Steps Towards Uncertainty Assessment for Calculated Atomic and Molecular Data

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The Atomic and Molecular Data Unit at IAEA is responsible for databases in the area of atomic and molecular processes (and plasma-material interaction processes too) for nuclear fusion. The Unit encourages data development primarily through the mechanism of IAEA coordinated research projects (CRP) and among our recent CRPs has been one on processes of light elements in fusion plasma, one on collisional and radiative processes of tungsten ions and one on atomic and molecular processes of hydrogen and helium. We aim to provide evaluated and recommended data and this in turn requires an assessment of uncertainties in the data. Cross sections and rates for state-resolved collision processes are almost always calculated and therefore the community is faced with the problem of obtaining uncertainty estimates for calculated scattering data [1].

In the present contribution we look at the problem of uncertainty estimates for calculated atomic scattering data in the context of other areas of scientific computing where uncertainties are being studied. On one side of the spectrum lies the established science of numerical analysis, where one deals with precisely specified problems and one develops a theory of discretization error and rounding error. On another side of the spectrum lies the emerging science of Uncertainty Quantification (UQ) for simulation of complex systems [2]; generally systems for which 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.

Atomic and molecular scattering processes occupy their own territory different from numerical analysis and from complex systems. Atoms and small molecules are not complex systems, but they are computationally hard because their description relies on many-body quantum mechanics. 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. We discuss possible approaches including the Unified Monte Carlo (UMC) method [3] to estimate uncertainties and their correlation structure. We also note rigorous lower-bound methods for electronic structure and their possible role in uncertainty estimation.

[1] Joint IAEA-ITAMP Technical Meeting on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data, ITAMP, Cambridge, Massachusetts, USA, 7-9 July 2014.
https://www-amdis.iaea.org/meetings/ITAMP/.

[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 neutron cross section data evaluation." Nuclear Data Sheets 109 (2008) 2768-2773.