Monday, November 9th, 9:00 am - 9:45 am, Invited Talk

Internationally Coordinated Activities of Uncertainty Quantification and Assessment of Atomic, Molecular and Plasma-Surface Interaction Data for Fusion Applications

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Abstract
The Atomic and Molecular (A+M) Data Unit at IAEA aims to provide evaluated and recommended databases in the area of A+M processes and plasma-material interaction (PMI) processes too for nuclear fusion and other plasma applications. As needs grow for comprehensive, complex and sophisticated data sets for A+M and PMI processes, available data are predominantly and unavoidably calculated data. Unfortunately, there is no tradition of estimating uncertainties in calculated data and there is no accepted formal procedure for evaluating and recommending such data. Recently, an editorial standard of Physical Review A requires that certain classes of atomic data must be published with uncertainty information and it specifies that advances in techniques for the evaluation of data and assessment of uncertainties qualify as "new physics" [1]. Therefore the community is beginning to recognize that uncertainty assessment and evaluation and recommendation of theoretical A+M data is an independent scientific interest.

The science of uncertainty assessment for theoretical A+M collision data may be viewed from the perspective of Uncertainty Quantification (UQ) for simulation of complex systems [2], but there are important differences. The field of UQ has strongly emphasized complex systems such as the coupled atmosphere-ocean system or large engineering systems, for which in many cases the basic equations are not well established, involve poorly known parameters and functional dependencies, include stochastic elements and give rise to chaotic behavior. A mathematical core of UQ, polynomial chaos, is concerned with uncertainty propagation for dynamical systems.

Atoms and small molecules may not be complex systems, but it is computationally hard to solve the many-body quantum mechanics governing the system. For these simple physical systems that are of high computational complexity a new science of uncertainty assessment needs to be developed, or at least a new branch of the developing science of UQ. Possible approaches include the Unified Monte Carlo (UMC) method [3] to estimate uncertainties and their correlation structure, which is intensively used for nuclear scattering data.

The A+M Data Unit is encouraging work to develop guidelines for critically assessing theoretical atomic and molecular structure and collision data, taking into account the process and the quantity of interest as well as specific theoretical methods employed in calculations. A joint ITAMP-IAEA workshop was organized in July 2014 [4] to discuss sources of uncertainty in the physical models and computational methods employed for studying processes of our interest: electron collisions with atoms, ions, and molecules, heavy-particle collisions, and also electronic structure of atoms and molecules as input in a collision calculation. We also begin to collaborate with researches in the PMI fields of electronic structure calculations, molecular dynamics and multi-scale modeling to address UQ issues. The progress towards guidelines for evaluation of theoretical A+M collision data and internationally coordinated activities at IAEA towards the UQ sciences of A+M/PMI data will be reviewed.

References
[1] Editorial in Phys. Rev. A 83, 040001 (2011).
[2] National Research Council Committee on Mathematical Foundations of Verification, Validation, and Uncertainty Quantification: "Assessing the reliability of complex models: mathematical and statistical foundations of verification, validation and uncertainty quantification." NAP Press, 2012. http://www.nap.edu/openbook.php?record_id=13395.
[3] R. Capote and D. L. Smith. "An investigation of the performance of the Unified Monte Carlo method of neu-tron cross section data evaluation." Nuclear Data Sheets 109 (2008) 2768-2773.
[4] Joint IAEA-ITAMP Technical Meeting on Uncertain-ty Assessment for Theoretical Atomic and Molecular Scattering Data, ITAMP, Cambridge, Massachusetts, USA, 7-9 July 2014. https://www-amdis.iaea.org/meetings/ITAMP/.

Biography

Hyun-Kyung Chung graduated from Seoul National University, Republic of Korea, in 1992 and received a Ph.D in 1998 at University of Wisconsin-Madison in the Department of Nuclear Engineering and Engineering Physics on the topic of atomic processes in plasmas. She did her postdoctoral work at Harvard-Smithsonian Center for Astrophysics, Institute of Theoretical Atomic Molecular Optical Physics (ITAMP) on the topic of line broadening of high pressure sodium vapor and worked at Lawrence Livermore National Laboratory in the field of high energy density physics before joining the atomic and molecular data unit of the nuclear data section at IAEA (International Atomic Energy Agency) in 2009.

Main research topics are studies of atomic processes to understand extreme plasma states produced in laboratory and astrophysical objects. Her time-dependent collisional-radiative code FLYCHK, available at the NIST website (http://nlte.nist.gov/FLY), is widely used by the plasma community for spectroscopic analysis. She is one of the recipients of 2015 John Dawson Award for Excellence in Plasma Physics Research. At IAEA, she coordinates research projects for atomic, molecular and plasma-material interaction data for fusion applications and serves in the editorial board of an open access journal Atoms and the journal of Atomic Data and Nuclear Data Tables.