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International Code Centres Network

Summary Report of the Technical Meeting

IAEA Headquarters, Vienna, Austria

27–28 September 2010

Prepared by

H.-K. Chung

International Atomic Energy Agency, Vienna, Austria

January 2011

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Abstract

Fifteen international experts on computational aspects of atomic, molecular and particle surface interaction data for fusion energy research participated in the 2nd technical meeting of the International Code Centres Network. Participants reported on the research on data production and computational tools at their institutions. Experts in the field of plasma modeling of magnetic fusion research joined this meeting to present the data needs and to bring the perspective of data users. The interaction and discussion among data producers and data users in this two-day meeting led to an agreement that the scope and function of Code Centres Network should be reformulated to serve the needs of fusion community in a more effective way.

January 2011

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1. Introduction

The 2nd Technical Meeting to discuss the activities of an “International Code Centres Network” was held on 27-28 September 2010 at IAEA Headquarters, Vienna and was joined by all the attendees of the 1st meeting except for D. Stotler (PPPL). Participants reviewed research activities and computational tools for atomic, molecular and particle surface interaction (AM/PSI) data relevant to the fusion research community. As suggested in the previous meeting, new participants were invited to the network: M. Klapisch of HULLAC atomic physics codes and R. Schneider of SDTrimSP plasma-surface interaction physics code. Participants of the meeting on “Data Needs for Plasma Modeling” held on 29-30 September 2010 were invited to this meeting to present their work on plasma modeling in magnetic fusion research and to offer a perspective on data needs from users of AM/PSI data. (See Appendix 1 for the list of participants.)

After the presentations participants discussed current data needs for the fusion research and the future direction of the International Code Centres Network (CCN). The interaction between data users and data producers was found extremely useful on both sides as data users had a chance to obtain information on both the computational capabilities and limits of available data and data producers to obtain information on the current needs directly from data users. Data users expressed the importance of evaluated and recommended data sets in the modeling. They also noted the lack of information on the uncertainties of available data and hence the concerns over unevaluated data sets generated by inexperienced users of online codes. Other methods to distribute numerical data sets were discussed and finally the scope of the CCN was suggested to be reformulated to enhance the collaboration between data producers and data users as well as among the data producers themselves.

2. Presentations and Proceedings

R. Forrest as Section Head of the Nuclear Data Section welcomed the participants on behalf of the IAEA. He acknowledged that the Code Centre Network (CCN) is rather new, but that it could become one of the key activities of the Unit. He emphasized the important role of code development in assisting fusion energy research by complementing the database development and wished participants a productive meeting. B.J. Braams as Unit Head of the Atomic and Molecular Data Unit reviewed the proposed agenda, which was accepted without change (see Appendix 2 for the agenda).

During the first day-and-a-half participants gave summary presentations of relevant research within their institutes (see Appendix 3) and specific code centre activities such as online computing and code or data sharing activities. Discussions then took place on the progress of recommendations and resolutions of the last meeting and the future functions of the CCN.

D. Coster of the Max-Planck-Institut für Plasmaphysik reviewed the activities of the ITM-TF (Integrated Tokamak Modeling Task Force) and the use of atomic, molecular, nuclear and surface/solids data in European codes. Requirements, challenges and immediate needs in the data used for the modeling were described. Data should be robust, comprehensive, easy to use, efficient and able to address special needs. Version control, expert validation, standardized input and output are important for data modules used in the integrated tokamak modeling. A list was provided for missing or not verified data sets and immediate needs. Isotope-resolved atomic and plasma-surface interaction data and differential cross sections are among the immediate needs. Current activities to incorporate atomic, molecular and plasma-surface interaction data sets in the ITM database were described.

D. Elder of the University of Toronto, Canada, reviewed the OEDGE suite of plasma modeling codes relevant to fusion research. The OEDGE suite used for modeling the behavior of the edge plasma of magnetic fusion devices is composed of several elements: an Onion Skin Model (OSM), the EIRENE Monte Carlo code and the DIVIMP Monte Carlo plasma impurity code. Results of simulations are compared to spectral measurements, plasma condition measurements by Thomson scattering and probes and other diagnostics. OEDGE uses a broad range of atomic, molecular and surface data at a relatively processed level. Dr. Elder described the data requirements for these codes: ionization and

recombination rate data for hydrogen as well as all charge states of the impurity species, rate data for hydrogen molecules and the line emission data for both hydrogen and impurity species. Surface sputtering data for both impurity species as well as hydrocarbon molecules are required (see Appendix 3 for more details).

R. Schneider of Ernst-Moritz-Arndt University Greifswald, Germany, reviewed the tools and strategies for the description of plasma-wall interaction. The complex and varied nature of the physics requires a combination of methods and the real structure of the material is important. Molecular dynamic simulations and simpler models can complement each other and more fundamental understanding of model systems are needed for validation. Dr. Schneider described several versions of the code TRIM, which calculates the sputtering of a surface exposed to a flux of energetic ions. The TRIM code calculates the sputtering yield of a projectile of an ion of a volatile (recycling) element similar to experimental results. If the projectile is a solid-state (non-recycling) ion then the dynamic change of surface by projectile implantation is important and it can be treated with 1D-TRIM (TRIDYN, later SDTrimSP). As the surface roughness may increase the sputtering yield by as much as a factor of 5, the calculation is extended to 2D and 3D grids in lateral dimensions for rough surface problems. An example of a Si pitch grating exposed to 6 keV Ar ions shows that the SDTrimSP-2D code predicts the results with a good accuracy. Another extension includes the chemical sputtering and the code reproduces experimental observation such as a hydrocarbon surface bombarded with neon and in parallel exposed to thermal hydrogen influx. (See Appendix 3 for more details.)

J. Abdallah of Los Alamos National Laboratory (LANL), USA, reviewed the recent activity in his institute. The LANL contribution to the IAEA Atomic and Molecular Data Code Centre is the online version of atomic physics codes. These codes are accessed remotely by users to perform atomic structure calculations, including excitation and ionization cross sections, for arbitrary ions and configurations. A brief description of the online capabilities was presented. A short summary of the ATOMIC plasma modeling code was also provided. Recent improvements to the CATS code were discussed, in particular, the recently developed parallel computing capability. Several examples of the use of the LANL suite of atomic physics codes to applications of interest to magnetic fusion were discussed including recent boron power loss calculations and preliminary results for modeling low temperature tungsten plasmas.

F. Koike of Kitasato University and NIFS, Japan, reported the activities in the study of atomic structure and dynamics calculations using the GRASP (General purpose Atomic Structure Program) family of codes and related activities at NIFS. The projects include analysis of visible M1 lines in Tungsten ions, collisional-radiative model for W ions, a code development for single electron capture by H nucleus from metal surface, and studies of $K\alpha$ radiation from low charge chlorine heated by an ion beam for plasma diagnostics. (See Appendix 3 for more details.)

L. Vainstein of the Lebedev Physical Institute, Moscow, Russia, described his work on calculations of ionization cross sections for W I and W II and reviewed the codes ATOM and MZ for atomic calculations. There are good experimental data for W II single and double ionization and no direct cross section measurements for W I. Therefore the calculations started with the ionization of W II and the results were tested by comparison with experimental data hoping that accuracy for neutral W would be similar. The cross sections are calculated by the code ATOM in Coulomb-Born approximation (CB) with exchange and correction for the normalization by the reduced K-matrix approximation. For highly charged ions calculations, the code MZ is used. It relies on a $1/Z$ expansion method and computes energies, wave lengths, spontaneous emission rates and photo-ionization cross sections and autoionization rates.

M. Klapisch of ARTEP Inc. (USA) and Institute for Particle Physics, ETH, Switzerland, reported on the activities of HULLAC code suite. The first version of HULLAC (Hebrew University Lawrence Livermore Atomic Code) dates back to the 1980's when Dr. Klapisch was at the Hebrew University, Jerusalem, Israel, and received support of LLNL. The concept is to generate a consistent atomic model by using the same wave functions for computing all atomic processes relevant to plasma spectroscopy. These wave functions are obtained by solving the Dirac equation in a parametric potential. The central

field model enables a convenient decoupling of the angular momentum algebra for all processes, including electron collisions, for which the factorization-interpolation method is introduced. Recently, the whole code was re-written in a more modern way and extensively checked. It now includes a collisional radiative solver with a special scaling for improved convergence, a new fit for the cross section, the ability to use the mixed transition arrays (MUTA), and to model the effect of an external radiation field. The latter capability was used to compare with a recent experiment on the transmission of Fe at $T_e = 156$ eV, with excellent agreement. The latest version is used by several groups, whose feedback is used to constantly improve and/or correct the code. (See Appendix 3 for more details.)

I. Bray from Curtin University of Technology, Australia, reported on considerable progress in the development of the Convergent Close-Coupling (CCC) theory. The major extension has been to institute a new parallelism paradigm. This utilizes a hybrid OPENMP/MPI combination with the main V-matrix being calculated across several nodes. Within each node the original OPENMP parallelism is used. Then, using MPI, the matrix is distributed in a block cyclic form across all the available cores suitable for solving the linear equations via the ScaLAPACK suite of routines. Consequently the CCC code is now able to be run across many nodes of memory sharing multiple cores. Both the original non-relativistic CCC and the recently developed relativistic RCCC codes have been parallelized this way. Additionally, the RCCC code has been extended to quasi two-electron targets, and highly charged ions, including Breit or Møller corrections. Recent applications of the CCC method include electron impact ionization of helium and electron-impact excitation of mercury and highly charged uranium ions. Currently the CCC method is being used to calculate electron-impact excitation and ionization of the He-like Li ion.

P. Fainstein from Centro Atómico Bariloche, Comisión Nacional de Energía Atómica (CNEA), Argentina presented their most recent calculations of different processes employing the non-relativistic Continuum Distorted Wave - Eikonal Initial State (CDW-EIS) approximation at intermediate and high energies. These include single and multiple ionization of atoms by ion impact including post collisional processes, and single ionization and electron capture in collisions between ions and molecules of biological interest. The calculations employ the independent electron model, initial and final states which verify the correct asymptotic conditions for Coulomb potentials and the straight-line version of the impact parameter approximation which is valid at high impact energies. Recent calculations for single and double ionization of He with a new version of the Exponential Model, modified to treat collisions with highly charged ions, were presented.

D. Reiter of Forschungszentrum Jülich GmbH, Institut für Plasmaphysik (IPP), Germany, presented plasma code activities mainly focused on the outer layers (edge plasma) of magnetically confined fusion plasmas. The suite of codes ranges from dedicated local erosion-redeposition transport codes (ERO) or drift fluid turbulence codes (ATTEMPT), up to integrated edge codes such as B2-EIRENE (operated and maintained jointly with ITER-IO, Cadarache), EMC3-EIRENE (jointly with IPP Greifswald, mainly for stellarators, LHD, W7X), OSM-EIRENE (with ITER) and EDGE2D-EIRENE (at JET). The atomic, molecular and surface data are integrated into these models mostly via the kinetic Monte Carlo code module EIRENE. Most of the integrated edge modeling activities at FZ Jülich are under ITER contracts; this includes EIRENE stand alone (first wall fluxes, diagnostic mirrors), EMC3-EIRENE (3D rmp effects) and B2-EIRENE (2D code benchmarks internally within SOLPS family). EIRENE resorts to a combination of external databases for which interfaces to EIRENE exist, internal (default) atomic data and collisional radiative codes integrated into the EIRENE source. The web based database and toolbox HYDKIN (www.hydkin.de) serves to publicly expose the A&M data used by EIRENE obtained from earlier IAEA CRP's, or as a non-LTE collisional radiative code. It is also used for sensitivity analysis via analytical solutions of linearized equations for sensitivity parameters. With respect to surface data EIRENE resorts to a kinetic reflection database (under www.eirene.de) based on TRIM code calculations. Distinct from other surface databases the EIRENE database format choice was driven by the need to preserve full information regarding all angular dependencies as well as energy spectra, as needed by kinetic plasma models (e.g., Monte Carlo), rather than only averaged quantities. (See Appendix 3 for more details.)

I. Rabadan of Universidad Autonoma de Madrid, Spain, presented a summary of the methodologies assembled there to treat ion-atom and ion-molecule collisions. Some of these methodologies can deal with systems having more than two active electrons, which is particularly important for the intermediate range of collisional energies (around 1 keV/u). At the same time, they developed methods to treat complex systems (many electrons) using one-electron wavefunctions and/or classical mechanics. A chart of codes with a brief summary of their capabilities was presented, alongside a few examples showing recent results on isotope effects in beryllium collisions with hydrogen and collisions with molecules like CH₄. The possibility of other users accessing the codes was discussed.

A. Dubois of Laboratoire de Chimie Physique Universite Pierre et Marie Curie (Paris VI), France, presented theoretical models used to evaluate cross sections of various electronic processes occurring in ion-atom and ion-molecule collisions. Lattice representation calculations are illustrated by the presentation of results for ionizing ion-molecule collisions. For atomic targets results were shown of double capture to autoionizing states cross sections computed by spectral methods. Finally, the work on the implementation of the codes at the IAEA web site was described.

M. Capitelli of Universita di Bari, Italy, reviewed the activity in the Plasma Chemistry group in Bari focused on state-to-state kinetic modeling of systems of interest for technological applications ranging from fusion (negative ion sources) to aerospace. Tools for the investigations on the dynamics of elementary processes were described in detail. For the simulation of plasm-chemical systems two existing codes have been coupled: the collisional-radiative model for an atomic hydrogen plasma under shock-wave condition, and the code for calculation of synthetic hydrogen spectrum, deriving plasma optical properties. The effect of non-equilibrium internal distribution on the spectrum is investigated for different positions of the shock. Thermodynamics and transport of plasmas have been studied. In particular, thermodynamic properties have been calculated in the frame of a novel approach that reduces complex systems of levels to an equivalent system of two or three levels by means of grouping. The quantum problem of levels for hydrogen atom confined in a spherical box has been investigated in the frame of solution of divergence of the internal partition function. Modules for transport coefficients calculations have been implemented including the effects of different choices of cut-off criterion and of electronically excited states in the mixture. (See Appendix 3 for more details.)

Yu. Ralchenko of the Atomic Spectroscopy Group, National Institute of Standards and Technology, USA, presented a set of atomic structure and plasma kinetics codes that are being developed or hosted at NIST. The most advanced methods in atomic structure theory are implemented in non-relativistic Multiconfiguration Hartree-Fock (MCHF) and relativistic Multiconfiguration Dirac-Fock (MCDF) codes. Both these packages as well as some simpler codes are available for free download from the NIST web site. The NIST Atomic Spectroscopy Group also develops sophisticated collisional-radiative models for calculation of plasma population kinetics and emission characteristics. The NOMAD code is used for calculation of spectral patterns in EBIT experiments with highly-charged ions of tungsten and other heavy elements. This detailed code is also used for simulations on neutral beam spectroscopy in fusion machines, e.g., charge exchange recombination spectroscopy and motional Stark effect. Another advanced collisional-radiative code, FLYCHK, developed by LLNL researchers and available for online calculations on the NIST site is used by hundreds of researchers, including specialists in fusion plasmas, for calculations of ionization distribution, radiative power losses and other important parameters. (See Appendix 3 for more details.)

H. Chung of the International Atomic Energy Agency reviewed databases and online capabilities hosted by the IAEA Atomic and Molecular data unit. The unit hosts ALADDIN, a numerical database of collisional data of atomic and molecular processes and plasma-surface interaction data, AMBDAS, a bibliographical database and GENIE, an online search engine of 9 spectroscopic databases and 6 collisional databases worldwide. The unit has simple online codes to calculate heavy particle collisional data, electron impact cross sections and collisional-radiative charge state distribution and radiated power in a steady state plasma. More recently, comprehensive atomic data for argon, chlorine and silicon calculated by the group at Los Alamos National Laboratory (LANL) and charge distributions calculated by FLYCHK codes have been made available in addition to access to the LANL Atomic Physics Codes and to FLYCHK at NIST.

V. Lisitsa of the Russian Research Centre “Kurchatov Institute”, Russia, described fast codes for calculations of radiative-collisional processes in collisions between electrons and many-electron ions. The codes are based on quasiclassical approximation for electron motion in atomic potentials described by statistical models of the atoms (ions). Specific calculations are presented for Bremsstrahlung and radiative recombination spectra for complex ions as well as for dielectronic recombination rates for Li-like carbon ions and the Mg^{+1} ion. Detailed comparisons with quantum calculations were presented that show quite good agreements between quasiclassical and quantum numerical data. Several advantages of quasiclassical codes were discussed. Quasiclassical codes can decrease sharply the computing time as compared with quantum calculations, resulting in the possibility of their combinations with more complex plasma modeling codes, such as EIRENE or ASTRA transport codes. The codes can be used to establish quasiclassical scaling laws for probabilities of radiative-collisional processes. The precision of quasiclassical codes is quite good for most of plasma applications such as radiation background in tokamak plasmas as well as radiative and dielectronic recombination rates. (See Appendix 3 for more details.)

3. Discussions and Recommendations

The progress in meeting recommendations from the previous meeting was reviewed after the presentations. As recommended, an IAEA webpage was created to list basic information about the current code capabilities of Code Centre Network (CCN) members with a link to individual web pages at participating institutes. It was reported that the network has provided good interaction among code developers and the visibility of the network served well in attracting students to fusion related research. Feedback from online code users to code developers and increases in collaboration opportunities were recognized as important benefits of CCN. Providers of the plasma-surface code SDTrimSP and the suite of atomic physics codes HULLAC were invited to the network as a way of expanding the network.

A recommendation for code developers to consider an xml output utilizing XSAMS (xml schema for atomic, molecular and solids, <http://www-amdis.iaea.org/xsams>) was found to be premature as XSAMS remains under active development. The recommendation that code developers should attempt to estimate the accuracy of calculations in a similar manner to that of numerical databases was found difficult to meet. This led to a considerable amount of discussion on the role and future activities of the Code Centres Network.

There were general concerns over the accuracies of data computed with online code capabilities. Codes can provide unavailable data sets to meet comprehensive modeling needs even though the accuracies of these computed data sets are unverified and generally limited. While the accuracy should be determined by the code developers, it is almost impossible to determine the accuracies of all data sets generated by the code. More often than not, code documentation is not good enough to train the code users and hence unevaluated data sets generated by inexperienced users may lead to an erroneous result when applied. In order to avoid such an adverse effect, it was suggested that either the codes should be available in collaboration with code developers to meet specific data needs of data users or only the data sets calculated by code developers with accuracy information should be available through data centres.

Participants exchanged ideas of how the CCN can contribute to the community in addition to generating new data sets. They agreed that the CCN activities should benefit the code developers as in the case of the DCN (Data Centre Network) through which data centres improve their databases by activities such as collaboration, technical help and visits. Several ideas were proposed as future activities to directly help CCN members. One proposal is to organize focused meetings where code developers in the CCN can work on a formulated physics problem together. As an example, at the series of NLTE (non-local thermodynamic equilibrium) kinetics code comparison workshops, code developers compare their results together on a pre-defined problem, identify sources of discrepancies among results, and improve their codes. Such a workshop on a focused topic will improve the accuracy of calculated data and validate the codes.

The other proposal is to develop the CCN into a structured network of data producers, data producers and experimentalists on request. Participants found the interaction with a wide range of science through the CCN useful as one finds a significant overlap among atomic, molecular and plasma-surface interaction physics. The greater visibility from the larger network with members from diverse background will be an important benefit since it will offer more collaborative opportunities and also help with recruiting young scientists.

This was the first CCN meeting to invite researchers from the plasma modeling community who extensively use atomic, molecular and plasma-surface data in their calculations. Data users had a chance to acquire clear information on the capabilities and limits of available data and the needs of a variety of consumer level codes and the understanding of what is needed by these codes. On the other hand, data producers had a chance to understand how their data sets are implemented in the applications. They found it necessary to establish a priority list of data needs so that they can focus more to produce unavailable data sets or improve the important data sets in fusion research. Data accuracies and validations were an important subject in this meeting and the information on the quality and availability of needed data sets are not easily obtainable. To meet the needs of both data users and producers it was proposed to develop a decision tree of available data sets and quality information. The proposed decision tree may provide a means to categorize available data sets and make it easier to prioritize data needs.

All participant agreed that this meeting was extremely productive and they supported the idea that the CCN should expand its activities with a balance between computational tools and scientific interaction among participants. A DAFF (DATA For Fusion) mailing list was proposed to be used as the communication method among CCN participants. Code developers were motivated to develop and update online codes regularly with the need for information about accuracy in mind. More representation of plasma surface interaction codes in the CCN was recommended.

4. Summary

This was the second meeting in the code centre network, an important meeting to discuss the future direction of the network. Data users from the plasma modeling community were invited to join the discussion with code developers and participants felt that this combined meeting was very productive. It was proposed that the network should expand to a more structured network of data users, data producers and possibly experimentalists. Data users expressed concerns over the quality of available data sets from online codes and proposed that the codes should be made available with expert help or that only the data sets generated by experts should be available online. A decision tree was proposed as a means to obtain information on available data with accuracy information. Data producers found the interaction with data users useful in terms of understanding the needs of the plasma modeling community and suggested that there should be a priority list of important data.

IAEA Technical Meeting on International Code Centres Network

27–28 September 2010, IAEA Headquarters, Vienna, Austria

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IAEA Technical Meeting on International Code Centres Network

27–28 September 2010, IAEA Headquarters, Vienna, Austria

Agenda

Monday, 27 September

Meeting Room A04-78

09:30 – 09:40 Opening, Adoption of Agenda, R. Forrest, B. Braams

Session 1: Reports I

Chairman: D. Reiter

09:40 – 10:10 D. Coster: Use of atomic, molecular, nuclear and solids data in European codes: new developments

10:10 – 10:40 D. Elder: The OEDGE code and interpretive modeling

10:40 – 11:00 *Coffee Break*

11:00 – 11:30 R. Schneider: Tools and strategies for the description of plasma-wall interaction

11:30 – 12:00 J. Abdallah: Recent developments with the Los Alamos atomic physics codes

12:00 – 12:20 F. Koike: Atomic structure and dynamics calculations using the GRASP family of codes, and an introduction of some activities in NIFS

12:20 – 12:40 L. Vainshtein: Ionization cross sections for W I and W II and the ATOM and MZ codes

12:40 – 14:00 *Lunch*

Session 2: Reports II

Chairman: J. Abdallah

14:00 – 14:30 M. Klapisch: Latest updates of HULLAC theory and applications

14:30 – 14:50 I. Bray: Recent applications of the CCC method

14:50 – 15:10 *Coffee Break*

15:10 – 15:30 P. Fainstein: Recent advances in distorted-wave calculations of ion impact single and multiple ionization of atoms and molecules

15:30 – 16:00 D. Reiter: HYDKIN: towards online hydrogen and hydride kinetics to publicly expose A+M data in particular edge modeling applications

16:00 – 16:20 I. Rabadan: Theoretical treatment of ion-atom and ion-molecule collisions

16:20 – 16:40 A. Dubois: One- and two-electron processes in multi-center collisional systems

16:40 – 17:00 M. Capitelli: State to state kinetics of molecular and atomic hydrogen plasmas

Tuesday, 28 September

Session 3: Reports III

Chairman: D. Coster

- 09:00 – 09:20 Yu. Ralchenko: NIST simulations for support of fusion research
09:20 – 09:40 V. Lisitsa: Fast codes for modeling fusion plasma radiative properties
09:40 – 10:00 H.-K. Chung: Code capabilities at IAEA
10:30 – 11:00 *Coffee Break*

Session 4: Review

Chairman: D. Coster

- 11:00 – 12:30 All: What do we wish to get out of the CCN
12:30 – 14:00 *Lunch*

Session 5: Plans and Recommendations

Chairman: Y. Ralchenko

- 14:00 – 15:30 All: Progress and plans towards goals of CCN
15:30 – 16:00 *Coffee Break*
16:00 – 17:00 All: Recommendations for IAEA
17:00 – *Adjourn*

ABSTRACTS AND SUMMARIES**The OEDGE code**

J. David Elder, University of Toronto, Canada

The OEDGE code suite is used for modeling the behavior of the edge plasma of magnetic fusion devices. The OEDGE code is composed of several elements. An Onion Skin Model (OSM) can be used to create a background plasma solution for the edge plasma. This includes solving for edge plasma density, temperature, flow velocity and electric field on a 2D grid representing the poloidal magnetic structure of the fusion device. OEDGE typically assumes toroidal symmetry. OEDGE can also load a plasma solution provided by other plasma solvers in use by the fusion modeling community. After an initial plasma solution is obtained, OEDGE runs the EIRENE Monte Carlo code to obtain the distribution and magnitude of hydrogenic source terms: ionization, recombination, power and momentum loss terms. These are then fed back to the OSM and the process is iterated until a stable plasma solution is found. OEDGE then uses the DIVIMP Monte Carlo plasma impurity code to model the impurity production, transport and deposition including such things as estimates of core impurity content, self-sputtering at surfaces and many other physics effects. The end result is a simulation of the fusion edge plasma including both hydrogenic and impurity behavior.

The input to these simulations is usually the density and temperature of the plasma at the target plates as measured by Langmuir probes. The simulation results are compared to measurements of hydrogenic and impurity spectral emissions, plasma condition measurements from Thomson scattering and reciprocating probes, neutral pressure measurements from in-vessel pressure gauges and many other diagnostics. Discrepancies between the simulation and experimental measurements are then investigated to determine whether physics not presently incorporated in the simulations could be the cause of the discrepancy. In this way, the OEDGE code is used to understand complex experiments with fusion edge plasmas and offers a tool giving insight into the physics underlying the experiments.

In terms of fundamental data used by the OEDGE code, there is a substantial body of data required by both EIRENE and DIVIMP in order to accomplish a simulation of this type. These codes require ionization and recombination rate data for hydrogen as well as the impurity species being modeled. The impurity species examined range from lithium to tungsten. These data are required for all charge states of the impurity species. Typically in DIVIMP, the code assumes a Maxwellian electron velocity distribution which then means that the code uses rate data as opposed to cross section data. The EIRENE code also uses data for hydrogen molecules as well as atoms and ions. In addition, these codes also need line emission data for both hydrogen and specific lines for each impurity species. The specific lines are those examined experimentally so they may vary from one fusion device to another depending on the diagnostic choices made. The spectral atomic data are combined with the impurity density calculated by the code to obtain a photon emission rate for each element in the simulation. These data are then combined with diagnostic geometry data loaded into the code to generate a simulated diagnostic measurement which takes into account such things as field of view of the instrument.

Finally, DIVIMP also makes use of surface sputtering data for both impurity species as well as hydrocarbon molecules. This includes both chemical and physical sputtering as well as primary (background ion) and self sputtering data. These data are used to calculate the source impurity particle distribution in the simulation. As a data consumer, OEDGE uses a broad range of atomic, molecular and surface data at a relatively processed level since the code only produces particle density estimates in the simulation and does not, at present, track the population of excited states.

As a result of the CCN meetings good information was acquired on capabilities and limitations of data available in the atomic physics community. In addition, the needs of a variety of consumer level codes were explained so the understanding of what is needed by these codes was clarified. This may result in improvement of the data currently available for fusion edge plasma modeling.

Tools and strategies for the description of plasma-wall interaction

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1. General considerations

PWI modeling has to deal with very complex and different problems such as arcs (field emission coefficients), NNBI (surface ionization, effect of Cs layers) and hot spots (SEE coefficients for ions and electrons). Therefore, interaction with other fields is needed and multi-scale physics requires a combination of methods. The real structure of the material is quite important, because it determines diffusion and impurities can strongly affect surface binding energies. Molecular dynamic simulations can help to overcome some shortcomings of simpler models, but they are only as good as the quality of the interaction potentials. Also, they can deal mostly with idealized systems and have problems for realistic fusion wall materials (mixed materials with a lot of damage and impurities). For fundamental understanding model systems are needed for validation.

2. SDTrimSP

Sputtering of a surface exposed to a flux of energetic ions is one of the best studied effects of ion-surface interactions. The details of ion-surface interactions depend greatly on the target-projectile combination. When the projectile is an ion of a volatile (recycling) element then sputtering usually dominates and the surface is eroded. In this case experiments are well described theoretically. The sputtering yield is the main parameter that is used to validate theoretical models against experiments. Existing models such as the TRIM code show good agreement with experiment for many target-projectile combinations.

If the projectile is a solid-state (non-recycling) ion then its interaction with the surface can lead to implantation if the ion, after penetration and deceleration in the solid, remains in the surface. This leads to formation of a mixed surface of target and projectile atoms. The properties of the mixed surface may deviate significantly from the properties of original materials. Additionally, the surface composition is dynamically changed by sputtering and implantation. The study of such interactions cannot be described just by the sputtering yield behavior; it depends strongly on the elemental composition of the surface, which is, in turn, modified continuously by ion bombardment. Similar difficulties are encountered when volatile ions interact with compounds or when a surface is exposed to a mixed flux of volatile and solid-state ions. To solve this problem a dynamic version of the TRIM code called TRIDYN (later re-written as SDTrimSP) was developed. This is a 1D version of TRIM, where the distance from the surface into the solid is discretized on a grid and dynamical change of the surface composition along the depth due to implantation of projectiles and relocation of recoils during collisional cascades are considered. There have been a number of studies comparing experiments with TRIDYN simulations showing generally good agreement.

The existing models assume that a plane and perfectly smooth surface exists and they demonstrate good agreement with experiments if well-polished specimens are used. Surface roughness is prone to increase the sputtering yield by up to a factor of 5. There were a few approaches to predict sputtering yields of rough surfaces. Ruzic suggested considering the surface to have a fractal geometry, and Kuestner *et.al.* assumed that the surface can be represented as aggregates of simple surfaces at tilted angles. These approaches yield reasonable agreement, but their intrinsic limitations have prevented further development of the models. One of the limitations is their inability to simulate surface morphology changes by deposition and implantation.

The limitations of the approaches can be overcome by extending the grid of the existing model into the second and third lateral dimensions. The first step in this direction has been made in developing the SDTrimSP-2D code, which is capable to treat the interaction of ions with a 2D surface. An example of such a surface is a diffraction lattice. The code belongs to the TRIM family and it incorporates the same physical model, but due to existing of second lateral dimension, it requires also an advanced

relaxation mechanism. It has been shown that the code predicts the evolution of a Si pitch grating exposed to 6 keV Ar ions with a good accuracy. Although this system is rather simple and governed mainly by sputtering and relaxation, the agreement between the experiment and numerical simulation demonstrates the validity of the basic physics included in the model. The code has also been used to evaluate the effect of the surface roughness of W exposed to C and C+D flux.

Another extension of the code is the inclusion of chemical sputtering by combining the local chemistry model of Mech et al. (based on work by Küppers et al.) with the experimental flux scaling from Roth et al. and the concept of escape probabilities for hydrocarbons depending on the distance to the surface (see Jacob et al.). This code reproduces a large number of experiments including the observation that a hydrocarbon surface bombarded with Neon (producing damage) and in parallel exposed to thermal hydrogen influx shows strong chemical sputtering.

Recent developments with the Los Alamos atomic physics codes

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The LANL contribution to the IAEA Atomic and Molecular Data Code Centre is the online version of atomic physics codes. These codes are accessed by remote users to perform atomic structure calculations, including excitation and ionization cross sections, for arbitrary ions and configurations. A brief description of the online capabilities was presented. A short summary of the ATOMIC plasma modeling code was also provided. Recent improvements to the CATS code were discussed, in particular, the recently developed parallel computing capability. Several examples of the use of the LANL suite of atomic physics codes to applications of interest to magnetic fusion were discussed including recent boron power loss calculations and preliminary results for modeling low temperature tungsten plasmas.

Atomic structure and dynamics calculations using the GRASP family of codes, and an introduction of some activities in NIFS

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We have briefly reported on the activities in the study of atomic structure and dynamics calculations using the GRASP (General purpose Atomic Structure Program) family codes and also on some activities at NIFS. We have introduced the following items: 1. Analysis of Visible M1 Lines in Tungsten Ions, 2. Collisional-radiative model for W ions, 3. Code development for single electron capture by H nucleus from metal surface, 3. $K\alpha$ radiation from low charge chlorine heated by an ion beam for plasma diagnostics, 4. Code Availability. And we have summarized the talk.

The visible light emitted from highly charged tungsten ions are of special interest; they are mainly realized by magnetic dipole transitions between the fine structure levels of ions and therefore they suffer less self-absorption by surrounding plasma providing us with a great advantage for the diagnostics of core plasma. We have studied the source of these visible line emissions in terms of accurate non-empirical atomic structure calculations and of population kinematics analyses. The GRASP package [1] for multi-configuration Dirac-Fock atomic structure calculation have provided us with the transition energies that are accurate enough to discriminate the states and the charges of tungsten ions. We tried, further, to reproduce the emission spectra by modifying a population kinetics code that has been used for the analysis of boron-like ion plasmas [2]. We have assigned new visible emission lines. We have shown that the use of the GRASP family of codes is quite effective for the spectroscopy of the visible line emissions of tungsten ions and for the diagnostics of MCF plasmas.

We have extended a CR model calculation code [2] to include the case of tungsten ions in plasma; the atomic data have been calculated using HULLAC code. We have applied the code to the analysis of W^{35+} to W^{37+} in plasma. The code is still under development. We have now under development a code

for single electron capture by H nucleus from a metal surface. The features of the theoretical method implemented in the code are: 1. semi-classical treatment of H nucleus colliding with metal surface, 2. static linear density response of target electron gas induced by external nuclear charge, 3. direct numerical solution of time-dependent Schrödinger equation of electron wave-function, 4. adiabatic expansion of wave-function, and 5. B-spline method and discrete-variable-representation of the adiabatic state function. We have obtained the level populations created by electron capture from molybdenum surfaces. It is found that the code can be improved substantially (e.g. more realistic target description, beyond jellium model), and that validation of theoretical methods implemented in the code requires more comparison with experimental results. This code is, at present, not ready to be open to the public.

We have investigated the $K\alpha$ radiation from low charge chlorine heated by an ion beam for ICF plasma diagnostics. In those plasmas, many $K\alpha$ lines are distributed over photon energy according to the ionization state and, therefore, $K\alpha$ photon energies show the characteristic charge state of plasmas. $K\alpha$ with M-shell electrons may be useful for the diagnostics of lower temperature plasmas. In ions with K-shell vacancies many Auger channels compete with radiative processes and they are indispensable to estimate $K\alpha$ yield.

We have discussed the availability of computer codes for open computing. We have listed out the following codes that are to be considered. 1. GRASP and GRASP2, 2. GRASP92 + RATIP, 3. GRASP2K, 4. CR-Model Code based on HULLAC, 5. Code for single electron capture by H nucleus from metal surface.

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Ionization cross sections for W I and W II and the ATOM and MZ codes

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The problems of ionization of the atom W and ion W^+ are of similar complexity. There are good experimental data for W^+ single and double ionization and no direct cross section measurements for W. For this reason we start with the ionization of W^+ and test the calculations by comparison with experimental data hoping that the accuracy for neutral W is similar. Most of the calculation details are the same (or at least similar) for the atom W and ion W^+ . Ionization of W^+ can be produced either by direct ionization (DI) or through excitation of inner shells followed by autoionization (EA). Ionization from the inner shells (IA) is followed by autoionization and therefore results in double ionization. The cross sections are calculated by the code ATOM in the Coulomb-Born approximation (CB) with exchange and correction for the normalization effect (account for the electron flux conservation) by the reduced K-matrix approximation. This considerably improves the results due to consideration of strong virtual excitations. The contribution of EA through $4f^{13}5d^5$ and $5p^55d^5$ and the double ionization due to ionization from those shells followed by autoionization (IA) are calculated. The double ionization cross section can be directly measured in beam experiments. On the other hand, in calculations of the ionization equilibrium and other plasma kinetic problems the double ionization should be included in the total ionization rate. In addition to the cross sections we calculated the rate coefficients $\langle v\sigma_{iz} \rangle$ for Maxwell electron energy distribution with the temperature T as well as 3 adjusted parameters for fitting formula.

The calculated $\sigma_{iz}^{(1)}$ overestimate the cross section by 20% at the cross section maximum. For such complicated ion as W^+ this accuracy is rather good. Without the correction for normalization the error is twice as much. Ionization of atoms W I was considered in the way similar to W II.

Latest updates of HULLAC theory and applications

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The first version of HULLAC (*Hebrew University Lawrence Livermore Atomic Code*) dates back to the 1980's when M. K. was professor at Hebrew University, Jerusalem, Israel, and got the support of LLNL. The concept is to generate a consistent atomic model, by using the same wave functions for computing all atomic processes relevant to plasma spectroscopy. These wave functions are obtained by solving the Dirac equation in a parametric potential [1]. The central field model enables a convenient decoupling of the angular momentum algebra [2] for all processes, including electron collisions, for which we introduced the factorization-interpolation method [3]. Recently, the whole code was re-written in a more modern way [4] and extensively checked. It now includes a collisional radiative solver with a special scaling for improved convergence, a new fit for the cross sections [5], the ability to use the mixed transition arrays (MUTA) [6], and to model the effect of an external radiation field. The latter capability was used to compare with a recent experiment on the transmission of Fe at $T_e=156\text{eV}$ [7], with excellent agreement [8]. The latest version is used by several groups, whose feedback is used to constantly improve and/or correct the code.

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Recent applications of the CCC method

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There has been considerable progress in the development of the Convergent Close-Coupling (CCC) theory. The major extension has been to institute a new parallelism paradigm. This utilizes a hybrid OPENMP/MPI combination with the main V-matrix being calculated across several nodes. Within each node the original OPENMP parallelism is used. Then, using MPI, the matrix is distributed in a block cyclic form across all the available cores suitable for solving the linear equations via the ScaLAPACK suite of routines.

Consequently the CCC code is now able to be run across many nodes of memory sharing multiple cores. Both the original non-relativistic CCC and the recently developed relativistic RCCC codes have been parallelized this way. Additionally, the RCCC code has been extended to quasi two-electron targets, and highly charged ions, including Breit or Møller corrections.

Recent applications of the CCC method include electron impact ionization of helium and electron-impact excitation of mercury and highly charge uranium ions. Currently the CCC method is being used to calculate electron-impact excitation and ionization of the He-like Li ion.

Recent advances in distorted-wave calculations of ion impact single and multiple ionization of atoms and molecules

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I will present our most recent calculations of different processes employing the non-relativistic CDW-EIS approximation at intermediate and high energies. These include single and multiple ionization of

atoms by ion impact including post collisional processes, and single ionization and electron capture in collisions between ions and molecules of biological interest. We employ the independent electron model, initial and final states that verify the correct asymptotic conditions for Coulomb potentials, and the straight-line version of the impact-parameter approximation, which is valid at high-impact energies.

Recent calculations for single and double ionization of He using a new version of the Exponential Model, modified to treat collisions with highly charged ions, will be also presented.

HYDKIN: towards online hydrogen and hydride kinetics to publicly expose A+M data in particular edge modeling applications

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The FZ Juelich plasma codes activities are mainly focused on the outer layers (“edge plasma”) of magnetically confined fusion plasmas. The suite of codes ranges from dedicated local erosion-redeposition transport codes (ERO) or drift fluid turbulence codes (ATTEMPT), up to “integrated” edge codes such as B2-EIRENE (operated and maintained jointly with ITER-IO, Cadarache), EMC3-EIRENE (jointly with IPP Greifswald, mainly for stellarators, LHD, W7X), OSM-EIRENE (with ITER) and EDGE2D-EIRENE (at JET).

The atomic, molecular and surface data are integrated into these models mostly via the kinetic Monte Carlo code module EIRENE. Most of the integrated edge modeling activities at FZ Juelich are under ITER contracts: EIRENE stand alone (first wall fluxes, diagnostic mirrors), EMC3-EIRENE (3D rmp effects), B2-EIRENE (2D code benchmarks internally within SOLPS family). With respect to numerical data EIRENE resorts to a combination of:

1. external databases for which interfaces to EIRENE exist. Some of these are homemade and web-based (HYDKIN, AMJUEL), others are obtained from database centers (ALADDIN, ADAS);
2. internal (default) atomic data;
3. collisional radiative codes integrated into the EIRENE source.

The web based database and toolbox HYDKIN (www.hydkin.de) serves to publicly expose the A&M data used by EIRENE obtained from earlier IAEA CRP's, as “non LTE collisional radiative” code as well as for sensitivity analysis using analytic solutions of linearized equations for sensitivity parameters.

With respect to surface data EIRENE resorts to a kinetic reflection database (under www.eirene.de), based on TRIM code calculations. Distinct from other surface databases the EIRENE database format choice was driven by the need to preserve full information regarding all angular dependencies as well as energy spectra, as needed by kinetic plasma models (e.g. Monte Carlo), rather than only averaged quantities. This is achieved by storing the multidimensional data in form of conditional quantiles (loc. cit.).

Theoretical treatment of ion-atom and ion-molecule collisions

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I presented a summary of the methodologies that we have assembled to treat ion-atom and ion-molecule collisions. Some of these methodologies can deal with systems with more than two active electrons, which is particularly important for the intermediate range of collisional energies (around 1 keV/u). At the same time, we have developed methods to treat complex systems (many electrons) using one-electron wave functions and/or classical mechanics.

A chart of codes with a brief summary of their capabilities was presented, alongside a few examples showing recent results on isotope effects in beryllium collisions with hydrogen and collisions with molecules like CH₄. The possibility of other users using the codes was also discussed.

One- and two-electron processes in multi-center collisional systems

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In the presentation, we present briefly the theoretical models used to evaluate cross sections of various electronic processes occurring in ion-atom and ion-molecule collisions. Lattice representation calculations are illustrated by the presentation of results for ionizing ion-molecule collisions. For atomic targets, we show double capture to autoionizing states cross sections computed by spectral methods. Finally, before some conclusive remarks, the presentation of our partners is done together with the implementation of the codes at the IAEA web site.

State-to-State Kinetics of Molecular and Atomic Hydrogen Plasmas

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The activity in the *Plasma Chemistry* group in Bari is focused on state-to-state kinetic modeling of systems of interest for technological applications ranging from fusion (negative ion sources) to aerospace. Concerning the tools for the derivation of information on the dynamics of elementary processes, recent results include:

- the implementation of a simplified theoretical approach, the *similarity function*, for the calculation of cross sections for electron-impact induced vibronic excitation in diatomic molecules with resolution on internal degrees of freedom, giving results that compare well both to theory and experiments in the case of e-H₂ excitation and avoiding the high computational load of more accurate methods;
- new implementation of the code for resonant processes in electron-molecule collisions (resonant vibrational excitation and dissociative attachment) for the investigation of isotopic effects, considering the different role for the three relevant resonances in e-H₂ scattering;
- the inclusion of non-adiabatic effects, due to coupling among different potential energy surface, in the QCT (quasi-classical trajectory) code for the treatment of H⁺+H₂ system, representing a new frontier including quantum effects in the dynamics;
- the implementation of a numerical tool based on the Downhill Simplex Method for the deconvolution of rate coefficients to cross sections, validated in the case of well-known systems as H+H₂;
- the code for the semi-classical treatment of heterogeneous processes of atom recombination at surfaces has been used for the investigation of isotopic effect in the Eley-Rideal mechanism of deuterium on graphite.

For the simulation of plasm-chemical systems, two existing codes have been coupled, the collisional-radiative model, for an atomic hydrogen plasma under shock-wave condition, and the code for calculation of synthetic hydrogen spectrum, deriving plasma optical properties, i.e. emissivity and absorption coefficient. The role of non-equilibrium in internal distribution in affecting the spectrum is investigated in different position of the shock.

Finally thermodynamics and transport of plasmas have been studied. In particular, thermodynamic properties have been calculated in the frame of a novel approach that reduces complex systems of levels to an equivalent system of two-three levels by means of grouping. Moreover the quantum problem of levels for hydrogen atom confined in a spherical box has been investigated in the frame of solution of divergence of internal partition function.

Modules for transport coefficients calculation have been implemented including the effects of different choices of cut-off criterion and of electronically excited states (EES) in the mixture.

Atomic and plasma codes at NIST

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We present a set of atomic structure and plasma kinetics codes that are being developed or hosted at NIST. The most advanced methods in atomic structure theory are implemented in non-relativistic Multiconfiguration Hartree-Fock (MCHF) and relativistic Multiconfiguration Dirac-Fock (MCDF) codes. An example of an MCDF code is provided by the GRASP2K package which is being maintained and improved by C. Froese Fischer in collaboration with several researchers from other countries. C. Froese Fischer also develops the MCHF code. Both these packages as well as some simpler codes are available for free download from the NIST web site. Yu. Ralchenko presented some examples of recent highly accurate results obtained with MCHF and GRASP2K codes for atoms and ions of relevance to fusion research.

The NIST Atomic Spectroscopy Group also develops sophisticated collisional-radiative models for calculation of plasma population kinetics and emission characteristics. The NOMAD code is used for calculation of spectral patterns in the EBIT experiments with highly-charged ions of tungsten and other heavy elements. This detailed code is also used for simulations on neutral beam spectroscopy in fusion machines, e.g., charge exchange recombination spectroscopy and motional Stark effect. Another advanced collisional-radiative code FLYCHK developed by LLNL researchers and available for online calculations on the NIST site is used by hundreds of researchers, including specialists in fusion plasmas for calculations of ionization distribution, radiative power losses and other important parameters.

Fast quasiclassical codes for radiative-collisional processes

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Fast codes for calculation of radiative-collisional processes in collisions of electrons with many-electron ions are presented. The codes are based on a quasiclassical approximation for electron motion in atomic potentials described by statistical models of the atoms (ions). Specific calculations are presented for Bremsstrahlung and radiative recombination spectra for complex ions as well as for dielectronic recombination rates for Li-like carbon ions and the Mg^{+1} ion. Detailed comparison with quantum calculations is presented showing quite good agreement between quasiclassical and quantum numerical data.

The advantages of quasiclassical codes are as follows:

1. Quasiclassical codes can decrease sharply the computing time as compared with quantum calculations, resulting in the possibility of their being combined with more complex plasma modeling codes, such as EIRENE or ASTRA transport codes;
2. The codes discover quasiclassical scaling laws for probabilities of radiative-collisional processes pointed above which are followed by quantum numerical data as well; it makes it possible to propose universal scaling laws for the processes applicable for every kind of multi-electron ions.

The precision of quasiclassical codes is quite good for most of plasma applications such as radiation background in tokamak plasmas as well as radiative and dielectronic recombination rates.

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