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

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Outline

- IAEA A&M Data Unit Activities
- Critical Assessment of Data for Fusion
- Uncertainty Quantification of Data

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IAEA Atomic and Molecular (A+M) Data Unit to support for fusion program worldwide

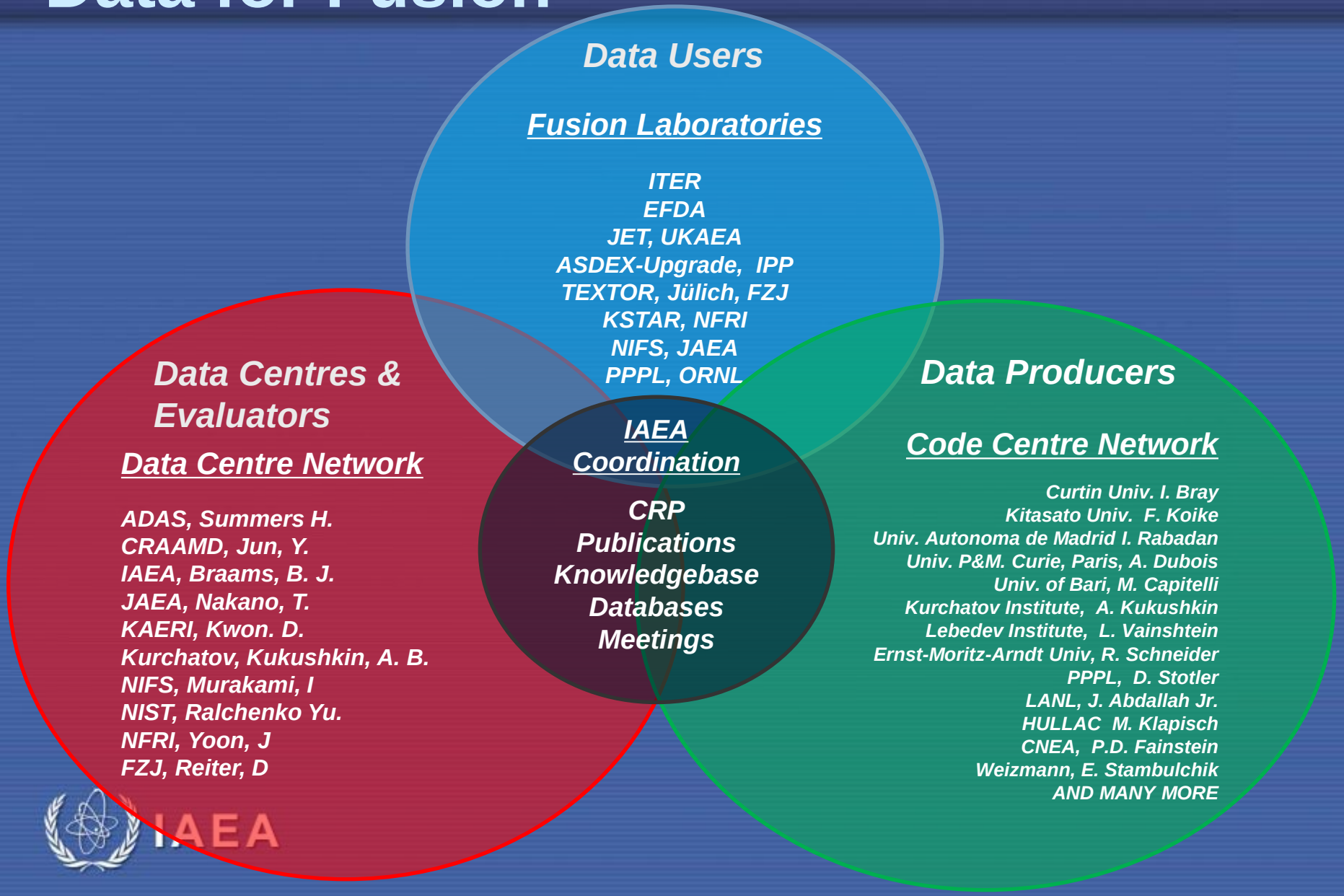
We say that we will put the sun into a box. The idea is pretty. The problem is, we don't know how to make the box. -- *Nobel prize winner Pierre-Gilles de Gennes*

Fusion research requires huge amounts of material data – AM/PSI data

- IAEA A+M Unit formed in 1977
- Review progress and achievements of *Atomic, molecular and plasma-surface interaction (A+M/PSI) data for Fusion programme* worldwide
- Stimulate international cooperation in measurement, compilation and evaluation of A+M / PSI data for fusion

Coordinated Research Projects
Publications
Knowledgebase
Databases
Meetings

Network Collaboration for AM/PSI Data for Fusion



Meetings and Publications (2003-2014)

- 88 meetings have been organized by the Unit for 12 years on average of 7.3/year. (TM, CM, RCM, Cooperation, WS)
- 76 INDC(NDS) reports have been published.
- 6 volumes of the series Atomic and Plasma-Material Interaction Data for Fusion (“Green Books”) have been published for CRPs.
- 8 volumes of the series International Bulletin on AM Data for Fusion have been published.
- 5 Special issues have been published or arranged for journal publication from the CRP, meetings and workshops (CCN, SLSP, ICTP, Tungsten)
- A book was published : Nuclear Fusion Research: Understanding Plasma-Surface Interactions (edited by R.E.H. Clark and D.H. Reiter, Springer, 2005)

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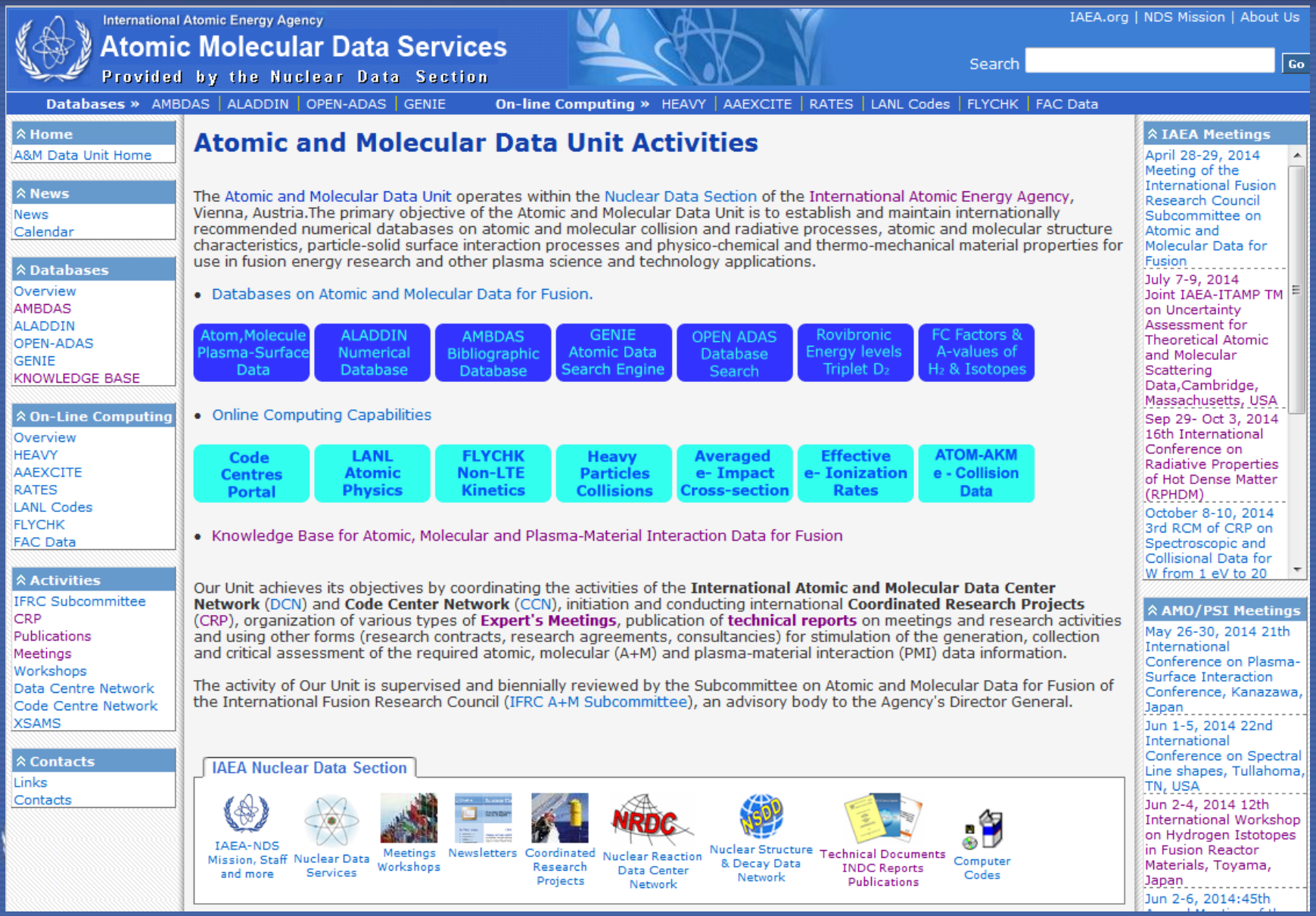
IAEA AMD Unit Home Page (AMDIS)

http://www-amdis.iaea.org



Code Centre Network (CCN)

http://www-amdis.iaea.org/CCN

Joint effort to gather and provide access to any information relevant for modellers in fusion plasma science

Purpose: To provide solutions to anyone willing AM/PSI data which can not be easily accessed on the web or which simply do not exist.

Tools: Online computing, Downloadable codes, Direct contacts for any expertise

Flexible group of participants

- Utilize CCN as a network for the coordination and collaboration on code activities
- Larger network with diverse background desirable (Codes, Models, Experiments)

CCN Interests:

- Uncertainties of code calculations
- An integrated database of recommended data and code capabilities
- Provision of complete sets and/or recommended data
- Activities to benefit code developers directly
  - Code comparison workshops (eg. NLTE7, SLSP)

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Atomic, molecular and plasma-surface interaction data

CRITICAL ASSESSMENT OF DATA FOR FUSION

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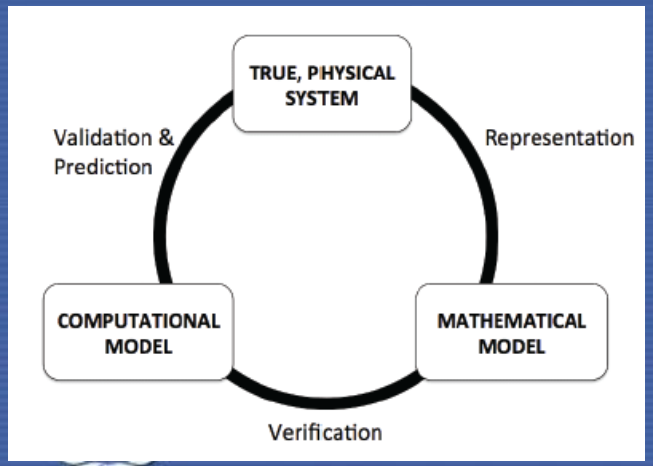
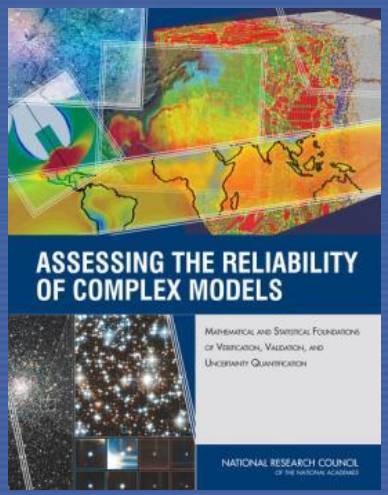
Critical Assessment for Modeling of Physical Processes (optimized based design)

- 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"

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UNCERTAINTY QUANTIFICATION OF DATA

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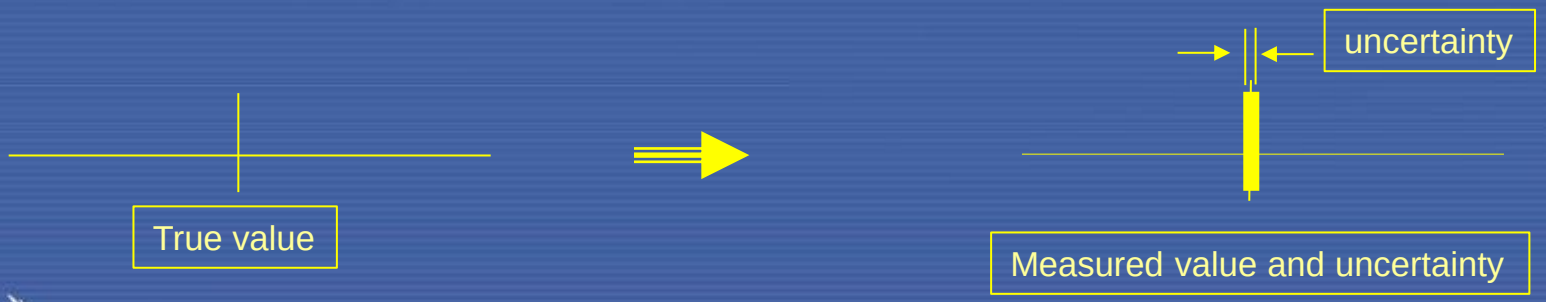
Uncertainty Quantification

- Terminology in metrology adopted by international communities
  - VIM (Vocabulaire International de métrologie, Bureau Int. des Poids et Measures)
  - 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)



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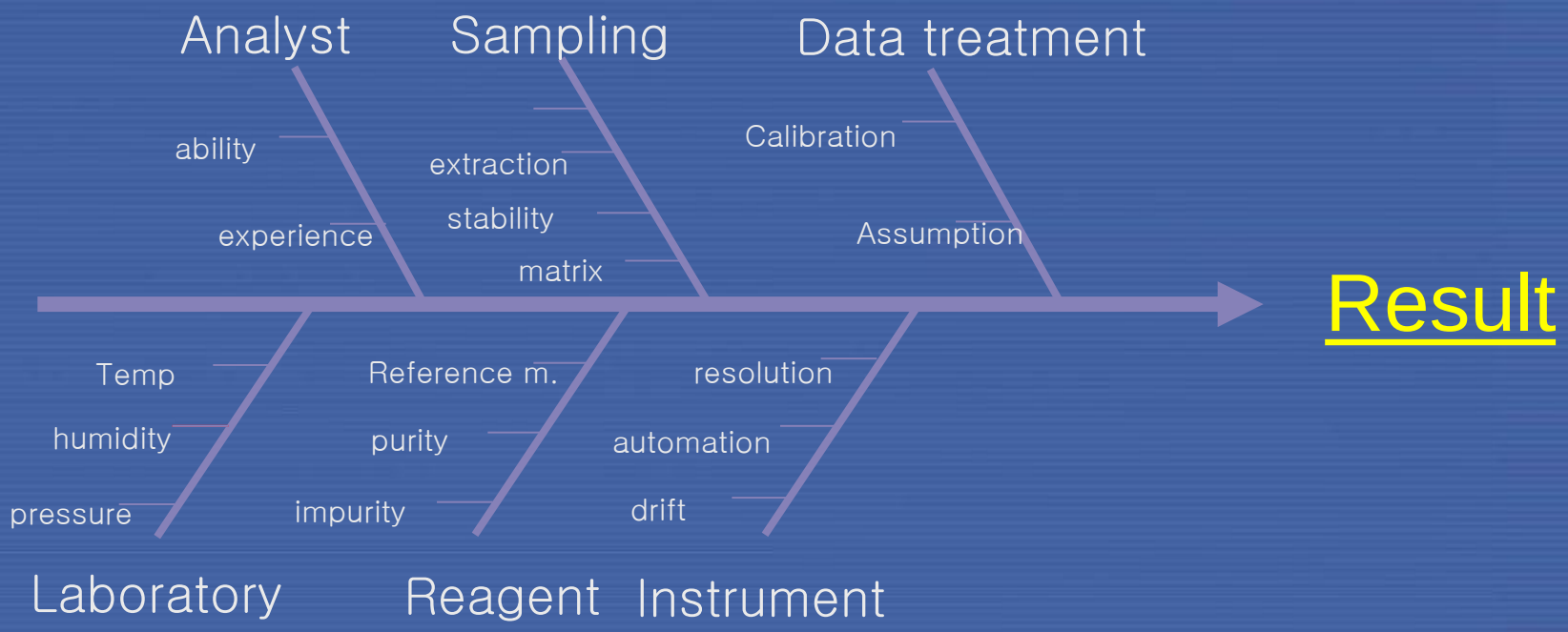
Uncertainty Evaluation

Guide to the expression of Uncertainty in Measurement (GUM),
BIPM,IEC,IFCC,ISO, IUPAC, IUPAP, OIML



Variation of each parameter

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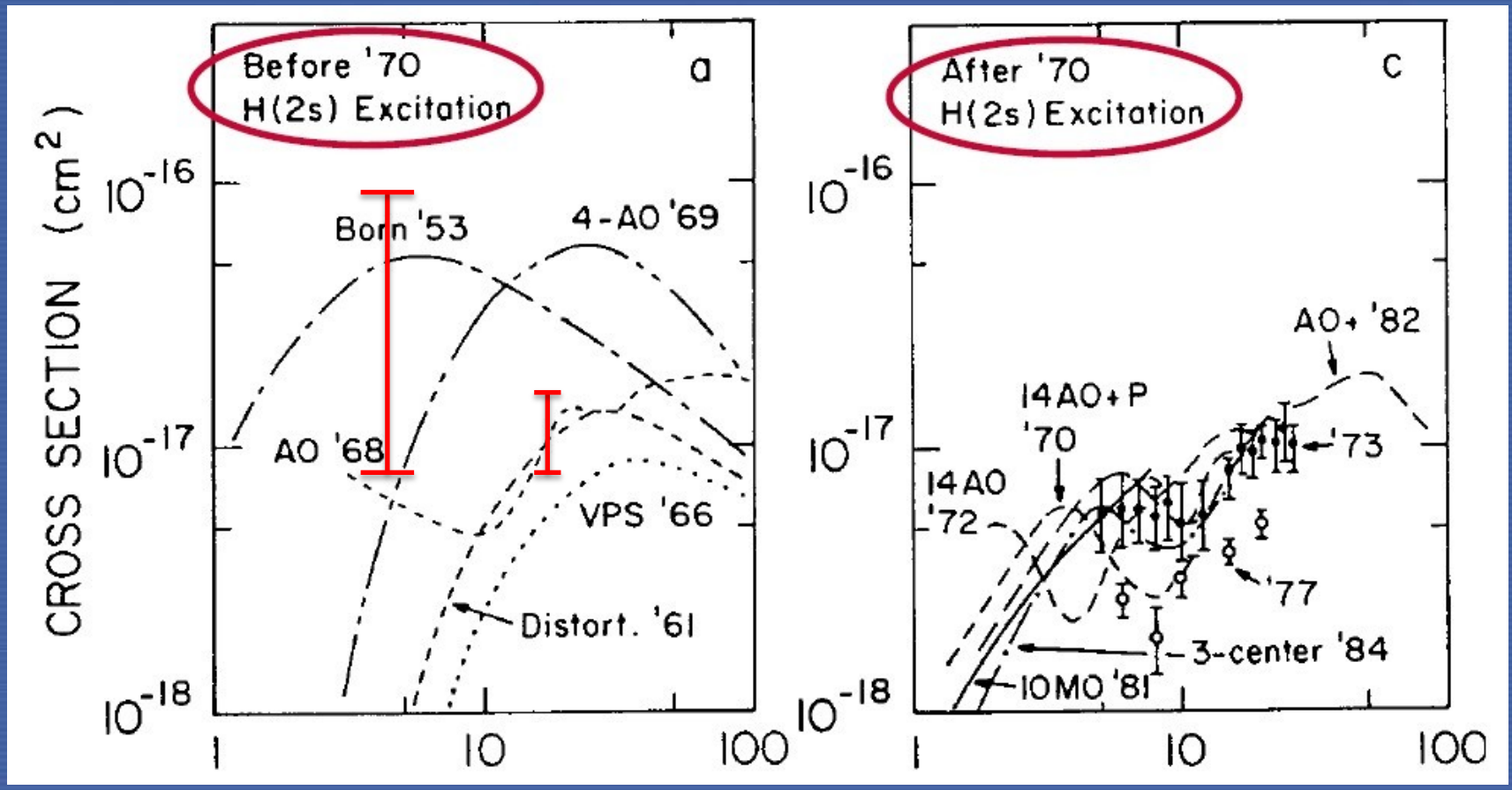
Theoretical cross-sections without uncertainty estimates

"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?

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.
- Output → Guidelines for estimating uncertainties of theoretical atomic and molecular data
- *Publication in preparation*

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4th Code Centre Network TM 2013

- Expand the UQ activities to the field of theoretical Plasma-Material Interaction data.
- Discuss the current status 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
  - Density Functional Theory simulations
  - Molecular Dynamics simulations
  - Kinetic Monte Carlo simulations
  - Rate simulations

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International cooperation

- International Workshop on Models and Data for Plasma-material Interaction in Fusion Devices, May 2015
  - A follow-up of the ICTP-IAEA Conference on Models and Data for Plasma-Material Interaction in Fusion Devices in 3-7 November 2014
- BIPM Workshop on Measurement Uncertainty, June 2015
  - Revision of the Guide to the expression of uncertainty in measurement (GUM) and discussion on its impact on various metrological aspects
- Workshop on Uncertainty Quantification in Physics and Chemistry, November 2015
  - Organized by the Institute for Advanced Computational Science, Stony Brook University

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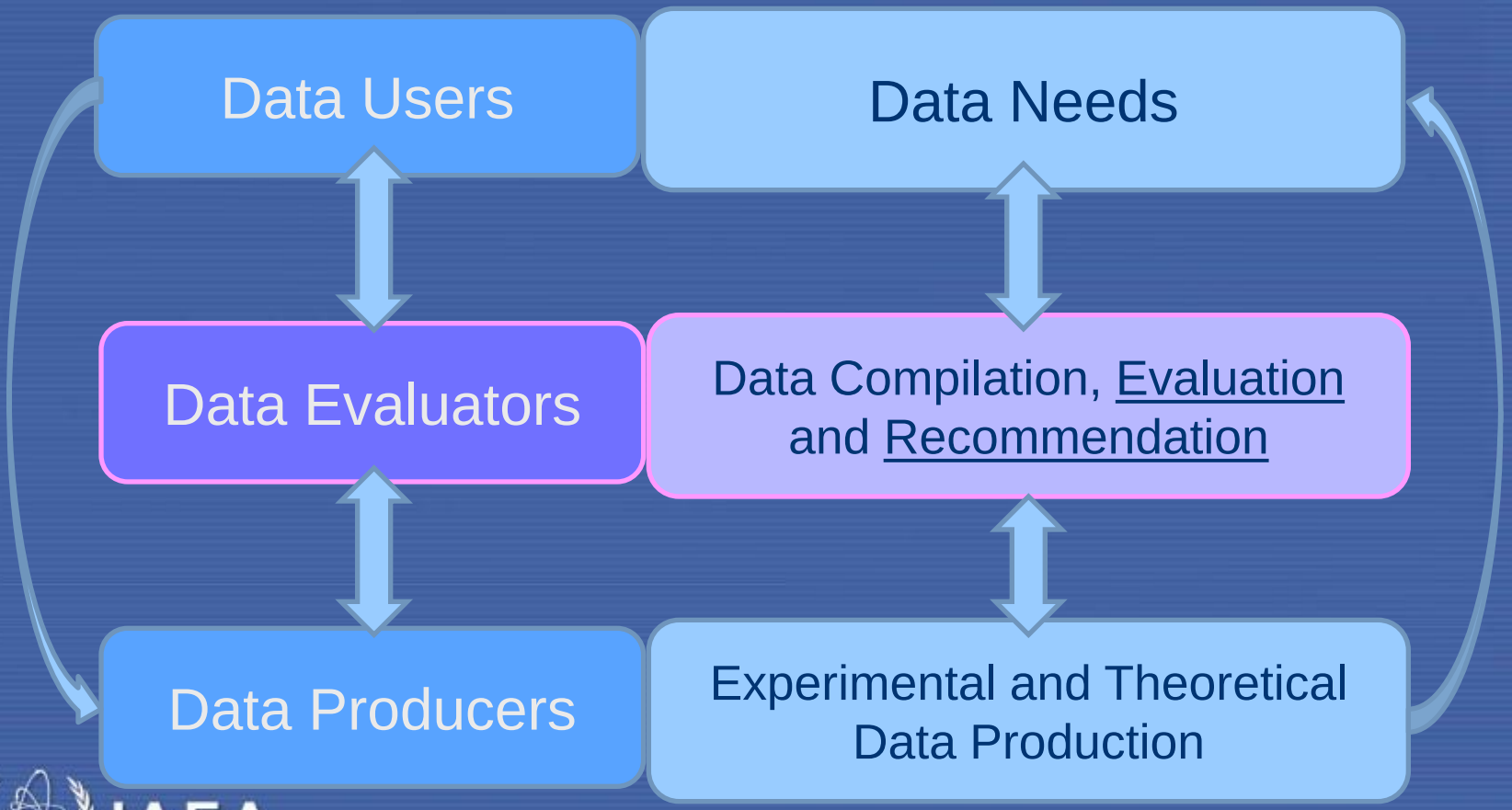
Long-term goal….

Global Network towards the *Internationally Agreed Data Library* for Fusion and other Plasma Applications



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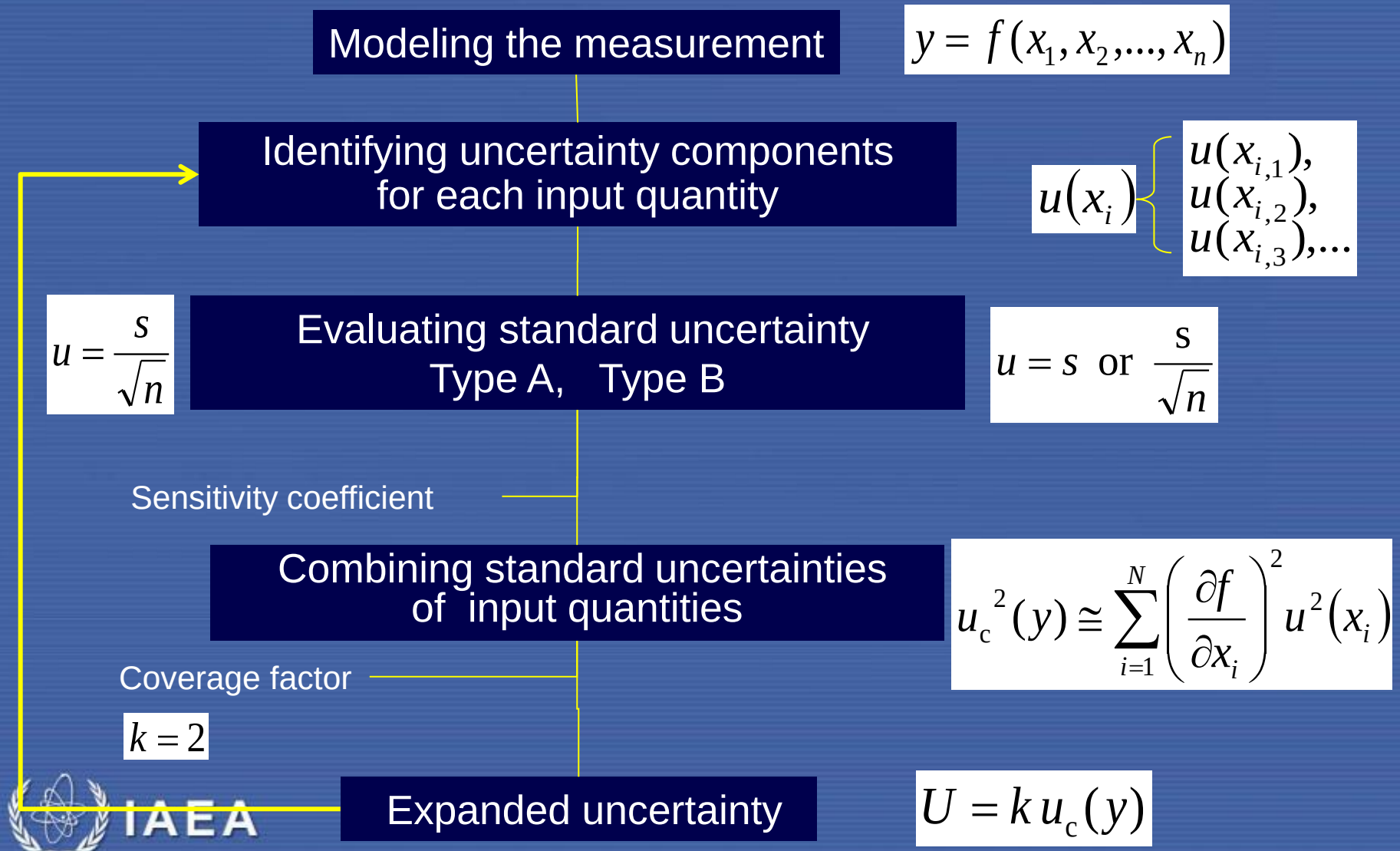
5 Steps in Uncertainty Evaluation