

Internationally Coordinated Activities of Uncertainty Quantification of Atomic, Molecular and Plasma- Surface Interaction data for Fusion applications

H.-K. Chung and B. J. Braams

IAEA Nuclear Data Section, Atomic and Molecular Data Unit

Consultants' Meeting on Recommended Data for Atomic Processes of Tungsten Ions
September 14-16, 2015, KAERI, Republic of Korea



IAEA

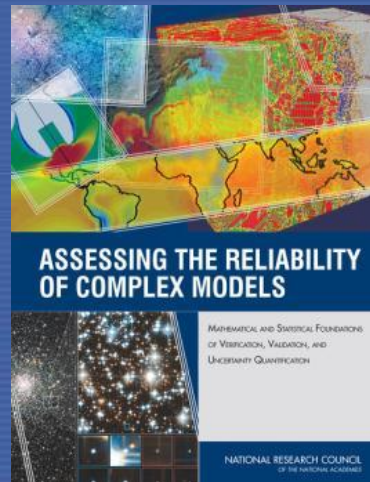
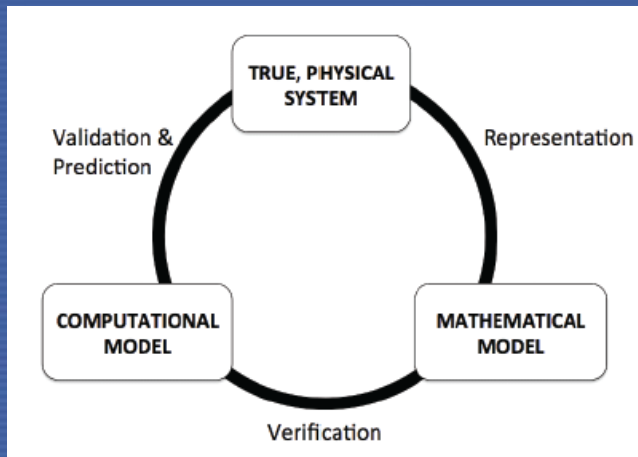
International Atomic Energy Agency

Atomic, molecular and plasma-surface interaction data

CRITICAL ASSESSMENT OF DATA FOR FUSION

Critical Assessment for Modeling of Physical Processes (optimized based design)

- **Verification.** The process of determining how accurately a computer program (“code”) correctly solves the equations of the mathematical model.
- **Validation.** The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model
- **Uncertainty quantification (UQ).** The process of quantifying uncertainties associated with model calculations of true, physical QOIs, with the goals of accounting for all sources of uncertainty and quantifying the contributions of specific sources to the overall uncertainty.



NSF Division of Mathematics and Physical Sciences should encourage interdisciplinary interaction between domain scientists and mathematicians on the topic of **uncertainty quantification, verification and validation**, risk assessment, and decision making. (2012)

Coordination Meetings for Evaluation

<http://www-amdis.iaea.org/DCN/Evaluation/>

Feb 12

- CM on Procedures for Evaluation of AM/PMI Data for Fusion: Current status & future coordination (Japan)

Jun 12

- CM on Data Evaluation & Establishment of a Standard Library of AM/PMI Data for Fusion (IAEA)

Sep 12

- TM on Data Evaluation for AM/PSI Processes in Fusion (Korea)

May 13

- TM (CCN) on General Guidelines for Uncertainty Assessments of Theoretical Data

Dec 13

- CM on Evaluation of Data for Collisions of Electrons with Nitrogen Molecule and Nitrogen Molecular Ion

Jul 14

- Joint IAEA-ITAMP TM on Uncertainty Assessment for Theoretical Atomic Molecular Scattering Data

Jun 15

- CM on Guidelines for Uncertainty Quantification of Theoretical Atomic and Molecular Data

Jul 15

- CM on Evaluation & Uncertainty Assessment for Be, C, Ne
- TM (CCN) on Simulation of PMI Experiments

Sep 15

- **CM on Recommended Data for Processes of Tungsten Ions**

TM on Data Evaluation 2012

<http://www-amdis.iaea.org/meetings/NFRI2012/>

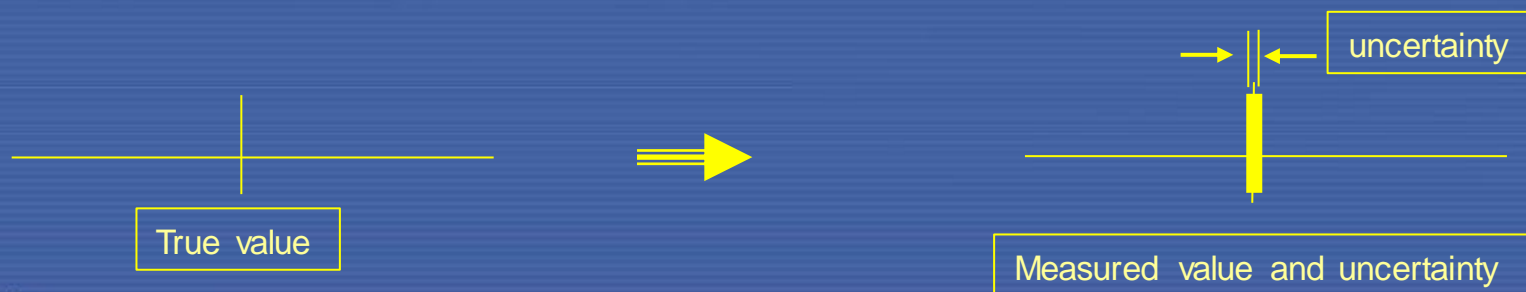
- More than 20 Participants from 11 countries
- Proceeding papers published at Fusion Science and Technology (2013)
- Community Consensus needed to produce evaluated/recommended data
 - Disseminate standard definitions of TERMINOLOGIES adopted internationally
 - Disseminate materials with the CRITICAL ANALYSIS SKILLS → NRC report
 - Involve COMMUNITY in data evaluation → eMOL, Group evaluation
- Technical Issues
 - Assessment for THEORETICAL data → UNCERTAINTY ESTIMATES
 - Assessment of EXPERIMENTAL data → Self-consistency checks
 - ERROR PROPAGATION and SENSITIVITY ANALYSIS → Uncertainties in “Data” & “Data Processing Toolbox”

International Code Centre Network

UNCERTAINTY QUANTIFICATION OF DATA

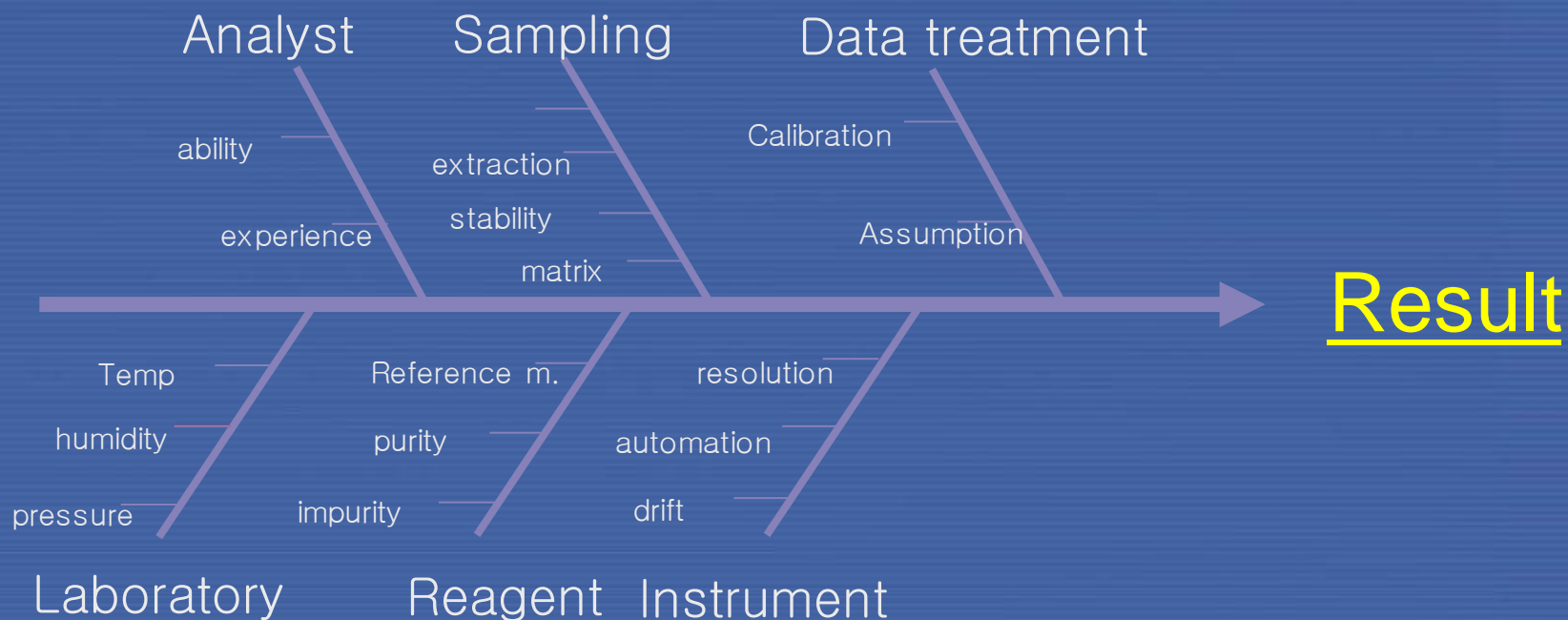
Uncertainty Quantification

- Terminology in metrology adopted by international communities
 - VIM (Vocabulaire International de métrologie, Bureau Int. des Poids et Mesures)
 - GUM (guide to the expression of uncertainty in measurement) 2008
- Conceptual Changes of Values and Uncertainties
 - True Value (Error Approach, ~ 1984) → A measure of the possible *error* in the estimated value of the measurand as provided by the result of a measurement
 - Measured Value (Uncertainty Approach) → A parameter that characterizes the dispersion of the quantity value that are being attributed to a measurand, based on the information used (VIM 3)



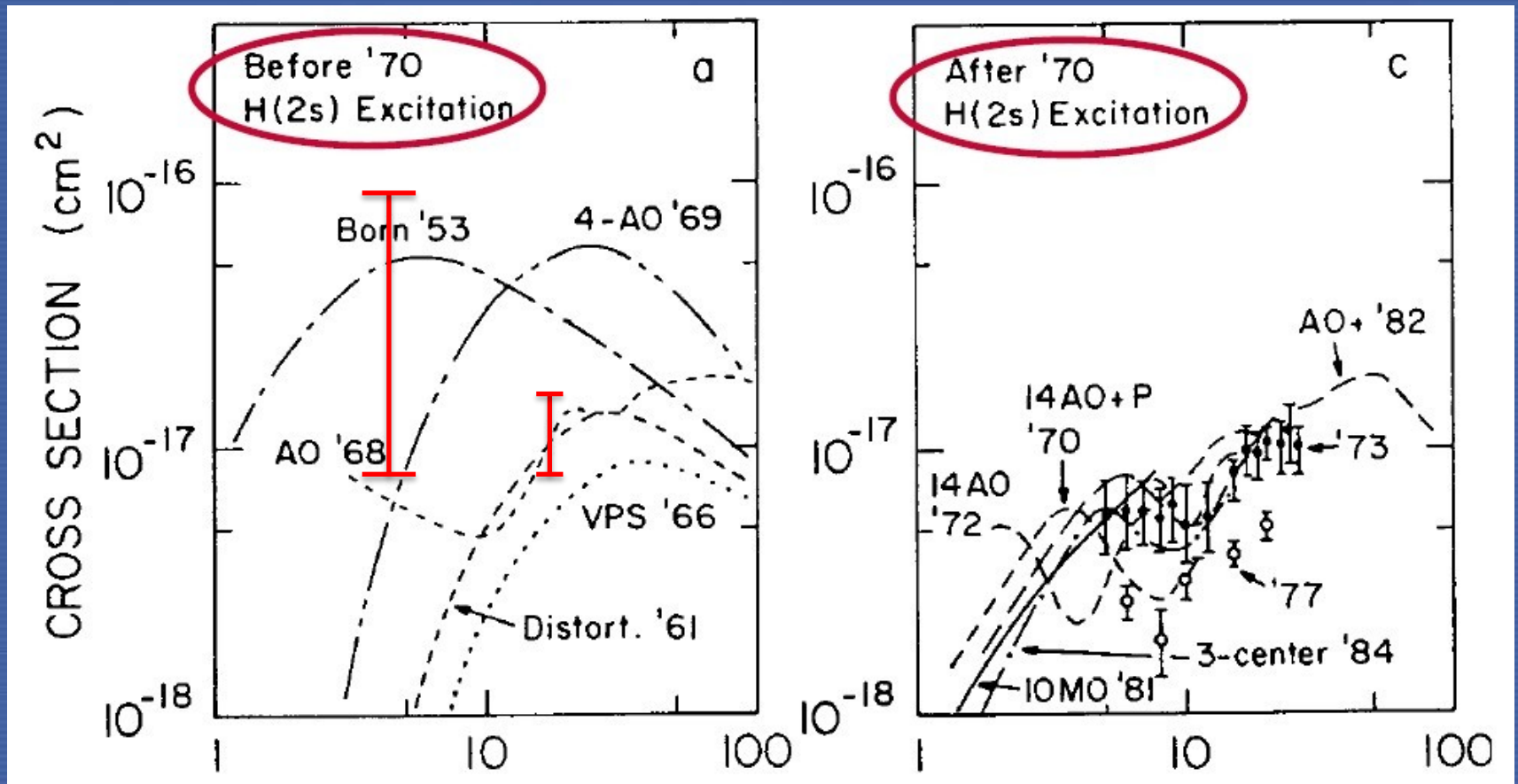
Uncertainty Evaluation

Guide to the expression of **U**ncertainty in **M**easurement (GUM),
BIPM, IEC, IFCC, ISO, IUPAC, IUPAP, OIML



Theoretical cross-sections without uncertainty estimates

"The Low-Energy, Heavy-Particle Collisions—A Close-Coupling Treatment"
Kimura and Lane, *AAMOP*, 26, 79 (1989)



What is the best way to assess the quality of theoretical data without physical measurements?

3rd Code Centre Network TM 2013

- Strategies to develop guidelines for the uncertainty estimates of theoretical atomic and molecular data
 - Depend on Target, Resolution, Observable of interest (QOI in NRC)
 - Atomic structures
 - State descriptions, operators, basis sizes, basis parameters, sensitivity
 - Special volume in “Atoms” journal – 5 papers on the topic
 - Atomic collisions
 - Highly accurate, computationally intensive codes vs production codes
 - Benchmark results, basis sets, different methods, consistency check
 - Molecular collisions
 - Target, resonances, different methods, consistency check

IAEA-ITAMP TM 2014 : Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data

- Bring together a number of people who are working on electron collisions with atoms, ions, and molecules, heavy-particle collisions, and electronic structure of atoms and molecules (~ 25 Participants)
- Come up with reasonable uncertainty estimates for calculations using the various methods of collision physics: perturbative, nonperturbative, time-independent, time-dependent, semi-classical, etc.
- Output → Guidelines for estimating uncertainties of theoretical atomic and molecular data
- *Publication in preparation*

Quantification of Theoretical Atomic and Molecular Data

- The maturity of physics and calculation procedures vary depending on the target system of the data. A UQ method should be established based on the physics “models” appropriate for the target.
- UQ methods are developed based on the applications or the quantity of interest (QOI).
- A quantity of interest (QOI) determines the resolution of measuring system. In some cases, calculated data with most details are needed and in other cases, averaged data are adequate for applications.

Uncertainty Quantification of Theoretical Electron-Atom Collision Data

Sources of Errors/Uncertainties

- Errors in the N-electron structure (energy levels, oscillator strengths, polarizabilities) can be expected to propagate into the collision problem.
- Errors associated with the cut-off in the close-coupling expansion, or the use of a perturbative method (plane-wave, distorted-wave to first or second-order).
- Approximations made in the treatment of relativistic effects.
- Numerical approximations (e.g., integration/discretization schemes, use of an R-matrix box etc.)

Uncertainty Quantification of Theoretical Electron-Atom Collision Data

Addressing and Estimating Errors/Uncertainties

- Purely numerical errors (space and time mesh, partial-wave convergence, etc.) should be negligible for "expert users".
- Structure problems are real, but they can, and should be, accounted for to the extent possible.
- The importance of relativistic effects can be tested by performing calculations in different models: non-relativistic with angular-momentum recoupling into a relativistic scheme; semi-relativistic (Breit-Pauli); and full-relativistic (in practice Dirac-Coulomb).
- Convergence checks of the close-coupling expansion, including the systematic use of pseudo-states to account for coupling to the ionization continuum.
- Suitability checks of (likely) more approximate methods by checking the matching of their predictions to those from (likely) more accurate methods.
- Comparison with experiment.