Evaluation Activities

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TM on "Technical Aspects of A & M Data Processing and Exchange
23rd Meeting of the A & M Data Centres Network"
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International Atomic Energy Agency

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 (Korea)

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"

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Community Role: Consensus Building

- Change of notions: Databases → Data research
- Enlighten young generation (in early career) that data evaluation is a critical part of scientific work
- Provide materials to teach "Critical Analysis Skills"
- Disseminate the standard definitions of terminologies adopted by international organizations (IAEA, IUPAC, IUPAP, BIPM, ISO, WHO, FAO, etc)
  - VIM (Vocabulaire International de métrologie, Bureau Int. des Poids et Measures) 2007
  - GUM (guide to the expression of uncertainty in measurement) 2008
- Agree on the procedure of evaluation towards a standard reference data

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Evaluation by the Community

- Group Evaluation: 4-5 panelists including young and senior people like the editorial board for a journal with the broad backgrounds (experimentalists, theoreticians, producers and users)
- eMOL project
  - Project to develop methodology for analysing, validating and recommending electron molecule collision data sets.
  - Each evaluation is a small group project by 4-7 people.
  - Aim to provide recommended datasets self-consistent and complete
- NFRI (National Fusion Research Institute, Korea) group evaluation
  - e-methane collisional data evaluation
- IAEA Consultant meetings
  - CM on e-N_2 collision data evaluation with eMOL project (Dec. 2013)
  - CM on Evaluation & Uncertainty Assessment for Be, C, Ne
  - CM on Recommended Data for Processes of Tungsten Ions

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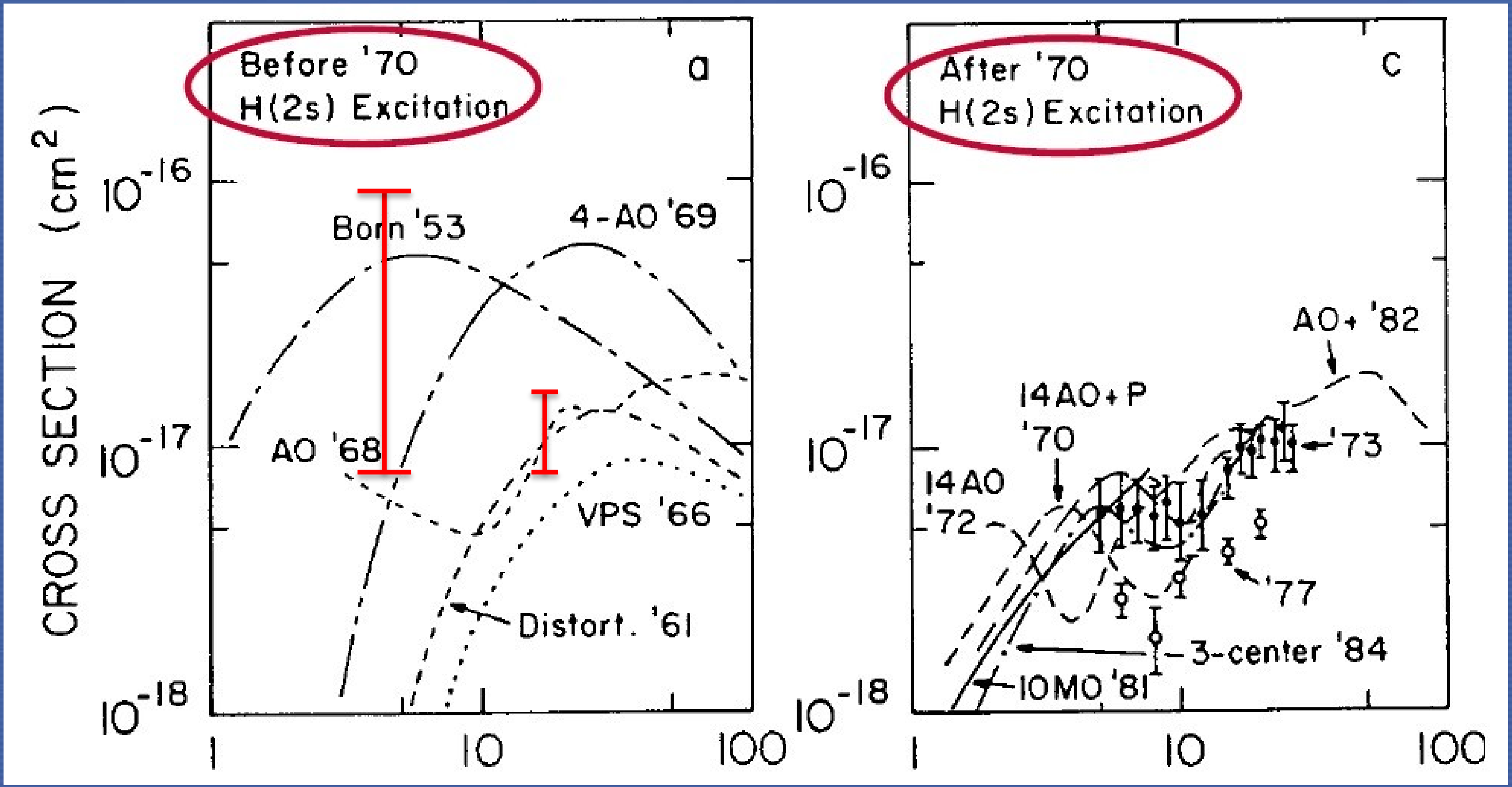
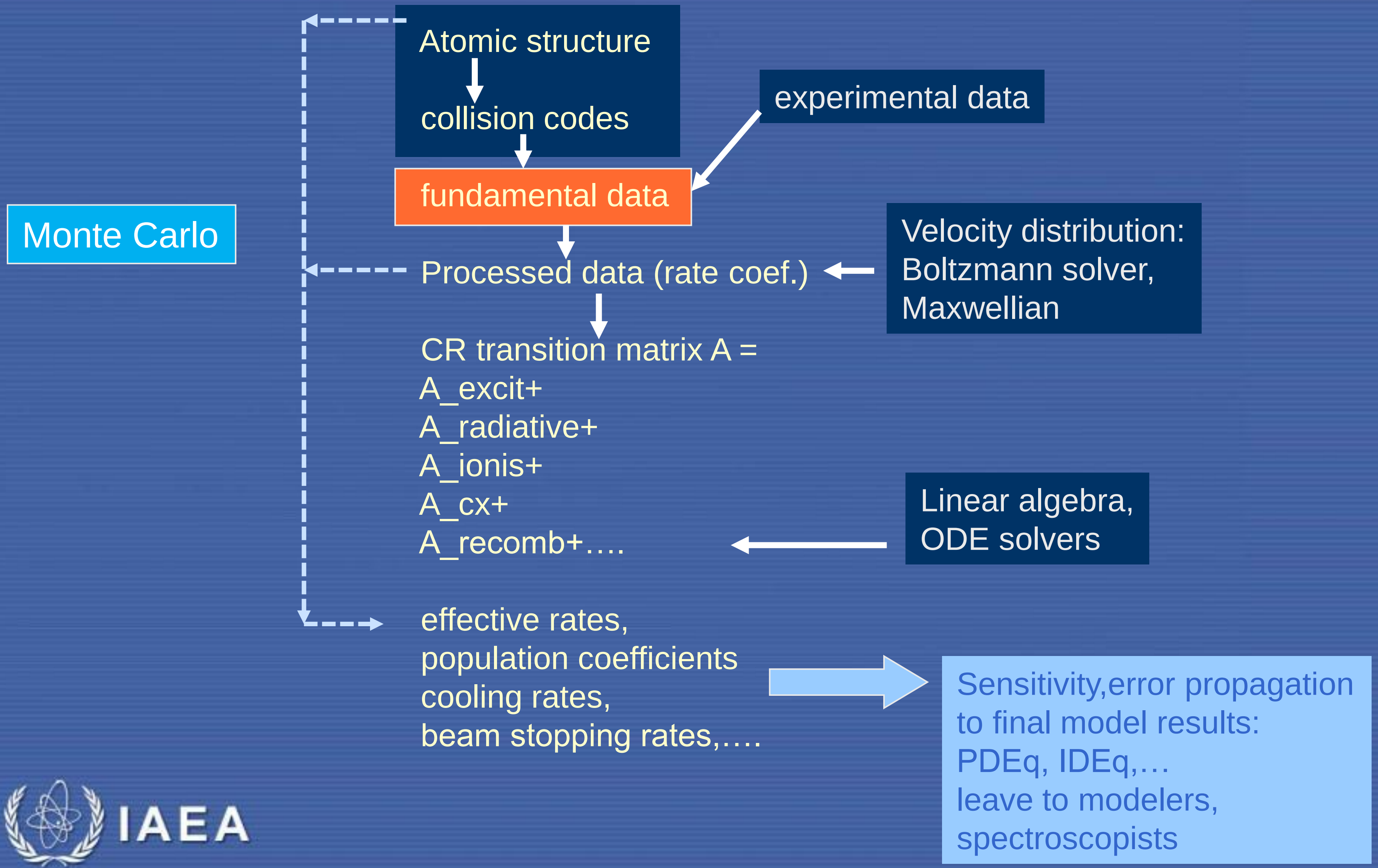
Theoretical cross-sections without uncertainty estimates

"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?

Error Propagation and Sensitivity Analysis:
Uncertainties in “Data” & “Data Processing Toolbox” ?



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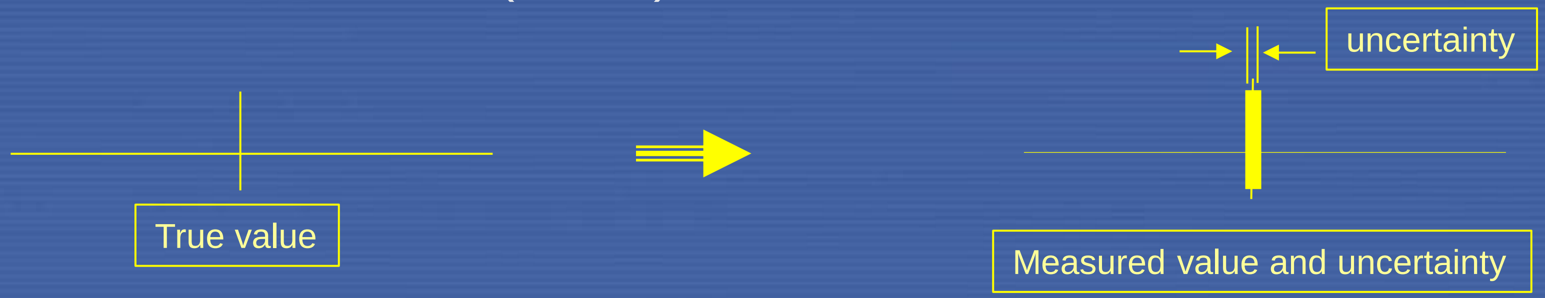
Uncertainty Quantification

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)



Critical assessment and evaluation of data became uncertainty quantification of data

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

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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.
- The concept of UQ was new to most participants and the meeting was valuable in drawing an attention from prominent physicists in the field of atomic and molecular collisions.
- Output → Guidelines for estimating uncertainties of theoretical atomic and molecular data
- *Publication in preparation*

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IAEA-ITAMP TM 2014: General Strategies

- 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.
- 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. UQ methods are developed based on the applications or QOI.
- A comprehensive bibliography and compilation of data led to comparisons of available data and hence evaluation of data.
- Evaluation of the data for conformance with expected physical behaviors and inter-comparison amongst theoretical and experimental results were possible if a large number of results exist and this methodology allows quantification of uncertainty of the recommended result to a certain extent.
- For cases in which only a single data set exists, such an approach is largely not applicable.

IAEA-ITAMP TM 2014: UQ of theoretical electron-atom 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.)

IAEA-ITAMP TM 2014: UQ of theoretical electron-atom data (cont'd)

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
- 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.

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IAEA-ITAMP TM 2014: UQ of theoretical electron-Molecule data

Molecular processes: Elastic scattering, rotational, vibrational and electronic excitation, dissociative recombination or attachment and Impact dissociation.

Consistency Check: Usually elastic scattering and electronic excitation calculations are performed within the fixed nuclei approximation. While rotational and vibrational excitation and dissociative recombination/attachment require specially developed methods for treating nuclear motion effects.

Source of Uncertainties:

- target model: It is straightforward to estimate uncertainties in structures (dipole moments etc) by systematic theoretical studies (focal point method) and/or comparison with measurement. The biggest issue is the quality of the target wavefunctions
- scattering model: the major source of (unquantified) uncertainty in electron scattering calculations. The most promising approach is probably represented by systematic studies using pseudo-state methodology. It would be helpful to have some benchmark studies on a number of exemplar problems.
- code/theoretical formalism: inter-comparison between major codes such the R-matrix (UKRMol), Schwinger and Kohn codes suggest that these implementations give very similar results for the same model

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4th Code Centre Network TM 2015

- Expand the UQ activities to the field of theoretical Plasma-Material Interaction data.
- Discuss the current status, challenges, open issues and future directions of the UQ activities for theoretical PMI data.
- Focus PMI fields to be directly related to hydrogen retention and migration physics
- Relevant topics
  - Interatomic potential constructions
  - Electronic Structure simulations (Density Functional Theory)
  - Molecular Dynamics simulations
  - Kinetic Monte Carlo simulations
  - Rate simulations

4^{th} Code Centre Network TM 2015 (cont'd)

Currently, UQ of theoretical PMI data are difficult due to

- Incomplete model descriptions for the systems of interest – it is unknown which physical processes have to be included etc. -- More interaction with experimentalists needed
- QUI determined by processes bridging many orders of magnitude in time & space and hence averaging processes at several levels are mandatory.
- Input parameters of limited or unknown accuracy

MD simulations are key simulation techniques for PMI, however, limited:

- When there is a need to resolve atomic vibrations (phonons) of the fs time scale, and simulation time is limited to nanoseconds
- Externally provided interaction potentials are of unknown accuracy
- MD potentials depends on accuracy of DFT simulations, which depend on the arbitrarily chosen exchange functionals.

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4th Code Centre Network TM 2015 (cont'd)

A global sensitivity approach may be only feasible way to multiscale-models

- Because tracing the uncertainties through all model stages is very challenging

Potential role of IAEA to promote UQ and PMI modeling

- A repository for DFTB (Slater-determinants) could be useful
- A similar meeting with experimentalists assessing the reliability/uncertainty of exp. Results in the PMI field
- Compilation of a best practice sheet for the exp. data preparation to establish a common standard
- Emphasize and support the up-stream incorporation of UQ techniques into the PMI modeling codes (TRIDYN, SOLPS, WallDyn, etc)

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CM on Guidelines for Uncertainty Estimates for Theoretical Atomic, Molecular Data

- Objective: Write a paper on Uncertainty Estimates for Theoretical Atomic, Molecular Data
- Participants: K. Bartschat, A. G. Csaszar, J. Tennyson & S. Kokooline, T. Kirshner, G. Drake
- Uncertainty Quantification (UQ) for:
  - Structure calculations: atoms and molecules
  - Electron collision calculations: atoms and molecules
  - Charge transfer calculations
- UQ in scattering calculations.
  - Target properties (energy levels, polarizability, dipole) associated with quality wavefunctions used.
  - Model contributions, including:
    - treatment of N-electron target vs. (N + 1)-electron collision problem
    - accounting for the nuclear motion effects
- Numerical uncertainty

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CM on Evaluation & Uncertainty Assessment for Be, C, Ne

- Objective: evaluate the current status of electron collisional data for Be, C and Ne atoms and recommend the best available data sets.
- Participants: K. Bartschat, C. Ballance, D. Fursa and Yu. Ralchenko
- Summary
  - B-spline R-matrix method, variants of CCC (Convergent Close Coupling) methods and RMPS (R-matrix Pseudo States) methods were compared
  - For e-Be scattering data, three codes agree within less than 10% and agree with oscillator strengths for optically allowed transitions.
  - Methods are mature enough for Be atoms and ions and for us to recommend the best e-Be collision data for use by the fusion community.
  - Recommended data using the CCC method and their uncertainties based on the comparison with results of B-spline R-matrix method and RMPS method calculations will be published.

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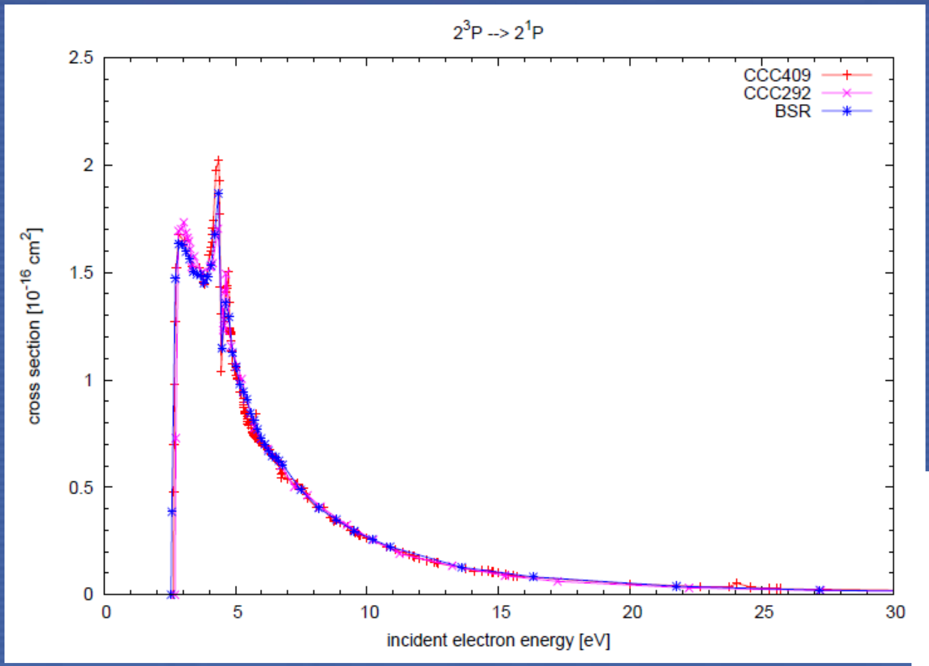
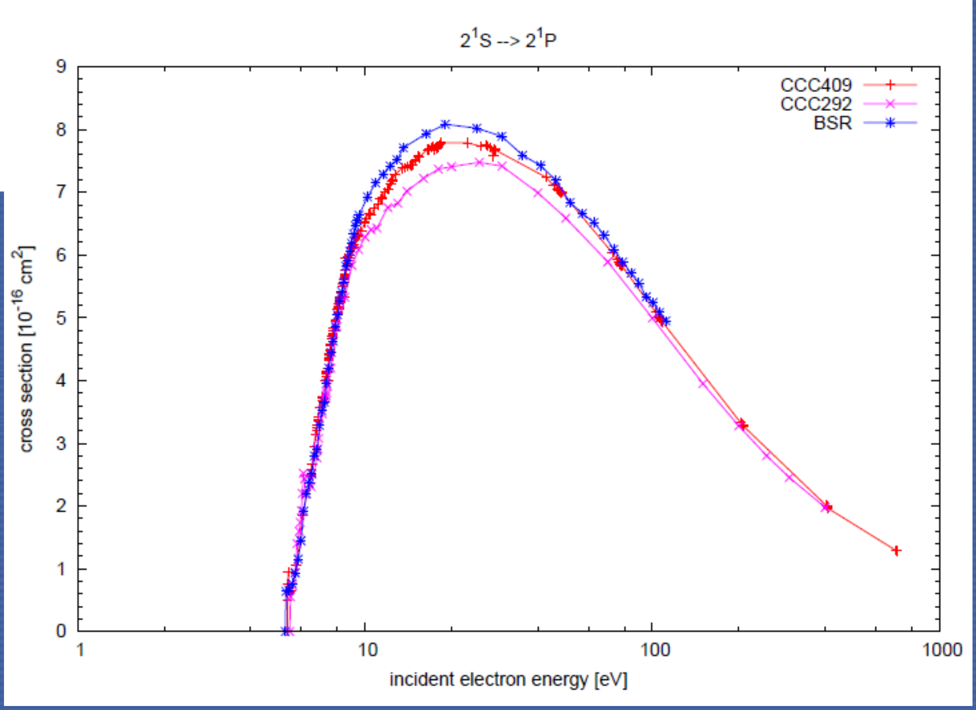
CM on Evaluation & Uncertainty Assessment for Be, C, Ne (cont'd)





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CM on Recommended Data for Processes of Tungsten

- Currently, there is a reliable set of ionization rate coefficients available for the community, however, a consistent and comprehensive set of dielectronic recombination (DR) rate coefficients is not available for all charge states of tungsten.
- Recognizing the need, the evaluation of total Maxwellian averaged dielectronic recombination (DR) data and recommend a data set from currently available data was the main topic of discussion
- Participants:
  - Bowen Li of Lanzou University, China
  - Xiaobin Ding of Northwest Normal University, China
  - Tomohide Nakano of Japan Atomic Energy Agency, Japan
  - Ehud Behar of Technion Israel Institute of Technology, Isarel
  - Connor Ballance of Queen’s University of Belfast, UK
  - Simon Preval of University of Strathclyde
  - Duck-Hee Kwon and Won-Wook Lee of Korea Atomic Energy Research Institute, Korea

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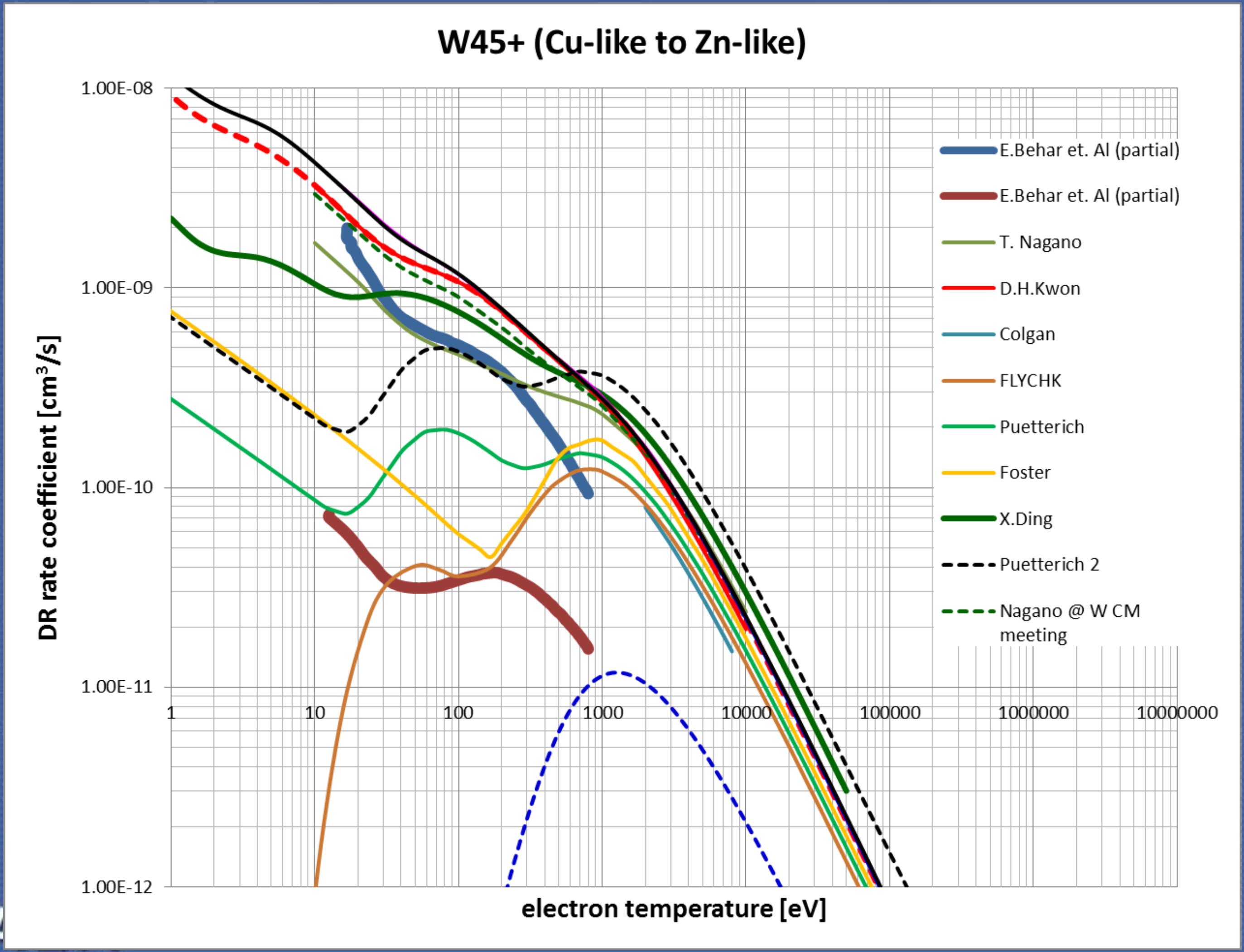
CM on Recommended Data for Processes of Tungsten (cont'd)



Future Work

- IAEA Atomic and Molecular (A & M) data unit is committed to work with atomic, molecular and plasma-material interaction (AM/PMI) data community on data evaluation and uncertainty quantification (UQ).
- There is more consensus in the atomic and Molecular data communities that an evaluation of data is a critical part of research (PRA and other journal policies).
- Researchers begin to see the value of the evaluation and UQ research as a validation of their work and an opportunity for a new physics.
- The understanding of UQ is still at the elementary level and there needs an established procedure of UQ.
- A systematic approach for UQ of AM/PMI data is required and it will require to collaborate with mathematical and computational sciences in the future.
- IAEA A& M data unit will continue to engage researchers in AM/PMI fields for UQ science and expand our network effort to other relevant interdisciplinary sciences in order to pursue the UQ science in data research.

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