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Establishment of A+M Computer Code Network

Summary Report of IAEA Technical Meeting

IAEA, Vienna, Austria

23 – 25 May 2005

Prepared by

R.E.H. Clark

January 2006

IAEA NUCLEAR DATA SECTION, WAGRAMER STRASSE 5, A-1400 VIENNA

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Abstract

Eleven international experts on computational aspects of atomic and molecular data for fusion energy research participated in a technical meeting arranged to discuss the establishment of an A+M Computer Code Network, and held at IAEA Headquarters on 23-25 May 2005. Each participant reviewed the current status of their own speciality and current lines of research, as well as anticipated needs in new data for nuclear fusion energy research. A preliminary method for making these valuable resources more readily available was outlined, and implementation will proceed. Several of the computational tools presented are already available through Internet connections. All the goals of the meeting were achieved, and every participant indicated a desire to see more collaboration and cooperation in fulfilling the A+M data needs for fusion. The discussions, conclusions and recommendations of the meeting are briefly described in this report.

January 2006

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1. Introduction

A Technical Meeting on the "Establishment of A+M Computer Code Network" was held on 23-25 May 2005 at IAEA Headquarters, Vienna. The purpose of this meeting was to review current status and research activities in computational tools related to Atomic and Molecular (A+M) data research, and co-ordinate these research activities with anticipated data needs for nuclear fusion energy research. Discussions were expected to yield a specific proposal for a network of institutions with computational capabilities in the A+M areas of relevance to fusion energy research.

Eleven experts on various aspects of computational A+M data participated in the meeting. 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 outline for a network of computer codes was formulated and will be implemented in the near future.

2. Meeting Proceedings

A. Trkov, Deputy Section Head of the Nuclear Data Section welcomed the participants on behalf of the IAEA. He expressed the hope that the expertise represented in the meeting would be organized into a useful network to make more computational tools for A+M available to the fusion community. R. Clark (IAEA Scientific Secretary) reviewed the proposed agenda, which was accepted without change.

During the course of the first day and a half, each participant gave a summary presentation of relevant on-going research activities within their institutes. All presentations were collected on CD and distributed to the meeting participants during the course of the meeting. At the end of the presentations, the current capabilities of each centre were summarized.

Relevant studies within Princeton Plasma Physics Laboratory (PPPL) were presented by D. Stotler. PPPL has a MC neutral transport code for fusion plasmas (DEGAS 2). The DEGAS-2 system includes a dedicated program for transforming data in Aladdin-format files to the internal format of DEGAS 2, integrating cross sections to give reaction rates if needed. This code utilizes extensive CR model data for H and He, as well as data for elastic scattering for D_2, He and D on D^+. These data files and the data manipulation program are currently available for download over the Internet as part of the DEGAS 2 distribution.

I. Bray from Murdoch University in Australia discussed the convergent close-coupling method for excitation and ionization cross section calculations. The method is currently working on one and two-electron over closed shell systems, and can serve as a benchmark for calculations of such cross sections using faster, but less accurate methods. Some work on making existing databases more accessible remains to be done. The codes require a high level of expertise to run, but specific requests are welcome. Since the code requires on the order of one week for a complete calculation, the hoped is that requests should be only those requiring the power of this method for resolution.

A. Dubois of the Laboratoire de Chimie Physique - Matière et Rayonnement presented work on collisions between heavy particles (atoms, ions and molecules). Existing codes calculate cross sections for ionization, excitation and charge transfer, especially for one- and two-electron systems. Codes using semi-classical (SC) and classical approaches are available with

a lower limit of approximately 0.1 keV/amu. One code is on the Web (IAEA, hydrogenic systems, SC), while others run in-house. The next versions may also be added to the Web, but can result in extensive calculations that require approximately one day for the calculation of all kinds of cross sections at one velocity.

Ismanuel Rabadan of the Departamento de Quimica Universidad Autonoma de Madrid presented recent research on collisions between heavy particles (atoms, ions and molecules). Codes exist for the calculation of cross sections for ionization, excitation and charge transfer, with no restrictions using the close-coupling method on multi-electron systems, including vibrational resolution. Both quantum-mechanical and Monte-Carlo (MC) (one-electron) codes have been developed for charge exchange and ionization. Currently, the codes can be used to calculate cross sections by request, with some delay possible depending on the difficulty of the case; systems such as ion-molecule collisions are more time-consuming.

Los Alamos National Laboratory (LANL) was represented by J. Abdallah, Jr. Two atomic structure codes have been developed at LANL, one semi-relativistic and the other fully relativistic. These structure codes are used to calculate the atomic structure parameters, which are later used for cross section calculations. Separate codes are available for calculating excitation and ionization processes. The results of the atomic data calculations are used in an atomic kinetics code. The semi-relativistic atomic structure, excitation and ionization codes can now be run through an interface on the Web. There are no plans to make the fully relativistic codes nor the kinetics codes available publicly; however, requests for specific calculations will be considered.

M. Capitelli of the Dipartimento di Chimica, Università di Bari, Italy described work on collisions involving molecules. Calculations have been carried out for for electron-molecule excitation-dissociation involving vibrationally excited molecules H_2, D_2, O_2, N_2 as well as atom-diatom excitation, dissociation and recombination. Vibrational deactivation and recombination of molecules and atoms on surface (C, graphite, Cu) have also been calculated. Transport cross sections involving electronic excited states can also be calculated. A Boltzmann MC code for EEDF has been developed. A particle-in-cell (PIC) MC code for transport of ions is also available. Negative ion source modelling (two codes) can be carried out. These codes must be run in-house. It us expected that in about two years a database for the first two items will be on the Web. Atom-surface interaction is much more difficult and time-consuming; transport cross sections of electronically excited states in H are available on demand; BMC, PIC MC can be run on demand; e-molecule collisions from threshold to 100 eV, for atom-mol up to 3 eV can be calculated.

D. Reiter represented the Institute for Plasma-Physics, FZ-Jülich, Trilateral Euregio Cluster. He has worked on the development of a MC neutral particle and radiation transport code. There are currently some facilities for using and calculating atomic data (CS, rates). There is a set of collisional-radiative (CR) model data for H, H_2, He, N and N_2. Hydrocarbon and silane databases also exist, as well as data for elastic scattering (classical interaction potentials) for D^+ on D_2, He and noble gases. All of the data, some processing and visualization of data, and code documentation are online at URL http://www.eirene.de. The code has been installed at many locations.

D. Kato of the National Institute for Fusion Science (NIFS), Japan discussed work on electron transfer and emission in ion-solid collisions. Energy shift and level broadening of H can take place above metal surfaces. The development of an SC code for the calculation of single-electron transfer between proton and metal surface is in progress; ionization probability and

occupation probability for outgoing particles can also be calculated. An MC code for secondary electron emission by electron impact 100 eV – 10 keV (Dr. Ohya, Tokushima University) is also being developed. Some further improvements are required (under development) before the code is ready for general use. Important targets will include W, Mo and Be.

Fumihiro Koike of Kitasato University discussed work on many electron atoms relevant to plasma analysis, as well as the GRID system developed by the EUVL team and others. The electronic states and dynamics of multiply-charged ions with multiple electrons are calculated using GRASP-92 and RATIP (Fritszche). Calculations can currently be undertaken on demand for some cases. These many-electron systems may require significant computing for completion. Although GRASP is available, this code requires great care in running. Issues such as convergence may be an issue.

V. Lisitsa of the Nuclear Fusion Institute, Russian Research Center "Kurchatov Institute", Moscow, Russia presented work on a simplified universal numerical node for radiative losses at arbitrary plasma parameters. Compton-Born tables are available for the ionization of neutral atoms and spectral line shapes (SLS) for transition between highly-excited states (astrophysical applications, radiolines). Currently, the code can be run in-house, and is still undergoing testing. Compton-Born has been tested for several atoms with more extended comparison necessary. The SLS data table is available for $H_{n\alpha}$, $H_{n\beta}$ spectral lines.

Y. Ralchenko of the National Institute of Standards and Technology (NIST) presented work on atomic and plasma spectral modeling. NIST has atomic structure codes (MCDF, MCHF), codes for ionization and excitation of neutral species (BEB method), and for CR modelling of non-Maxwellian plasmas. Online calculation of plasma emission under Saha/LTE conditions can be carried out. Atomic structure databases (evaluated and recommended data) are available. Structure codes (MCHF, GRASP) can be downloaded, the Saha/LTE code runs on-line, collisional cross sections and/or CR calculations can be undertaken on demand, and more CR codes are to appear soon for on-line calculations.

3. Recommendations and Conclusions

After summarizing current status, discussion focused on areas requiring further work. The following areas would benefit significantly from increased development work:

1. Extensive calculations of power loss results from plasmas for comparisons.
2. Total electron-impact ionization cross sections for neutral atoms (Compton data), including excited states.
3. Development of scaling laws for a large variety of atomic processes (some development has taken place, but much more work is needed).
4. Experimental data for many processes - experiments are often expensive and time consuming, but are essential to validate theoretical methods.
5. Modularity of application codes (atomic, transport, …….) for comparison purposes.
6. Common repository of datasets.
7. Development of XML schema for atomic and molecular data.
8. Development of standardized test cases for sensitivity studies of plasma modelling codes with respect to different data sets.

Hopefully, participants will be able to address some if not all of these issues.

All attendees agreed that a code centre network would be a valuable addition to fusion energy research, and were willing to participate. After much discussion, it was proposed that members of such a network would make a commitment to assist fusion-related research through a number of avenues.

A commitment to data generation would be a major part of the network. Members with data production capability will set priorities for data generation, generate such data as needed within constraints at the home institute, continue to make resources available on line, and undertake code verification. Data dissemination would be carried out through formation of web-based databases and through coordination with existing data centres. Code improvement and development would take place in response to feedback from data users. A web page for the Network will be developed in collaboration with all members. Each member will submit material that summarizes their capabilities and includes links to the code centre. Instructions for either running the codes on-line, or for requesting a specific calculation should be made available. There is also the need for increased membership of the network to ensure a wider coverage of plasma processes, particularly for plasma-surface interactions.

Appendix 1

IAEA Technical Meeting:
Establishment of A+M Computer Code Network

23-25 May 2005, IAEA Headquarters, Vienna, Austria

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Appendix 2

IAEA Technical Meeting:
Establishment of A+M Computer Code Network

23-25 May 2005, IAEA Headquarters, Vienna, Austria

Agenda

Monday, 23 May **Meeting Room: F-05-79**

09:30 - 09:45 Opening (R.E.H. Clark, Head, A+M Data Unit, A. Trkov, NDS)
Adoption of Agenda

Session 1:.*Current Activities of Potential Code Centres*

Chairman: M. Capitelli

09:45 - 10:30 D. Stotler
Atomic & Molecular Data Usage in the DEGAS-2 Monte-Carlo Neutral Transport Code

10:30 - 11:00 *Coffee Break*

11:00 - 11:45 I. Bray
The Convergent Close-coupling Method for Electron-atom Scattering

11:45 - 12:30 A. Dubois
Closed Channel Calculations in Ion-atom/molecule Collisions

12:30 - 14:00 *Lunch*

Session 2: *Current Activities of Potential Code Centres (Continued)*

Chairman:I. Bray

14:00 - 14:45 I. Rabadan
Calculation of Cross Sections for Ion-atom and Ion-molecule Collisions

14:45 - 15:30 J. Abdallah, Jr.
Los Alamos National Laboratory (LANL) Atomic Physics Codes on the Internet

15:30 - 16:00 *Coffee Break*

16:00 - 16:45 M. Capitelli
Dynamics and Modeling of Negative Ion Sources

16:45 - 17:30 D. Reiter
Atomic and Molecular Data Issues for ITER, and the Status of Databases for the EIRENE Code

17:30 - *Meeting Dinner, to be announced*

Tuesday, 24 May

Session 3: *Current Activities of Potential Code Centres (Continued)*

Chairman: A. Dubois

09:00 - 09:45 D. Kato
Program Code Activity at the NIFS for Electron Transfer and Emission in Ion-solid Collision

09:45 - 10:30 F. Koike
Calculations of Many Electron Atomic Ions Relevant to the Analysis of Various Plasmas

10:30 - 11:00 *Coffee break*

11:00 – 11:45 V. Lisitsa
Universal Kinetic Code for Radiative Losses at Arbitrary Plasma Parameters

11:45 – 12:30 Y. Ralchenko
Atomic and Plasma Spectrum Modelling at NIST

12:30 - 14:00 *Lunch*

Session 4: *Summary of Code Capabilities*

Chairman: J. Abdallah, Jr.

14:00 - 15:30 Summarization of Current Status of Code Capabilities (all participants)

15:30 - 16:00 *Coffee Break*

16:00 - 17:30 Discussion Continued

Wednesday, 25 May

Session 5: *Discussion of Data Centre Network*

Chairman: D. Reiter

09:00 - 10:30 Goals of the Network; Proposal for Framework; Recommended Participants

10:30 - 11:00 *Coffee Break*

11:00 - 12:30 Discussion, Continued

12:30 - 1400 *Lunch*

Session 6: *Meeting Conclusions and Recommendations*

Chairman: D. Stotler

14:00 - 15:30 Formulation of Meeting Conclusions

15:30 - 16:00 *Coffee Break*

16:00 - 17:30 Discussion, Continued

17:30 - *Adjournment of Meeting*

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