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Technical Aspects of Atomic and Molecular Data Processing and Exchange, 21st Meeting of the A+M Data Centres Network

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

7–9 September 2011

Prepared by

Hyun-Kyung Chung

November 2011

IAEA Nuclear Data Section, Vienna International Centre, A-1400 Vienna, Austria

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Abstract

This report summarizes the proceedings of the IAEA Technical Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (21st Meeting of the A+M Data Centres Network) on 7-9 September 2011. Fourteen participants from 12 data centres of 7 Member States and 2 International Organizations 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.

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1. Introduction

The IAEA Technical Meeting on “Technical Aspects of Atomic and Molecular Data Exchange and Processing” (21st Meeting of the Atomic and Molecular Data Centres Network) was held at the IAEA headquarters, Vienna, Austria from 7th to 9th September 2011. The objectives were to review progress in A+M data related activities in the data centres and to review and coordinate the work plans related to data issues for the next period.

Fourteen participants attended the meeting and three data centers were not represented. Dr Konstantinos Katsonis of GAPHYOR (France) and Dr Wolfgang Eckstein of IPP Garching (Germany) are retired and Dr Guiseppe Mazzitelli of ENEA (Italy) indicated that the ENEA is no longer functioning as a data centre. The newly elected member of ADAS (UK) was represented by Dr Martin O’Mullane. Dr Jung-sik Yoon of NFRI (Korea) and Dr Detlev Reiter of FZJ (Germany) were invited as candidates of new data centres.

Two observers attended the meeting. Dr Nigel Mason of VAMDC (EU) and Dr Yuri Ralchenko from NIST (USA) were invited for their expertise on data exchange and database tools including XSAMS. The Agency was represented by Dr Meera Venkatesh, Dr Bas Braams and Dr Hyun-Kyung Chung. Dr Stanslav Simakov (IAEA, Nuclear Data Section) was invited as a special guest speaker.

The full list of participants and related data centers is available in Appendix 1.

The meeting was opened by Dr Bas Braams (Head, A+M Data Unit, Nuclear Data Section), and Scientific Secretary Dr Hyun-Kyung Chung (Physicist, A+M Data Unit, Nuclear Data Section). Participants introduce themselves and the agenda was adopted (see Appendix 2). Dr Meera Venkatesh (Director, Division of Physical and Chemical Sciences, IAEA), absent in the morning to accompany the Director General of IAEA for an official function, came to welcome all participants in the afternoon and addressed the importance of data in the nuclear sciences and applications and the usefulness of this Technical Meeting to the Data Centre Network (DCN).

The meeting covered the following topics:

- Current Activities of the A+M Data Centres and invited talks
- Data Issues: Data Exchange Format
- Data Issues: Bibliographical Data Compilation
- Data Issues: Data Evaluation
- Data Needs for Fusion Research
- Data Centre Database Demonstration
- Membership in the network
- Meeting conclusions and recommendations

2. Proceedings of the Meeting

The presentations at the meeting are available on the A+M Data Unit web site http://www-amdis.iaea.org/DCN/ via the link to Meeting Reports and Presentations.

This 21st meeting was held at a time of many changes. It was the first meeting organized by the current IAEA A+M Data Unit since Dr R. Clark and Mr D. Humbert were replaced by Dr B. Braams and Dr H. Chung in 2009. There are foreseeable changes in data centre members. Many data centres have seen their representatives retiring after several decades of services and three data centres of GAPHYOR (France), IPP Garching (Germany) and ENEA (Italy) did not participate in this meeting for the first time in a few decades. The activities at the CFADC (Controlled Fusion Atomic Data Centre) at Oak Ridge National Laboratory, USA, are being phased out after 52 years of service. On the other hand, with the advent of construction and commissioning of new fusion devices internationally, new data centres have become established and existing projects have taken on new roles. The Atomic Data and Analysis Structure (ADAS) project had become of member of the Data Centres Network in 2009 and was again represented at the present meeting. The NFRI (Korea) Data Center for Plasma Properties was invited to this meeting for the first time and the Russian Federal Nuclear Centre All-Russian Institute of Technical Physics (RFNC VNIITF) spectroscopic data center was invited but could not participate in the meeting. Dr D. Reiter of FZJ (Germany) was invited in view of the important role of the EIRENE database for ITER modeling.

This meeting provided a timely opportunity to introduce the network activities to the potential members and to reformulate and coordinate them to accommodate changes in data use and data exchange. Dr Braams reviewed the first three meetings of the network from 1977 to 1982 in which the role of the network was developed, and presented the meeting objectives. Since its inception in 1977 the network has been devoted to the development and maintenance of bibliographical and numerical databases, the development of standards for data exchange and the coordination of activities in data production and data evaluation. The network has been successful in providing A+M/PSI data to support scientists and engineers of Member states working on fusion research and technology. The role of the network is even more important now because of the need for internationally accepted and recommended data in the modern designs of fusion reactors and power plants in the pursuit of energy use of nuclear fusion. The objectives of meetings of the Data Centres Network have been 1) to exchange information about activities in the Centres, 2) to coordinate work among the Centres to assess priorities in data evaluation and production and make plans for specific evaluations, and 3) to evaluate and revise procedures for collection and exchange of bibliographical and numerical data. These objectives were also adopted for the present meeting and sessions were established accordingly.

2.1 Current Activities of the A+M Data Centres

The first meeting session was dedicated to the progress reports of data centres on the data activities in the period of September 2009-August 2011. Representatives of data centres presented the work done on data compilation, evaluation and generation, web developments, data centre publications produced during the reporting period, and the status of ongoing programmes and future plans. The presentations are summarized here and the abstracts are attached in the Appendix 3.

W. Wiese, NIST, USA

Dr Wiese described the work of the Atomic Spectroscopy Data Center team at the National Institute of Standards and Technology (NIST) in Gaithersburg, MD, USA during the last two years. He reported the data centre activities on the annotated bibliographic databases and numerical databases as well as the NIST reference data program.

During the two years, atomic energy levels and wavelengths are completely tabulated for hydrogen and its isotopes (H, D, T), for argon (Ar II through Ar XVIII), cesium (Cs I through Cs LV), barium (Ba III through Ba LVI) and tungsten (W III through W LXXIV) and the atomic transition probabilities of hydrogen and its isotopes (H,D,T), for helium(He I and He II), for lithium (Li I through Li III), beryllium (Be I through Be IV), boron (B I through B V), sulfur (S I through S XVI), cesium (Cs I through Cs LV), and barium (Ba III through Ba LVI) are completed. Compilation of energy levels and spectral lines are in progress on neon (Ne IV), chlorine (Cl I through Cl XVII), and nickel (Ni I through Ni VIII) while their data assessments and compilations of atomic transition probabilities were completed. Additional compilations of atomic transition probabilities for the higher fluorine and neon ions (F V through F IX, Ne VI through Ne X), chlorine (Cl I through Cl XVII) and nickel (Ni I through Ni VIII) are in progress.

There was the major improvement of the Atomic Spectra Database (http://physics.nist.gov ASD Version 4.0 in September 2010, with an update 4.1.0 in May 2011). The ASD database is completely integrated with the two NIST bibliographies on atomic energy levels and spectra, and on atomic transition probabilities and the original papers of the data can be directly accessed by users. The NIST data tables contain only the reference data, i.e. data of a certain minimum quality, and only one numerical value is presented for the wavelength, transition probability, and lower and upper energy levels of a given spectral line. For atomic transition probabilities, explicit accuracy ratings are given and the uncertainties of calculated data are estimated. The number of tabulated digits indicates the accuracy for wavelengths and energy levels.

Dr Wiese expressed a concern over the lack of funding on data activities and sustainability of researchers in the reference data evaluation. It is important to develop a new way of data exchange and validation and to retain and train young researchers in the field. He informed that NIST will host the 8th International Conference on Atomic and Molecular DAta and Their Applications (ICAMDATA September 30 - October 4, 2012) in Gaithersburg, MD, USA.

J. Yan, CRAAMD, IAAMD, China

Dr Yan described the recent activities of the Chinese Research Association on Atomic and Molecular Data (CRAAMD) members during the years of 2010 and 2011. The CRAAMD initiated in 1987 has currently 11 groups working on topics of atomic spectra data collection and compilation, argon data and electron broadening, calculation of cross-sections for heavy particle collisions and stopping power of alpha particles in gold plasmas. He showed the CRAAMD webpage and demonstrated the CAMBD databases (http://www.camdb.ac.cn).

The groups collected and compiled about 2700 lines of atomic spectra for Au, Cr Ti, Fe, Si, Al and Br ions. Data calculation and evaluation have been carried out for argon in the framework of multichannel quantum defect theory where energy levels, radiative transition and collision processes based on the eigenchannel quantum defect, the transformation matrix and the generalized oscillator strength (GOS) to eigenchannels are obtained. Electron broadening calculations of spectral lines of Be-like N, O, F and Ne ions were reported. Cross sections of heavy particle collisions (excitation, ionization and charge transfer) using AOCC theory were calculated for H^{+}+Li, $Be^{2,3+}$+H, $B^{3,4+}$+H, N^{5+}+He, O^{6+}+He, H^{+}+He, N^{5+}+H, O^{6+}+H, as well as their collisions in Debye plasmas. Finally the stopping power calculations for α particles in gold plasmas were presented.

D.R. Shultz, CFADC, ORNL, USA

Dr Shultz of the Controlled Fusion Atomic Data Center (CFADC) in the Oak Ridge National Laboratory reported the current status of the center, and review recent activities and the history of the data centre. The CFADC was founded in 1959 by C. F. Barnett with the mission to “identify, compile, evaluate, and recommend data on atomic and molecular collision processes which are important in fusion energy research”. The principal activities included producing a published and later an on-line annotated bibliography used to answer data requests and as a foundation for data evaluation, publishing the two principal series of “Redbook” volumes of recommended data and participating in the IAEA ALADDIN and DCN network and CRPs (Coordinated Research Projects).

He presented the data centre activities in the last two years carried out within an overarching atomic physics research group through an active experimental and theoretical science program. The production of an annotated bibliography of AM&PSI literature relevant to plasma science continues to be among the most important activities of the data centre, forming the basis for the CFADC on-line bibliographic search engine and a significant part of the IAEA A+M Data Unit’s “International

Bulletin on Atomic and Molecular Data for Fusion." Other important activities included responses to specific data requests from the plasma science community, leading to either rapid feedback using existing data resources or long term data production projects, as well as participation in IAEA Coordinated Research Programs including "Data for Surface Composition Dynamics Relevant to Erosion Processes", "Atomic and Molecular Data for Plasma Modelling", and recently "Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma" and "Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions".

He reported the news from the US Department of Energy that it plans to close the program after a ramp down of funding in 2012, following a distinguished 52-year history of contributions to the US and international fusion research efforts by the data centre.

J.S. Yoon, NFRI, Korea

Dr Yoon of National Fusion Research Institute (NFRI) participated in a DCN meeting for the first time. He summarized the work conducted at the Data Center for Plasma Properties (DCPP) in the NFRI over last 5 years on the systematic synthesis and assessment of fundamental knowledge on low-energy electron interactions with plasma processing gases.

The NFRI is the host of the Korean fusion reactor KSTAR which generated the first plasma in 2008. The DCPP is one of the R&D (Research and Development) centres hosted by the NFRI. The DCPP project (http://dcpp.nfri.re.kr) was initiated in 2006 to produce the National Standard Reference Data (NSRD) for low temperature plasmas using a database hosting *more than half a million* A+M data sets for industrial plasma applications (http://plasma.kisti.re.kr) developed by the KISTI (Korea Institute of Science & Technology Information). It is the part of the Asia-Pacific Atomic data Network (APAN) and of the Data User Network (DUN) of university-industry-research institute joint collaboration. The APAN consists of researchers from Korea, Japan, Australia, India, Russia and China and it is expected to conduct and promote the measurement and calculation of A+M data of relevance to plasma applications, provide a mechanism for the efficient compilation, assessment and critical evaluation and provide a link between researchers in A+M physics and data users.

Currently, the DCPP centre has 12 people (6 theoreticians, 4 experimentalists and 2 IT people) working on A+M data research for plasma simulation, data evaluation and dissemination. Dr Yoon reported on the theoretical work on ion-neutral atom collision, electron-ion collision and plasma spectroscopy, the experimental work on electron-impact total cross-section and the data evaluation activities. The group published evaluated cross-sections for electron collisions with hydrogen molecules. They are actively carrying out evaluations of plasma-surface interaction data for industrial applications using both measurements and simulations. The centre invests heavily in the construction of an information system for plasma applications including the conceptual design of information management system for DEMO fusion reactor.

I. Murakami, NIFS, Japan

Dr Murakami of National Institute for Fusion Science (NIFS) presented the current activities of the Atomic and Molecular Processes group (Fusion Systems Research Division), including development and maintenance of databases, research activities related to atomic and molecular data and the publication of 6 NIFS-DATA-reports during the last two years. The NIFS databases of collision processes (http://dbshino.nifs.ac.jp) contain 476,048 entries in total (as of Aug. 23, 2011) and the new server started in March 2011. The databases consist of AMDIS (electron impact ionization, excitation, and recombination cross sections and rate coefficients), CHART (charge transfer of atom – ion collisions cross sections), AMDIS MOL or AMOL (electron collision with molecules), CHART MOL or CMOL (heavy particle collision with molecules), SPUTY (sputtering yield of solid) and BACKS (reflection coefficient of solid surface). During the last two years, new data were added mainly for

AMDIS and CHART. Currently, there is no need to log in to the databases with a user account and password and the AMDIS database is accessible through the GENIE search engine. The queries via GENIE constitute 20%-27% of the total.

In addition to the main collisional databases there are small databases developed for specific processes. For example, databases of rate coefficients of electron dissociative attachment of molecular hydrogen, differential cross-sections of molecules by electron impact, differential ionization cross-sections of hydrogen by proton impact, sputtering yields, photo-absorption cross-sections are available. A new database of bibliography and cross-section compilation and evaluation for 67 atoms and molecules done by Prof. M. Hayashi is in progress.

There are two main research activities related to A+M data: 1) A collaboration group has started for research on A+M processes in plasma using the Large Helical Device (LHD) and 2) a new project on tungsten has started with atomic physicists and plasma physicists in Japan. Projects include EUV and visible spectral measurement of W ions in Tokyo-EBIT, CoBIT and LHD, atomic structure calculations and collisional-radiative model of W ions and sputtering experiments of W target. EUV spectra of Ga, Nd and Fe ions are measured with LHD while the Fe EUV spectra are also measured with EBIT/CoBIT. A collaboration group is organized with atomic physicists from Japanese universities to study atomic data, spectra and collisional-radiative models for W ions.

D. Reiter, FZJ, Germany

Dr Reiter of Forschungszentrum Jülich GmbH (FZJ, Institut für Plasmaphysik) was invited to the DCN meeting for the first time with the expectation that his group may provide molecular databases for fusion and help improving collaboration between data users and data producers. He presented the work on the EIRENE online database (www.eirene.de) for surface and A+M data in fusion edge plasma modeling. The edge plasma simulations require data ranging from detailed data sets such as differential cross-sections for microscopic erosion redeposition modelling to compressed and processed data for macroscopic core plasma simulations. Therefore the microscopic and macroscopic A+M/PSI data are integrated into fusion edge plasma codes via kinetic (Monte Carlo) solvers, for example, DEGAS-2 (USA), NIMBUS, NEUT2D (Japan) and EIRENE (EU). EIRENE is a Monte-Carlo neutral particle, trace ion (He^+, C^+, C^{++}) and radiation transport code and the integrated edge plasma codes based on the EIRENE are B2-EIRENE, OSM, EDGE2D, EMC3 and FIDAP.

The atomic and molecular data in EIRENE code are publically available through the database maintained at FZ Juelich (www.eirene.de) and through publications. The data sets can be condensed into collisional-radiative (CR) rate coefficients using the online database and data analysis tool box, HYDKIN (www.hydkin.de). The HYDKIN code can provide online sensitivity analysis for plasma chemistry at given plasma conditions as well. Surface data are stored for EIRENE in a format (www.eirene.de/surface-data/TRIM) that provides kinetic information of backscattered and sputtered particles. Global quantities such as particle, energy and momentum reflection coefficients can be readily obtained from the multi-differential distributions.

Dr Reiter emphasized the role of the international network of A+M/PSI physicists in establishing recommended data sets. For computationally intensive edge plasma simulations (2-3 month per case), the backward compatibility of codes and databases is important, at least for design applications to ITER and DEMO (much less so for interpretative applications to current experiments) and the upgrades/changes of the underlying A+M/PSI data ought to be limited. Currently, there is no standard set of data, let alone a community to recommend modifications of the data. Since the ITER project is carried out with an international collaboration, the Data and Code Centre Network as established at IAEA should play the more prominent role to connect the ITER project with the world wide A+M/PSI physicists and individual data centres and establish a standard set of data for design applications.

Y. Rhee, KAERI, Korea

Dr Rhee of Korea Atomic Energy Research Institute (KAERI) presented the work on the Atomic Molecular and Optical Database Systems (AMODS, http://amods.kaeri.re.kr) database and the research activities on atomic physics and high energy density sciences. Research activities on atomic physics include calculations of 1) atomic structure and transitions calculations using the relativistic MCDF (Multi Configuration Dirac-Fock) code, 2) electron impact ionization processes of W, Mo, Be, C, etc., based on BEB (Binary Encounter Bethe) model and MCDF code, 3) spectra of highly charged ions of W, Xe, and Si and 4) dielectronic recombination process of Fe ions. Online calculations of direct ionization cross-section based on the BEB model are also possible in AMODS for W and Mo.

Dr Rhee's group has established a broad collaboration network with laser facilities world-wide for high energy density sciences (HEDS). He presented 1D radiation hydrodynamics simulations using the HYADES code for HEDS experiments performed at the following facilities: 1) GEKKO laser facility (Japan) for X-ray photoionization of low temperature Si plasma, 2) VULCAN laser facility (UK) for two dimensional compression of cylindrical target and investigation of hot electron transport in the compressed target plasma, 3) LULI laser facility (France) and TITAN laser facility (USA) for one dimensional compression of aluminum targets with different laser energies, and 4) PALS facility (Czech Republic) for "Laser Induced Cavity Pressure Acceleration" to understand the shock ignition process of laser fusion. He emphasized that the A+M data is crucial to the HEDS since the radiation hydrodynamics simulations depend on the equation of state (EOS) and opacity data of plasmas.

Yu.V. Martynenko, Kurchatov Institute, Moscow, Russian Federation

Dr Martynenko presented the activities on the atomic, molecular and plasma-surface interaction data at the Kurchatov institute mainly in the data generation and the development of a data acquisition system+ (DAS+, http://cpunfi.fusion.ru/dassql/dasweb2.dll/showgl). The DAS+ operates with experimental data such as discharge parameters or diagnostics data of various fusion devices (T-10, GTB, PN-3, S300, L-2M, Tuman, Globus), which are stored, transmitted, processed and represented. It allows one to create a database for experimental data to be used for fusion research.

He reported the new data sets produced at the centre by measurements, theory and codes: 1) direct observation $D^- + D^- \rightarrow D_2^-$ related to neutral beam heating, 2) tungsten erosion measurement in D_2 plasmas in presence of carbon, 3) analytical and numerical calculations of growth in the deposited film, 4) studies of dust mobilization, film exfoliation and fragmentation in tokamaks, 5) measurement of angular distribution of atoms sputtered from Mg, Al, Cu, Ag, Ta, Pt, Au, Ti, Cr, Zn, Zr, Nb polycrystalline targets, 6) tungsten experiments in QSPA-T for melting, crack formations and dynamics, surface structure changes and erosion products deposition studies, 7) beryllium erosion studies at QSPA-Be facility, 8) quasi-classical calculations of Bremsstrahlung gaunt factors and rates of radiative and dielectronic recombination processes, 9) development of fast codes for tokamak plasmas (nl-KINRYD of collisional radiative kinetics of Rydberg atomic states, and ESMEABRR of Bremsstrahlung and radiative recombination).

T. Nakano, JAEA, Japan

Dr Nakano of the Japan Atomic Energy Agency (JAEA) reported the research activities in the areas of 1) data compilation of chemical sputtering yields, 2) data production of charge exchange cross-sections and dissociative recombination cross-sections and 3) data evaluation of cross-sections of He-collision systems and data evaluation of ionization and recombination rate coefficients of highly charged tungsten ions.

Chemical sputtering yield data for hydrogen isotope collisions on CFC materials have been compiled in 2009 following the chemical sputtering yield data of impurity doped C and C by O^+ ions in 2007 and 2008. The state selective charge transfer cross-section data of Be^{4+}, C^{4+} and C^{6+} by collision with

H(n = 2) in the collision energy range between 62 eV/amu and 6.2 keV/amu have been calculated with a molecular-bases close-coupling method and the data of C^{4+} was implemented in a collisional-radiative model code for C^{3+}. The state-specific (principal quantum number) cross-section data of dissociative recombination (DR) and excitation of HD^+, D_2^+, DT^+, T_2^+, $^3HeH^+$ and $^4HeH^+$ were calculated. The analytical expressions for the cross-section data for 26 processes of He-collision systems were evaluated and compiled, and will be available at the web site http://www-jt60.naka.jaea.go.jp/engish/JEAMDL/. The ionization rate of W^{44+} and the radiative and the dielectronic recombination rates of W^{45+} were calculated with the FAC code and compared with the ratios inferred from the line ratio measured at the JT-60U. The calculated ratio of the recombination rate of W^{45+} to the ionization rate of W^{44+} agrees with the inferred ratio within the experimental uncertainty (~30%).

The A+M data activities in JAEA have been pursued in collaboration with Japanese universities, and other department of JAEA through research commissioning. Dr Nakano remarked that all the commissioned research projects, the key element of the JAEA activities for more than 20 years, are cancelled after the disaster in 2011. Now, the JAEA will seek a way to resume the commissioned researches under another framework.

M. O'Mullane, ADAS, UK

Dr O'Mullane of university of Strathclyde presented an overview of the ADAS project (Atomic Data and Analysis Structure, http://www.adas.ac.uk/) and of OPEN-ADAS (http://open.adas.ac.uk/). ADAS is maintained as a self-funding consortium of fusion laboratories. The project provides an interconnected set of computer codes and data collections for modeling the radiating properties of ions and atoms in plasmas. The ADAS data fall into 3 broad classes: 1) Fundamental data such as A-values, cross-sections and effective collision strengths obtained from ADAS collaborators, the literature or data centres. 2) Derived data processed for modeling such as electron temperature and density dependent effective emission coefficients, effective ionization/recombination rates, radiated power and spectral emissivities. 3) Driver data which allow complete regeneration of all ADAS derived data in conjunction with the various ADAS codes. ADAS data uses high quality data as well as baseline data for fall-back when high quality data is not available. The data is mostly embedded in codes and the update without expert help is problematic. The ADAS data formats (adf) are precisely defined and Fortran codes are supplied to read the data sets for easy access. IDL can be used for interactive manipulation.

The OPEN-ADAS project is a joint development between the ADAS Project and the IAEA to make the extensive fundamental and derived atomic data for fusion more widely available. It is designed to appeal to both plasma modelers and those interested in the detailed atomic physics. It has been searchable through the Google Scholar and appears in citations, which gives greater visibility and credits to the data producers. The OPEN-ADAS server was replaced due to a series of attacks since June 2011 and was off-line for 8 weeks. The new service removed the registration requirement and hence the user statistics is limited.

H. Chung, IAEA

Dr Chung summarized the activities of atomic and molecular data unit in the nuclear data section, IAEA on the data generation, exchange and transfer. The coordinated research project (CRP) is the main mechanism by which the unit encourages generation of new data by bringing international experts from 10 to 15 institutes to jointly work on the atomic, molecular and plasma surface interaction data for fusion. The generated data sets are published and are hosted by the IAEA databases. During the last two years, the five CRPs have had the research coordination meetings (RCM) on topics of "Data for Surface Composition Dynamics Relevant to Erosion Processes", "Characterization of Size, Composition and Origins of Dust in Fusion Devices", "Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions", "Spectroscopic and Collisional Data for W from 1 eV to 20 keV" and "Data for kinetic modelling of molecules of H and He and their isotopes in fusion plasma". In addition to the RCMs, there have been consultant meetings (CM) on "XML Schema for Atomic and Molecular Data" and technical meetings (TM) on "International Code Centres Network" and "IFRC Sub-committee on A+M data for fusion research". The meeting reports and presentations are available at the unit webpage (http://www-amdis.iaea.org). In addition to the IAEA-INDC(NDS) reports, the volumes of International Bulletin on Atomic and Molecular Data for Fusion and the Atomic Plasma-material Interaction data for Fusion (APID) are published.

The unit maintains numerical and bibliographical databases of ALADDIN and AMBDAS, routinely uploaded with data sets provided by CRP participants and DCN members. The newest update to the AMBDAS is the assignment of the DOI numbers (digital object identifier). The GENIE search engine has been expanded to include nine databases for radiative properties and six databases for collisional data. The GENIE mirror site at GAPHYOR is closed. The first version, version 0.1, of the XSAMS (XML Schema for A+M/PSI Data) was released in 2009 and the second version, 0.1.1, with bug fixes was released in 2010. The source files are available at the Source forge project (http://sourceforge.net/projects/xsams/) and sub-versions are currently being developed by groups of VAMDC for the description of molecular data sets. Recently, the unit built web pages to host the complete sets of argon, chlorine and silicon atomic data calculated by the LANL group as a part of the heavy element CRP (http://www-amdis.iaea.org/LANL), which is too large in the size (~ 2 GB) to fit well into the ALADDIN data base. Another new dataset separate from ALADDIN provides the charge state distributions calculated by the FLYCHK code (http://www-amdis.iaea.org/FLYCHK) as a function of temperature and density for all elements up to gold.

While maintaining databases for many different classes of A+M/PSI processes used for a variety of applications, some limitations were noticed in data collection and dissemination. For example, the extensive sets of LANL atomic data used for plasma modelling are easier to use if one can download them all as a whole in a structured data format than retrieve individual transitions from a database. In addition to numerical data, images and diagrams are important forms of plasma-wall interaction data. In order to present various data types to the community in more coherent and efficient way, the unit developed a wiki-based knowledge base for A+M/PSI data for fusion (http://www-amdis.iaea.org/w). The knowledge base consists of sections of data needs, data sources and data exchanges and provides links to the numerical databases of the DCN members, on-line capabilities of the CCN members, summaries of the CRP presentations and meeting reports. The unit hopes that the knowledge base will serve as an entry point to access data information for fusion research and eventually increase the visibility of data activities for the fusion and A+M/PSI physics community.

2.2 Other Presentations

N. Mason, VAMDC Consortium

Dr Mason of Open University, UK presented an overview on the VAMDC (Virtual Atomic and Molecular Data Centre, http://www.vamdc.eu) project. The VAMDC is a consortium of atomic and molecular data centres of mostly European countries with Venezuela and USA and it is funded under the "Combination of collaborative Projects and Coordination and Support Actions" Funding scheme of the Seventh Framework Program of European Union with 3.2 million euros. The project runs from July 2009 to December 2012. The VAMDC project will provide a scientific data e-infrastructure enabling easy access to A&M resources, and currently some 17 databases plan to participate in the common portal of a single point entry developed by the project.

The VAMDC project will develop and extend standards for interoperability of A&M resources to provide a uniform access and build an e-science network built on the existing Euro-VO and Grid infrastructures. The current XML schema (XSAMS) is extended to include solid, surface spectroscopy, large molecules and the line shapes. Dictionaries and protocols retrieving different types of resources are in development: numerical data, libraries, documentation and references. A general query language (Xquery) will be used to allow users to access and retrieve A+M data. Registries provide a mechanism with which applications can discover and select resources. Finally, the tools for manipulation of data sets will be developed to return data in an organized way that the scientific concept attached to the data will be produced. The VAMDC also organises a series of Networking Activities (NAs). NAs are specifically aimed at engaging data providers, coordinating activities among existing database providers, ascertaining and responding to the needs of different user communities and providing training and awareness of the VAMDC across the international A&M community and other use communities such as the radiation chemistry community.

The funding for the current VAMDC project is ending soon in 2012 and the consortium should find a way to sustain the project. The need for access to A+M data, for data compilation and evaluation still remains. The partnership between IAEA and VAMDC may be considered for the continuing work on systems (portals/language/registries) and for the data evaluation and recommendations. The VAMDC project is establishing itself as leading data source in AMO science and it may be supported through a subscription sponsorship and advertising.

Yu. Ralchenko, NIST, USA

Dr Ralchenko of the National Institute of Standards and Technology (NIST) reported on the recent developments in XSAMS (XML Schema for Atoms, Molecular and Solids). The XSAMS was proposed at the DCN meeting in 2003 and was developed by a team of DCN participants and external participants. Since its start in 2009 the VAMDC group played an important role in the XSAMS development. The development group (steering committee) meets typically twice a year, most recently at NIFS and at IAEA. The next meeting will be at NIST in October 2011. The XSAMS source files are available at the IAEA official XSAMS webpage (http://www-amdis.iaea.org/xml/) as well as Sourceforge.net (http://sourceforge.net/projects/xsams/) where also sub-versions can be stored for development. Currently, there are two branches other than the official version: the nist-branch and the vamdc-branch.

XSAMS contains descriptors of physical objects (atoms, molecules, solids and particles), physical processes (radiative, collisional and non-radiative), environment and other items (data production methods, data sources, etc.). The original idea was to provide a complete classification of atomic and molecular processes and this was largely achieved for atomic processes. However, the molecular part is so complex that more practical approach has been proposed and adopted by VAMDC. The vamdc-branch has a significant separate development in the molecular part (where a case-by-case approach is developed, coordinated by Christian Hill of UK) and in the solid parts. The implementation is under way in almost all VAMDC member institutes. The spectroscopic databases are in a better shape than the collisional databases in terms of XSAMS implementation. Currently only a couple of DCN members have adopted the XSAMS output in their databases and the DCN members should be encouraged to adopt it in the future.

S.P. Simakov, IAEA

Dr Simakov of Nuclear Data Services Unit in the Nuclear Data Section (NDS) gave a brief overview of the data compilation and evaluation activities in the nuclear data community: experimental nuclear reaction data (EXFOR, http://www-nds.iaea.org/exfor/) and evaluated nuclear reaction data (ENDF, http://www-nds.iaea.org/endf).

The International Network of Nuclear Reaction Data Centres (NRDC) coordinated by NDS includes 14 Centres in 8 Countries (China, Hungary, India, Japan, Korea, Russion, Ukraine, USA) and 2 International Organizations (NEA, IAEA). It had the first meeting of four core centres (Brookhaven, Saclay, Obninsk, Vienna) in 1966 and the EXFOR was adopted as an official data exchange format. In 2000, IAEA implemented the EXFOR database as a relational multiform database and the EXFOR is a trusted, increasing and living database with 19100 experimental works (as of September 2011) and 141600 data tables. The EXFOR provides a compilation control system for selection of articles and compilation of data and the NRDC home page provides manuals, documents and codes. The nuclear data can be retrieved by the web-retrieval system or distributed on a DVD on request.

The EXFOR data play a critical role in the development of evalulated nuclear reaction data. There are several major general purpose libraries: ENDF (US), CENDL (China), JEFF (EU), JENDL (Japan) and RUSFOND (Russia). In addition, there are special libraries for particular applications: EAF (European Activation File), FENDL (Fusion Evaluated Nuclear Data Library for ITER enutronics), IBANDL (Ion Beam Analysis Nuclear Data Library for surface analysis of solids), IRDF, DXS (Dosimetry, radiation damage and gas production data) and Medical portal. Dr V. Zerkin of NDS demonstrated the data retrieval from the EXFOR database and the ENDF library.

3. Data Issues

There were several issues discussed in the meeting regarding the data centre activities. The main topics for discussion included the data exchange format, bibliographical data compilation, data evaluation and the priorities in A+M data compilation and evaluation for fusion. This chapter summarizes remarks and statements during the discussion.

3.1 Data Exchange Format

Developing a common data exchange format for the A+M data centres has always been one of the core activities of the data centre network. In the 1980s the ALADDIN format was adopted and promoted by data centres as the data format for plasma modeling. However, there were many data users outside fusion modeling and the ALADDIN format was not generally adopted by plasma modelers who rather invented data formats specific to their own codes. Eventually ALADDIN lost ground to the relational databases supported by online activities. As more and more data are available through web interfaces, a common exchange format for the data transfer through web applications gained attention and the XSAMS project was started by DCN members and coordinated through IAEA Consultants' meetings since 2003. The 1st version of the XSAMS was released in 2009. Currently XSAMS is actively implemented and further developed by members of the VAMDC consortium with international coordination through IAEA consultants'meetings and the DCN.

Over the same period of time, since about 2000, many DCN members chose to use GENIE, the search engine maintained by the IAEA A+M unit, to present users with the collection of data retrieved from the databases of the network through the engine. The collection of relevant outputs from a few databases is impressive and yet, the output page shows data in different formats as the search engine retrieves data from individual databases in arbitrary order. The results are not sorted and a user quickly discovers that it can be overwhelming to go through the multiple data sets from a query. If the databases had outputs in a common format, one would be able to generate an output page from the retrieved data sets in more consistent and informative way.

Even though the DCN members played a critical role in launching the XSAMS project and have been very supportive of the activity, the implementation of XSAMS on their databases has been slow. The barrier for entry in the implementation of XSAMS turns out to be high and there is no separate funding available for implementation. As an alternative option to the XSAMS format, the ADAS format was mentioned in this meeting since it is widely accepted by plasma modelers particularly for the ITER design campaign. The ADAS has long been available to the astrophysical communities and fusion communities and has a large user base. Since many fusion codes have an interface to the ADAS files, any data set in the ADAS format may be readily available to modelers. It is of simple tabular forms in an ascii file with a few lines of data description and hence the barrier for entry is considerably lower than for XSAMS.

While the ADAS format offers a simple solution for the time being, it was noted that the format may be too simple and unstructured to be used as a data “exchange” format or a “common” format for the GENIE output. It will offer numerical data effectively, however, not the relevant information such as authors, sources and other crucial information for data compilation and evaluation since the inputs are less structured in the ADAS format. In addition, some plasma modelers with a serious interest in the A+M/PSI data invent their own data formats, which means that they should translate the ADAS format into their own format. The better solution seems to implement the XSAMS format and then one develops conversion tools to translate the XSAMS formatted data to the ADAS formatted or to any format specific to codes. In this way, users will have an easy access to data from the DCN and VAMDC databases in the multiple options of output formats including the ADAS format directly applicable to some plasma modeling codes.

The DCN members came to the same conclusion as before that they should start implementation of XSAMS on their databases. There was a view that the XSAMS may not be mature enough yet to be implemented. Nevertheless, with the success of VAMDC project, they agreed that it is a good time to start implementation even for limited data sets. In order to overcome the high barrier of entry and the lack of funding it was proposed that training workshops should be organized. It was announced that there will be a training workshop planned in the VAMDC project in 2012 where the DCN members may join. Future workshops in collaboration with VAMDC project were proposed. The session ended with the note that OPEN-ADAS, CRAAMD, JAEA, NFRI, AMODS and ALADDIN will actively explore the option of producing XSAMS output.

3.2 Bibliographical Data Compilation

One of the main activities of the DCN is the collection and dissemination of bibliographical records for the A+M/PSI data for fusion research. Though the search engines such as Google, Google scholar or the Web of Knowledge offer a great deal of search options, the results are often too general and inadequate to find records that contain “numerical” data. The AMBDAS was initially developed to provide a source for data evaluation to be maintained by the contributions of the DCN members. If the material includes numerical data sets, private communications and reports were included as well as journals since not all data is published through literature, particularly because journals limit data-only papers. The compilation of bibliographical data has been carried out carefully by experts in the field.

For more than 3 decades, the bibliographical data for collisional processes have been collected by the CFADC (ORNL) and distributed to all the other data centres. As the future of the CFADC and their bibliographic data compilation activities is uncertain, the DCN should consider an alternative way to collect these data. The best solution is to find a way to support the experts at the CFADC to continue the excellent work on the compilation. However, such a proposal may take a while, even a few years and there is a fair chance that it won’t happen after all. While the DCN strongly supports the proposal, it has no choice but seek an alternative solution, that is, to organize the compilation activities among the data centres.

The bibliographical data compilation is fairly complicated and time-consuming work by experts in the field and it is a costly project for one group to carry out. There are several components required for this task: 1) the guidelines or filters for relevant records should be established by experts in the field, 2) the experts in the field should be involved in the collection of records (it is not considered suitable work for graduate students), 3) the distribution of tasks to the participating data centres or individuals should be made based on several factors such as subscription status of journals and relevance of the field, 4) the collected records should be reviewed by editorial staffs, 5) there should be a leader to supervise the project to deliver the final version and 6) finally, the cost to carry out this task should be estimated.

The DCN members expressed their support for the continued compilation of bibliographical data for fusion research. Already several DCN members have their own compilation activities of the bibliographical data. In order to organize a collaborative project the guidelines and procedures should be first established and regularly updated. The classification list should be reviewed and publicized. The priority in the short term should be to re-invigorate the compilation of data for atomic and molecular collision. Achieving comprehensive compilation of plasma surface interaction data will take longer due to its complexity in classification. It was suggested that the DCN should look for collaboration with other communities in the fields of electron-molecules collisions, plasma surface interaction physics and heavy particles collisions.

3.3 Data Evaluation

The importance of evaluated and/or recommended data for fusion research has been echoed in almost every meeting held by the IAEA A+M data unit, from a meeting of data producers involved in a CRP to a meeting of data users in the plasma modeling community or the DCN meetings. However, there rarely exist definite sets of recommended A+M/PSI data, except for the atomic spectroscopic data maintained by NIST. There are collisional data evaluation activities going on in data centres as reported in this meeting, however, only a small set of collisional data is evaluated and there are multiple sets available so that a user needs to select a set eventually. The integrated modeling used for the ITER designs takes weeks and months for a simulation and arbitrary variations due to choice of material properties databases should be avoided. That is why the integrated modeling community is strongly interested to have well-defined evaluated and recommended standard datasets for the required processes, with properly structured and coordinated database maintenance.

In spite of all the requests and demands from the fusion community, not much has been done for systematic coordinated data evaluation. The biggest difficulty in data evaluation activities has to do with the lack of man-power. As the funding situation deteriorated over the years, many data centres downsized the activities on the compilation and evaluation in order to focus more on the production of new data. Experts are either retiring or leaving the field and there are very few young people in the field.

Technically, data evaluation is a difficult task. First, multiple sets of data should exist for an evaluation. It is still hard to do a benchmark experiment for collisions and theoretical data are ever more popular to fill in. Secondly, error bars on evaluated data sets should be available, but the uncertainties are hard to estimate especially for theoretical data. Uncertainties of theoretical data may be made on the formulations of theory and the comparison with a few quality experimental data as demonstrated by Dr Wiese in his presentation on radiative life times in this meeting. However, the implementation of the formulation should be carefully considered since the rate of convergence by adding configurations for theoretical calculations is very slow.

Even with the constraints and challenges, the participants were motivated to change course and discussed the ways to increase data evaluation activities. They concluded that the data evaluation activities should be a community effort to establish a standard set of recommended data for fusion applications. There are several aspects to achieve the goal through collaboration: 1) data should be collected and available for evaluation, 2) evaluation guidelines for experimental and theoretical data sets should be established in the community, 3) data evaluation activities should be organized within the community and 4) a list of recommended data sets should be available as a final product with a direct impact on the ITER project.

The first step is the collection or compilation of data sets in a centralized location. As an example, the nuclear data community stores all the experimental data sets in the EXFOR database (http://www-nds.iaea.org/exfor/) and the evaluators have an access to the EXFOR database for data sets. Similarly, the A+M/PSI data evaluation will require a central location for data collection. Currently, several data centers run databases with A+M/PSI data sets, which need to be coordinated to provide the data sources for evaluation. The compilation of some A+M data sets such as data of highly charged ions or charge transfer is in the better shape than PSI data sets.

Secondly, the international guidelines for evaluation and standardization should be established. The topics for a guideline are diverse, ranging from the technical aspects to the terminology definitions. The evaluation procedures for theoretical data are not well established unlike those for experimental data. Nor is the definition of uncertainties of theoretical data sets. Terminologies issues of differentiating evaluated data from recommended data or preferred data should be discussed. If no data is available, the guideline of generating new data sets is crucial for establishing a comprehensive set. The maintenance and updates of the guidelines should be discussed.

Participants expressed commitment towards the success of data evaluation activities by actively collaborating on the collection and compilation of data sets and the management of international evaluation guidelines. NIFS and NFRI are actively engaged in the data evaluation through the APAN and JAEA suggested the EBIT machine to be used for data evaluation. Kurchatov described their activities to aid the evaluation procedures. Participants suggested a series of focused meeting on the organizational and technical aspects of data evaluation. CRAAMD, NIFS and NFRI offered to host workshops and meetings on the topic. NIST is willing to collaborate with other data centres to transfer their knowledge in atomic spectroscopic data sets.

The importance of having standard data for fusion research was continually emphasized, particularly for the ITER project. The data evaluation activities should be aimed at producing the list of standard or recommended data for the relevant plasma applications. It was proposed that the IAEA A+M data unit should develop closer collaborative relationship with the ITER project for their needs while the relevant work is carried out by the DCN members. The DCN should play a role as an entry point for data activities for the ITER project and make a direct impact on the fusion research. The unit should also work more closely with the IFRC (International Fusion Research Council) subcommittee on atomic and molecular data for fusion (http://www-amdis.iaea.org/IFRC/) in order to increase the visibility and impact of the local activities of the DCN in their own countries as well as the international fusion research community.

3.4 Priorities in A+M Data Compilation and Evaluation for Fusion

The long-term priorities in A+M/PMI data compilation, evaluation and generation were reviewed during the IAEA Technical Committee Meeting on "A+M Data for Fusion Reactor Technology" held in October 12-16, 1992 in Cadarache, France (IAEA Report INDC(NDS)-277 and "Atomic and Plasma-Material Interaction Processes in Controlled Thermonuclear Fusion", R. K. Janev and H. W. Drawin, editors, Elsevier Science Publishers B.V., Amsterdam, 1993). The list was reviewed and updated at IAEA Advisory Group Meetings held on 10-11 July 1995 (IAEA Report INDC(NDS)-339), 21-22 July 1997 (IAEA Report INDC(NDS)-339), 13-14 September 1999 (IAEA Report INDC(NDS)-410), 10-11 September 2001 (IAEA Report INDC(NDS)-430), 6-7 October 2003 (IAEA Report INDC(NDS)-449), 10-11 October 2005 (IAEA Report INDC(NDS)-489), 3-5 October 2007 (IAEA Report INDC(NDS)-527), 7-9 September 2009 (IAEA Report INDC(NDS)-563).

Produced almost two decades ago, the list of long-term priorities in A+M/PMI data compilation, evaluation and generation served as a reference for the A+M/PSI data producer to understand the data needs of direct importance to plasma community. As the ITER project and new fusion projects developed, research topics of plasma modeling have changed and so have the A+M/PSI data needs. However, the current list is considered to be too general and broad for data producers to meet the specific needs of data users. It is desirable to provide source information on the available sets. The IAEA A+M Data unit proposed to compose a new list of data needs discussed in various technical meetings and research coordination meetings. Participants agreed that the review of the long-term priorities in A+M/PMI data compilation, evaluation and generation should be deferred to later meetings so that inputs from the data user community can be incorporated to the list. A new format should be discussed that provides information on both the data needs and the available data sources.

4. DCN Membership

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

As data centre activities of GAPHYOR, ENEA and IPP-Garching data centres diminished, they will not be invited to the DCN meetings in the future. The new data centres of NFRI and FZJ will submit a proposal in the next meeting. As old data centre representatives approach the retirement and the new data centres are established the DCN membership of existing data centres will be reviewed regularly. New research organizations with data centre activities will be actively sought out.

5. Data Centres Web Interface and Software Presentations

This session gave an opportunity to demonstrate new tools, interfaces or databases developed by the data centres available on the web.

Dr Hyun-Kyung Chung, IAEA showed the new knowledge base on the A+M/PSI data for fusion. It contains information on the data centre network activities such as the list of data centres, the list of code centres as well as the list of data needs. It also contains the summaries of the CRPs as well as the summaries of presentations. Participants were invited to contribute to the knowledge base.

Dr Yuri Ralchenko, NIST, showed the new version 4 of NIST atomic spectra database. The new version provides the information on the history and the updates of the versions. The information is provided for the additions and corrections on the energy levels and spectral lines. In the new version, the energy levels for isotopes are available.

Dr Jung-Sik Yoon, NFRI, presented the database at http://plasma.kisti.re.kr in Korean which hosts 500,000 data published in literature in the field of A+M/PSI data for plasma applications. The literature data are scanned by 100 people for 3 years and available to the public. The database at NFRI, http://dcpp.nfri.re.kr, hosts the subset of the data selected for data evaluation and publically available in both Korean and English.

Dr Detlev Reiter, FZJ, presented the EIRENE database, http://www.eirene.de, which includes the A+M/PSI data currently used in the plasma edge physics codes. He also demonstrated the HYDKIN, http://www.eirene.de/eigen/ the online reaction kinetics analysis tool for hydrocarbon in hydrogen plasmas consisting of a Monte Carlo linear transport solver with the hydrocarbon data sets.

6. Meeting Conclusions and Recommendations

The meeting was held at a critical time of many changes in the data centre network. Three old data centres retired and three data centres including the VAMDC project are invited as observers. Both staff members of the IAEA A+M data unit were replaced during the last two years. It was timely for DCN members to review the objectives of the network and make the work plans to benefit both DCN and the fusion community. The DCN members discussed topics on data exchange format, bibliographical data compilation, data evaluation and the following action items were agreed upon at the end of the meeting and after the meeting:

6.1 Data Exchange Format

- Open-ADAS, CRAAMD, JAEA, NFRI, AMODS and ALADDIN will actively explore the option of making XSAMS available as an output format.
- Training workshops will be organized in collaboration with DCN and/or VAMDC. (There is a VAMDC conference/workshop on February 21-24 in Vienna)
- IAEA will work with data centres in developing an output conversion tool in order to demonstrate the advantages of XSAMS output to facilitate better data comparisons.
- *(discussion after the meeting)* NFRI will establish the new database based on the XSAMS.

6.2 Bibliographical Data Compilation

- IAEA will review the ORNL procedures and coordinate the updates of guidelines and procedures with other DCN members.
- IAEA looks forward to collaborate with other community outside DCN (e-molecules, PSI, heavy-particle collisions) for bibliographical data collection
- The data classification list and the template of bibliographic data collection should be made easily available and should be reviewed.
- An immediate priority is placed for AM collisions in order to fill the gap since 2009.
- It is recognized that while it is a high priority to collect PSI data, it will take longer to achieve.
- NFRI & APAN network will actively participate in this effort.

6.3 Data Evaluation

- IAEA A+M Unit wishes to organize a series of technical meeting involving data evaluation activities (Plasma-material interaction data as a starting point, December 12-13, 2011)
- CRAAMD will organize an international workshop on data evaluation next years (2012-2013) in China in collaboration with the DCN members. (Possibly with the connection to ICAMDATA (NIST) or/and ICPEAC (Lanzhou))
- IAEA CRPs will include data evaluation activities and consider an evaluated data list as a final production.
- DCN should encourage national labs or data centres to do more evaluation work.

- IAEA will contact ITER to identify its and DCN's possible role in data recommendation / evaluation, specification of standards to meet the needs of ITER.
- International standards of A+M/PSI for fusion data evaluation should be established (take NFRI guidelines as a starting point).
- *(discussion after the meet ing)* NIFS will host a consultants' meeting on data evaluation in February 2012 and NFRI will host a joint technical meeting on data evaluation in September 2012.

6.4 Status of Priorities in A+M Data Compilation and Evaluation for Fusion

- As the list of data needs and priorities was briefly reviewed and the improvement of the current list on its effectiveness and impact was discussed, the discussion on its reformulation was deferred to the next meeting.
- IAEA technical meetings, consultants' meetings, coordinated research programmes and individual consultancies will be used to propose a list of priorities in A+M data compilation and evaluation for fusion.

This meeting was very productive and the collaboration and communication between datacentres and the A+M Data Unit were very useful. The communication continued shortly after the meeting on the collaboration on various topics, in particular, on the data evaluation as summarized above.

IAEA Technical Meeting on Technical Aspects of Atomic and Molecular Data Processing and Exchange (21st Meeting of the A+M Data Centres)

7-9 September 2011, IAEA Headquarters, Vienna
Scientific Secretary: Hyun-Kyung Chung

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Appendix 2

IAEA Technical Meeting on Technical Aspects of Atomic and Molecular Data Processing and Exchange (21st Meeting of the A+M Data Centres)

7-9 September 2011, IAEA Headquarters, Vienna
Scientific Secretary**:** Hyun-Kyung Chung

Agenda

Wednesday, 7 September **Meeting Room: F0879**

09:30 – 10:15	Opening (Meera Venkatesh, Director of NAPC) Introduction of Participants and Adoption of Agenda B. Braams (IAEA): Review Meeting Objectives
Session 1:	Current Activities of the A+M Data Centres
Chairman:	T. Nakano
10:15 – 10:40	W.L. Wiese (NIST): Activities 2009-2011 at the Atomic Spectroscopy Data Center at the National Institute of Standards and Technology (NIST)
10:40 – 11:05	J. Yan (CRAAMD): Activities at CRAAMD
11:05 – 11:30	*Coffee break*
11:30 – 11:55	D.R. Schultz (ORNL): The ORNL Controlled Fusion Atomic Data Center
11:55 – 12:20	J.S. Yoon (NFRI): Current Activities of Data Center for Plasma Properties
12:20 – 14:00	*Lunch*
Session 2:	Current Activities of the A+M Data Centres (Continued.)
Chairman:	J. Yan
14:00 – 14:25	I. Murakami (NIFS): Atomic and Molecular Data Activities at NIFS in 2009-2011
14:25 – 14:50	D. Reiter (FZJ): The EIRENE.DE On-line Database for Surface and A&M Data in Fusion Edge Modelling
14:50 – 15:15	Y. Rhee (KAERI): AMODS and High Energy Density Sciences
15:15 – 15:45	*Coffee break*
15:45 – 16:10	Yu. Martynenko (Kurchatov Institute): Report A+M/PSI Data Centre NRC "Kurchatov Institute"
16:10 – 16:35	T. Nakano (JAEA): Atomic and Molecular Data Activities for Fusion Research in JAEA
16:35 – 17:00	M. O'Mullane (ADAS): The OPEN-ADAS approach to atomic data provision
17:00 – 17:25	H. Chung (IAEA): IAEA Atomic and Molecular Unit Activities
19:30	*Social Dinner*

Thursday, 8 September

Session 3: Data Needs: Data Exchange Format

Chairman: I. Murakami

09:00 – 09:45	N. Mason (VAMDC): VAMDC - The Virtual Atomic and Molecular Data Centre A New Era in Database Collaboration
09:45 – 10:10	Yu. Ralchenko (NIST): Some Topics in A&M Data Exchange
10:10 – 11:00	Data Exchange Format (all participants)
11:00 – 11:25	*Coffee break*

Session 4: Data Needs: Bibliographical Data Compilation

Chairman: B. Braams

11:25 – 11:45	B. Braams/H. Chung (IAEA): IAEA AMBDAS Activities
11:45 – 12:45	Data for the International Bulletin on Atomic and Molecular Data for Fusion (all participants)
12:45 – 14:00	*Lunch*

Session 5: Data Needs: Data Evaluation

Chairman: W. Wiese

14:00 – 14:30	S. Simakov (IAEA): Experimental (network) and Evaluated Nuclear Reaction Data at NDS
14:30 – 15:30	Coordinated Activities on Data Evaluation (all participants)
15:30 – 16:00	*Coffee break*

Session 6: Data Needs for Fusion Research

Chairman: D.R. Schultz

16:00 – 17:30	Priorities in A+M data Compilation and Evaluation (all participants)

Friday, 9 September

Session 7: Review on Data Needs

Chairman: B. Braams

9:00 – 12:30 Plan of DCN activities for the future

- Data Exchange Format
- Data for the Int. Bulletin on Atomic and Molecular Data for Fusion
- Data Evaluation Network
- Membership Issues

12:30 – 13:30 *Lunch*

Session 8: Demonstrations

Chairman: H. Chung

13:30 – 15:30 Data Centre WWW Database and Software Demonstrations

15:30 – 16:00 *Coffee break*

Session 9: Meeting Conclusions and Recommendations

Chairman: H. Chung

16:00 – 17:00 Formulation of Meeting Conclusions and Recommendations (Round-Table)
Date of Next meeting

17:00 – ***Adjourn of the Meeting***

Abstracts of Presentations

The abstracts are given below for the meeting presentations available at http://www-amdis.iaea.org/DCN/Presentations.

Review of Meeting Objectives

B. J. Braams
International Atomic Energy Agency, Vienna, Austria

This is the 21st meeting of the International Atomic and Molecular Data Centres Network. The traditional DCN meeting objectives are: to exchange information about activities in the Centres and review progress; to coordinate work in the Centres; to assess priorities in data evaluation and data production; to make plans for specific evaluations; and to evaluate and revise procedures for collection and exchange of bibliographical and numerical data. All of these are objectives for the present meeting too. In addition to the presentations from DCN and prospective DCN members we have two participants from outside the field of fusion data: Dr N. Mason will tell us about coordination of the Virtual Atomic and Molecular Data Centre and Dr S. Simakov will describe the manner in which nuclear structure and cross-section database development is coordinated by our colleagues in the Nuclear Data Section.

In the discussions on Thursday and Friday there are two topics that need special attention this year: the future of our bibliographical data compilation and ways in which we can strengthen data evaluation activities, all with emphasis on collison processes and plasma-material interaction.

The first 3 Data Centre Network meetings were held in 1977, 1980 and 1982 and the reports of those meetings make interesting reading and can still provide inspiration for the present meeting. I show some excerpts in the presentation.

In 1977 the emphasis was on the coordination of the bibliographical database, AMBDAS, and a collision data index, CIAMDA, as the initial activities of the Network and of the newly formed IAEA A+M Data Unit. In 1980 the central topic of discussion at the meeting shifted to the numerical database and to data evaluation. The Network recommended that numerical data be reviewed by a selected group of scientists and that no unevaluated numerical A+M collision data should be distributed by the IAEA. The report of the meeting in 1982 shows that the bibliographical database work and the index to numerical data was at that time well established; the key ongoing work was the development of an exchange format for numerical data.

In subsequent meetings of the Data Centres Network the issue of data evaluation and of associated selection criteria for inclusion in what became the ALADDIN database are recurring themes, and they are themes for us again at the 21st meeting. The sense of the A+M Data Unit is that we do not want to restrict ALADDIN to offer only evaluated data; however, we do want to strengthen data evaluation activities and provide recommendations about data quality. We hope that the present DCN meeting will help with those objectives.

Summary of the Activities of the NIST Atomic Spectroscopy Data Center for 2009 to 2011

W. L. Wiese
National Institute for Standards and Technology, Gaithersburg, MD, USA

The work of the Atomic Spectroscopy Data Center team at the National Institute of Standards and Technology (NIST) in Gaithersburg, MD USA centered in the last two years on two main subjects:

First, the data center completed and issued a new, significantly improved version of its principal product, the Atomic Spectra Database (ASD Version 4.0 in September 2010, with an update 4.1.0 in May 2011). These versions contain new data for a good number of additional spectra as well as new, better quality and more extensive data replacing the earlier material. They are also for the first time completely integrated with the two NIST bibliographies on atomic energy levels and spectra, and on atomic transition probabilities. The sources of the material selected in ASD for the various spectra and transitions are identified there by their numbers in the respective bibliographies, so that the original papers can be directly accessed by users if they desire more background material.

Secondly, new tabulations of atomic energy levels and wavelengths were completed for hydrogen and its isotopes (H, D, T), for argon (Ar II through Ar XVIII), cesium (Cs I through Cs LV), barium (Ba III through Ba LVI) and tungsten (W III through W LXXIV). Compilations of energy levels and spectral lines are in progress on neon (Ne IV), chlorine (Cl I through Cl XVII), and nickel (Ni I through Ni VIII). Data assessments and compilations of atomic transition probabilities were completed for hydrogen and its isotopes (H,D,T), for helium(He I and He II), for lithium (Li I through Li III), beryllium (Be I through Be IV), boron (B I through B V), sulfur (S I through S XVI), cesium (Cs I through Cs LV), and barium (Ba III through Ba LVI). Additional compilations for the higher fluorine and neon ions (F V through F IX, Ne VI through Ne X), chlorine (Cl I through Cl XVII) and nickel (Ni I through Ni VIII) are in progress.

As in all our earlier work, the NIST data tables are limited to reference data, i.e. data of a certain minimum quality. Only one numerical value is presented for the wavelength, transition probability, and lower and upper energy levels of a given spectral line. This value may be either from a single source, evaluated to be the most accurate one, or from an average of several sources of about equal reliability. For atomic transition probabilities, explicit accuracy ratings are given. For wavelengths and energy levels, the number of tabulated digits indicates their accuracy.

CRAAMD Activities 2010-2011

J. Yan
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The recent activities of the Chinese Research Association on Atomic and Molecular Data (CRAAMD) members in 2010-2011 will be introduced. About 2700 lines of atomic spectra was collected and compiled for Au, Cr Ti, Fe, Si, Al and Br ions. Data calculation and evaluation for Ar atom in the framework of multichannel quantum defect theory will also introduced, which is convenient to get the properties of energy levels, radiative transition and collision processes based on the eigenchannel quantum defect, the transformation matrix and the generalized oscillator strength (GOS) to eigenchannels. Cross sections of heavy particle collisions (excitation, ionization and charge transfer) are calculated for H^{+}+Li, $Be^{2,3+}$+H, $B^{3,4+}$+H, N^{5+}+He, O^{6+}+He, H^{+}+He, N^{5+}+H, O^{6+}+H, as well as their collisions in Debye plasmas. I will show the examples of data application to calculate the electron broadening width for atomic spectra and stopping power for α particle in Au plasmas.

The ORNL Controlled Fusion Atomic Data Center: Overview of Activities 2011

D. R. Schultz
Controlled Fusion Atomic Data Centre, Oak Ridge National Laboratory, Oak Ridge, TN, USA

The Controlled Fusion Atomic Data Center (CFADC) of the Oak Ridge National Laboratory continued operation aimed at collecting, evaluating, and disseminating atomic, molecular, and particle-surface interaction (AM&PSI) data needed by both the U.S. and international plasma science communities. This work has been carried out within an overarching atomic physics research group which produces much of the required data through an active experimental and theoretical science program. The production of an annotated bibliography of AM&PSI literature relevant to plasma science continues to be among the most important activities of the data center, forming the basis for the CFADC on-line bibliographic search engine and a significant part of the IAEA A+M Data Unit's "International Bulletin on Atomic and Molecular Data for Fusion." Also chief among the data center's activities are responses to specific data requests from the plasma science community, leading to either rapid feedback using existing data resources or long term data production projects, as well as participation in IAEA Coordinated Research Programs including recently "Data for Surface Composition Dynamics Relevant to Erosion Processes" and "Atomic and Molecular Data for Plasma Modeling." Highlights of recent data production projects include the following: Experimental and theoretical data for inelastic electron-hydrocarbon reactions, large scale computational results for particle reflection from surfaces, measurements of chemical sputtering from carbon, inaugural experiments considering molecular ion collisions with neutral hydrogen, and expansion of the database of elastic and related transport cross sections calculated for intrinsic and extrinsic impurities in hydrogen plasmas. Progress is being hampered owing to news from the US Department of Energy that it plans to close out the program after a ramp down of funding in 2012, following a distinguished 52 year history of contributions to the US and international fusion research efforts by the data center.

Current Activities of Data Center for Plasma Properties

J.-S. Yoon
Data Center for Plasma Properties, National Fusion Research Institute, Daejeon, South Korea

The study of atomic and molecular physics using electron, ion and neutral has been an active area of experimental and theoretical research for several years. Since, the interactions with various atomic and molecular targets play an important role in many areas, such as nuclear fusion, semiconductor manufacturing, lighting, propulsion, environmental remediation and material processing. Also, Plasma modeling now becomes a necessary engineering tool in the design of new semiconductor, display equipment and in process control. However, we suffer from lack of theoretical and experimental cross section data for plasma gas (A+M data).

Thus, in my talk, the work conducted at the Data Center for Plasma Properties (DCPP) over last 5 years on the systematic synthesis and assessment of fundamental knowledge on low-energy electron interactions with plasma processing gases is briefly summarized and discussed.

Atomic and Molecular Data Activities at NIFS in 2009-2011

I. Murakami
National Institute for Fusion Science, Toki, Japan

We open and maintain the NIFS atomic and molecular numerical databases. Numbers of data records increase to 476,048 in total (as of Aug. 23, 2011) and mainly new data are added for AMDIS (electron impact ionization, excitation, and recombination cross sections and rate coefficients) and CHART (charge transfer of atom – ion collisions cross sections) during last two years. A collaboration group has started for research on atomic and molecular processes in plasma using the Large Helical Device and we measure visible and extreme ultraviolet spectra of W and rare earth elements. We also organize a collaboration group with atomic physicists from Japanese universities for research on W to study atomic data, spectra and collisional-radiative models for W ions.

The EIRENE.DE Online Database for Surface and A+M Data in Fusion Edge Modelling

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In magnetic fusion plasma modelling no unique optimal data format for atomic, molecular and surface data exists, because the level of detail (condensation, pre-processing) of raw data is highly case and application dependent. Microscopic erosion redeposition modelling requires, in principle, multi-differential cross sections, whereas macroscopic core plasma simulations can be based on strongly reduced (compressed and processed) A&M data, even charge stage bundling might be an option here. Integrated edge plasma modelling (e.g for ITER divertor design studies) has both important microscopic and macroscopic components (and a related wide spectrum of requirements for AMS data formats). The B2-EIRENE code (aka: SOLPSx.y) is a prominent example of such an integrated edge plasma code.

The AMS database maintained at FZ Juelich (www.eirene.de) is set up to publicly expose the database available for this codes system as used in the current ITER design. It is a database tailor-made for this particular code system, but it is (partially) used by other edge modelling codes as well. In that sense it acts as a data centre for edge transport codes.

The database covers the full range of microscopic data (interaction potentials for elastic neutral-ion collision, differential cross section soon to be added as an alternative), total cross sections, rate coefficients. Also condensed rate coefficients (so called "collisional radiative (CR) rate coefficients"), are based on quasi-steady state assumptions for a large subset of states, mostly excited states. These are parameterized and stored as well. An issue with these CR model databases is the number of independent parameters: e.g already for the H2 molecules, due to the near resonant charge transfer of H2(v=4) with protons, independent variables for effective dissociation or ionisation rates are at least: n_e, n_p, T_e, T_p and E, the energy of the H2 molecules, leading to five dimensional tables or fits already without considering isotopically correct datasets for a mixture of H-molecules.

A feature enabled by the rapidly growing computing power is therefore that the full dataset for the EIRENE neutral particle Monte Carlo transport code now also comprises CR model codes (rather than pre-processed data) themselves, which allow to evaluate CR coefficients on the fly within the transport calculation, retaining all necessary dependencies. Furthermore an interface between EIRENE and the online database analysis tool HYDKIN (www.hydkin.de) is currently developed (and in place for hydrocarbons) with the goal to pre-process and condense the raw data of the database specifically as part of the modelling application itself. The HYDKIN code is based on a spectral analysis of rate equation matrices and therefore also capable of direct online (linear) sensitivity analysis regarding the plasma chemistry at given plasma conditions.

Surface data are stored for EIRENE (and other kinetic edge plasma codes) in a particular "conditional quantile function" format (see www.eirene.de/surface-data/TRIM), which allows to retain the kinetic information of backscattered and sputtered particles. Global quantities such as particle, energy and momentum reflection coefficients can be readily obtained from the multi-differential (in velocity space of re-emitted particles) distributions, but these microscopic distributions themselves can (and are) readily directly used in kinetic Monte Carlo simulations, thus eliminating frequently made approximations here.

Due to the ongoing ITER (and forthcoming DEMO) design process, and the very computing intensive edge plasma simulations (2-3 month per case) **backward compatibility of code and databases** is a key ingredient, at least for design applications to ITER and DEMO (much less so for interpretative applications to current experiments). Upgrades/changes of the underlying AMS databases are to be kept at an absolute minimum. Perhaps, ITER being a world wide project, they should be carried out only if a worldwide community consensus regarding the need for an upgrade/modification of underlying AMS data is achieved.

It is anticipated that the role of an international Data and Code centre **network**, as established at IAEA, could become far more central once ITER has evolved from its current construction phase to a joint world-wide scientific endeavour. It is argued that IAEA with its networks might be in the position of acting in a prominent way as "gateway" for ITER into the world-wide AMS community and to various individual data centres, **and vice versa**.

AMODS and High Energy Density Sciences

Y.-J. Rhee
Lab for Quantum Optics, Korea Atomic Energy Research Institute, Daejon, South Korea

Following a brief introduction to the Lab for Quantum Optics (LFQO) in KAERI, which has been devoted to the research on atomic spectroscopy for more than 20 years with precision measurement of atomic parameters such as isotope shift, hyperfine structures, autoionization levels and so on as well as with theoretical analysis of atomic systems by developing relativistic calculation methodologies for laser propagation and population dynamics, electron impact ionization, radiative transitions of high Z materials, etc for the application to isotope separation, the AMODS (Atomic Molecular and Optical Database Systems) which was established in 1997 and has been a member of International Data Center Network of IAEA since then is explained by giving an information on the data sources and internal structure of the compilation of AMODS. Since AMODS was explained in detail during last DCN meeting, just a brief introduction is given this time.

Then more specific research themes carried out in LFQO in conjunction with A+M data are discussed, including (1) electron impact ionization processes of W, Mo, Be, C, etc, (2) spectra of highly charged ions of W, Xe, and Si, (3) dielectronic recombination process of Fe ion. Also given are the talk about research activities about the simulations of high energy density experiments such as those performed at (1) GEKKO laser facility (Japan) for X-ray photoionization of low temperature Si plasma, which can explain the unsolved arguments on the X-ray spectra of black holes and/or neutron stars, (2) VULCAN laser facility (UK) for two dimensional compression of cylindrical target and investigation of hot electron transport in the compressed target plasma to understand the fast ignition process of laser fusion, (3) LULI laser facility (France) and TITAN laser facility (USA) for one dimensional compression of aluminum targets with different laser energies, and (4) PALS facility (Czech Republic) for “Laser Induced Cavity Pressure Acceleration” to understand the shock ignition process of laser fusion. The importance of A+M data in these simulations is emphasized since those hydrodynamic simulations are based on the EOS/opacity data which is directly related to atomic and molecular characteristics of target materials.

It is also mentioned that AMODS of KAERI will continue to be the main source of atomic and molecular data in Korea for nuclear applications either in fission or fusion (IFE/MFE) as long as KAERI is in charge of the research on nuclear power in Korea .

Report A+M/PSI Data Centre NRC “Kurchatov Institute”

Yu.V.Martynenko
Institute for Fusion Research, Scientific Research Centre "Kurchatov Institute", Moscow, Russian Federation

The main activities on A+M/PSI DATA in Kurchatov institute are
1. New Data generation. (Experiment, theory, codes).
2. Data Acquisition System + (DAS+) http://cpunfi.fusion.ru/dassql/dasweb2.dll/showgl, which is to operate with experimental data of various devices (T-10, GTB, PN-3, S300, L-2M, Tuman, Globus) of controlled nuclear fusion (storage, transmission, processing and results representation).

The presented new data are following.
1. Direct observation $D^- + D^- \rightarrow D^{2-}$.
2. Quasiclassical calculation: bremsstrahlung (W ion (different charge Z_i) + 5 keV electron); radiative and dielectronic recombination rates for Cr3+, Mg1+.
3. Fast codes: (i) *n,l* collisional-radiative kinetics of Rydberg atomic states, (ii) Bremsstrahlung + Radiative Recombination.
4. Data for surface Composition Dynamics Relevant to Erosion Processes. C addition in D plasma increases W erosion yield, surface structure development and adds C in deposit

5. Conditions (temperature T and deposition rate q) for different deposited films structure
6. Calculation of grains size in deposited film.
7. Condition of dust mobilization in tokamaks
8. Condition of deposited film exfoliation and size of fragmented films.
9. Angle distribution of atoms sputtered from Mg, Al, Cu, Ag, Ta, Pt, Au, Ti, Cr, Zn, Zr, Nb polycrystalline targets
10. Testing of W at plasma accelerator QSPA-T (edges melting, cracks formation and dynamic, surface structure, erosion products deposition)
11. Plan for Be samples study at QSPA-Be facility. Testing of Be samples by D plasma pulses and by Ar and Ne plasma radiation. Investigation of erosion products. Comparison of Be grades.

Atomic and Molecular Data Activities for Fusion Research in JAEA

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The Japan Atomic Energy Agency (JAEA) has been producing, collecting and compiling cross-section data for atomic and molecular collisions and spectral data relevant to fusion research. In this talk, an overview of our activities since the last meeting in September 2009 will be presented.

The state selective charge transfer cross-section data of Be^{4+}, C^{4+} and C^{6+} by collision with H($n = 2$) in the collision energy range between 62 eV/amu and 6.2 keV/amu have been calculated with a molecular-bases close-coupling method. The calculated charge transfer data of C^{4+} was implemented in a collisional-radiative model code for C^{3+}[1], and it is shown that in some cases the charge transfer from C^{4+} to H(n=2) populates predominantly C^{3+} (n = 6, 7). The cross-section data of dissociative recombination and excitation of HD^+, D_2^+, DT^+, T_2^+ $^3HeH^+$ and $^4HeH^+$ were produced by theoretical calculation. The principal quantum number of dissociated H atom isotopes was also given. The analytical expressions for the cross-section data for 26 processes of He-collision systems were produced in order to facilitate practical use of the data. The compiled data are in preparation for the web site at the URL of http://www-jt60.naka.jaea.go.jp/engish/JEAMDL/. The chemical sputtering yield data of CFC materials with hydrogen isotope collisions have been compiled. The ionization rate of W^{44+} and the radiative and the dielectronic recombination rates of W^{45+} were calculated with FAC. The ratio of these rates was compared with experimentally measured ratio of W^{45+} density to W^{44+} density in JT-60U, showing that the calculated ratio of the recombination ratio of W^{45+} to the ionization rate of W^{44+} is accurate within the experimental uncertainty (~ 30%) [2].

The atomic and molecular data activities in JAEA are pursued in collaboration with Japanese universities, and other department of JAEA.

References
[1] Nakano T. Kubo H. *et al*., *J. Plasma Fusion Res.*, **80** (2004) 500.
[2] Nakano T. and the JT-60 team, *J. Nucl. Mater.*, in press (2011).

IAEA Atomic and Molecular Unit Activities

H.-K. Chung
Nuclear Data Section, Division of Physical and Chemical Sciences, IAEA, Vienna, Austria

Research on fusion energy devices requires a large amount of data for atomic, molecular and plasma-surface interactions. As current machines are updated and future machines are designed, data for a variety of different materials for a wide range of plasma parameters arise. The Atomic and Molecular (A+M) Data Unit of the International Atomic Energy Agency works to coordinate efforts to establish databases for this fusion research effort.

Current activities for database development include a number of Coordinated Research Projects (CRP), Technical Meetings, Consultant Meetings and a number of collaborations. These activities generate significant new data in support of fusion research. These data are published in journals as well as IAEA publications and are included in numerical databases ALADDIN accessible by all fusion researchers.

Historically a number of institutions have contributed to development of such databases and continue to participate in a Data Centre Network, supported by the A+M Unit. Members of this network maintain individual databases, many of which can be searched using the GENIE search engine. The A+M Unit host the OPEN-ADAS system that allows access to most of the numerical data stored within the ADAS system. An effort on development of an XML schema for data exchange among the databases is underway. .

Many numerical data for specific processes in fusion relevant materials are not available. In many cases computer codes exist with the capability of generating such data as needed. An informal network of institutions with such capabilities is in the process of formation to provide a means quickly generating such data. The A+M Unit maintains on-line code capabilities to generate atomic and molecular data and serves as an access point to LANL atomic physics codes and FLYCHK, Non-LTE kinetics codes at NIST.

Currently, a wiki-style knowledge base is under the development. It will host a wealth of information on atomic, molecular, plasma-surface data for fusion research performed through the CRP and other activities. The knowledge base will complement the numerical and bibliographical databases.

VAMDC - The Virtual Atomic and Molecular Data Centre: A New Era in Database Collaboration

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Atomic and molecular data (A&M) are of critical importance in developing models of radiation chemistry including track structures. Currently these vital and fundamental A&M data resources are highly fragmented and only available through a variety of often poorly documented interfaces. The Virtual Atomic and Molecular Data Centre (VAMDC) is an EU funded e-infrastructure (www.vamdc.eu) that aims to provide the scientific community with access to a comprehensive, federated set of Atomic and Molecular (A&M) data. These structures have been created by initiatives such as the Euro-VO (http://www.euro-vo.org) and EGEE (Enabling Grids for E-sciencE, (http://www.eu-egee.org/).

VAMDC will be built upon existing A&M databases. It has the specific aim of creating an infrastructure that on the one hand can directly extract data from the existing depositories while on the other hand is sufficiently flexible to be tuned to the needs of a wide variety of users from academic, governmental, industrial communities or even the general public.

Central to VAMDC is the task of overcoming the current fragmentation of the A&M database community. VAMDC will alleviate this by:

- developing the largest and most comprehensive atomic and molecular e-infrastructure to be shared, fed and expanded by A&M scientists,
- providing a major distributed infrastructure which can be accessed, referenced and exploited by the wider research community.

In fulfilling these aims, the VAMDC project will organise a series of Networking Activities (NAs). NAs are specifically aimed at

- Engaging data providers.
- Coordinating activities among existing database providers.
- Ascertaining and responding to the needs of different user communities.
- Providing training and awareness of the VAMDC across the international A&M community and other use communities such as the radiation chemistry community.

In this talk I will therefore outline the aims, methodology and mechanisms of the VAMDC project while giving examples of the datasets that it will provide access to that will be valued by the fusion community.

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