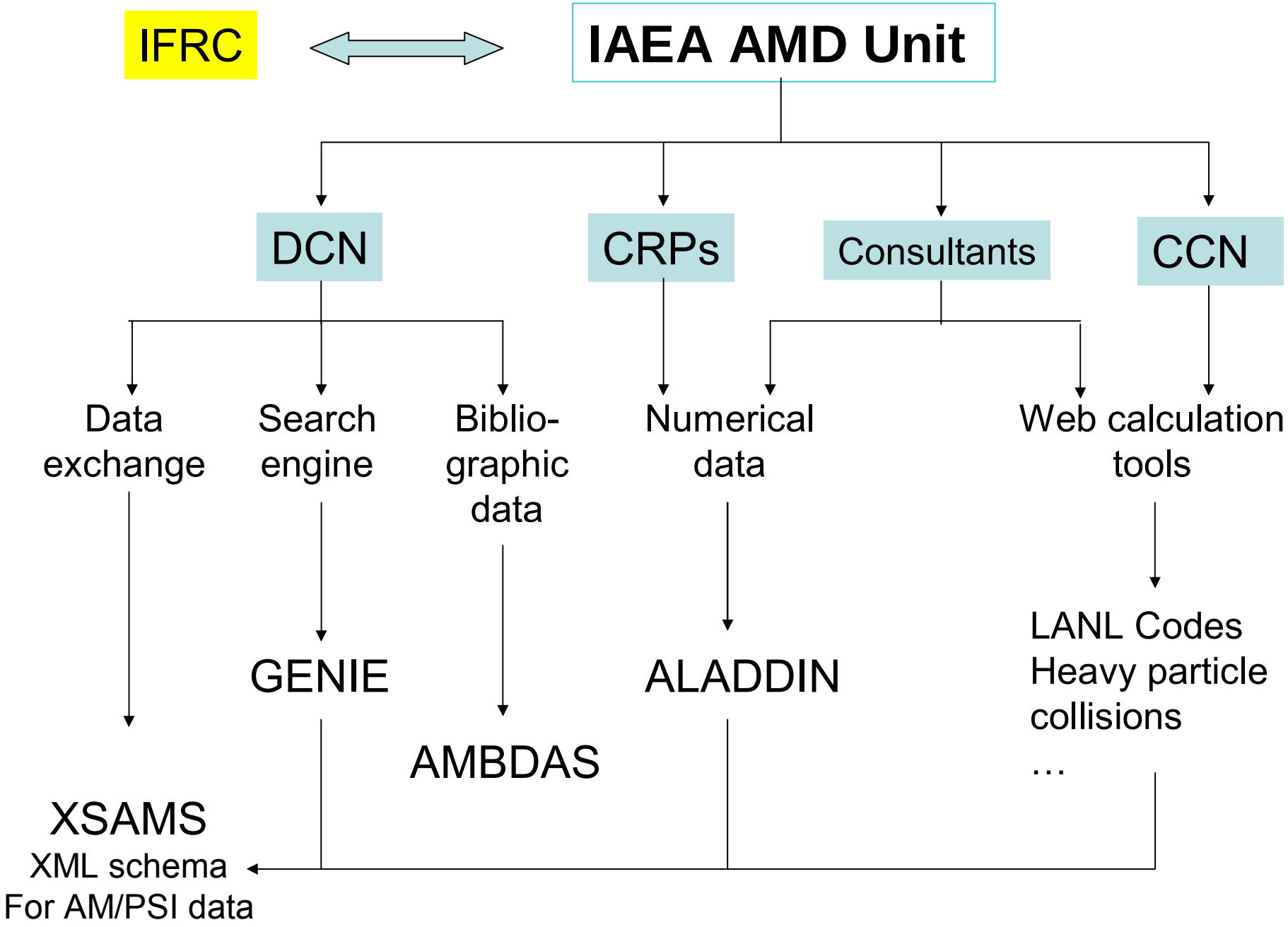
Output

Benchmark data for most important processes: transition probabilities, excitation and ionization cross sections, charge transfer and recombination

Ending 2009

Code Centre Network

- Establish a network to provide computational tools related to atomic, molecular and particle surface interaction data generation for use in fusion energy research
  - Web tools, download of codes, expertise
- Members
  - Web tools: NIST, IAEA, LANL, NIFS, FZ Juelich
  - Codes: Lebedev Physical Institute
  - Expertise: Curtin University (CCC and RCCC), Universidad Autonoma de Madrid
- Extension
  - R-Matrix community
  - HULLAC, FAC, AUTOSTRUCTURE…
  - PMI community: ORNL, IPP Garching
- Biennal meeting, December 2008 meeting:
  http://www-nds.iaea.org/reports-new/indc-reports/indc-nds/indc-nds-0548.pdf


IFRC
IAEA AMD Unit
DCN
CRPs
Consultants
CCN
Data exchange
Search engine
Biblio-graphic data
Numerical data
Web calculation tools
GENIE
ALADDIN
LANL Codes
Heavy particle collisions
…
AMBDAS
XSAMS
XML schema
For AM/PSI data

Conclusions

- With the DCN, attempt to coordinate international efforts on AM/PSI data for fusion energy research
- WWW is the main support of the information
- Focus on structured databases with a web interface
- Development of web calculations tools
- Data exchange issues, XSAMS
  - Huge amount of data disseminated on the web
  - Communication between applications
  - Attempt to codify the whole field of AM/PSI physics