IAEA
International Atomic Energy Agency

INDC(NDS)- 0622
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INDC International Nuclear Data Committee

Data Evaluation and the Establishment of a Standard Library of Atomic, Molecular and Plasma-Material Interaction Data for Fusion

Summary Report of an IAEA Consultants' Meeting

IAEA Headquarters, Vienna, Austria

20 – 22 June 2012

Prepared by

B. J. Braams

August 2012

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Printed by the IAEA in Austria

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Abstract

Seven experts in the field of atomic, molecular and plasma-material interaction (A+M+PMI) data and data evaluation for fusion plasma physics met with IAEA A+M Data Unit staff at IAEA Headquarters to provide advice towards the establishment of an evaluated and recommended library of A+M+PMI data for fusion. The proceedings and conclusions of the meeting are summarized here.

August 2012

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1. Introduction

The Atomic and Molecular Data Unit (AMDU) in the Nuclear Data Section at IAEA is responsible for the development and maintenance of internationally validated and recommended data for atomic, molecular and plasma-material interaction (A+M+PMI) processes in fusion. In carrying out this work the unit coordinates an international network of A+M data centres, the DCN. At a recent meeting members of the DCN agreed that data evaluation needs new impetus and it should be coordinated by AMDU. The purpose of the Consultancy Meeting was to advise the Unit about strategy for evaluation of theoretical data in general and of A+M collision data and PMI data in particular and for coordinating the establishment of a standard library of atomic, molecular and plasma-material interaction data for fusion. The CM should provide policy and technical advice about unit activities in the next 3-5 years on the coordination of data evaluation and about evaluation of theoretical A+M collision data, evaluation of PMI data and establishment of a network of data evaluators.

Appendix 1 provides the list of participants and Appendix 2 provides the meeting agenda. The roadmap towards the establishment of a standard library, as revised during the discussions, is provided in Appendix 3.

2. Presentations

Robin A. Forrest and Bas Braams: Opening.

Dr Forrest, head of the Nuclear Data Section, briefly reviewed the mission of the section and described the manner in which nuclear cross section, structure and decay data are assembled and evaluated and standard libraries are produced. As a topic of special interest for fusion he noted the Fusion Evaluated Nuclear Data Library (FENDL), which is now being revised to include charged particle and neutron cross sections at energies up to 60 MeV in view of the needs of IFMIF. He welcomed the participants to Vienna and wished for a productive meeting. Dr Braams extended his welcome and recalled the core objective of the meeting to contribute to the development of a standard recommended library of atomic, molecular and plasma-material interaction data for fusion. He noted on the one hand the similarity of aims with FENDL and on the other hand the challenge that in the A+M+PMI field calculated data have a much larger role than in the nuclear field and therefore the evaluation procedures are quite different.

Hyun-Kyung Chung: IAEA Data Centre Network activities on data evaluation for fusion applications

Dr Chung reviewed the mission of the atomic and molecular data unit at IAEA and its recent activities on data evaluation. The unit was formed in 1977 with the purpose to stimulate and coordinate international work on the measurement, compilation and evaluation of atomic, molecular and plasma-surface interaction data for fusion. The unit manages coordinated research projects and technical and consultancy meetings, maintains numerical (ALADDIN) and bibliographical (AMBDAS) databases and a database search engine (GENIE), contributes to standardization of database formats for A+M data (XSAMS) and publishes reports (INDC series and the Bulletin) and an in-house journal (APID).
International cooperation of data centres is supported by biennial meetings of the Data Centre Network (DCN) since the start of the unit and more recently also of a Code Centre Network (CCN). The latest meetings of the DCN and the CCN both emphasized strongly the need for a Standard Data Library containing critically evaluated and recommended data. The discussions in the DCN meeting of 2011 and a subsequent consultancy meeting at NIFS in Feb 2012 provided recommendations for a new organization of data evaluation work in the DCN community. The database infrastructure needs to be renewed to support evaluation work, experts in data evaluation need to be attracted to the work and their knowledge needs to be transmitted, and procedural guidelines for data evaluation must be established, especially and most urgently for evaluation of theoretical data sets. A Joint IAEA-NFRI Technical Meeting on data evaluation for A+M+PMI processes in fusion is planned to be held in Daejeon, Korea, 4-7 September 2012, focussed on uncertainty estimation, error propagation and

sensitivity to errors as well as database management and data recommendation, all primarily for reaction data. The long term goal is the development (and ongoing maintenance) of an internationally agreed and recommended data library for fusion and other plasma applications.

The meeting at NIFS developed a Roadmap towards establishment of such a standard library and one objective of the present meeting is to refine that roadmap. (Please refer to the Discussion and to Appendix 3.)

Jong-Oh Choi: Measurement and uncertainty

Dr Choi, head of the Center of Standards and Quality Management at the Korea Research Institute of Standards and Science (KRISS) reviewed the international standard vocabulary on measurement and uncertainty as laid out in the International Vocabulary of Basic and General Terms in Metrology (VIM) and in the Guide to the expression of Uncertainty in Measurement (GUM). The present instance (2007) of VIM uses an operational approach with focus on observed variability that is captured in the concept of "uncertainty"; it avoids the concepts of true value and an associated "error". Precisely, VIM describes *measurement* as the process of experimentally obtaining one or more quantity values that can reasonably be attributed to a quantity, *traceability* as the possibility to relate a measurement result to a stated metrological reference through a documented unbroken chain of calibrations of measuring systems, and *measurement uncertainty* as a parameter that characterizes the dispersion of the quantity values that are being attributed to a measurand, based on the information used.

The GUM provides detailed recommendations and standards for evaluating and expressing the uncertainty in measurements. The Standard Uncertainty has Type A and Type B components. Type A is the familiar measure based upon repeated measurements and evaluation of a standard deviation. Type B uncertainty evaluation involves previous measurement data, general knowledge of the behavior and properties of relevant materials and instruments, manufacturer's specifications, data provided in calibration and other certificates, and uncertainties assigned to reference data taken from handbooks. (This topic was elaborated in Dr Choi's second presentation later in the meeting.)

David Coster: Using AMNS data within an Integrated Tokamak Modelling environment

Dr Coster described the use and management of atomic, molecular, nuclear and surface/solids (AMNS) data by the European Fusion Development Association (EFDA) Task Force (TF) on Integrated Tokamak Modelling (ITM). This task force coordinates the development of a coherent set of validated simulation tools for core and edge plasma physics and plasma-wall interaction. The codes are meant to provide a comprehensive simulation package for ITER and DEMO plasma that is benchmarked on present experiments. The work of the TF requires a centralized source of AMNS data. Version control is mandatory (it must be possible to recover previously used data even if they are superseded) and the provenance of the data is an integral part of the database.

The standardization efforts by the ITM Task Force concern the code interface rather than the database itself; the codes will work with different database formats so long as the required code interface is provided. The ITM Task Force insists that all use of AMNS data by ITM-TF codes be done through the standard interface. The interface is still evolving, but the basic paradigm has been developed and implemented in Fortran with C bindings; a Python interface is due next and there is also interest in C++, Matlab and Java. Data are viewed as Consistent Physical Objects (CPOs) and each CPO is described by an XML Schema. Some examples of the Schema and the interface are shown in the presentation. Note that this ITM-TF standardization effort is quite different than familiar database standard formats for A+M data such as ALADDIN, ADAS and XSAMS.

The ITM Task Force emphasises the importance of data that have been given a stamp of approval by an expert. However, at this time the TF does not itself manage a programme of evaluation of AMNS data. Data selection is driven by the requirements of the models, which may imply the need for fully differential cross sections resolved with respect to excited states. The Task Force works with data consumers (code users), code authors, data providers (A+M+PMI researchers) and database developers. The work is not always well synchronized and it is in any case under stress; there is a quite limited group of expert data providers. The ITM TF would really need some full time experts in the A+M+PMI area rather than experts on 20% time

.

With respect to data evaluation activities, having an IAEA recommended data set will make the ITM-AMNS job of selecting data easier. It will help if the IAEA data is in a standard format including information on the provenance of the data. Decisions on how the data are categorized and stored in the IAEA database may affect the organization within ITM.

Steve Lisgo: ITER A/M/PMI data requirements and management strategy

Dr Lisgo started his presentation by emphasizing the very large size of ITER and the long time scale in design and construction. The divertor is the key area for A+M+PMI data. The ITER Baseline has a mixed tungsten and carbon fibre composite (W/CFC) divertor, but at present the option to start immediately with a full-W divertor is favoured. The main wall is made of beryllium. For tungsten the main concern is plasma contamination and for beryllium it is erosion and wall lifetime and also tritium retention. A complicating concern is material migration from the main wall to the divertor, leading to a W/Be mix in the divertor. In order to limit the production of tungsten impurities it is essential to operate in detached plasma mode with about 75% of the power that enters the divertor being converted to radiation. This heat flux mitigation requires active, controlled impurity seeding. The radiating agent can be C in the baseline scenario or N, Ne or Ar for the all-tungsten divertor.

Detailed plasma modelling including A+M+PMI physics is carried out with use of the SOLPS code and the ERO code primarily. In addition to the basic atomic physics data (rate coefficients for ionization, recombination and radiated energy loss) the A+M data needs for ITER include collisional radiative data for hydrogen molecules, photo-ionization and photo-dissociation rates, radiation transport data for hydrogen and also in connection with massive gas injection for disruption mitigation, data for helium molecules (He_2^+, HeH^+) and data for beryllium hydride.

ITER will have an extensive system of diagnostics. For A+M+PMI processes in the divertor the most important diagnostic system is the two-dimensional visible spectroscopy system that is intended to measure the basic plasma parameters (n_e, T_e, T_i, $v_{//}$), plasma recycling flux, impurity concentrations in the divertor and (via source spectroscopy) the impurity influx from the wall. In addition a divertor VUV spectroscopy system is being developed for tungsten measurements. For A+M processes in the main plasma there will be a dedicated main chamber spectroscopy system and a charge exchange recombination spectroscopy (CXRS) system that relies on a 100 keV diagnostic neutral beam. There are many A+M+PMI challenges still for ITER diagnostics especially for the plasma boundary region and the neutral beam effects.

The ITER A+M+PMI management strategy is under development and it involves primarily Integrated Modelling (IM) and Computer Services (CODAC). The primary IM tool is the "ITER Integrated Modelling Analysis Suite", or IMAS. The data model for IMAS (under development) is a universal API that sits above all of the ITER data served by CODAC. It represents a single point of entry; all data must be supplied through this API. Data tracking (origins, version, etc.) will be part of the Data Model, i.e., it will be self-documenting. The atomic, molecular and plasma-material interaction data used by ITER must all belong to this data model. It appears that the EU-ITM CPO structure (described by D. Coster at this meeting) may be a good starting point for defining the details of the data model. At the present time the discussions are still at the conceptual level.

Jung-Sik Yoon: Data compilation and evaluation at National Fusion Research Institute (NFRI)

Dr Yoon described the work on atomic, molecular and plasma-material interaction data in the Data Center for Plasma Properties (DCPP) at NFRI. The Center has 14 staff at present: a theory group that is concerned with A+M+PMI data and plasma simulation and an experimental group for cross section measurements. The Center maintains international collaborations through the Asia-Pacific Atomic Data Network (APAN).

At first the DCPP concentrated on producing a database from published literature. Atomic and molecular data from a large collection of articles were scanned and digitized and assembled into a database at the Korea Institute of Science and Technology Information (KISTI). This database was oriented towards processes in industrial plasma and the database is in the Korean language. The A+M data in the database are freely accessible and in addition simulation tools are offered that require a login.

Subsequently the DCPP expanded to carry out cross section measurements in collaboration with Chungnam National University in Daejeon and also with Australian National University. The Asia-Pacific Atomic data Network was created to foster collaboration on the measurement and calculation of atomic data relevant to discharge and plasma physics, materials science and biomedical science. APAN aims also to coordinate compilation and evaluation of data and to provide a link between producers and users of A+M data.

At present the DCPP also has an extensive programme in data evaluation, concerned with data for reactions in plasma processing and also reactions in the near-wall plasma in fusion devices.

David Schultz: Experience with data compilation and evaluation at the Controlled Fusion Atomic Data Centre (CFADC)

Dr Schultz discussed the history of the CFADC at Oak Ridge National Laboratory and the evolution of A+M data evaluation activities there and elsewhere. The CFADC was founded in 1959 by C. F. (Barney) Barnett with the mission to “identify, compile, evaluate, and recommend data on atomic and molecular collision processes which are important in fusion energy research”. This work included the publication and maintenance of an annotated and classified bibliographical database of literature that provides A+M data and the creation of the series of “Redbook” volumes of evaluated data. From the founding of the CFADC through the early 1990s the work took place in an environment of strong interaction between fusion energy research and atomic and molecular physics: atomic data for fusion benefited from a fundamental interest in collisions and spectroscopy and atomic physics was inspired by data from fusion plasma experiments.

The traditional data evaluation process at CFADC and elsewhere often began with compilation of an annotated bibliography. Relevant articles were reproduced, data extracted via scanning and digitizing of graphs, and a group of experts evaluated the available data and with the aid of scaling laws, semi-empirical formulae, known asymptotic behaviours, etc., deduced a recommendation synthesizing the results. This paradigm changed from about the mid-1990s on with the need for much larger, more finely resolved data (state resolved data and associated elastic and transport cross sections) that are much more than before based on calculations (e.g. the ADAS work) and are less amenable to traditional evaluation efforts. An example from the 1990s is the CFADC elastic scattering database for hydrogen and helium that was incorporated into the IAEA “Greenbook” (APID) volume 8 (1998) and that contains some 250 integral and 3000 differential cross sections. A more recent example of the need for very detailed state resolved data is the interpretation of charge exchange recombination spectroscopy (CHERS) data which needs complex density matrix values for hydrogen excitation by various collision processes.

The change in data needs from broad experimental data to finely resolved calculated data is one factor that affects the work at data centres. Another factor is the changing landscape in atomic, molecular and optical physics where production of collisional and spectroscopic data, with collateral benefit for applications, is not viewed with much interest. It is not possible at this time, in many countries anyway, for fusion energy science to rely on the natural interests of AMO scientists for the production of needed new data, let alone the critical evaluation of existing data. The greatest impact will most likely come from closely integrated efforts by fusion energy researchers and atomic physics experts.

Gordon Drake: Policies on uncertainty estimates for theoretical data and their implementation

Dr Drake described the experience with a recent new editorial policy at Physical Review A concerning uncertainty estimates for theoretical papers. The editors recognize that extensive tabulations of data may be very useful to plasma physicists and astrophysicists, but they insist that a critical assessment of uncertainties be provided in order for such an article to meet the acceptance criterion of providing new physics. This is laid out in an editorial on uncertainty estimates that appeared in 2011 [1]. In general papers presenting the results of theoretical calculations are expected to include uncertainty estimates whenever practicable, and especially if (a) the authors claim high accuracy, or improvements on the accuracy of previous work; (b) the primary motivation for the paper is to make comparisons with present or future high precision experimental measurements; or (c) the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

In the implementation of this policy manuscripts may be returned to the authors prior to review with a request to add an assessment of uncertainties; this happens frequently and the response by the authors has been very positive. Dr Drake notes that the policy has influenced standard software packages (GRASP, Desclaux code, RMBPT, CI etc.) to retain information needed for uncertainty estimates. As an illustration of careful uncertainty estimates in a theoretical article the publication [2] was highlighted and several others were listed in the talk. (It should be noted that these articles are almost all in the area of electronic structure. Some more effort is needed to achieve the same standard for calculations of scattering processes.)

[1] Editorial: Uncertainty Estimates. http://pra.aps.org/pdf/PRA/v83/i4/e040001

[2] M. S. Safronova and U. I. Safronova, “Blackbody radiation shift, multipole polarizabilities, oscillator strengths, lifetimes, hyperfine constants, and excitation energies in Ca^{+}”. http://dx.doi.org/10.1103/PhysRevA.83.012503

Joachim Roth: Plasma-wall interaction data base and associated uncertainties

Dr Roth described the status of the database for physical sputtering and chemical erosion and procedures for evaluation of uncertainties. The processes and methods of calculation were briefly reviewed. Physical sputtering is the ejection of surface atoms by incident energetic ions or atoms, either directly or via a collision cascade. Due to the surface binding energy there is a threshold energy for the incident particle, which can be hydrogen or an impurity ion in fusion applications. Chemical erosion results from the formation and release of volatile molecules, e.g. hydrocarbons, in the interaction of incident plasma particles and target atoms. Chemical erosion strongly depends on the surface temperature and does not have threshold energy.

Physical sputtering is primarily modeled using the binary collision approximation (BCA); the SDTrim.SP Monte Carlo code is widely used. This code follows a collision cascade, including secondary energetic particles. Projectiles and recoil particles lose energy in elastic collisions with nuclei and in collisions with electrons. The behaviour is rather well understood. Heavy ion projectiles create a large collision cascade with isotropic velocity distribution whereas light ion projectiles undergo few nuclear collisions and mainly slow down by electron collisions. Dr Roth showed the development of a universal fitting formula with just a few free parameters that provides an adequate fit to calculated data over a wide range of projectile energies. However, there is much larger scatter (factor of 2 or more) in experimental data and this needs to be understood in order to assess the accuracy of calculated data.

Possible reasons for scatter in experimental data for physical sputtering include experimental limitations and surface conditions. The experimental limitations are most severe for hydrogen due to its low sputter yield. The sputter yield is measured via target weight loss and experiments may have to run in a stable way for several days in order to be able to measure the yield with accuracy of about 15%. The problem of surface condition is more severe; for example, it is found that an oxide layer on a Fe surface reduces the sputter yield for H by more than a factor 10. Therefore one needs excellent vacuum conditions in order to measure sputter yields for clean surfaces, and one needs to characterize the surface condition in order to obtain relevant sputter yields depending upon the surface treatment. Besides oxidation also surface roughness is relevant and morphology can account for a factor of 2-3 reduction in sputter yield.

Chemical erosion is much more difficult to simulate than physical erosion as the BCA approximation is not applicable and MD has not, in general, provided adequate simulations. However, detailed experiments have clarified all steps of the underlying processes and this is incorporated in an analytical formula. The scatter about the best fit is large and there are several factors that are not well represented including the effect of surface temperature and that of bulk impurities.

Similar limitations exist for the data base on hydrogen retention in different first wall materials. Surface oxide layers may act as diffusion barriers influencing hydrogen retention and details of the crystalline structure of the material also change the retention behavior. Interpretation of excessive data scattering and reliable extrapolation to realistic surface conditions in fusion devices require very detailed parameter studies and data analysis.

Jong-Oh Choi: General procedures for data evaluation

In a brief second presentation Dr Choi reviewed in more detail the steps laid out in the Guide to the expression of uncertainty in measurement (GUM) for quantifying uncertainty. The steps are summarized in Section 8 of GUM essentially as follows.

1. Express mathematically the relationship between the measurand Y and the input quantities X_i on which Y depends: $Y = f(X_1, X_2, ..., X_N)$. The function f should contain every quantity, including all corrections and correction factors, that can contribute a significant component of uncertainty to the result of the measurement.
2. Determine x_i, the estimated value of input quantity X_i, either on the basis of the statistical analysis of series of observations or by other means.
3. Evaluate the standard uncertainty $u(x_i)$ of each input estimate x_i. For an input estimate obtained from the statistical analysis of series of observations, the standard uncertainty is evaluated as described for Type A evaluation of standard uncertainty. For an input estimate obtained by other means, the standard uncertainty is evaluated as described for Type B evaluation of standard uncertainty.
4. Evaluate the covariances associated with any input estimates that are correlated.
5. Calculate the result of the measurement, that is, the estimate y of the measurand Y, from the functional relationship f using for the input quantities X_i the estimates x_i obtained in step 2.
6. Determine the combined standard uncertainty $u_c(y)$ of the measurement result y from the standard uncertainties and covariances associated with the input estimates. If the measurement determines simultaneously more than one output quantity, calculate their covariances.
7. If it is necessary to give an expanded uncertainty U, whose purpose is to provide an interval $y - U$ to $y + U$ that may be expected to encompass a large fraction of the distribution of values that could reasonably be attributed to the measurand Y, multiply the combined standard uncertainty $u_c(y)$ by a coverage factor k, typically in the range 2 to 3, to obtain $U = ku_c(y)$. Select k on the basis of the level of confidence required of the interval.
8. Report the result of the measurement y together with its combined standard uncertainty $u_c(y)$ or expanded uncertainty U. Describe how y and $u_c(y)$ or U were obtained.

3. Discussion and Conclusions

The discussions covered two broad topics: a review of methods for assigning uncertainties to calculated data and a set of procedural recommendations to coordinate the development of a standard library.

Following the presentation by Dr Drake and due to the high accuracy of experimental spectroscopic data it appears that methods for assigning uncertainties to atomic structure calculations are in good shape. It is more challenging to obtain good estimates for accuracy of electron-atom scattering calculations and it requires expert understanding of the codes. For example, for R-matrix calculations the convergence behaviour as function of basis size can be oscillatory and depend on resonances; one cannot simply increase the basis size and derive an error estimate that way. In addition one needs to understand how the uncertainty in the atomic structure part or the neglect of certain terms, e.g. relativistic corrections, propagates to the scattering cross section. Comparison between R-matrix calculations and distorted wave (DW) calculations isn't very helpful for error estimates because these methods have different regions of validity (high energy for DW, lower energy for RM).

It would be valuable to locate some model papers that contain careful electron scattering calculations together with a credible estimate. Maybe there exists such work for a simple system such as e^- + He or e^- + H_2, but we are not sure of it.

For electron-atom collisions there are several widely distributed codes, including FAC and HULLAC, but this community doesn't have such widely shared codes for heavy particle collisions. The main problem with molecular collision experiments is to know the excitation state of incoming and outgoing molecules. The fully differential "COLTRIMS" reaction microscope measurements at storage rings provide the best experimental benchmarks.

Particle surface interaction data are more difficult yet due to anomalies such as oxide layers, surface morphology and redeposited surface layers. For sputtering the work-horse are the BCA calculations and these have uncertainties even within their simple model due to the choice of surface potential and pairwise interaction potential. One might wish to view MD as a tool to provide a benchmark for BCA, but the molecular dynamics calculations don't have that quality at present. Like BCA the MD calculations suffer from unknown defects due to possible poor quality of the interaction potential and neglect of quantum effects. Therefore, for calculations of sputtering and reflection the benchmark has to be experiment, and one has to overcome the problems of characterizing the precise state of the surface and the bulk. It is noted that plasma-material interaction is a huge issue; the erosion lifetime and the tritium retention properties of the ITER main wall are really not adequately understood today.

The discussion moved to policy or procedural recommendations and one important item of advice is for the Unit to discover and document precisely which data sets are used throughout the fusion modelling community. In connection with the work of the ITM-TF Dr Coster developed a questionnaire for the key participants about their use of AMNS data and this looks like a good starting point for a more detailed and more widely distributed questionnaire by the Unit. It should ask for precise datasets that are used for all the important A+M+PMI processes. Some names were collected of plasma modellers and authors of widely used modelling codes and the Unit will pursue this questionnaire.

Another policy issue for the Unit is the organization of future code comparison workshops similar to the successful series of non-local LTE workshops (most recently NLTE-7 in Vienna) and a first spectral lineshapes in plasmas (SLSP) code comparison workshop. A code comparison workshop on problems in particle surface interaction could be valuable; one would choose a few precisely defined problems and have contributions from various BCA, MD and other codes. The Code Centre Network should also consider a code comparison exercise for heavy particle collisions or electron-molecule collisions.

Appendix 1

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Appendix 2

Agenda

Wednesday 20 June 2012 Room: B0482

09:30 – 09:50	**Robin Forrest, Bas Braams**: Welcome, introductions, review of meeting objectives, adoption of the agenda
09:50 – 10:30	**Hyun-Kyung Chung**: IAEA Data Centre Network activities on data evaluation for fusion applications
10:30 – 12:30	**Jong-Oh Choi**: Measurement and uncertainty
12:30 – 14:00	*Lunch*
14:00 – 14:50	**David Coster**: Using AMNS data within an Integrated Tokamak Modelling environment.
14:50 – 15:40	**Steve Lisgo**: ITER A/M/PMI data requirements and management strategy
15:40 – 16:30	**Jung-Sik Yoon**: Data compilation and evaluation at National Fusion Research Institute (NFRI)
16:30 – 17:20	**David Schultz**: Experience with data compilation and evaluation at the Controlled Fusion Atomic Data Centre (CFADC)
19:00 –	*Social dinner*

Thursday 21 June 2012 Room: B0482

09:00 – 09:50	**Gordon Drake**: Policies on uncertainty estimates for theoretical data and their implementation
09:50 – 10:40	**Joachim Roth**: Plasma-wall interaction data base and associated uncertainties
10:40 – 12:00	Discussion: Uncertainty estimation in practice for A+M+PMI data
12:00 – 13:30	*Lunch*
13:30 – 14:30	**Jong-Oh Choi**: General procedures for data evaluation
14:30 – 15:30	Discussion: Management of compiled data, evaluated data, recommended data
15:30 – 17:00	Discussion: Data evaluation for A+M+PMI processes

Friday 22 June 2012 Room: B0482

09:00 – 10:00	**Gordon Drake, David Schultz and All**: Publication policies and issues for uncertainty estimation and data evaluation
10:00 – 12:00	**All**: Meetings, workshops, data centre network, code centre network and other activities to support data evaluation and establish an evaluators network
12:00 – 13:30	*Lunch*
13:30 – 16:00	Review of roadmap; draft of documents for the TM in September
16:00	*Close of meeting*

Revised Roadmap

Phase 0: Inventorise the AM/PSI Data Collection used by Fusion/Plasma Community

● Priority list of critical data needs and data sets currently used by data users

- There are a variety of A&M/PSI data sets required for fusion applications.
- A users' network of intensity data applications should be established to provide and update the priority list of critical data needs for fusion applications.
    - Draft of the present data sets used by data user community
    - Absolute grand canonical list of presently used data sets
    - What is the most critical and urgent need?
    - Reiter, Coster, Jet, Zagorski?, Borodin, 10 (Europe) 5 (US), 5(Far east)—30 people
    - What is the A+M/PSI data set used for fusion applications.
    - World Draft AM/PSI Data Collection
        - Questionnaires (ITM)
        - Working group formation
        - Reconcile, remediate and upgrade/expand/complete data library
    - Standard Data Format: Easy Data Access

Phase 1: Establishment of infrastructure for evaluated data library

● IAEA Atomic and Molecular Unit: Development of database to host the standard data library

- It is understood that the IAEA A+M data unit will host two databases: 1) the internationally agreed standard (recommended) data library and 2) the evaluated data library.
- The standard data library is the final goal which gives a single recommended data set as the best data of the given process at the time of determination.
- The evaluated data library is the intermediate database where evaluated data sets are collected before standardization (recommendation) and there may be more than one evaluated data set for the given process. The version of data sets can be traced through the evaluated data library.
    - Evaluated data is a data set reviewed and having uncertainties assigned by an expert.
    - There may be another class of datasets, which was previously recommended.
    - The establishment of the evaluated library may involve interactions with providers of data sets
- The data format and the maintenance of databases should be determined as the first step.
    - XSAMS-Lite may be useful for output tools/export tools
    - Full XSAMS should be used for data description
    - The description of PMI/PSI data needs further work
- The unit should make efforts to emphasize the importance of data evaluation activities to the member states for more support at the government level.

● Data Centers: Compilation of relevant data for evaluation

- It was suggested that there should be a unified database available for evaluators. Prominent sources of A+M data include NIFS, Open ADAS(Open), NFRI and VAMDC. For PMI data the PWI group at IPP Garching has been the principal source.

- A meeting should be organized to discuss the location of the database, the coordination of data collection, the decision of data format for this data storage.
    - Theoretical data needs to include code descriptions

● Data Centers and Evaluators: Establishment of data evaluators' network

- Data evaluator's network should be established to coordinate effectively evaluation activities in the community level.
- The network will train younger generation and facilitate the knowledge transfer from seasoned evaluators.
    - Collisional-radiative model descriptions
    - Processed data description (documents?)
    - If there is only one set, how would you evaluate it? – guidelines needed (threshold behaviors, asymptotic behaviors, simpler model comparison, semi-empirical fit comparison…)

● Data Evaluators: Guidelines of evaluation methods

- Evaluation methods should be agreed among data evaluators and standardized.
- Meetings should be organized for evaluators to discuss the guidelines of evaluation methods for each category of processes.

● Data Producers: Guidelines of uncertainty estimates

- There is a need of internationally agreed standards for theoretical data uncertainties.
- Meetings should be organized to draw a consensus among data producers and to find the methods to determine the uncertainties.
- Excessive scattering in experimental data needs to be interpreted in view of hidden parameters influencing individual data values

Phase 2: Establishment of evaluated data library

● IAEA: Establishment / maintenance of databases to host the evaluated data library

- IAEA will host the database to contain the evaluated data sets in coordination with data centers and evaluators.
- IAEA will organize meetings for evaluation activities

● Data Centers: Coordination of data evaluators' network activities

- The designated committee of the network will work with evaluators to assign an evaluation task to the corresponding expert.
- The committee will collect evaluated data sets in the evaluation data library and will publish the volume of evaluated data sets.

● Data Evaluators: Evaluation of data sets

- Designated evaluators will evaluate data sets and maintain/improve the guidelines of evaluation methods
- Evaluators will review the previously evaluated data sets on regular basis

● Data Producers: Guidelines of scaling laws / fit expressions

- Evaluated data sets need to be extended to ranges where no data sets are available.
- Data producers, especially of theoretical data will be able to provide the scaling laws or physically consistent fit expressions.

● Data Users: Development of data format compatible to applications

- Evaluated data sets will be used for modeling and the common data format will make it easier to transfer data sets from the evaluated library to the modeling code.

Phase 3: Establishment and maintenance of standard data library

● IAEA: Establishment / maintenance of databases to host the standard data library

- IAEA will host the database to contain the standard data sets in coordination with data centers and evaluators.
- IAEA will organize meetings for evaluation activities

● Data Evaluators and Data Centers: Coordination of Technical Committees

- Data centers and evaluators will work together to form technical committees to recommend the evaluated data as the internationally agreed standard data.

● Data Producers: Feedback on data sets (production of missing data, data improvement)

- The standard data library will provide an overview of the quality of the data required for fusion and data producers may provide a feedback on data sets.

● Data Users: Feedback on data sets

- Data users will update the data lists required for plasma applications and may give the feedback about the quality of the standard data sets after applications to modeling work

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