

**IAEA**

International Atomic Energy Agency

# Technical Meeting on Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications

International Atomic Energy Agency  
Vienna, Austria

19-21 December 2016

Ref. No: IAEA-A9-TM-52452

## Information Sheet

### A. Background

Computer simulations play a critical role in understanding physical and chemical systems. In the last decades verification, validation and uncertainty quantification (VVUQ) of computer simulations has become an important research topic in the physical and chemical sciences and engineering. In support of optimization-based design of fusion reactor and high precision diagnostics of plasmas in fusion devices the IAEA atomic and molecular data unit has been pursuing VVUQ activities for theoretical atomic and molecular (A+M) data. Our objective is to encourage and support the data development community to provide data users with reasonable uncertainty estimates for calculated A+M data. After a series of meetings and discussions with theoretical atomic physicists organized by the Unit it has become clear that the VVUQ methods for theoretical data should develop in collaboration with experimental physicists and benchmark experiments.

### B. Objectives

The meeting is meant to advance data-oriented research on A+M processes and properties that are important for fusion plasma simulation, fusion plasma diagnostics and fusion energy technology. Leading theoretical and experimental A+M physicists are invited along with plasma physicists using

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A+M data to discuss uncertainty assessments and benchmark experiments for A+M data that are important for fusion studies. The discussion topics are as follows:

- Target uncertainties of A+M data for fusion applications.
- Prioritization of A+M data needs for fusion applications.
- Experimental methods and systems to benchmark theoretical A+M data.
- Uncertainty quantification methods for theoretical A+M data.
- Network of A+M physicists doing benchmark experiments and computations.

Among other things the meeting will identify the most important data needs for fusion applications, decide what can be done to benchmark those data and formulate a plan of action among experimental and theoretical A+M physicists to carry out this benchmarking and perform the associated uncertainty assessment. Questions to be addressed include:

- How can benchmarking measurements be organized taking into account the most recent developments in the experimental as well as theoretical areas?
- How can detailed measurements of the reaction dynamics, as benchmarks for theory, help to improve reliability of theoretical calculations for a given collision system?

The discussions should lead to specific proposals for measurements to set new benchmarks for prioritized data. These measurements will obviously be very difficult in some cases, but they will set the standard. Along with the discussions about new benchmark experiments there will be discussions and proposals about suitable theoretical methods to compute these data, and how and by whom this can be done. Obviously these calculations should be accompanied by a full discussion of the inherent uncertainties.

## C. Format

The meeting will feature invited and contributed oral presentations, a poster session and discussion sessions. It is expected that the duration of invited talks will be 20 minutes and that of contributed talks will be 12 to 15 minutes. An electronic projector connected to a computer with a slot for a USB flash drive or memory stick will be available for the presentations (PDF or Power Point format).

Discussion sessions will be dedicated to data research needs for atomic and molecular processes; priorities for data development and evaluation, recommendations for benchmark experiments and calculations, and procedures for uncertainty assessment.

Please refer to the meeting web page (see below) for current information about invited speakers and for a tentative meeting schedule.

The working language of the meeting will be English. All communications must be sent to the IAEA in English.

## D. Participation

### (a) Submission of abstracts

Participants wishing to present a paper during this meeting must submit an abstract to the organizers. A one-page abstract must be submitted as an email attachment before 15 August 2016. The abstract

submission email must contain the author's name, affiliation and email address. The filename should be in the following format: Lastname.Initials.ShortTitle filetype. The abstract should be submitted by email to: H.Chung@iaea.org.

Please use page size A4 (21 cm by 29.7 cm), vertical orientation and margins of 25 mm on all sides. Please use Times New Roman (TNR) font throughout and then:

- Title: centered, single-spaced, 14-point size, bold, first letters capitalized
- Authors: centered, single-spaced, 12-point size, bold
- Affiliation: centered, single-spaced, 12-point size, italics
- Text: single spaced, 12-point size

The length is limited to one page. Authors must make sure that the files do not include copyrighted fonts or other impediments to reproduction. Authors are urged to make use of the Abstract template available from the IAEA web page for the meeting (see below).

### **(b) Acceptance of papers/posters**

Authors will be informed by 1 September 2016 as to whether their abstract has been accepted by the Scientific Advisory Committee. At the same time, authors will be advised as to whether their paper has been accepted for oral presentation or for presentation as a poster.

### **(c) Expenditures**

No registration fee is charged to participants.

As a general rule, the IAEA does not pay for travel and living expenses of participants. However, limited funds are available to help meet the cost of attendance of selected specialists, mainly from developing countries with low economic resources. If governments wish to apply for a grant on behalf of one of their specialists, they should address specific requests to this effect to the Scientific Secretary of the meeting. Governments should ensure that applications for grants:

- are received by the IAEA before 24 August 2016;
- are accompanied by a duly completed and signed Grant Application Form (Form C); and
- are accompanied by a duly completed and signed Form for Submission of a Paper (Form B) and abstract.

Awards will be announced after 15 September 2016.

### **(d) Documents and Publications**

A preliminary programme of the meeting will be made available on the meeting web page. The final programme and the Book of Abstracts will be available upon registration at the meeting.

A meeting report will be produced on the basis of the proceedings of the meeting. The report will summarize presentations, discussions and recommendations contributed by the meeting participants.

## **E. Venue and Accommodation**

The meeting will be held at IAEA Headquarters (conference room M2). Detailed information on accommodation and other administrative details will be made available on the meeting web page (see below) well in advance of the meeting.

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Designated participants who require a visa to enter Austria should submit the necessary application to the nearest diplomatic or consular representative of Austria as soon as possible. The official letter of invitation from the IAEA usually serves to assist with visa arrangements.

## F. Key Deadlines

- Submission of Abstracts (one page, sent to organizers): 15 August 2016
- Submission of Forms A and B (transmitted to IAEA via national authority): 24 August 2016
- Notification of acceptance of papers/posters: 1 September 2016

## G. Scientific Advisory Committee

- H.-K. Chung (Scientific Secretary), IAEA; B. J. Braams, IAEA;
- R. Bartschat, Drake University, Des Moines, IA, USA;
- S. Buckman, Australian National University, Canberra, Australia;
- I. Murakami, National Institute for Fusion Science, Toki-City, Japan;
- D. R. Schultz, University of North Texas, TX, USA;
- J. Tennyson, University College London, UK;
- D. Reiter, Forschungszentrum Jülich, Germany;
- A. Wolf, Max Planck Institute for Nuclear Physics, Heidelberg, Germany.

## H. Meeting Web Page

Please visit the following IAEA web page for new information regarding this meeting:

<https://www-amdis.iaea.org/meetings/UO2016/>