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Technical Aspects of Atomic and Molecular Data Processing and Exchange, 24th Meeting of the A+M Data Centres Network

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

4-6 September 2017

Prepared by

Christian Hill and Hyun-Kyung Chung

October 2018

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Prepared by

Hyun-Kyung Chung

Abstract

This report summarizes the proceedings of the IAEA Technical Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (24th Meeting of the A+M Data Centres Network) on 4-6 September 2017. 12 participants from 11 data centres of seven Member States attended the three-day meeting held at the IAEA Headquarters in Vienna. The report includes discussions on the data issues, meeting conclusions and recommendations and the abstracts of presentations presented in the meeting.

October 2018

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1. Introduction

The 24th IAEA Technical Meeting (TM) of the Atomic and Molecular Data Centres Network (DCN) on "Technical Aspects of Atomic and Molecular Data Exchange and Processing" was held at the IAEA Headquarters in Vienna, Austria, from 4 to 6 September 2017. Participants from national data centres are invited to review progress in atomic, molecular and plasma-surface interaction (A+M/PSI) data related activities in the data centres in the last two years and to discuss data issues for the next period.

The activities of nine of the data centres currently participating in the DCN were presented: by Yu. Ralchenko of NIST (National Institute of Standards and Technology, USA), I. Murakami of NIFS (National Institute of Fusion Science, Japan), M. O'Mullane of ADAS (Atomic Data and Analysis Structure project, UK), P. Goncharov of SPBSTU (Peter the Great Polytechnic University, Russia) on behalf of A. B. Kukushkin (NRC Kurchatov Institute, Russia), D. Reiter of FZJ (Forschungszentrum Jülich GmbH, Institut für Plasmaphysik, Germany), T. Nakano of QST (National Institutes for Quantum and Radiological Science and Technology, Japan), M.-Y. Song of NFRI (National Fusion Research Institute, Korea), H. Chung of IAEA and D.-H. Kwon of KAERI (Korea Atomic Energy Research Institute, Korea). The representative from the Chinese Research Association on Atomic and Molecular Data at Institute (CRAAMD) of the Institute of Applied Physics and Computation Mathematics (IAPCM, Beijing, China) could not attend the meeting due to difficulties with the nomination.

Two experts were invited to discuss their work in atomic, molecular and plasma-surface interaction data: C. Ballance of Queen's University of Belfast, UK and Raúl Barrachina of Comisión Nacional de Energía Atómica, Argentina. Their data centres are considered as the new members of the DCN and the membership status will be formally accepted in the next DCN meeting in 2019 after a review.

A. Koning (Section Head, Nuclear Data Section) and H. Chung (Head of Atomic and Molecular Data Unit and Scientific Secretary) represented the IAEA. The previous Unit Head, B. J. Braams retired in November, 2016 and H. Chung, who took the Unit Head position from December 2016, will also leave the Agency by the end of September under the staff rotation policy. The new Unit Head from October 2017 is Christian Hill from University College London, UK.

Discussions were held on the following topics:

- Exchange of information on data centre activities.
- Data evaluation: experiences, plans and encouragement.
- Data exchange format: status of XSAMS development and implementation.
- Cooperation on the maintenance of bibliographical databases.
- Funding for atomic and molecular data for fusion applications.
- Priorities for data development and evaluation, new meetings and information exchange.

The proceedings of the meeting are summarized in Section 2 and the summary of technical discussions on the above topics and recommendations on future work plans are presented in Sections 3 and 4 in this report. The full list of participants is available in Appendix 1 and the adopted agenda is listed in Appendix 2. Presentations are summarized in Appendix 3.

2. Proceedings of the Meeting

The head of the Nuclear Data Section, A. Koning welcomed participants and emphasized increasing interest and need for atomic and molecular data. He acknowledged the progress made in the uncertainty quantification activities that DCN has supported. He described the crowdsourcing project that IAEA is pursuing to use a massive amount of material simulation data to be hosted by the Unit. An investigation is on the way to use the material data for global estimates of radiation damage. Participants introduced themselves and the agenda in Appendix 2 was adopted without change. H. Chung reviewed meeting objectives.

The meeting proceeded with presentations by data centres on their current activities and by the experts on atomic and molecular data research. On the first day, participants discussed the current status and future plans for the bibliographic database AMBDAS. On the second day, presentations were given on two data centres viewed as the new members to the DCN. The new unit head, C. Hill, presented a talk on online databases, which was followed by two sessions on the topic of databases and data exchange. In the afternoon, two talks were presented on the topic of data needs for fusion applications and participants discussed the issue of funding for data. Discussions on data evaluation activities were postponed to the last day when discussion took place for previous and future DCN activities.

Slides of presentations are available on the Unit web site http://www-amdis.iaea.org/DCN/ via the link to Meeting Reports and Presentations. Detailed summaries of presentations are provided in Appendix 3. Discussion sessions are summarized in Section 3.

2.1 Current Activities of Atomic and Molecular Data Centres

Seven data centres presented progress reports on their activities on data compilation, generation and evaluation or web developments, publications in the period of 2015-2017 and future plans on the first day.

Yu. Ralchenko described the status of the atomic data program at NIST which hosts the Atomic Spectra Database (ASD) with 258 000 spectral lines and 110 000 energy levels, and three bibliographic databases of 20 018 references for energy levels and spectra lines, 9 380 for transition probabilities and 6923 for line shapes and broadening. A new database for LIBS (Laser Induced Breakdown Spectroscopy) was introduced and activities on data compilation, collisional-radiative modeling and EBIT measurements were presented as well as collaboration activities with other data centers.

I. Murakami reported the development and maintenance of NIFS databases containing 770 745 collisional data in total (as of 3 August 2017). The relational database management system has been changed from Oracle/MySQL to PostgreSQL. Collaborative research on tungsten ions and heavy atom ions as well as data relevant for divertor applications was described.

M. O'Mullane reported on recent updates to the ADAS atomic database and new developments in ADAS data production and atomic models. A project to calculate state selective dielectronic recombination (DR) rates for all tungsten ions is described and the effort to improve parameter-driven spectral features was described.

P. R. Goncharov reviewed developments in Russia in the past two years in the field of atomic, molecular and PMI data. The review includes (a) new results pertaining to generation of atomic and molecular data for fundamental science and controlled fusion; (b) use of atomic and molecular data in con-trolled fusion research, with the emphasis on the data needs for ITER diagnostics being developed in Russia and for Russian domestic research programme; (c) recent works in Russia on plasma-material interaction data.

M.-Y. Song reported on the activities of Data Centre for Plasma Properties (DCPP); the new database system of 26 518 data records, contribution to IAEA AMBDAS bibliographic database. The centre manages the data evaluation project by a group of scientists and produces experimental and theoretical data for electron-atom and electron-molecule collisions.

H. Chung summarized the activities at IAEA A+M Data Unit, which include CRP (Coordinated Research Projects), meeting organizations, book and report publications as well as the maintenance and development of databases and online codes. Much of the unit's activities has been focused on promoting data evaluation and uncertainty quantification activities in the atomic, molecular and plasma-surface interaction data communities.

D. Kwon presented the recent progress of the KAERI atomic and molecular data centre. The activities consist mainly of two parts: 1) state-of-the-art calculations for the electron-impact ionization and recombination, and photoionization data which are essential in modeling for laboratory and astrophysical plasmas and 2) Spectroscopic measurement in plasma devices and the modeling for analysis on the measured spectra since 2012.

2.2 Proposed Data Centre Activities

Two data centres, potentially joining the DCN, presented their data activities. Their membership will be reviewed prior to the 2019 DCN meeting.

C. P. Ballance reported on the atomic and molecular data production and evaluation activities by the CTAMOP collision group at Queen's University Belfast. The electron-impact collision data sets have been applied to magnetically confined fusion diagnostics and modeling, for example, in support of the Compact Toroidal Hybrid (CTH, Auburn University) and DIII-D Tokamak (General Atomics), as well as ITER.

R. O. Barrachina reported activities in many laboratories in Argentina working on Atomic, Molecular and Surface Physics in Argentina. They include the Bariloche Atomic Centre, a research facility of the National Atomic Energy Commission (CNEA), the Institute of Astronomy and Space Physics or IAFE, the Rosario Institute of Physics (IFIR) and the Southern Physics Institute (IFISUR) consisting of more than 50 researchers and graduate students working in a large range of processes, with different projectiles (ions, electrons, positrons, photons, etc.), targets (atoms, molecules, surfaces, etc.) and outgoing channels (elastic and inelastic collisions, charge exchange, ionization, transfer ionization, etc.). There is a plan to create a data centre within the structure of CNEA and the objectives will be to provide fundamental data for nuclear and non-nuclear science and technological projects, and to coordinate the generation, collection and critical assessment of the required data by the different groups in Argentina.

2.3 Databases and Data Exchange

The new Unit Head C. Hill presented recent developments in several online atomic and molecular databases: 1) VAMDC, the Virtual Atomic and Molecular Data Centre: an EU-funded project to build a network of databases and data services around a common query language and output format, 2) HITRAN, a major database of molecular spectroscopy data, 3) ExoMol a database of *ab initio* molecular line lists for high temperature applications. 4) QuantemolDB, a database of electron collisional cross section processes and heavy particle reaction Arrhenius parameters. Future directions and challenges for AM databases were also described.

The database and software demonstrations by data centres followed the presentation and data exchange formats were discussed. The discussions are summarized in Section 3.3, below.

2.4 Data Needs for Fusion Research

D. Reiter summarized ongoing and pending database activities at FZJ for existing databases (molecular and surface reflection databases) used in fusion edge plasma modelling, including:

- the kinetic Monte Carlo Code EIRENE (www.eirene.de);
- the molecular database HYDKIN (http://www.hydkin.de);
- a surface reflection database based on the BCA (binary collision approximation): see (http://www.eirene.de/html/surface_data.html); and
- an online sensitivity analysis tool, also available at www.hydkin.de, which facilitates uncertainty propagation (UP) in fusion codes.

In addition, major issues related to AM data used in edge plasma modelling codes were reviewed.

T. Nakano reviewed the current data needs for ITER tungsten divertor. Data needed for lowly ionized W ions in divertor/SOL plasmas (10 eV < Te < 200 eV) and highly ionized W ions in core plasma (1 keV < Te < 20 keV) were reviewed. Data needs for radiative divertor modelling with impurity seeding are also reviewed for light elements such as C, N, Ne and Ar in divertor/SOL plasmas (10 eV < Te < 200 eV). Finally, the data needs for sub-divertor region (where no plasma exist) were also reviewed.

3. Technical Discussions

Issues related to data research and data centres were discussed: bibliographical data compilation, data evaluation, data exchange, database development, and priorities for data development and evaluation for fusion applications.

3.1 Bibliographic Data Compilation

The following points were raised during discussion about the compilation of bibliographic information on atomic and molecular data:

- The Harvard ADS system (http://ads.harvard.edu/) works well and is widely used in the astrophysics community;
- The A+M Unit's own AMBDAS bibliographic database has grown to 50 162 entries, but is currently under-used and its interface is in need of an upgrade. Its advantage is that, in many cases, it contains the numerical data in addition to citation information (including DOI) for each entry.
- NIST maintains several well-used bibliography databases, including:
  - the NIST Atomic Energy Levels and Spectra Bibliographic Database (https://physics.nist.gov/cgi-bin/ASBib1/ELevBib.cgi);
  - the NIST Atomic Transition Probability Bibliographic Database (https://physics.nist.gov/cgi-bin/ASBib1/TransProbBib.cgi); and
  - the NIST Atomic Spectral Line Broadening Bibliographic Database (https://physics.nist.gov/cgi-bin/ASBib1/LineBroadBib.cgi).
- NFRI has numerical data to be linked to bibliographical data; it would be desirable to obtain this data for AMBDAS.
- The previously-available ORNL web page, the "red book", is now no longer available.

3.2 Data Evaluation and Uncertainty Quantification

IAEA data evaluation activities have been coordinated by the DCN and a series of meetings have been organized since 2012 including consultants' meetings (CM) and technical meetings (TM) as well as collaboration workshop with ITAMP (Institute of Theoretical Atomic, Molecular and Optical Physics, at the Harvard-Smithsonian Center for Astrophysics). At the 1st TM on data evaluation held in Daejeon, in 2012, participants identified the issues such as lack of uncertainty quantification for theoretical data, lack of self-consistency checks in experimental data sets or lack of qualified data evaluators in the community. After the meeting, IAEA has promoted activities on uncertainty quantification (UQ) of theoretical data and data evaluation by a group of scientists of a form of an editorial board. There were a few group data evaluation projects developed, such as the eMOL group project (headed by Nigel Mason), NFRI group project on e-methane data and IAEA CM project on tungsten dielectronic recombination rate coefficients. In December 2016, more than 50 participants attended the TM on "Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications", one of the largest TM that the unit organized. It shows that the data evaluation and UQ activities are shaping up nicely in the community within 5 years of DCN collaboration.

The validation for thermal desorption spectroscopy (TDS) data is under way. The TDS technique is critical to the measurement of hydrogen trapping and retention in material. However, the measured data have never benchmarked. IAEA organized the round-robin experiments in collaboration with IPP-Garching and Osaka University to validate the TDS data and recommend the best practices of TDS measurements. In addition, a workshop to compare codes to interpret TDS measured data is to be organized.

A review paper was published on the uncertainty estimates of atomic and molecular data under the IAEA collaboration with community (2016 *J. Phys. D: Appl. Phys.* **49** 363002), which shows that the atomic and molecular data physics community is beginning to recognize the value and significance of the UQ activities. Recently, the importance of UQ is recognized for the optimization-based design of complex systems, such as fusion divertor designs. If the user community requests the target accuracy of necessary data, the UQ activities of theoretical data will be more active. Particularly, the joint effort with mathematical and computational sciences is foreseen in the quest of UQ activities, as shown at the 2015 workshop on sensitivity, error and uncertainty quantification for atomic, plasma and material data hosted by Stony Brook University, Institute for Advanced Computational Science. The community is seeking the more systematic and objective way to quantify uncertainties associated with atomic and molecular data.

The IAEA wants to expand this kind of network effort to other relevant scientific areas.

A report from the National Research Council of the US National Academy of Sciences in 2012 titled as "Assessing the Reliability of Complex Models: Mathematical and Statistical Foundations of Verification, Validation, and Uncertainty Quantification" outlines mathematical and rigorous ways to compute uncertainties of model results. A method such as surrogate model or subset model may be applied to assess the accuracy of calculated cross-sections of complex atoms and molecules and a CM may be organized to address such a UQ method. Monte Carlo approach of sensitivity analysis or uncertainty propagation of atomic structure and collision data on the final results of ionization and population distributions has been started. *UQ in this area is complex because there exists a correlation between atomic structure and collisional data.* A Consultancy Meeting may be organized to address UQ issues for highly complex atomic structure and cross-sections. A suggested possibility is a CM on surrogate (simplified) model for error propagation (atomic structure to collision cross section: sensitivity analysis).

IAEA unit's activities on UQ and data evaluation have changed the views in the community. However, there is a concern on financial support to continue the activities and publicize them. DCN members have been major supporting forces for the IAEA unit to pursue data evaluation activities. The IAEA DCN is expected to continue to play an important role in the quest of data evaluation and uncertainty quantification.

The Integrated Modeling community is seeking to apply VVUQ (Verification, Validation and Uncertainty Quantification) workflow principles to its activities. IAEA has helped with organized meetings, but not held a CRP on the topic as yet. *A CRP may be considered for UQ issues*: such an activity would be addressed at users, producers and people from mathematical and computational communities. Tungsten collisional data provides a case in point: researchers have been doing tungsten studies individually, but the CRP held 2010-2015 initiated a series of coordinated activities and organized comparison, benchmarking, and consensus-building of data amongst groups.
A round robin type of exercise would be useful (in the CRP); for example, adding arbitrary errors for propagation, or doing code comparison workshops. An example of non-LTE kinetics code comparison workshops is useful. In the neutral beam CRP, a code comparison workshop of cross-sections was discussed, which can lead to UQ. It was considered that funding will eventually come if everyone finds it important; visibility is also important.

Outcome of evaluation activities will be journal publications, which might be expected to be highly-cited. The IAEA would host the evaluated data after the data evaluation activity is done. Eventually, we should provide a "reference" set recommended by the data community, which will provide a single set for user community.

Currently a coverage is better than the standard data, and data centres provide multiple data sets for a process (that is why ADAS keeps old data sets).

For Applications, it is important to ascertain what the target uncertainty is to be. Users should establish a list of important processes what is tolerated uncertainty etc. Integration of user and producer communities is very important.

Outreach issues:

- IAEA has no mechanism of bringing new students etc. unless it involves developing countries.
- Atomic data are fundamental and many user communities require atomic data.

- The ICAMDATA conference is a good medium to bring the issues.

For nuclear data, it is a common practice to use Bayesian approach for UQ estimates. We should ask experimentalists to measure data, especially for simple atoms. In this context, the knowledgebase on researchers in atomic and molecular collisions that will form part of the upcoming Experimentalists' Nework will be useful.

3.3 Databases and Data Exchange

The development of XSAMS (XML Schema for Atoms, Molecules and Solids) was transferred to the VAMDC (Virtual Atomic and Molecular Data Consortium: http://www.vamdc.org/) which issued an official release of the Schema in 2012 and several minor updates since then. Work has recently focused on the development of tools to transform data in the XSAMS format into other formats for use in existing software tools and for comparison purposes. A single "portal" website, giving access to all 33 databases in the consortium was also released and is undergoing active development (https://portal.vamdc.eu/vamdc_portal/home.seam). The next annual meeting of the VAMDC will be held at the Paris Observatory, 23 – 25 May 2018.

A subset of the IAEA's ALADDIN database is available using the protocols of the VAMDC; other relevant databases not in the Data Centres Network include:

- LXCat, a collection of data and online tools relevant to modeling low-temperature, non-equilibrium plasmas (http://fr.lxcat.net/home/).
- BEAMDB, electron interaction cross-sections for elastic scattering, electron excitation, ionization and total scattering (http://servo.aob.rs/emol/).
- IDEADB, the Innsbruck Dissociative Electron Attachment Database: this database contains information about dissociative electron attachment upon interaction with low energy electrons (http://ideadb.uibk.ac.at/).
- STARK-B, a database of calculated widths and shifts for isolated lines of neutral and ionized atoms due to electron and ion collisions (http://stark-b.obspm.fr/).
- BASECOL, a database devoted to collisional ro-vibrational excitation of molecules by colliders such as atoms, ions, and molecules (http://basecol.obspm.fr/).
- CHIANTI, an atomic database for spectroscopic diagnostics of astrophysical plasmas (http://www.chiantidatabase.org/).

3.4 Data Needs for Fusion Research

A brief summary of the main data areas discussed is given here.

- BeH, H_2, HD, etc. → H* + D etc. (P. Goncharov).
- Be^{q+} transition probs. (P. Goncharov; NFRI staff have some BeH calculations).
- Be^{4+} etc. as impurities due to neutral beam penetration, of particular relevance to JET and ITER.
- BeD data: this has been measured by various fusion experiments (band heads detected).
- Experimental data for beryllium. Unfortunately, such measurements can currently only be done one place (UCSD PISCES).
- In many cases, the formation mechanism of molecules is not clear; the concentration of atoms consisting the molecules should be high enough to make a molecule.
- Sn^{q+} (for liquid metal divertors, vapour shielding); note that the AMD Unit will initiate a CRP on fundamental data for vapour shielding soon.
- Data for modelling of "killer" pellets.
- Data for runaway electron mitigation purposes.
- For ITER: NH_3 data is important: N_2 puffed into the plasma to cool it is converted to NH_3 in the subdivertor region, which enters the cryopumps):

- Arrhenius parameters only in the list they have compiled already;
- There is a need for surface data relating to the formation of NH_3: sticking coefficients;
- Reaction frequencies, E_{ads}, etc. are also required;
- See D. Reiter, preliminary report for ITER.

The IAEA and the Data Centres Network can assist in community building to aid the coordinated calculation, measurement and evaluation of relevant data.

3.5 Funding for A&M data for fusion applications

A brief summary of the main points discussed is given here.

- Funding from EUROfusion: their focus is on running JET, MAST, etc.
- There is difficulty obtaining funding for uncertainty quantification activities.
- It is necessary to use the correct “buzzwords” in any grant application.
- The perception to funding applications from outside the community is that fusion is already very well-funded (therefore, it is hard to get further external money).
- DoE funding is not critical to NIST (they get funding directly from the US Federal budget).
- Russia funding possible: ~$500k to an individual (difficult to obtain, need an h-index greater than 30 – 40).
- Can AM research for fusion appeal to non-fusion (e.g. medical) applications?
- Can uncertainty quantification (UQ) be presented as a *safety* issue?

3.6 Data Centres Network Membership Issues

The terms of reference for the AM/PSI Data Centre Network are as follows: The domain is atomic and molecular physics and particle surface interactions (AM/PSI). Data should be strongly relevant to fusion. A participating data centre should have established programs in one or more of the following:

- Collection of data
- Dissemination of data
- Calculation and/or measurement of data
- Assessment/evaluation of data

Two new data centres are expected to join the Data Centres Network by the time of its next meeting: the Centre for Theoretical Atomic, Molecular and Optical Physics (CTAMOP) at the School of Mathematics and Physics, Queen’s University Belfast, UK and the Bariloche Atomic Centre, Argentina, part of the Comisión Nacional de Energía Atómica (CNEA), represented at this meeting by Raúl Barrachina.

As old data centre representatives approach retirement, or their research groups shift focus, and the new data centres are established, the DCN membership of existing data centres will continue to be reviewed regularly.

4. Future Activities of Data Centre Network

The following notes refer to planned or desired activities that can be promoted within the DCN.

- A network or database of AM/PSI experimentalists would be useful: an IAEA Consultancy Meeting could be held to help find relevant research groups.
- As ever, coordinated activities on data evaluation should be promoted: it was considered to approach Jonathan Tennyson (UCL) and Nakamura Nobuyuki (ILS-UEC) in connection with this.
- Coordinated data collection is needed for AMBDAS; with respect to PMI data, again, a Consultancy Meeting could be held.
- XSAMS implementations on existing databases should be encouraged; the AMD Unit will continue to offer its support to the VAMDC in its activities in setting and implementing standards in data exchange.
- Coordinated activities to establish a list of critical data needs for fusion:
    - The DCN has only relatively few contacts in fusion community: these could be expanded by hiring an expert, such as a retired specialist or ITER contact as a consultant for a short period of time.
    - There will be an ITER meeting on divertor design (to be held at the IAEA)
    - ITER now sponsors code comparison for neutral beam transport (cf CRP): the aim here is to propagate uncertainties with relatively simple codes.
- Proposed meetings and workshops:
    - See above (CMs, TMs).
    - Outreach (e.g. ICTP advanced schools).
    - It would be particularly helpful to build links in China and Brazil.
- Outreach to AM/PMI scientists outside our community:
    - medical plasmas.
    - plasma for waste disposal (though there is little actual fundamental data used here; a lot of the work is empirical).
    - In-country Workshops; it is noted that Russia in particular is currently encouraging outreach of this nature.

Appendix 1

List of Participants

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Appendix 2

AGENDA

Monday, 4 September **Meeting Room: C0343**

09:30 – 10:00	Opening (Arjan Koning, Nuclear Data Section Head) Introduction of Participants Review Meeting Objectives Adoption of Agenda
Session 1:	Current Activities of Data Centres
Chair:	D. Reiter
10:00 – 10:30	Y. Ralchenko (NIST): Recent Developments of the NIST Atomic Data Program
10:30 – 11:00	I. Murakami (NIFS): Atomic and Molecular Data Activities at NIFS in 2015-2017
11:00 – 11:20	*Coffee break*
11:20 – 11:50	M. Song (NFRI): A+M Data Center Activities in National Fusion Research Institute
11:50 – 12:20	M. O'Mullane (ADAS): Recent updates to the ADAS atomic database and new developments in ADAS data production and atomic models
12:30 – 14:00	*Lunch*
Session 2:	Current Activities of Data Centres (Continued)
Chair:	I. Murakami
14:00 – 14:30	D. Kwon (KAERI): Aspects and Prospects of KAERI Atomic Data Center
14:30 – 15:00	P. Goncharov (SPBSTU): Update on atomic, molecular and PMI data activity in Russia
15:00 – 15:30	H. Chung (IAEA): Current activities of IAEA atomic and molecular data unit
15:30 – 15:50	*Coffee break*
Session 3:	Bibliographical Data Compilation
Chair:	H. Chung
15:50 – 17:00	Coordinated activities on bibliographical data compilation (all participants)
18:30	*Social Dinner*

Tuesday, 5 September

Session 4:	Proposed Data Centre Activities
Chair:	C. Hill
09:00 – 09:30	R. Barrachina (CNEA): Atomic and Molecular Data Activities in Argentina
09:30 – 10:00	C. Ballance (QUB): R–matrix electron–impact excitation and ionization calculations in support Mo I and W I diagnostics
10:00 – 10:30	*Coffee break*
Session 5:	Databases and Data Exchange
Chair:	Yu. Ralchenko
10:30 – 11:00	C. Hill (UCL): Online Atomic and Molecular Databases
11:00 – 11:30	Data centre WWW database and software demonstrations
11:30 – 12:00	Data exchange format: xsams, adas, genie, (all participants)
12:00 – 13:30	*Lunch*
Session 6:	Data Needs for Fusion Research
Chair:	M. O'Mullane
13:30 – 14:00	D. Reiter (FZJ): AMS Data: data types and formats, and data needs for fusion edge plasma modelling
14:00 – 14:30	T. Nakano (QST): A&M data needs for fusion plasma research
14:30 – 15:30	Discussion on funding for A&M data for fusion applications (all participants)
15:30 – 15:50	*Coffee break*
Session 7:	Data Evaluation and Uncertainty Quantification
Chair:	H. Chung
15:50 – 16:20	H. Chung (IAEA): IAEA evaluation activities
16:20 – 17:00	Coordinated activities on data evaluation (all participants)

Wednesday, 6 September

Session 8: Data Needs for Fusion Research (Continued)

Chair: D.Reiter

09:00 – 10:30 Priorities in A+M/PMI data compilation and evaluation (all participants)

10:30 – 10:50 *Coffee break*

Session 9: Review on Data Centres Network Activities

Chair: H. Chung

10:50 – 11:10 Membership Issues

11:10 – 12:30 Plan of DCN activities for the future

- Network of AM/PSI Experimentalists
- Coordinated activities on data evaluation
- Coordinated data collection for bibliographical database AMBDAS
- XSAMS implementation of DCN members
- Coordinated activities to establish a list of critical data needs for fusion
- Proposed meetings and workshops on AM/PSI
- Outreach to A+M/PMI scientists outside our community

12:30 – 14:00 *Lunch*

Session 10: Meeting Conclusions and Recommendations

Chair: H. Chung

14:00 – 16:00 Formulation of meeting conclusions and recommendations
Date of next meeting

16:00 – ***Adjournment of the Meeting***

Appendix 3

SUMMARY OF PRESENTATIONS

Current status of the atomic data program at NIST

Yu. Ralchenko
National Institute of Standards and Technology

Yu. Ralchenko described the status of the atomic data program at NIST. The main collection of evaluated data, the Atomic Spectra Database (ASD) version 5.4 (released in Sep 2016), contains about 258,000 spectral lines and 110,000 energy levels. A new release is planned for October 2017. Also three bibliographic databases of more than 20,000 references for energy levels and spectral lines, 9380 for transition probabilities and 6923 for line shapes and broadening are maintained and regularly updated. A new database for Laser Induced Breakdown Spectroscopy (LIBS) was reported. Also activities at the NIST Atomic Spectroscopy Group on calculation and evaluation of atomic data (energy levels and spectral lines, collisional cross sections including charge exchange for fusion-related processes) were described in detail.

Atomic and Molecular Data Activities at NIFS in 2015-2017

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National Institute for Fusion Science (NIFS)

We have continuously worked on atomic and molecular database and research related atomic and molecular data collaborated with atomic physicists and plasma physicists in 2015-2017. We have maintained, updated and opened public the NIFS atomic and molecular database via internet. We reconstructed our database system in 2016 and the relational database managing system is changed from Oracle to PostgreSQL. User interfaces do not changed, however, internal systems are newly developed. New functions are added to show selectable tables of elements with charge states or processes with projectile and target atom/molecules for simpler search. These changes allow user to find easily what they want to see.

Many collaborative researches have been carried out mostly on tungsten ions and heavy atom ions. We measured visible and extreme ultraviolet (EUV) spectra of tungsten ions in LHD and compact EBIT (CoBIT) plasmas. M1 visible lines of W^{26+} and W^{27+} ions were measured to estimate spatial distribution of tungsten ions in LHD plasmas [1], which agree with calculated abundance distribution with ADAS ionization and recombination rate coefficients. With using CoBIT, we succeeded to measure EUV spectrum of W^{26+} and W^{27+} ions with high resolution [2], and identified the EUV spectral lines for their charge states from W^{6+} to W^{13+} ions [3]. Precise measurement of the wavelength for M1 visible line between fine structure levels of the ground state of W^{7+} ion can be used for benchmark of atomic structure calculation [4]. We have constructed a collisional-radiative model for W^{27+} ion including recombination processes for the first time [5]. We have measured EUV spectra for lanthanide ions in LHD for high and low temperature plasmas and obtained Z-dependence of EUV spectra for them [6]. As a result, some lines of Tm^{40+} and Tm^{22+} ions have been identified experimentally for the first time [7]. We have calculated atomic structure and opacities for low-charged high-Z elements, mostly lanthanides, for astrophysical application purpose [8].

Related to atomic and molecular processes in divertor plasmas, we measured absolute generalized oscillator strength distribution for ionization and dissociation processes of H_2 and D_2 [9]. Various collaborative research related to fusion and other plasmas with domestic and oversea researchers are very important for us to keep activities related to atomic and molecular data.

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Developments in ADAS and OPEN-ADAS since the 23rd DCN meeting

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The ADAS release schedule is yearly and OPEN-ADAS is updated at the same time. The data in ADAS can be classified as either fundamental or derived: the former has a purely atomic nature while the derived data depends on macroscopic plasma parameters. ADAS population codes are developed to process relevant fundamental data into derived data suitable for plasma modelling and diagnostic interpretation. OPEN-ADAS, a public repository with no login requirements, contains a wide range of fundamental and derived atomic data suitable for fusion research needs.

Atomic data for tungsten has been the primary focus for ADAS since the last DCN meeting. A project to calculate state selective dielectronic recombination (DR) rates for all tungsten ions (funded by the UK research body, EPSRC) is on-going and data for W^{38+}–W^{73+} is now archived in ADAS and OPEN-ADAS in the ADAS adf09 data format. Compatible radiative recombination rates, in adf48 format, were calculated at the same time. The goals of the project, methodologies and results are given in journal papers: S P Prevel et al, Phys. Rev. A 93, 042703 (2016) and S P Prevel et al, J. Phys. B 50, 105201 (2017). Data for the next set of ionization stages is currently being calculated.

At the 23rd DCN meeting we outlined a method to develop a rule based system to optimize the line emission radiated power. The choice of configurations is key and the relative importance of the different rules depends on the element and ionization stage. Line power coefficients, in ADAS data format adf11/plt, are available for Ar, Fe, Kr, Xe and W in ADAS and OPEN-ADAS and a full description of the method is outlined in S S Henderson et al, Plas. Phys. Control. Fus., 59, 055010 (2017). The excitation data, in adf04 format, underlying this analysis is also available from ADAS and OPEN-ADAS.

One of the first systematic ADAS projects was to calculate state selective DR rates for each iso-electronic sequence (N R Badnell et al, Astron. Astrophys., 406, p1151 (2003)). The Al-like stage is the latest set of data produced (Sh. A. Abdel-Naby et al, Astron. Astrophys., A40, p537 (2012)) and these rates are available as adf09 files. This may be the last sequence generated as part of the DR Project work since the size of the resulting files is becoming large and difficult to handle in the population codes. Rate data resulting from the tungsten DR calculations is archived in a more compact format and this will be preferred for future work.

Fundamental excitation data for selection iron ionization stages, photon emissivity coefficients for the hydrogen Balmer and Paschen series, as well as selected ions (eg Ca^{19+}, Ni^{27+} and O^{2+}) have been added as a result of specific requests. Charge exchange emissivity coefficients (adf12) for lithium have also been produced to support liquid metal wall studies.

Generally fundamental atomic data comes from either a bespoke single ion calculation or a less targeted sequence consideration. The latter is classed as baseline in ADAS and improving the quality of this baseline data is a guiding principle of ADAS. The line power optimization work has shown the value of a systematic approach. The completeness of the set of configurations resulting from that optimization is the basis for optimizing the structure calculations of AUTOSTRUCTURE, giving a corpus of distorted wave excitation data for arbitrary ionization stages. This elevated quality baseline data will then be used to drive spectral feature codes and generalized collisional-radiative models for any element of interest.

For medium to heavy species, data which is LS-resolved is no longer adequate and an intermediate-coupled (ie J-resolved) resolution becomes necessary. The electron impact excitation data (adf04) required is mostly present in IC resolution but ion impact collisions must be explicitly included in the population calculations. A new class of data, adf06, archiving ion impact effective collision strengths resulting from proton, and other colliders, is being developed. A baseline set of data has also been calculated and will be added to ADAS and OPEN-ADAS soon.

Update on atomic, molecular and PMI data activity in Russia

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A review of developments in Russia in the past two years in the field of atomic, molecular and PMI data has been presented, based on contributions from the NRC Kurchatov Institute, NRNU Moscow Engineering Physics Institute, Peter the Great St. Petersburg Polytechnic University, A.F. Ioffe Physico-Technical Institute, P.N. Lebedev Physical Institute, G.I. Budker Institute of Nuclear Physics, and other organizations. The review includes (a) new results pertaining to generation of atomic and molecular data for fundamental science and controlled fusion; (b) use of atomic and molecular data in controlled fusion research, with the accent on the data needs for ITER diagnostics being developed in Russia and for Russian domestic research programme; (c) recent works in Russia on plasma-material interaction data.

New results on interatomic potentials have been published, including the effect of electronic screening on the nuclear fusion cross-section for the D^+-D^0 system (A.N. Zinoviev 2017 Nucl. Instr. and Meth. in Phys. Res. B **406** part B 465), and a technique for determining the interaction potentials of He^+–W, Ta systems (A.N. Zinoviev et al. 2016 Journal of Surface Investigation **10** 576). The correctness of model potentials used in calculations of the interaction of H and He ions with multielectron atoms of impurities in nuclear fusion facilities was assessed in (V.V. Afrosimov et al. 2017 Tech. Phys. Lett. **43** 122) where cross sections of electron capture and electron capture with ionization of Ar by He^{2+} ions were studied at various impact parameters.

In (V.V. Afrosimov et al. 2017 Tech. Phys. Lett. **43** 351) and (V.V. Afrosimov et al. 2016 Tech. Phys. **61** 342) new studies of mechanisms of radiation damage of amino acid molecules were reported aiming to probe the intrinsic properties of the molecules and trace their chemical structure changes under the ion impact for the needs of biochemistry.

In (V.P. Shevelko et al. 2016 Nucl. Instr. and Meth. in Phys. Res. B **377** 77) and (L. Bozyk et al. 2016 Nucl. Instr. and Meth. in Phys. Res. B **372** 102) charge changing collisions of uranium ions with H_2, He, C, N_2, O_2, and Ar were investigated using BREIT computer code (Balance Rate Equations of Ion Transportation) recently described in (N. Winckler et al. 2017 Nucl. Instr. and Meth. in Phys. Res. B **392** 67). These contributions are relevant for fundamental scientific research at NICA and FAIR, including the use of heavy ion beams as drivers for inertial confinement fusion.

Total dielectronic recombination rates of heavy ions, including tungsten, calculated using a statistical model of atoms, were published in (D.S. Leontyev, V.S. Lisitsa 2016 Contrib. Plasma Physics **56** 846) and (D.S. Leontyev 2017 Problems At. Sci. Technol. **40** 19). This is one of effective channels for the recombination of heavy impurity ions in a fusion plasma.

The largest factual database Spectr-W^3 containing the information on spectral properties of multicharged ions was described in (I.Yu. Skobelev et al. 2016 Optics and Spectroscopy **120** 507). Specrt-W^3 node is directly accessible from the VAMDC data-request portal. Researchers from five Russian organizations contributed to VAMDC activity as indicated in (M.L. Dubernet et al. 2016 J. Phys. B: At. Mol. Opt. Phys. **49** 074003).

Progress on the development of ITER main chamber H-alpha (and Visible Light) spectroscopic diagnostic in Russia, reported in (A.B. Kukushkin et al. 2016 Fusion Sci. Technol. **69** 628) and (E.N. Andreenko et al. 2017 Fusion Eng. Des., in press), relies on extensive use of atomic and molecular data. The data needs include the treatment of (a) Beryllium ion transition probabilities in a strong magnetic field, (b) dissociation of Hydrogen isotope molecules with excited atoms as products, and (c) Beryllium hydride molecules.

Atomic data is used in numerical modelling for ITER neutral particle diagnostics being developed in Russia (S.Ya. Petrov et al. 2016 Problems At. Sci. Technol. **39** 68). It is desirable to revisit the model of fast neutral beam penetration into the plasma in order to (a) include updated cross sections where available, (b) take into account more impurity species and charge state distributions, and (c) clarify the isotope effect.

The activity on the selection and testing of materials for steady state operation and studies of the underlying PMI processes has been vigorous. This is partly due to the ongoing work on ITER and to the fact that the development of a fusion-fission hybrid system was mentioned among the priorities of Russian research programme on controlled nuclear fusion. 19th Russian Conference on Plasma-Surface Interactions (28-29 January 2016, Moscow, Russia) and 20th Russian Conference on Plasma-Surface Interactions (26-27 January 2017, Moscow, Russia) were mostly attended by domestic participants reporting on activities in Russia. Selected papers from the 19th Conference have been published in a special issue of Journal of Physics: Conference Series, vol. 748. A report on Deuterium removal from radiation damage in tungsten by isotopic exchange with hydrogen atomic beam was presented. A study on surface modification and deuterium retention in reduced-activation steels under low-energy deuterium plasma exposure was published in (O.V. Ogorodnikova et al. 2017 Nucl. Fusion **57** 036010) and (O.V. Ogorodnikova et al. 2017 Nucl. Fusion **57** 036011). Simulations of diffusion of hydrogen atoms in the lattice of tungsten were presented (N.N. Degtyarenko et al. 2016 Journal of Physics: Conference Series **748** 012010). The corrosion resistance of Mo, Nb and W in pure liquid tin was investigated at temperatures up to 1050°C for the selection of the alloy base material of in-vessel tokamak elements based on liquid tin capillary pore systems (I.E. Lyublinski et al. 2016 Journal of Physics: Conference Series **748** 012014).

Newest PMI activities in Russia and in the world were reported at the 23rd International Conference on Ion-Surface Interactions (21-25 August 2017, Moscow, Russia). Selected papers will be published in special issues of international peer-reviewed journals. More than 60 oral presentations were made, about 50% of them authored by researchers from Russia, and about 130 poster presentations. New experimental works on Hydrogen and Helium retention in tungsten under ion irradiation and Hydrogen trapping into and release from tungsten covered by Beryllium/Aluminum oxide layer under plasma irradiation were presented by Y. Gasparyan, L. Begrambekov et al. Removal of Deuterium implanted into graphite by consequent irradiation by ions of Hydrogen plasma was experimentally studied by A.A. Ayrapetov et al.

Experimental studies of PMI and behavior of materials under plasma loads in the multiple-mirror trap of the GOL-3 facility were described in the recent review paper (A.A. Shoshin et al. 2017 Fusion Eng. Des. **114** 157). The energy density in the extracted plasma stream varied from 0.5 to 30 MJ/m^2. A specialized test installation for research on material behavior under the impact of the powerful thermal shock was developed at the G.I. Budker Institute of Nuclear Physics (A.A. Vasilyev et al. 2016 Nuclear Materials and Energy, in press). It grants new capabilities for experimental simulation of transient heat loads corresponding to ITER-relevant ELMs type I.

In summary, generation of atomic and molecular data by experimental and computational methods in Russia in the past two years is reflected in a large number of publications in high-rank international journals. Studies are motivated by astrophysics, biochemistry, fundamental science and controlled fusion research. Development of neutral particle diagnostics and H-alpha spectroscopy for ITER in Russia has revealed new data needs. Strategic goals of Russian research programme on controlled nuclear fusion lead to vigorous activity on PMI data. Generation of new PMI data was reported at several conferences hosted by Russian institutions and published in international scientific journals.

A+M Data Center Activities in National Fusion Research Institute (2015~2017)

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Our database is built with cross section, rate coefficient by electron, heavy particle collision. The total amount of data is about 26000 recodes in this year.

DCPP web database system provides numerical and bibliographic data of atomic, molecular interaction. Also, the system provides functions for the efficient compilation, assessment, and grade evaluation process of atomic, molecular and plasma-material interaction data. We improved our system that focuses on user convenience. We plan to add plasma-surface reaction data in the near future.

We also collected 1000 papers from 170 journals a year to update AMBDAS. We need to change the data searching method to shorten the collection time, so we plan to find a way through the analysis of past search result

Our evaluation activities decided at the Joint IAEA-NFRI Technical Meeting (TM) on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion in September 2012.

We evaluated 3 molecules during 5 years and published it.

Our evaluation group strives to provide the data set as complete as possible. If there is no data, we are suggesting data studies to colleagues. We plan to make the Group data evaluation project for continuous activity.

We investigated ways to produce collisional scattering cross sections of atoms and molecules by electron collision, and established a direct data production base through experimental measurements and developed a measuring device and measured total scattering cross section for e – Ar, CH_4 collisions at low electron energies.

We have optimized the structure of CxFy using the Density Functional Theory DFT (wB97X-D/aug-cc-pVTZ) using the Gaussian 09 program and the optimized geometry is used for the calculation and calculated various cross sections at low energies along with the detection of resonances using ab initio R-matrix method through Quantemol-N.

Current Activities of IAEA Atomic and Molecular Unit Activities

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The IAEA atomic and molecular data unit manages data projects and network activities. For data projects, the unit organizes Coordinated Research Projects (CRP), technical and consultants' meetings and publications for public access to data. The unit also manages coordinated activities by data centre network of national data centres and code centre network of code developers. A CRP brings researchers to collaborate on a data-related topic and the main output includes publications, meeting presentations, reports and books. In the period of 2015-2017, 5 CRPs were managed as following:
2011-2016: Data for kinetic modelling of molecules of H and He and their isotopes in fusion plasma
2012-2016: Erosion and Tritium Retention for Beryllium Plasma-Facing Materials
2013-2017: Plasma-Wall Interactions with Irradiated Tungsten and Tungsten Alloys in Fusion Devices
2015-2019: Plasma-wall Interaction with Reduced-activation Steel Surfaces in Fusion Devices
2016-2020: Data for Atomic Processes of Neutral Beams in Fusion Plasma

The unit organized 9 meetings in 2015, 7 meetings in 2016 and 8 meetings in 2017. In December 2016, the TM on uncertainty assessment and benchmark experiments for AM data brought more than 50 scientists in the atomic, molecular, plasma-surface interaction and fusion physics community to discuss the uncertainty quantification of data for fusion. It was one of the largest TM that the unit organized and shows that the UQ activities promoted by the unit have generated substantial interests in the communities. The Joint ICTP-IAEA advanced school on atomic processes in plasmas held in February 2017 received more than 190 applications and was regarded highly successful by the participants.

The 70th volume of International Bulletin on Atomic and Molecular Data for Fusion and 2 volumes of Atomic and Plasma-Material Interaction data for Fusion (APID) were published. Two special issues are published with Atoms journals as a result of 2 CRPs.

The unit maintains several databases such as ALADDIN numerical database and AMBDAS bibliographical database and hosts online codes and code results. New databases on DFT (density functional theory) and MD (molecular dynamics) simulations are under the development.

Aspects and prospects of KAERI atomic data center

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Research activities of KAERI (Korea Atomic Energy Research Institute) atomic data center have focused on two parts: 1. State-of-the-art calculations for the electron-impact ionization and recombination, and photoionization data which are essential in modeling for laboratory and astrophysical plasmas. 2. Spectroscopic measurement in plasma devices and the modeling for analysis on the measured spectra since 2012.

Research activities during 2015-2017 and for future are as follows. We have calculated PEC for complex tungsten (W) ions W^{q+} (q = 5-48) by parallelizing radiative transition routine of original FAC (flexible atomic code). These data has been adopted to analyze measured W impurity spectra in KSTAR (Korea Superconducting Tokamak Advanced Research) by KAIST (Korea Advanced Institute of Science and Technology) team. We had compiled available DR data for W ions and provided the recommended data through IAEA and KAERI joint CM. We have calculated DR (Dielectronic Recombination) for W^{q+} (q =5-11, 44-46) and will calculate DR for W^{q+} (q = 30-34). We have installed a CCP (Capacitively Coupled Plasma) device and measured plasma temperature and density for Ar plasma with a Langmoir probe. OES (Optical Emission Spectroscopy) for Ar has also been carried out with Ocean Optics HR4000 which was absolutely calibrated. CR modeling including detailed collisional and radiative processes will be constructed and compared with measured spectra. Sensitivity of the modeled line intensity to underlying atomic data choices will be investigated which gives an indication of a validity of used atomic data. We have uploaded the calculated atomic data and the implemented the CR modeling for He I previously performed during 2015 and 2016 on our Web DB (http://pearl.kaeri.re.kr) in user friendly graphical forms as well as text format download. Parallelization for autoionization routine of FAC will be performed in near future to calculate DR for very complex ion stages efficiently and unitary correction for collisional excitation routine based on distorted wave approximation of FAC will be tried to improve the accuracy for near neutral atomic system.

R–matrix electron–impact excitation and ionization calculations in support Mo I and W I diagnostics

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The CTAMOP collision group at Queen's University Belfast presented some of their collision calculation capabilities in support of magnetically confined fusion diagnostics and modelling. We proposed two approaches to the generation of electron-impact excitation data. For comprehensive coverage along iso-electronic sequences we have developed a perl script that allows Maxwellian averaged collision strengths to be calculated in the well-known ADAS adf04 format from a simple list of atomic configurations. In contrast, more attention is given to heavy neutral systems, where greater effort is given to the atomic structure in order to achieve the greatest spectroscopic accuracy possible.

For electron-impact ionization the RMPS (R-matrix with Pseudostates) method was presented that allows for the ground and metastable ionisation of neutral and near-neutral systems. In this regard, it is accepted that species that are more than 4-5 times ionized, perturbative methods provided acceptable answers.

We illustrated that to provide usable rate coefficients that are a function of temperature and density, sometimes referred to as Generalised Collsional Rate (GCR) coefficients both the excitation and ionisation rates are both required. The example for neutral Lithium was provided in which an experimentally measured effective ionisation rate was compared with the theoretically calculated value. This confirmed the important role of metastable ionisation.

As an illustrative of our connection to ongoing fusion experiments, namely the Compact Toroidal Hybrid (CTH) [Auburn University] and DIIID[General Atomics] neutral molybdenum and neutral tungsten are both being investigated. The long-term goal is to provide theoretical predictions of the impurity influx for both these species.

Tungsten, remains the highest priority due to its use in the ITER experiment currently under construction in Cadarache, France. The final topic about the adoption and calculation of uncertainties for theoretical calculations was part of a wider discussion by the group, and should be encouraged strongly outside of DCN Meetings. Hopefully, this can achieve support at the National level.

Atomic, Molecular and Surface Research in Argentina

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There are many laboratories in Argentina working on Atomic, Molecular and Surface Physics in Argentina. The first one was created in 1960 by Prof. Wolfgang Meckbach at the Bariloche Atomic Centre, a research facility which depends on the National Atomic Energy Commission (CNEA) and is located in the city of San Carlos de Bariloche, a famous tourist resort at about sixteen hundred kilometers southwest from Buenos Aires, in the Northern part of Patagonia. This Laboratory counts with a 1.7 MeV Tandem accelerator with PIXE, RBS, ERDA and channeling capabilities, and a chamber for Cold Target Recoil Ion Momentum Spectroscopy (COLTRIMS). There are also 2 electrostatic accelerators of 100 and 300 keV, a time-of-flight system for ISS spectroscopy, a surface analysis equipment for XPS, UPS, AES and SIMS spectroscopy, and STM and atomic force AFM microscopes.

The Institute of Astronomy and Space Physics or IAFE (due to its acronym in Spanish) is located in Buenos Aires and depends on the University of Buenos Aires and the National Council of Scientific and Technical Research, or CONICET. A third group is located at Rosario, about 300 kilometers to the northwest of Buenos Aires. It is part of the Rosario Institute of Physics, or IFIR, which depends on the University of Rosario and CONICET. Finally yet importantly, at the Southern Physics Institute, or IFISUR, created in Bahía Blanca in 2008, there is a very active group. In total, more than 50 researchers and graduate students are working in this area of research in Argentina.

We study a large range of processes, with different projectiles (ions, electrons, positrons, photons, etc.), targets (atoms, molecules, surfaces, etc.) and outgoing channels (elastic and inelastic collisions, charge exchange, ionization, transfer ionization, etc.), usually at intermediate and large impact energies. We make purely basic research, but also pay special attention to a range of applications, as for instance in radiobiology.

From the theoretical point of view, we employ continuum distorted wave models, Classical Trajectory Montecarlo, Sturmian functions, and time-dependent close coupling, among other techniques.

We publish in the main scientific journal and attend the principal conferences of our area. Actually, we hosted the ICPEAC conference in 2005 in Rosario and the HCI conference in 2014 in Bariloche.

The proposal of our community is to create a Data Centre, within the structure of CNEA. Its objectives will be to provide fundamental data for nuclear and non-nuclear science and technological projects, and to coordinate the generation, collection and critical assessment of the required data by the different groups in Argentina.

We had and still have some links with the Atomic and Molecular Data Unit. For instance, Claudia Montanari from IAFE is responsible for the updating of the network created in 1990 by Helmut Paul for Stopping Power data; while Pablo Fainstein, from Bariloche, developed the CDW-EIS code that can be found in the AMDIS page.

Therefore, based on our 50 years of experience, we are willing to contribute with the international atomic and molecular data center network. We can certainly provide numerical and bibliographic data, direct contact for any expertise needed -especially in relation with ion impact atomic processes and surface science- and collaborate with the ongoing coordinated research project (CRP) on Atomic Processes of Neutral Beams in Fusion Plasma.

Online Atomic and Molecular Databases

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A summary of recent developments in atomic and molecular (AM) database services will be given, focusing on the following databases and topics.

1. VAMDC, the Virtual Atomic and Molecular Data Centre: an EU-funded project to build a network of databases and data services around a common query language and output format:

- Example queries to individual data "nodes";
- XSAMS, an XML-based format for representing a wide range of atomic and molecular data, initiated within the IAEA and subsequently further developed by the VAMDC consortium;
- The VAMDC portal, a service for simultaneously querying multiple database nodes.
- Recent developments to improve VAMDC technologies and services.

2. HITRAN, a major database of molecular spectroscopy data, recently implemented as a web based service with a relational database backend (HITRANonline).

3. ExoMol a database of ab initio molecular line lists for high temperature applications.

- Curation and management of very large scientific data sets
- A website with a flexible data schema for representing several relevant data types

4. QuantemolDB, a database of electron collisional cross section processes and heavy particle reaction Arrhenius parameters

- User authentication, authorisation and accounting (AAA) management issues
- Interactive functionality for visualising data sets
- Data upload functionality for approved users and community data evaluation
- API functionality

5. Future directions and challenges for AM databases

- Sustainability
- Security concerns
- Software tools for interconversion between data formats
- Time stamping and preservation of old data
- Distributed databases

AMS Data: data types and formats, and data needs for fusion edge plasma modelling

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FZ Jülich develops and hosts the kinetic Monte Carlo Code EIRENE (www.eirene.de) which, in magnetic fusion, is one of the most distributed community codes to quantify AM&S processes in context with plasma flow and plasma transport simulations, in the boundary region of both: tokamaks and stellarators.

This code takes atomic, molecular and plasma surface interaction data as primary input.

Past activities at FZ Jülich on establishing own atomic, molecular cross section databases for EIRENE, e.g. for collision processes between plasma electrons or protons and hydrocarbons up to C_3H_8 (and their ions) as well as of the Silane family SH_4 and smaller, have ended. But the databases are currently still maintained online under http://www.hydkin.de.

A similar attempt to build a database for breakup of BeH, BeH_2, and their ions in fusion plasma relevant conditions had been started some years ago. But despite the significant amount of cross section material meanwhile being available in published literature, a comprehensive, internally consistent, complete chain of cross sections and rate coefficients for all competing fragmentation channels, to be used in modelling codes, could not yet be established. This is due to lack of resources at FZJ, and the need for an evaluated and recommended Be – Be+ cross section database first, to which the molecules couple via dissociative excitation, ionization and recombination processes into excited atomic product states.

A similar atomic cross section database for the He—He^+ system is available, by the Ralchenko-Janev-Bray-deHeer et al. ADNDT 2008 database. The almost finalized similar data evaluation process for electron collisions on Be, Be^+, by the AMS data unit of IAEA, will soon provide such a reference dataset also for Be, Be^+. But the issue of keeping the underlying unprocessed data (cross section tables) in an internationally accessible repository has been raised, and the lack thereof for the mentioned earlier (2008) He reference data set clearly limits its applicability in fusion research today and leads to duplication of work.

The FZJ hosted surface reflection database based on the BCA (binary collision approximation), i.e. on various versions of TRIM-code results) is maintained under http://www.eirene.de/html/surface_data.html, and is continuously updated with further target projectile combinations upon request.

This database differs from other surface (reflection) databases by the fully retained resolution wrt. reflected energy and angles, by storing the full 3D velocity space distributions in a "conditional quantile format", (G. Bateman, PPPL report no. 1, 1980), which is particularly well suited for Monte Carlo transport code sampling of energy and angles of reflected (or sputtered) particles, for a given incident energy and angle.

Progress has been made on uncertainty propagation (UP) capabilities of fusion codes: The online sensitivity analysis tool www.hydkin.de provides analytic solutions to all sensitivity parameters in CR (collision-radiative) models, and hence also a linear uncertainty propagation from individual rate coefficients to condensed collisional radiative model parameters (such as line emissivities, for plasma spectroscopy). However, the underlying HYDKIN online code (Perl) has become legacy, and will either have to be re-written soon or be taken offline.

An UP study, from cross section data to finally responses (detector signals) via Monte Carlo simulation of incremental effects has been enabled in the EIRENE code, by utilizing the standard "correlated sampling" techniques (originally developed for nuclear Monte Carlo transport applications in the 50th or 60th of the last century). It is shown with EIRENE, using a multi-fluid, non-linear ITER reference simulation case (1573), that a 10% uncertainty in charge exchange cross section data can safely be progressed into final neutral particles fluxes, e.g. detector signals, with conventional CPU cost as common in today's applications to the chemically rather complex divertor plasma conditions.

Due to progress in computing speed and also transport code development the atomic/molecular data used in edge plasma modelling codes today can be far more detailed than before. This calls not necessarily for new raw data, but for less condensation, more independent parameters in so called "effective rate coefficients". E.g. already 5 independent parameters n_e, T_e, n_i, T_i, and E_0 are needed for an isotopically correct effective MAR (molecular activated recombination) rate coefficient. Major issues currently investigated are implementation of "physically correct" asymptotic behavior in all variables, proper behavior of the data when applied for the reverse processes (detailed balancing), either in case of fits or tables, and the possibility to directly integrate collisional radiative codes into transport modules completely without the intermediate step of multi-dimensional tabulation or fitting (i.e.: establishment of a CR model code library rather than multidimensional tabulated data).

A&M data needs for fusion research

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It has been decided that ITER (International Thermonuclear Experimental Reactor) will be operated with tungsten (W) divertor from the day one because of low tritium retention property of W. However, due to high atomic number (=74), W ions tend to accumulate at the plasma core, and strong line radiation from the W ions reduces the plasma temperature. Thus, one of the issues in plasma operation with W divertor is to prevent W ions from penetrating plasmas towards the core, and therefore, it is important to measure the W density at the core quantitatively as well as to determine W source flux at the divertor and W transport flux from the divertor toward the main plasma. For these purposes, following data needs are recognized;

- Lowly ionized W ions in divertor/SOL plasmas (10 eV < T_e < 200 eV):
  - Wavelengths with S/XBs for W II, III and up to ~ X. (Ex. W I 400.9 nm)
  - Evaluated cooling rate
- Highly ionized W ions in core plasma (1 keV < T_e < 20 keV):
  - Wavelengths of isolated and simple transition lines with evaluated excitation rates and A coefficients. (Ex. W XVI 4s-4p (6.2 nm))
  - Evaluated ionization and recombination rates in particular DR rates.
  - Charge exchange cross sections between W^{q+}(q~20-70) and D^0 (< 1 MeV)
  - Evaluated cooling rate
  - Similar data for liquid metals such as Sn

For mitigating heat load onto the divertor plates, radiative divertor with impurity seeding is one of the promising techniques. Because the biggest radiator is a Li-like ion such as C IV and Ne VIII [1, 2], it is important to measure spatial distribution of those ions in the divertor plasma, and to measure absolute intensity of radiation-responsible lines such as 2s-2p line. For these purposes, following data needs are recognized;

- Light elements such as C, N, Ne and Ar in divertor/SOL plasmas (10 eV < T_e < 200 eV):
  - Wavelengths for Δn=0 lines (visible range) such as Ne VIII 4s-4p
  - Evaluated excitation rates and A coefficients for 2s-2p lines of Li-like ions. (Ex. C IV 2s-2p)

Further, to evaluate pumping efficiency, it is necessary to simulate transport of neutrals such as D_2 in sub-divertor region, where neutral-neutral collisions such as D_2-D_2 collision are dominant processes because there is no plasma. Cross sections for atom-atom and atom-molecule collision are available, however, cross sections for molecule-molecule collisions are not available. For future devices, cross sections between molecules with T becomes important. Hence following data needs are recognized;

- Sub-divertor region (no plasma):
  - Total and differential cross sections of molecule-molecule collisions such as D_2-D_2, T_2-DT, and any combination.

Reference:
[1] T. Nakano, H. Kubo, etal., J. Nucl. Mater. 390-391 255 (2009)
[2] T. Nakano, N. Asakura, etal., J. Nucl. Mater. 438 Supplement S291 (2013)

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