IAEA
International Atomic Energy Agency

INDC(NDS)- 0548
Distr. LP,NE,SK

INDC International Nuclear Data Committee

Summary Report of an IAEA Technical Meeting

International Code Centres Network

IAEA Headquarters, Vienna, Austria
2–3 December 2008

Prepared by

R.E.H. Clark
International Atomic Energy Agency, Vienna, Austria

February 2009

IAEA Nuclear Data Section, Wagramer Strasse 5, A-1400 Vienna, Austria

Selected INDC documents may be downloaded in electronic form from
http://www-nds.iaea.org/indc_sel.html or sent as an e-mail attachment.
Requests for hardcopy or e-mail transmittal should be directed to *services@iaeand.iaea.org*
or to:
Nuclear Data Section
International Atomic Energy Agency
PO Box 100
Wagramer Strasse 5
A-1400 Vienna
Austria

Printed by the IAEA in Austria

February 2009

INDC(NDS)- 0548
Distr. LP,NE,SK

Summary Report of an IAEA Technical Meeting

International Code Centres Network

Prepared by

R.E.H. Clark

Abstract

Eleven international experts on computational aspects of atomic, molecular and particle surface interaction data for fusion energy research participated in a technical meeting to initiate an International Code Centres Network. The participants reviewed the capabilities and future directions in their computational efforts at their institutions. Different methods of accessing the computational facilities were discussed, and a proposed method of linking efforts was formulated. A consensus was reached on forming a flexible organization with the ability to adjust and adapt to future needs of the fusion community as new experimental devices are developed, requiring different priorities of data generation.

February 2009

TABLE OF CONTENTS

1. Introduction

A Technical Meeting to discuss the benefits and possibility of forming an "International Code Centres Network" was held on 2-3 December 2008 at IAEA Headquarters, Vienna. The purpose of this meeting was to review the current status and research activities in computational tools related to atomic, molecular and particle surface interaction (AM/PSI) data generation tools, and co-ordinate these research activities in the form of a network accessible by the fusion research community. Discussions took place on establishing guidelines for the operation of a network, with suggestions on setting up links from the Atomic and Molecular (A+M) Data Unit home page for access of individual centres.

Eleven experts on various aspects of computational AM/PSI data participated in the meeting (see Appendix 1). Each participant gave a summary of current work in their field of expertise, as well as active lines of research. The current capabilities of each centre were discussed and summarized, along with the means by which the expertise could be made available for fusion research. Finally, a preliminary table summarizing the code capabilities, institutions and contact persons was formulated.

2. Proceedings

A. Nichols, as Section Head of the Nuclear Data Section, welcomed the participants on behalf of the IAEA. He acknowledged the importance of developing a code-based network, and expressed hope that the result would be a powerful tool in assisting fusion energy research. He noted the success of the existing networks dedicated to atomic and nuclear databases, and the hope that the computational tools proposed for this new network would be a powerful complement to the atomic database network, filling data needs in the established databases. R. Clark (IAEA Scientific Secretary) reviewed the proposed agenda, which was accepted without change (see Appendix 2).

During the course of the first day, each participant gave a summary presentation of relevant on-going research activities within their institutes (see Appendix 3 for abstracts). All presentations were collected into a data file and distributed to participants during the course of the meeting. At the end of the presentations, the current capabilities of each centre were summarized. Discussions then took place on the initial operational functions of an appropriate code centres network.

I. Bray from Curtin University, Australia, discussed the convergent close-coupling method for excitation and ionization cross section calculations. Codes exist for both relativistic and non-relativistic calculations, and the methods used were discussed along with the systematic approach to their convergence. A number of comparisons with experiments have been carried out to validate the method, and there are no substantial discrepancies with experiment. Current calculations are limited to one and two valence electron systems, but work is underway to extend the method to other systems. These codes require large amounts of computational resources and expertise, necessitating experts running cases in response to specific requests.

F. Koike of Kitasato University, Japan, reviewed work on calculation of atomic structure and radiative transition probabilities. He described studies of electron correlation effects and going beyond the Dirac (Hartree) Fock approximation. Spectral features of Sn were compared with observed spectra. Work has been carried out to optimize all configurations and to take into account interference effects. Dielectronic recombination rates for Sn have been calculated using the FAC code, and comparisons have been made with and without configuration interaction. Spectroscopy of heavy and super-heavy elements have been investigated using the Grant code. Work at NIFS was also summarized, including collisional-radiative modelling and plasma-wall interaction simulation. A summary of the calculational tools was given with the web site for those tools.

I. Rabadan of Universidad Autonoma de Madrid, Spain, discussed calculations of ion-atom and ion-molecule cross sections. A chart of codes with a brief summary of their capabilities was presented.

Methods used include quantal calculations as well as semi-classical methods. Details of the flow of calculations and program inputs and outputs were presented, and a number of examples were given. Isotope effects in hydrogen collisions were also shown.

A. Dubois of Laboratoire de Chimie Physique-Matière et Rayonnement, Paris, France, described the work on computer implementation of cross-section calculations for ion-molecule collisions. The motivation is to understand and model the ultra-fast dynamics of atomic and molecular systems and to model the interplay of many open channels. He described the non-perturbative models used in different energy regimes, and cited examples for specific systems. A summary of methods with advantages and drawbacks was presented - collaboration with the A+M Unit has already made some of the calculational tools available through an on-line interface.

M. Capitelli of Bari University, Italy, summarized work on elementary processes and the modelling of plasmas for fusion applications. He reviewed some fusion regimes with plasmas in which molecular processes play an important role, and described relevant approximations for calculations in those regimes. A number of calculational tools and diagrammed interfaces to those codes were summarized. He described numerical experiments on plasma situations, such as particle-in-cell and Monte Carlo simulations. Calculations of large sets of cross sections for application to the modelling of current plasma problems were emphasized, such as negative ion sources.

A.B. Kukushkin of the Kurchatov Institute of Russia, presented calculations of escape probabilities for radiation transport. V.S. Lisitsa (together with colleagues in Marseille and Pierre and Marie Curie Universities) has worked on an ultra-fast method to calculate dynamic spectral line shapes by means of a kinetic frequency fluctuation method. The method has been applied to a number of systems, and the results show a good fit to observations. This approach is orders of magnitude faster than the FFM method alone, and greatly simplifies radiation transport modelling, of particular interest in the edge plasma and divertor regions in tokamaks. Further work on escape probability and benchmarking codes for electron cyclotron radiation power loss in tokamaks was summarized. A number of calculational tools are available as modules, and could be made available through the code centres network.

L. Vainshtein of the Lebedev Institute in Russia described work on the generation of atomic data and collisional-radiative modelling of plasmas. Codes of increasing sophistication have been developed for the calculation of the atomic data needed in the CR models. He proposed grouping codes by a grading system of sophistication, but there are many open questions on how to categorize specific codes in this manner. Different levels of accuracy may be needed in different regimes. Some transitions may require more accuracy than others in any particular regime. Several different levels of sophistication can be merged to produce a complete data set for modelling the complete plasma with good results.

D. Reiter of Forschungszentrum Jülich, outlined work on collisional-radiative modelling for ITER. Different machine sizes will change the calculational time needed for a model, with ITER requiring months of computer time for a complete CR model at the present time. Molecular processes dominate the models in the edge region, and can require a great deal of computational power. Separation of time scales is also an important issue: if certain modelling processes can be decoupled from others with different time scales, computation time can be greatly reduced. A tool called HYDKIN was described that is already available on-line, and allows the calculation of time scales for a number of processes in hydrocarbon molecules, as well as the presentation of data from the database. HYDKIN can be used in conjunction with the EIRENE code to produce a model of the plasma.

J. Abdallah, Jr. of the Los Alamos National Laboratory, USA, described a reduced detailed configuration accounting (DCA) model for non-LTE plasmas. The method starts with a large detailed model, and reduces the size by combining many levels into groups, based on a prescription from energy level considerations. The modelling requirement is for very fast CR capability, but with better accuracy found in average-atom scaled hydrogenic-type approximations. A DCA package is available in LANL, but is never used due to the large amount of computer time required. He showed a number of comparisons in which the reduced DCA method was demonstrated to give nearly the same answers

as the full DCA with orders of magnitude less computer time. Results are much better than the average atom approximation results, but do not require much greater computer resources.

Y. Ralchenko of NIST, USA, discussed work on atomic physics and plasma modelling. NIST has the multi-configuration Hartree Fock code of Froese-Fisher as well as the Grasp2k code for relativistic calculations. Comparisons with both codes are often made with the experimental database at NIST, providing good validation of both codes. NOMAD is also available (CR code), and can perform both time-dependent and steady-state calculations with non-Maxwellian electron distributions. Data can be collected from any available database or computer code calculations as needed. FLYCHK is also a CR model that uses approximation methods to generate on-line data. This code is available through the NIST website, and gives reasonable estimates for plasma parameters under a wide range of parameters. Ralchenko stressed the need for a universal data exchange format for all AM/PSI data, and pointed out the on-going development of XSAM, the XML-based data exchange.

D. Stotler of Princeton Plasma Physics Laboratory, USA, described advances in edge plasma simulation. A multi-institutional collaborative project (Centre for Plasma Edge Simulation) is attempting to build a new integrated predictive plasma edge simulation applicable to existing magnetic fusion facilities, while the Fusion Simulation Project (FSP) will get underway in the next year. Stotler reviewed the relevant physics of edge plasmas in tokamaks, including pedestal buildup, Edge Localized Mode instabilities, and the low (L) and high (H) confinement modes. He described the importance of the AM/PSI data that enter the models through the transport codes. Codes used to model the plasmas and the multi-scale approach to simulations were also noted. The interface between these large computer codes is quite complex, and is the subject of significant computer science research within the project.

3. Recommendations and Conclusions

After the presentations, discussion took place on how best to implement a Code Centres Network. Initial discussion focused on producing a concise listing of the capabilities of the participating institutions.

The listing includes the following:

Institution:	Curtin University
Contact:	I. Bray http://atom.curtin.edu.au/CCC-WWW/index.html
Codes:	CCC and RCCC
Description:	Convergent Close Coupling. Two independent implementations. NR version is more stable. First is applicable to electron, positron and photon collisions with quasi-one and two electron atoms and ions. Provides cross sections for excitation and ionization. (Link to page with more detailed information, references, etc. Use the page Yuri has set up)

Institution:	NIFS
Contact:	F. Koike http://dpsalvia.nifs.ac.jp/~katomasa/crmtest/
Codes:	CR model
Description:	CR model of He and He-like ions is available through web page. CR model for Fe ions will come on-line soon. Ion metal surface interaction code – Hydrogen ion–metal surface interaction is also in preparation and will appear soon.

Institution:	Universidad Autonoma de Madrid, Spain
Contact:	I. Rabadán
Codes:	MELDF*-TCAM, QUAN, SEIKON, CTMC
Description:	These codes perform calculations of electronic excitation, single and double charge transfer, molecular vibrational excitation, vibrationally-resolved charge transfer,

vibrationally-resolved electronic excitation, ionization of atoms and molecules. They can treat poly- and mono-electron systems over entire range of energies from 1.e-3 eV/amu to 1.e6 eV/amu. (Add link and web page with references, etc.)

Institution: Univ. Pierre Marie Curie – CNRS, France
Contact: A. Dubois and P.D. Fainstein (Centro Atomico Bariloche CNEA, Argentina), for the distorted waves code available at IAEA http://www-amdis.iaea.org/HEAVY/
Codes: CDW, VPN
Description: The CDW code calculates total and differential ionization cross sections for ion-atom collisions at high energy (MeV). Available on-line at the above IAEA web site. Target is either a hydrogen-like ion or neutral He, and the projectile is a bare nucleus. VPN code calculates charge transfer and excitation cross sections for similar targets and projectiles by means of close coupling for energies from 1 keV/amu to a few hundred keV/amu (available at the above web site). A two-electron, ion-atom or ion- molecule, quasi-two-electron system is in the process of development, which will also use close-coupling to produce total cross sections for charge transfer, excitation, and ionization for energies from 100 eV/amu to 500 keV/amu.
(Dubois to provide web page and link)

Institution: University Bari, Italy
Contact: M. Capitelli
Codes:
Description: Semi-classical impact parameter method is used to calculate vibrationally-resolved cross section for excitation and dissociation for spin–allowed transitions. Some of these calculated data are already available on the ALADDIN web page. The quasi-classical trajectory approximation has been used to calculate vibrational translational relaxation and dissociation for H, H_2, and isotopic variants. Calculations of atom-molecule gas surface interaction have been carried out, specifically for atomic hydrogen or deuterium on copper or graphite. Resonant charge transfer of electronically excited states in atom-ion, highly-excited atoms can be calculated. (Mario will provide a web page with details and actual contacts)

Institution: Kurchatov Institute, Moscow
Contact: A.B. Kukushkin, V.S. Lisitsa http://vo.nfi.kiae.ru/atomic_physics
Codes:
Description: Calculation of *n,l* collisional radiative kinetics of Rydberg atomic states and line intensities can be carried out. The specific application is for charge exchange recombination spectroscopy (CXRS). A modified version of the Frequency Fluctuation Method (FFM) for line shapes is available as a code module, particularly for Stark broadening, of hydrogen atoms (to be generalized to hydrogen like ions). A semi-analytical description of Bremsstrahlung and radiative recombination cross sections for collisions of electrons with many electron atoms and ions (up to fully stripped) is available. Rosmej has developed a dense plasma quantum kinetics code with application (with Lisitsa) to non-equilibrium plasmas.

Institution: Lebedev Physical Institute, Moscow
Contact: L. Vainshtein
Codes: ATOM, ATOM– AKM, GKU
Description: The ATOM code can calculate collisional ionization and excitation cross-section photo-ionization and radiative recombination for any atom and ion in the first order approximation. ATOM-AKM calculates excitation cross sections with inclusion of full channel interactions. GKU calculates populations of levels and ions in stationary and non-stationary conditions, particularly for beam diagnostics of plasmas.

Institution: Forschungzentrum Juelich
Contact: D. Reiter
Codes: HYDKIN
Description: HYDKIN is a computational tool containing molecular databases compiled over recent years, specifically for the hydrogen atom, and ethane, methane and propane molecules. There is access to the cross sections, and Maxwellian-averaged reaction rates can be calculated on-line. A master rate equation can be constructed and solved and an analysis of the time scales carried out, which is beneficial to modelling codes for reducing the number of species required in simulations. The databases are presently being extended towards tungsten. (Add link)

Institution: Los Alamos National Laboratory, USA
Contact: J. Abdallah, Jr.
Codes: LANL codes
Description: These codes calculate non-relativistic atomic structure (Hartree-Fock), cross sections (plane wave Born or distorted wave) for excitation and for electron and photon impact ionization, as well as auto-ionization rates for any atom or ion. They are freely available from the appropriate LANL web site. The ATOMIC code calculates CR models when linked to these data, incorporating the RDCA model to reduce the size of the CR model. At a later date, the RATS relativistic code may be incorporated into the on-line system.

Institution: National Institute of Standards and Technology, USA
Contact: Y. Ralchenko http://nlte.nist.gov/FLY/
Codes: MCHF, GRASP2K, FLYCHK, NOMAD
Description: MCHF and GRASP2K codes are non-relativistic and relativistic atomic structure packages, respectively, and are used to calculate energy levels, transition probabilities, isotope shifts and hyperfine structure. The FLYCHK code is an on-line CR code (non-Maxwellian plasmas, radiation field, opacity effects and mixtures) available at the above web site, and can produce the following output parameters: reaction rates, ionization distribution, power losses and UTA spectra. FLYCHK contains detailed data for hydrogen-, helium- and lithium-like atoms and ions and uses the hydrogenic approximation with screening parameters for other ions. The NOMAD code is similar to FLYCHK, but is more useful for spectroscopic diagnostics - data normally include detailed structure for all relevant ions, as well as non-Maxwellian ions, radiation field, opacity effects and mixtures. This code is applicable to CXRS problems, and there are plans to have a version on-line in the future.

Institution: Princeton Plasma Physics Laboratory, USA
Contact: D. Stotler, http://w3.pppl.gov/degas2
Codes: DEGAS databases
Description: H and He collisional radiative data are available as on-line tables. The DEGAS 2 User's Manual also provides a brief introduction to collisional radiative models suitable for novices in atomic physics.

Further discussion focused on formulating a uniform format that each participant would use for an initial web page. The following information will be included:

- Name of code.
- Responsible person – contact data.
- Description of code (including approximations and accuracy) and applications.
- References and recent applications.
- Link(s).
- Reference to Code Centre Network.
- Logo / link to Code Centre Network.

After much discussion the following recommendations were also agreed:

- An IAEA web page will be created to include the basic information from summaries of the current code capabilities.
    - The A+M Unit will create individual web pages as per the above guidelines. Staff will contact contributors annually to request updates to information on these web page(s).
    - Participants will create more extensive pages at their home institutes as needed, with links on the A+M Unit page.
    - After a one-year trial period, contact should be initiated with other code and data providers (specifically the R-matrix community, the PMI community, Auburn University, Krstic at ORNL, group at Belfast, Biemont, HULLAC, FAC, etc.).
- Code authors will attempt to assess the accuracy of their calculations in a similar manner to the numerical database estimate (e.g., graded as “A”, “B”, “C”).
- Code authors and data users should begin utilizing the XSAMS XML format for transmission and exchange of data.
- This group should meet periodically (e.g., every two years) to monitor progress and identify future needs.
- The Network should make the broader fusion community aware of the capabilities represented by this group (e.g., via presentations at fusion-oriented conferences).

The following conclusions were reached:

- This meeting had been extremely productive and informative, both for the participants and the A+M Data Unit.
- The meeting will lead to substantial new collaborations between the participants.
- The basis for the web page of the International Code Centres Network was established.
- The code centres network will constitute an informal federation in order to permit flexible membership.

Appendix 1

IAEA Technical Meeting: International Code Centres Network

2–3 December 2008, IAEA Heaquarters, Vienna, Austria

LIST OF PARTICIPANTS

Prof Igor Bray
ARC Professorial Fellow
Director, Institute of Theoretical Physics
Deputy Director, ARC Centre for
Antimatter-Matter Studies
Curtin University of Technology
GPO Box U1987
Perth WA 6845
AUSTRALIA
Tel.: +61-8-9266-4416; Fax: +61-8-9266-1972
E-mail: I.Bray@curtin.edu.au

Prof Alain Dubois
Laboratoire de Chimie Physique
Matiere et Rayonement
Universite Pierre et Marie Curie (Paris VI)
UMR du CNRS 7614
11, rue Pierre et Marie Curie
F-75231 Paris Cedex 05
FRANCE
Tel.: +33-1-44276631; Fax: +33-1-44276226
E-mail: ad@ccr.jussieu.fr

Prof Dr Detlev Reiter
Forschungszentrum Jülich GmbH
Institut für Plasmaphysik (IPP)
D-52425 Jülich, GERMANY
Tel.: +49-2461-61-5841; Fax: +49-2461-61-2970
E-mail: d.reiter@fz-juelich.de

Prof M. Capitelli
Centro di Studio per la Chimica de Plasmi
Departmento di Chimica
Universita di Bari
Via Orabona 4
I-70126 Bari, ITALY
Tel.: +39-80-544-2104; Fax: +39-80-544-2024
E-mail: mario.capitelli@ba.imip.cnr.it

Prof Fumihiro Koike
Physics Laboratory
School of Medicine
Kitasato University
Kitasato 1-15-1, Sagamihara
Kanagawa 228
JAPAN
Tel.: +81-427-78-8029; Fax: +81-427-78-8441
E-mail: koikef@kitasato-u.ac.jp

Dr Alexander Kukushkin
Russian Research Centre "Kurchatov Institute"
Nuclear Fusion Institute
Kurchatov Square, 1
123182 Moscow
RUSSIAN FEDERATION
Tel.: +7-495-1967334; Fax: +7-495-9430073
E-mail: kuka@nfi.kiae.ru

Prof L.A. Vainshtein
P.N. Lebedev Physical Institute
Leninsky pr., 53
119991 Moscow
RUSSIAN FEDERATION
Tel.:/Fax: +7-499-135-2429
E-mail: vainsh@sci.lebedev.ru

Dr Ismanuel Rabadan
Departamento de Quimica, C-9-602
Universidad Autonoma de Madrid
28049 Madrid, SPAIN
Tel.: +34-91-497-5259; Fax: +34-91-497-5238
E-mail: ismanuel.rabadan@uam.es

Dr Joseph Abdallah Jr.
Los Alamos National Laboratory
Group T-4, MS B212
Los Alamos, NM 87545
U.S.A.
Tel.: +1-505-667-7388; Fax: +1-505-665-6229
E-mail: abd@lanl.gov

Dr Yuri Ralchenko
Atomic Spectroscopy Group, Stop 8422
National Institute of Standards & Technology
Gaithersburg MD 20899-8422
U.S.A.
Tel.: +1-301-975-3210; Fax: +1-301-975-1350
E-mail: yuri.ralchenko@nist.gov

Dr Daren Stotler
MS27 C-Site A131
Plasma Physics Laboratory
P.O. Box 451
Princeton, New Jersey 08543-0451
U.S.A.
Tel.: +1-609-243-2063
E-mail: dstotler@pppl.gov

Dr. Robert E.H. Clark
IAEA Atomic and Molecular Data Unit
Wagramerstrasse 5
P.O. Box 100
A-1400 Vienna
AUSTRIA
Tel.: +43-1-2600-21731; Fax: +43-1-26007
E-mail: r.e.h.clark@iaea.org

Dr. Denis Humbert
IAEA Atomic and Molecular Data Unit
Wagramerstrasse 5
P.O. Box 100
A-1400 Vienna
AUSTRIA
Tel.: +43-1-2600-21729; Fax: +43-1-26007
E-mail: d.humbert@iaea.org

Appendix 2

IAEA Technical Meeting: International Code Centres Network

2–3 December 2008, IAEA Heaquarters, Vienna, Austria

AGENDA

Tuesday, 2 December **Meeting Room: F-07-04**

09:30 - 09:45	A.L. Nichols, R.E.H. Clark	Welcoming remarks, Adoption of Agenda

Session 1: Reports on current status

Chairman: L. Vainshtein

09:45 – 10:15	I. Bray	Convergent close-coupling approach to atomic collisions
10:15 – 10:45	F. Koike	Some efforts on precise calculations for atomic structures and transitions
10:45 – 11:15	*Coffee Break*	
11:15 – 11:45	I. Rabadan	*Ab inito* calculation of ion-atom and ion-molecule cross sections
11:45 – 12:15	A. Dubois	Computer implementation and use of non-perturbative methods for ion-molecule at intermediate and high impact energies
12:15 – 12:45	M. Capitelli	Elementary processes and modelling of plasmas for fusion applications
12:45 – 14:00	*Lunch*	

Session 2: Reports on current status II

Chairman: F. Koike

14:00 – 14:30	A. Kukushkin	Escape probability method for radiation transport in continuous spectra and the benchmarking of the codes for electron cyclotron power loss in tokamak reactors **and** Ultrafast method of calculating the dynamic spectral line shapes for integrated modelling of plasmas (V.S. Lisitsa)
14:30 – 15:00	L. Vainshtein	Atom-AKM-GKU codes for atomic and CR model calculations
15:00 – 15:30	D. Reiter	Collisional-radiative and transport modeling for ITER
15:30 – 16:00	*Coffee Break*	
16:00 – 16:30	J. Abdallah, Jr.	The reduced detailed configuration accounting (RDCA) model for NLTE plasma
16:30 – 17:00	Y. Ralchenko	Atomic and plasma codes at NIST
17:00 – 17:30	D. Stotler	Advances in US edge plasma simulation and computer science

Wednesday, 3 December

Session 3: Summary of current status and available tools

Chairman: D. Reiter

09:00 – 10:30 Summary of current status

10:30 – 11:00 *Coffee Break*

Session 3: Continued

11:00 – 12:00 Summary of available codes

12:00 – 13:30 *Lunch*

Session 4: Establishment of Code Centre

Chairman: Y. Ralchenko

13:30 – 15:00 All participants: Discussion of operation of code centre

15:00 – 15:30 *Coffee Break*

Session 4: Continued

15:30 – 17:00 All participants: Formulation of conclusions and recommendations

17:00 – *Adjournment of Meeting*

Appendix 3

ABSTRACTS

Convergent Close-Coupling Approach to Atomic Collisions

I. Bray, Curtain University, Australia

We review the applications of the convergent close-coupling (CCC) method to collisions involving electrons, positrons and protons with atoms and ions. The Laguerre basis is used to expand the target wave functions, and these are then applied to expand the total wave function of the collision system. Both, the non-relativistic and relativistic, implementations of the CCC formalism have been implemented. Considerable comparison with experiment will be presented and discussed.

Some efforts on precise calculations for atomic structures and transtions

Fumihiro Koike, Kitasato University, Japan

In relation to the increasing needs for precise and accurate data of atomic electronic structures and transitions, we have tried the use of sophisticated atomic codes. We present our recent several results of such efforts.

***Ab initio* calculation of ion-atom and ion-molecule cross sections**

Ismanuel Rabadan, Universidad Autonoma de Madrid, 28049-Madrid, Spain

Details of the present capabilities of the codes used by the TCAM group in Madrid will be discussed and illustrated with examples of recent calculations of cross sections in ion-atom and ion-molecule collisions, including electronic excitation, vibrational excitation, charge transfer and ionization

Computer implementation and use of non perturbative methods for ion-molecule at intermediate and high impact energies

Alain Dubois and Nicolas Sisourat, Laboratoire de Chimie Physique-Matière et Rayonnement, Université Pierre et Marie Curie - CNRS,, Paris, France

During the meeting we shall present new methods to describe electronic transition occurring during two-active-electron ion-molecule collisions at intermediate and high impact energies. A rapid overview of two specific computer implementations of semi-classical non perturbative treatments shall be shown : a totally numerical method in which the wave functions and Hamiltonian are discritized in space and a semi-analytical one where the total electronic wave function is expanded onto two-electron, 3-center basis set, expressed in terms of travelling Gaussian-Typed Orbitals. The use of these codes will be illustrated by two examples concerning ionization and double electron transfer from di-hydrogen molecular target.

Escape probability method for radiation transport in continuous spectra and the benchmarking of the codes for electron cyclotron power loss in tokamak reactors

A.B. Kukushkin, RRC Kurchatov Institute, Moscow, Russian Federation

The escape probability method originally designed for the radiation transport in atomic spectral lines was extended to the case of continuous spectra, and applied to the electron cyclotron (EC) radiation transport in hot strongly-magnetized plasmas in fusion reactor-grade tokamaks. The recent benchmarking of the codes for calculating the spatial profile of the EC power loss (US, EU, Russia) has shown good agreement of the fast-routine approaches with the Monte-Carlo modeling. Simplification of calculations due to the strong non-locality (non-diffusivity of transport) in the EC power loss in tokamak-reactors enabled us to produce a fast routine which is included to the transport code ASTRA for the integrated modeling of the ITER operation scenarios.

Ultrafast method of calculating the dynamic spectral line shapes for integrated modelling of plasmas

V.S. Lisitsa (presented by A.B. Kukushkin), RRC Kurchatov Institute, Moscow, Russian Federation

An ultrafast code for spectral line shape calculations is presented to be used in the integrated modelling of plasmas. The code is based on the close analogy between two mechanisms: (i) Dicke narrowing of the Doppler-broadened spectral lines and (ii) transition from static to impact regime in the Stark broadening. The analogy makes it possible to describe the dynamic Stark broadening in terms of an analytical functional of the static line shape. A comparison of new method with the widely used Frequency Fluctuating Method (FFM) developed by the Marseille University group (B. Talin, R. Stamm, *et al.*) shows good agreement, with the new method being faster than the standard FFM by nearly two orders of magnitude. The method proposed may significantly simplify the radiation transport modeling and opens new possibilities for integrated modeling of the edge and divertor plasma in tokamaks.

Atom-AKm-GKU codes for atomic and CR model calculations

L.A. Vainshtein, P.N.Lebedev Physical Institute, Moscow, Russian Federation

The set of codes Atom-AKM-GKU is used in the Spectroscopy Department of LPI (Lebedev Physical Institute). The code ATOM calculates different atomic characteristics:
- oscillator strengths,
- photo-ionization cross sections and photo-recombination rates,
- excitation and ionization cross sections by electrons,
- excitation and ionization cross sections by point heavy particles,
- auto-ionization cross sections.

The semi-empirical one-particle wave functions and 1st order perturbation theory for all processes are used. There are options for inclusion of the intermediate couplings and the configuration interaction with usage of eigenvector matrix from other codes or papers.

The AKM code transforms the collisional data from ATOM by K-matrix method to take into account the channels interaction and normalization effects.

Data obtained by ATOM-AKM are used to get the atomic database for the kinetic GKU code, which calculates the level populations and line intensities in plasmas for different electron temperatures T and densities N. Stationary and non-stationary models are possible. The non-stationary model is used for plasma beam diagnostics.

The Reduced Detailed Configuration Accounting (RDCA) model for NLTE plasma calculations.

J. Abdallah, Jr., M.S. Sherrill, C.J. Fontes, H.L. Zhang, J. Oelgoetz and D.P. Kilcrease, Los Alamos National Laboratory, USA

The motivation for this work is to provide a more accurate and cost-effective in-line NLTE capability for calculating plasma properties in large-scale radiation-transport hydrodynamic simulations. A method is developed to transform the large detailed atomic models to very small models that can be used for fast in-line calculations. An averaging technique reduces detailed models involving tens of thousands of states into just a few (10-40 states) per ionization state. The reduced model is more accurate than the average atom models conventionally used in such simulations. The averaging scheme is presented and results of the reduced model are compared to the original detailed model and the average atom model. Average ionization states of iron, gold and uranium plasmas under various conditions of material temperature, atom number density and radiation temperature are compared. Several spectral comparisons will also be presented.

Atomic and plasma codes at NIST

Yuri Ralchenko, National Institute of Standards and Technology (NIST), Gaithersburg, USA

We will present several advanced computer codes for atomic structure and plasma kinetics available at the NIST Atomic Spectroscopy Group. These codes include such programs as Multi-configuration Hartree-Fock (MCHF) and Multi-configuration Dirac-Fock (GRASP2K) structure codes, time-dependent collisional-radiative (CR) code NOMAD, and an on-line version of the CR code FLYCHK. Several examples of fusion-related applications including time-dependent simulations of charge-exchange recombination in tokamaks will be presented. We will also briefly discuss the on-going development of standards for exchange of atomic, molecular and particle-surface-interaction data.

Advances in US Edge Plasma Simulation and Computer Science

Daren Stotler, Princeton Plasma Physics Laboratory (PPPL), Princeton, NJ, USA

Several multi-institutional collaborative simulation projects dominate the US fusion simulation landscape. Initially, these Scientific Discovery through Advanced Computing (SciDAC) projects dealt with individual magnetic fusion energy problems, such as core micro-turbulence. These have been followed by a few more ambitious projects endeavoring to pave the way towards an all-encompassing "Fusion Simulation Project" (FSP). Among these proto-type FSP projects is the Center for Plasma Edge Simulation (CPES). Over the previous three years, CPES has made significant progress towards the primary objective of understanding the behaviour of the boundary of fusion plasmas. We will describe some of this progress and review the atomic and plasma material interaction data needs of the project. However, the computer science related aspects of CPES may be of even greater interest to this audience since they deal with the monitoring of computationally intensive simulations, as well as with the movement and visualization of data from those simulations.

Nuclear Data Section
International Atomic Energy Agency
P.O. Box 100
A-1400 Vienna
Austria

e-mail: services@iaeand.iaea.org
fax: (43-1) 26007
telephone: (43-1) 2600-21710
Web: http://www-nds.iaea.org