WWW Atomic and Molecular Data

Workshop on Atomic and Molecular Data for Fusion Energy Research

ICTP -Trieste

28 August-8 September 2006

Denis Humbert

IAEA

Content

- 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

- Bibliographic data
  - Databases
  - AMBDAS
  - Web search engines
  - Electronic publishers
  - Web libraries

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

- Annex 1: Database definition
- Annex 2: Exercises

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-solid 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

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

DCN

- The A+M/PMI Data Centre Network (DCN) includes 10 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

CRP: Co-ordinated Research Project

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

- Representatives from approximately 10 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 electronic database: http://www-amdis.iaea.org/ALADDIN/

Active and Planned CRPs

Title	Duration
Data for molecular processes in edge plasmas	2001-2005 *(ending)*
Tritium inventory in fusion machine	2002-2006
Atomic and molecular data for plasma modelling	2005-2008
Atomic data for high Z element impurities in fusion reactors	2005-2008
Data for surface composition dynamics relevant to erosion processes	2006-2009

CRP on Data for Molecular Processes in Edge Plasmas

Overall Objective:

To identify the specific molecular processes that are important to the plasma physics in the edge regions and to provide data for some of these processes

- Most important molecular species were identified as molecular hydrogen with all possible isotope distributions, CO, CO_2, CH_4, C_2-C_3 group hydrocarbons, silicates, nitrogen compounds and H_2O
- Major processes for which data are needed: ionisation, recombination, attachment, detachment, excitation, de-excitation, dissociation, charge transfer, chemical reactions, energy transfer and plasma wall interactions
- Final report will be published in APID 13. Data are included into ALADDIN as soon as available.

CRP on Tritium Inventory in Fusion Reactors

Overall Objective: Gather and generate new data relevant to the overall inventory of tritium in fusion reactors, with special emphasis on the interactions of tritium with plasma facing components and methods for tritium removal

- Removal of tritium will be an important issue for ITER
- Important materials include carbon, tungsten and beryllium
- Cannot be assumed that the first wall will be carbon free
- Effects of dopants are important, and dependent on particle and heat load
- Flux and fluence dependence of chemical erosion important in modelling
- Still some questions on erosion sources
- Electron-simulated desorption, glow discharge and laser heating are all being investigated for tritium removal
- Research has been initiated on all topics
- Last RCM in September 2006

CRP on A + M Data for Plasma Modeling

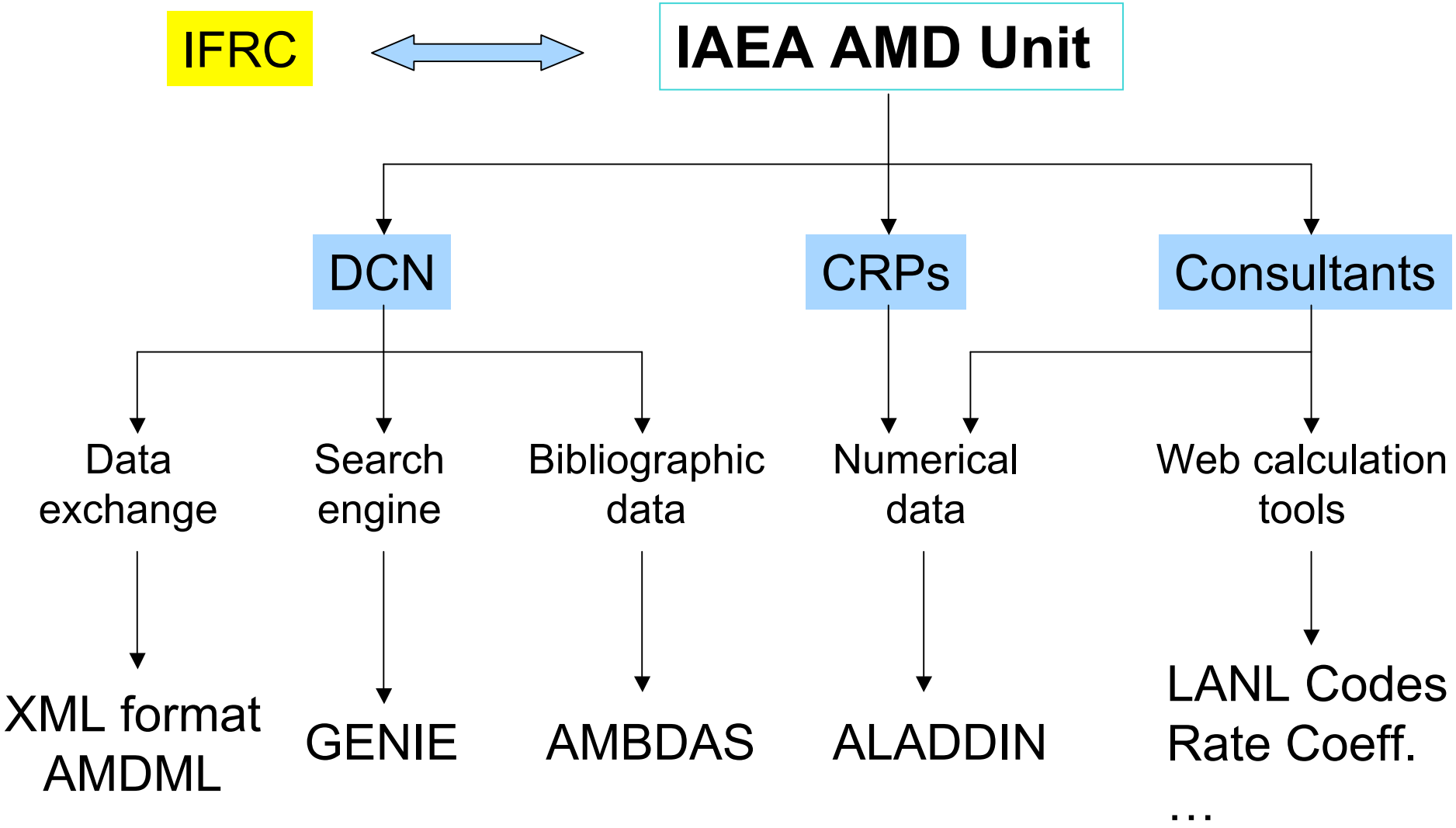
Overall objective: gathering and generating new data relevant to modeling the edge region of plasmas relevant to nuclear fusion energy devices

- 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
- First RCM in September 2005

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 lines
- Output: benchmark data for most important processes (transition probabilities, excitation and ionization cross sections, charge transfer and recombination)
- First RCM in November 2005


IFRC
IAEA AMD Unit
DCN
CRPs
Consultants
Data exchange
Search engine
Bibliographic data
Numerical data
Web calculation tools
XML format AMDML
GENIE
AMBDAS
ALADDIN
LANL Codes
Rate Coeff.
…

Bibliographic Data

Bibliographic Search

- Bibliographic databases
  - AMBDAS, IAEA
  - CFADC, ORNL Oak Ridge
  - GAPHYOR, University of Paris XI
  - FUSION, NIFS (subscript of INSPEC)
- Specialized databases
  - NIST: energy levels, transition probabilities, line broadenings
- Web search engines
  - General: Google, Yahoo…
  - Specialized: Crossref
- Electronic publishers

  AIP, IOP, …
- On line libraries: LANL, NASA

Bibliographic databases

- General Databases for A+M, PMI and Fusion Research
  - AMBDAS, IAEA, Vienna Austria
    http://www-amdis.iaea.org/AMBDAS
  - CFADC, ORNL, Oak Ridge USA
    http://www-cfadc.phy.ornl.gov/bibliography/search.html
  - GAPHYOR, Université Paris XI, Orsay France
    http://gaphyor.lpgp.u-psud.fr/gaphyor/gaphyor.html
  - FUSION (subset of INSPEC), NIFS, Japan
    https://dbshino.nifs.ac.jp/
    Logon ID : triesta Password : kXdb$nGy

- Specialized databases
  NIST Atomic Spectra Bibliographic databases
  http://physics.nist.gov/PhysRefData/ASBib1/index.html
  - Energy levels, wavelengths
  - Transition probabilities
  - Spectral line broadenings

GAPHYOR

http://gaphyor.lpgp.u-psud.fr/gaphyor/gaphyor.html

Domain: atomic and molecular physics

- Properties of atoms and molecules
- Photon collisions
- Electronic collisions
- Heavy particles collisions
- Macroscopic properties of gases
- Particle surface interactions

Interface and data structure

- No title
- Standard and advanced search

AMBDAS

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

IAEA bibliographic database: 112 000 records from 42 000 references

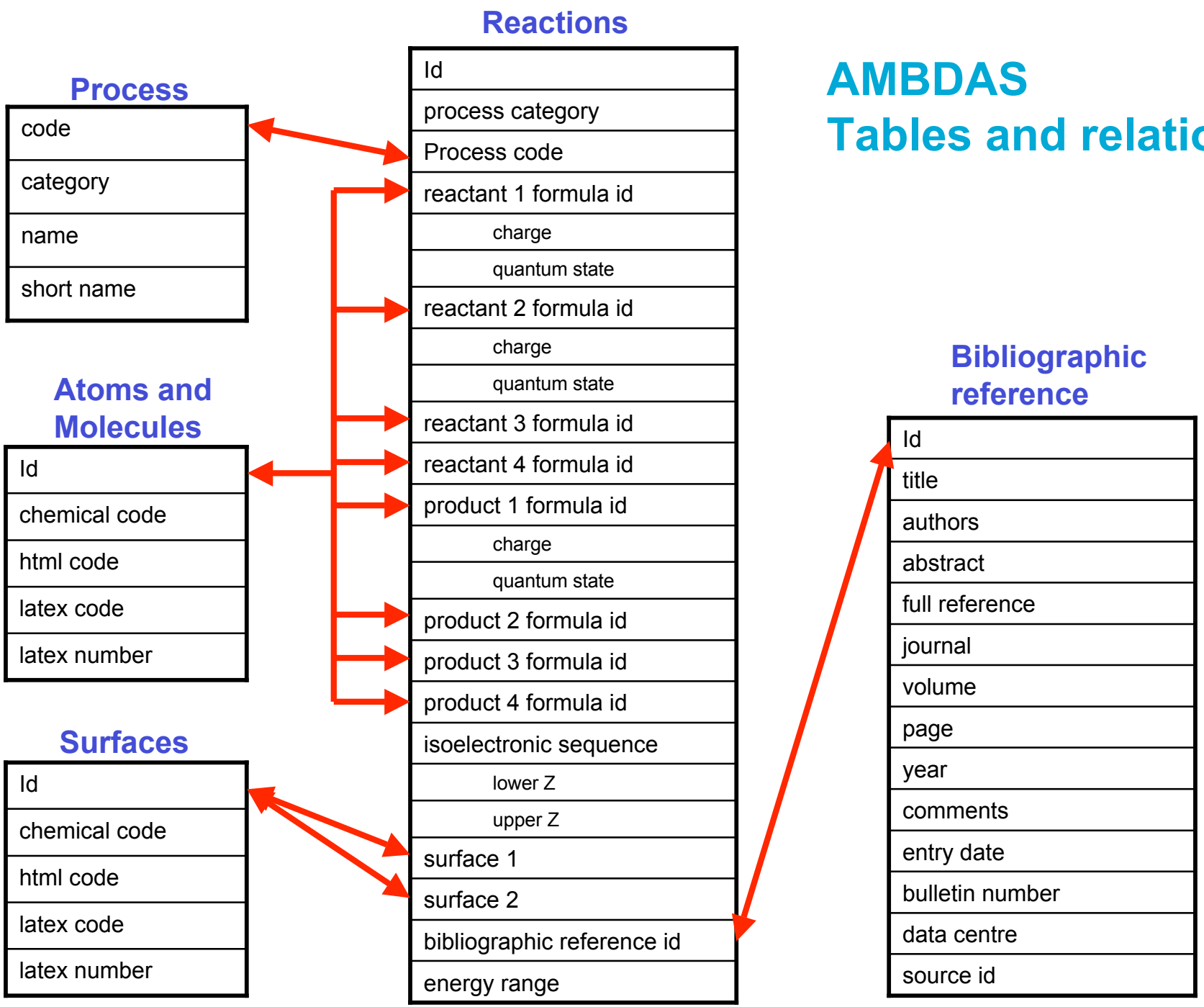
Domain covered: information of interest for fusion energy research

- Structure and spectra: transition probabilities, oscillator strengths, interatomic potentials, energy levels, wave lengths
- Atomic and molecular collisions
- Surface interactions
- Particle beam-matter interactions
- Fusion research of general interest

Data collected through the DCN

- NIST: structure and spectra
- ORNL, Oak Ridge: atom and molecular collisions, plasma interactions
- Other data centres: laboratory report, thesis…

AMBDAS
Tables and relations



AMBDAS Query

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

- Physical/chemical criteria
  - Process category
  - Process
  - 1 or 2 reactants with or without ionization stage
  - 1 product of reaction with or without ionization stage
  - 1 surface
  - 1 isoelectronic sequence
- Bibliographic criteria
  - Keywords on title
  - 1 or 2 authors
  - Journal/book/report

AMBDAS main journals

1.	Journal of Physics B	IOP
2.	Physical Review A	APS
3.	Nuclear Instruments and Methods in Physics Research section B	Science Direct
4.	Physica Scripta	IOP
5.	Surface Science	Science Direct
6.	Astronomy Astrophysics	EDP
7.	Journal of Nuclear Materials	Science Direct
8.	Chemical Physics Letter	Science Direct
9.	Physical Review B	APS
10.	Journal of Chemical Phys.	AIP
11.	Physical Review Letters	APS
12.	Astrophysics Journal, Part 1	University of Chicago

Electronic Publishers

- IOP http://www.iop.org/EJ/
  - Journal of Physics B, Physica Scripta…
- APS http://publish.aps.org/
  - Physical review A and B, Physical Review Letters..
- Elsevier (Science Direct) http://www.sciencedirect.com/
  - Surface Science, Chemical Physics Letter…
- AIP http://www.aip.org/pubs/
  - Journal of Chemical Physics
- EDP: http://www.edpsciences.org/index.cfm
  - Astronomy Astrophysics Journal (free)

⇩

CrossRef

Crossref

- This project is to implement full-text interpublisher searchability http://www.crossref.org/.
- CrossRef pilot launches a typical general web search but filters the result set to the scholarly research content from participating publishers, with the intent of reducing the noise produced by general web searches.
- Result is a cross-publisher citation linking system that allows a researcher to click on a reference citation on one publisher's platform and link directly to the cited content on another publisher's platform, subject to the target publisher's access control practices.
- CrossRef citation-linking network today covers millions of articles and other content items from several hundred scholarly and professional publishers.
- CrossRef is the official DOI registration agency for scholarly and professional publications.
- Crossref pilots:
  1. http://portal.acm.org/xrs.cfm
  2. http://www.iop.org/EJ/search_crossref
  3. …

DOI

- A Digital Object Identifier (DOI), is a unique string created to identify a piece of intellectual property in an online environment (http://www.doi.org/hb.html)

- A DOI in text or header information can be resolved by embedding it in an HTTP hyperlink to the DOI proxy, http://dx.doi.org. This redirects the DOI to the currently registered location for this content item:
  doi:10.1103/PhysRevA.71.022713 can be resolved as http://dx.doi.org/10.1103/PhysRevA.71.022713.

- To include the DOI in a citation to an article, simply append it at the end, prefaced by "doi:" as follows:

  Sheng-Guang Wang, Dong-Bo Cao, Yong-Wang Li, Jianguo Wang and Haijun Jiao
  "CH4 dissociation on Ni surfaces: Density functional theory study"
  Surface Science, **doi:10.1016/j.susc.2006.06.008**

Web Libraries

- The NASA Astrophysics Data System, digital library for Physics and Astrophysics
  - basic search and advanced search

    http://adswww.harvard.edu/

- LANL Library

  http://catalog.lanl.gov/F

Web Search Engines

- **Google**: http://www.google.com/
- Yahoo: http://www.yahoo.com/
- Alta Vista: http://www.altavista.com/
- Ask.com: http://www.ask.com/
- MSN: http://search.msn.com/
- **Dogpile**: http://www.dogpile.com/

- **CrossRef**

Numerical Data

Databases

Search engine: GENIE

Web calculation tools

Numerical data

- Data Centres with numerical data on line
  - NIST http://physics.nist.gov/PhysRefData
  - CAMDB http://www.camdb.ac.cn/e/
  - NIFS http://amdata.nifs.ac.jp/
  - IAEA http://www-amdis.iaea.org
  - ORNL http://www-cfadc.phy.ornl.gov
  - KAERI http://amods.kaeri.re.kr
  - *Open ADAS*

- Smaller websites

Data Quality

- Traceability
- Reference: published data, how and where
- Quality of the organisation originally reporting the data
- Year of publication / production
- Experimental / theoretical / compilation
- Method
- Accuracy
- Raw data / fitting function / interpolation

Spectroscopic Data
Atoms and Molecules Properties

- Atomic Spectra: waves lengths, energy levels, transition probabilities → GENIE
  - ASD 3.1, NIST, Atomic spectra http://physics.nist.gov/PhysRefData/ASD
  - KAERI AMODS Spectral lines http://amods.kaeri.re.kr/spect/SPECT.html
  - Kurucz's CD-ROM http://cfa-www.harvard.edu/amdata/ampdata/kurucz23/sekur.html
  - Atomic Line List v.2.04 http://www.pa.uky.edu/~peter/atomic
  - TOPbase (Opacity Project) http://heasarc.gsfc.nasa.gov/topbase/home.html
  - Kelly Atomic Line Database http://cfa-www.harvard.edu/amdata/ampdata/kelly/kelly.html
  - MCHF/MCDHF Collection http://atoms.vuse.vanderbilt.edu
  - CAMDB http://www.camdb.ac.cn/e/

- Molecular spectra
  - NIST Molecular Spectra Database http://physics.nist.gov/PhysRefData/MolSpec/
  - NIST Chemistry Webbook http://webbook.nist.gov/chemistry/
  - Finding Chemical Spectra and Spectral Data, University of Texas, Austin http://www.lib.utexas.edu/chem/info/spectra.html

- Ionization potentials, CAMDB http://www.camdb.ac.cn/e/

Collisional Data

- IAEA ALADDIN http://www-amdis.iaea.org/ALADDIN
- Atomic and Molecular Data, NIST
  http://physics.nist.gov/PhysRefData/contents-misc.html
- CAMDB http://www.camdb.ac.cn/e/
  - Electron impact ionization, excitation
  - Dielectronic recombination
  - Photon ionization, auto ionization
  - Ion molecules collisions
- AMDIS NIFS http://dbshino.nifs.ac.jp (login and password)
  Rate coefficients, cross sections
  - Atomic data: excitation, ionization, recombination
  - Molecular data
- CFADC, ORNL ALADDIN http://www-cfadc.phy.ornl.gov/aladdin/aladdin.html
- KAERI, total and differential cross sections by electron impact
  http://amods.kaeri.re.kr/impact/IMPACT.html
- *OPEN ADAS*

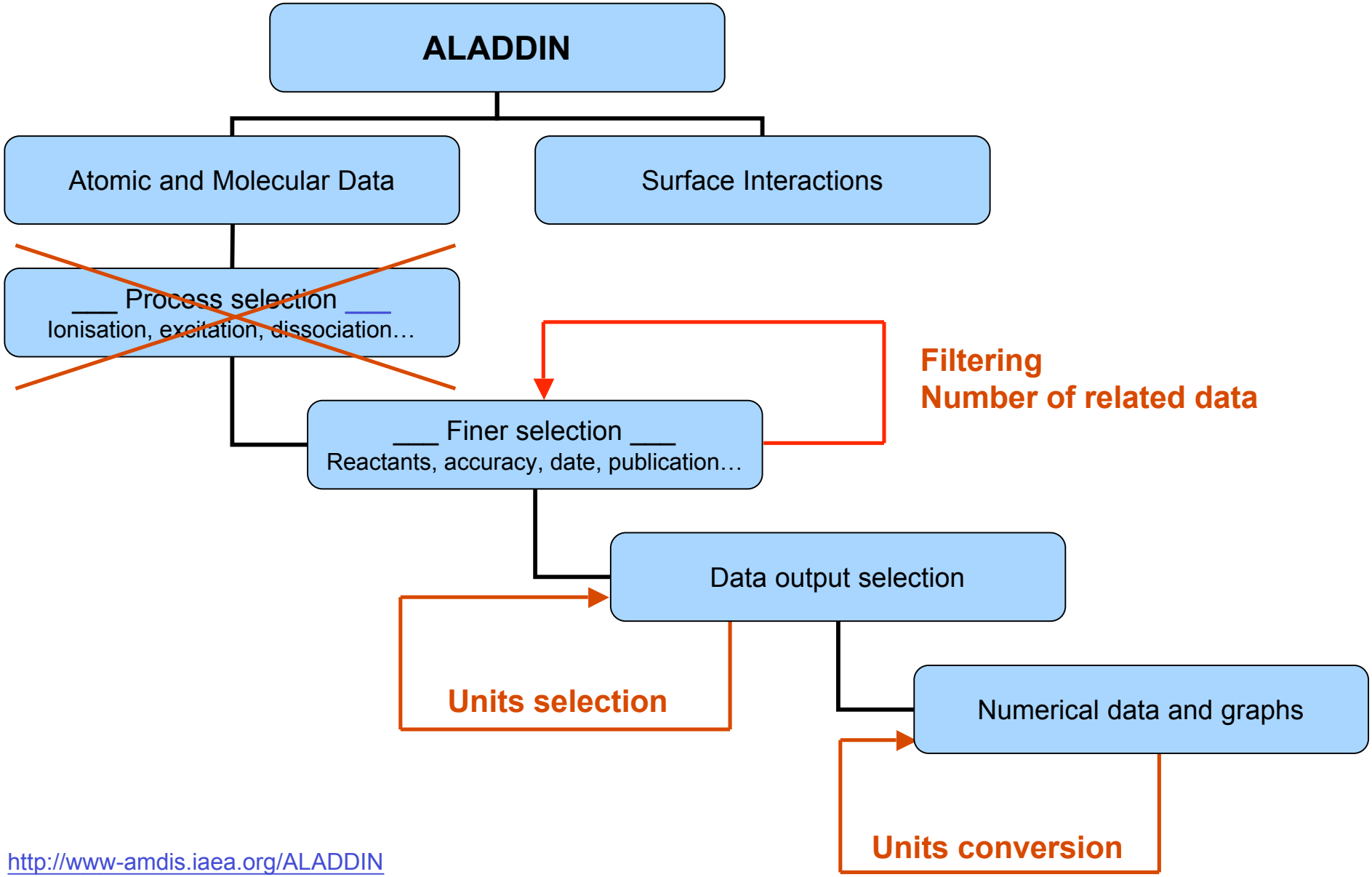
ALADDIN

Domain

- Atomic and molecular collisions (8000 data)
- Particle surface interactions (1500 data)

Search criteria (atomic and molecular data)

- process and category of processes
- 1 or 2 reactants, including possible ionization and quantum state
- 1 product, including possible ionization and quantum state
- data quantity: cross sections, rate coefficients differential cross sections
- data type: experimental, theoretical, derived
- data accuracy
- Bibliography: publication, author, date



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

OPEN-ADAS

ADAS is an interconnected set of computer codes and data collections for modelling:

- Radiating properties of ions and atoms in plasmas
- Analysis and interpretation of spectral measurements

Database scope: data for fusion and astrophysical application

ADAS accessible to members (fee), not WWW access

Project

To develop a free WWW access to ADAS data

Search Engine

GENIE

General Internet Search Engine

- http://www-amdis.iaea.org/GENIE/
- http://www2.lpgp.u-psud.fr/genie/ (mirror site)

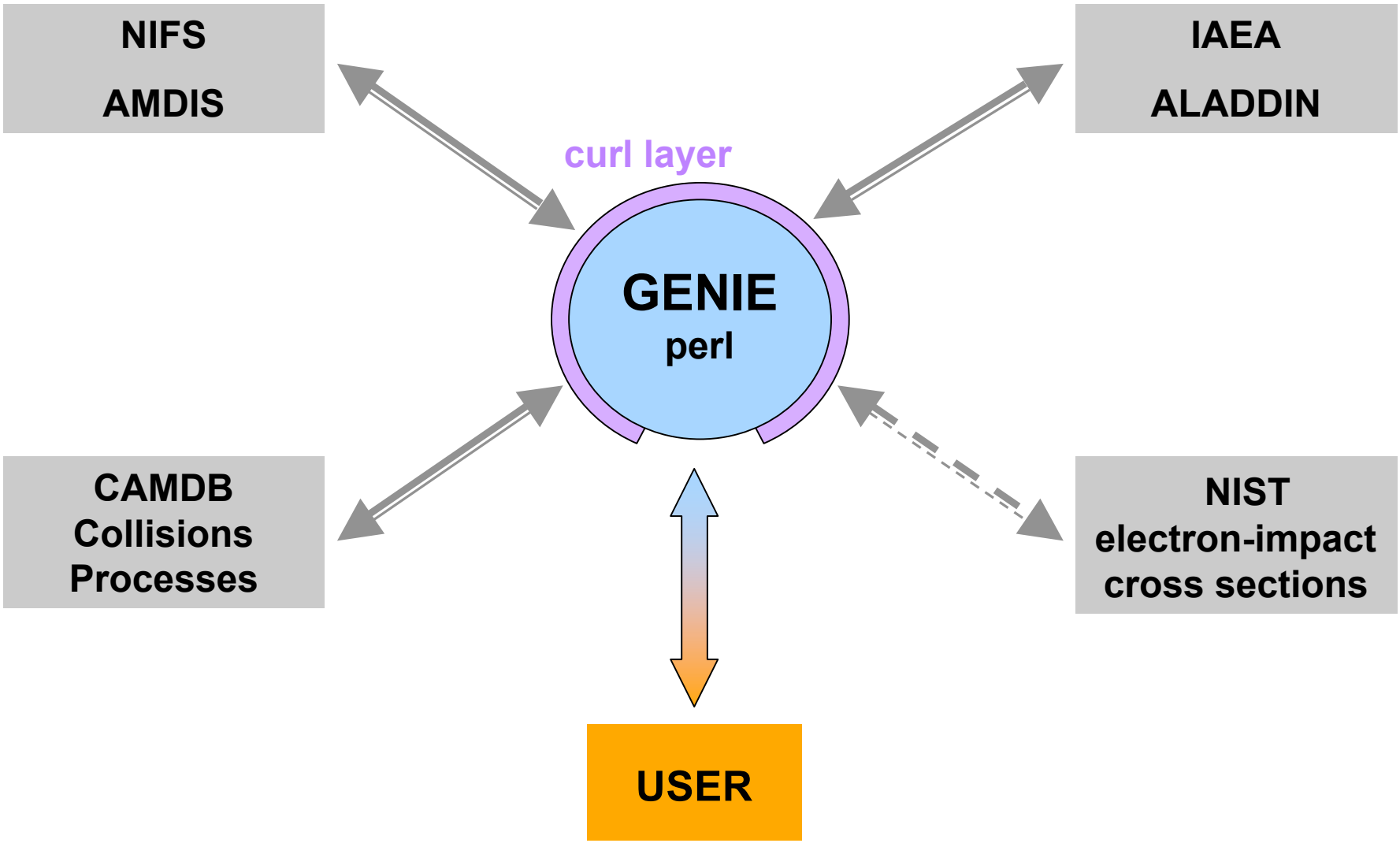
Spectroscopic data

- Oscillator strengths, transition probabilities and energy levels
- 8 databases

Electronic Collisions

- Electronic ionisation or excitation cross-sections and rate coefficients
- 4 databases

Excitation and Ionization Cross Sections



Web calculation tools

IAEA

- Cross sections of bare nuclei on hydrogenic ions:

  http://www-amdis.iaea.org/HEAVY/
- Average approximation for electron impact excitation of atomic ions:

  http://www-amdis.iaea.org/AAEXCITE
- Results from collisional radiative calculations of plasmas are available, as carried out with the Los Alamos modeling codes:

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

LANL

- Los Alamos atomic physics codes: an interface is available to run several Los Alamos atomic physics codes to calculate atomic structure and electron impact excitation, as well as ionization processes

  http://aphysics2.lanl.gov/tempweb/lanl/

Database definition

- Origin: computer science, but broadened to popular use even to non-electronic data collections.
- Possible definition: database is a collection of records stored in a computer in a systematic way, so that a computer program can consult it to answer questions
- A database implies:
  - Schema: definition of the different objects (tables and relations between tables)
  - Database model: the relational model is the most common one
  - Database management system (DBMS) to manage and query the data.

Exercises

Bibliographic data

Using different databases and CrossRef

1. Find a recent publication of Joshipura on excitation of CH_4
2. Find publications on “excitation cross sections for e, Fe^{13+} collisions” (3 more recent publications)
3. Make a biblio in your field of interest for the recent years

Numerical Data

Using different databases and GENIE

1. Looking for all excitation cross sections/coefficient rates for e, C^{4+}
2. Looking for a specific transition:

   e, C^{4+} [$1s^2$ ^1S] → e, C^{4+} [1s2p ^1P]

Bibliographic Data Links

General Databases for A+M, PMI and Fusion Research

- AMBDAS, IAEA http://www-amdis.iaea.org/AMBDAS
- CFADC, ORNL http://www-cfadc.phy.ornl.gov/bibliography/search.html
- GAPHYOR, LPGP http://gaphyor.lpgp.u-psud.fr/gaphyor/gaphyor.html
- FUSION, NIFS https://dbshino.nifs.ac.jp/
  Logon ID : triesta Password : kXdb$nGy

Specialized databases:

NIST Atomic Spectra Bibliographic database http://physics.nist.gov/PhysRefData/ASBib1/index.html

- Energy levels, wavelengths
- Transition probabilities
- Spectral line broadenings

Crossref pilots:

- http://portal.acm.org/xrs.cfm
- http://www.iop.org/EJ/search_crossref

….

Electronic publishers

- IOP: http://www.iop.org/EJ/ (Journal of Physics B, Physica Scripta…)
- APS: http://publish.aps.org/ (Physical review A and B, Physical Review Letters..)
- Elsevier (Science Direct) http://www.sciencedirect.com/ (Surface Science, Chemical Physics Letter…)
- AIP: http://www.aip.org/pubs/ (Journal of Chemical Physics)
- EDP: http://www.edpsciences.org/index.cfmAstronomy Astrophysics Journal (free)

Web Libraries

- The NASA Astrophysics Data System http://adswww.harvard.edu/
- LANL Library http://catalog.lanl.gov/F

Numerical data links

Collision Data

IAEA ALADDIN http://www-amdis.iaea.org/ALADDIN
CAMDB http://www.camdb.ac.cn/e/
Electron impact ionization, excitation, dielectronic recombination, photon ionization, auto ionization, ion molecules collisions
AMDIS NIFS http://dbshino.nifs.ac.jp Logon ID : triesta Password : kXdb$nGy
Atomic data: excitation, ionization, recombination
Molecular data
CFADCALADDIN, ORNL http://www-cfadc.phy.ornl.gov/aladdin/aladdin.html
Atomic and Molecular Data, NIST http://physics.nist.gov/PhysRefData/contents-misc.html

Spectroscopic Data

Atomic Spectra: waves lengths, energy levels, transition probabilities → GENIE
ASD 3.1, NIST, Atomic spectra http://physics.nist.gov/PhysRefData/ASD
KAERI AMODS Spectral lines http://amods.kaeri.re.kr/spect/SPECT.html
Kurucz's CD-ROM http://cfa-www.harvard.edu/amdata/ampdata/kurucz23/sekur.html
Atomic Line List v.2.04 http://www.pa.uky.edu/~peter/atomic
TOPbase http://heasarc.gsfc.nasa.gov/topbase/home.html
Kelly Atomic Line Database http://cfa-www.harvard.edu/amdata/ampdata/kelly/kelly.html
MCHF/MCDHF Collection http://atoms.vuse.vanderbilt.edu
CAMDB http://www.camdb.ac.cn/e/
Molecular spectra
NIST Molecular Spectra Database http://physics.nist.gov/PhysRefData/MolSpec/
NIST Chemistry Webbook http://webbook.nist.gov/chemistry/
Finding Chemical Spectra and Spectral Data, University of Texas, Austin
http://www.lib.utexas.edu/chem/info/spectra.html
Ionization potentials, CAMDB http://www.camdb.ac.cn/e/

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