



**IAEA**

*60 Years*

*Atoms for Peace and Development*

# Review of CRP and Meeting Objectives

**Hyun-Kyung Chung,**

**Atomic and Molecular Data Unit, Nuclear Data Section**

**CRP F43023 on Data for Atomic Processes of Neutral Beams in Fusion Plasma**

# IAEA A&M Data Unit support for fusion program worldwide

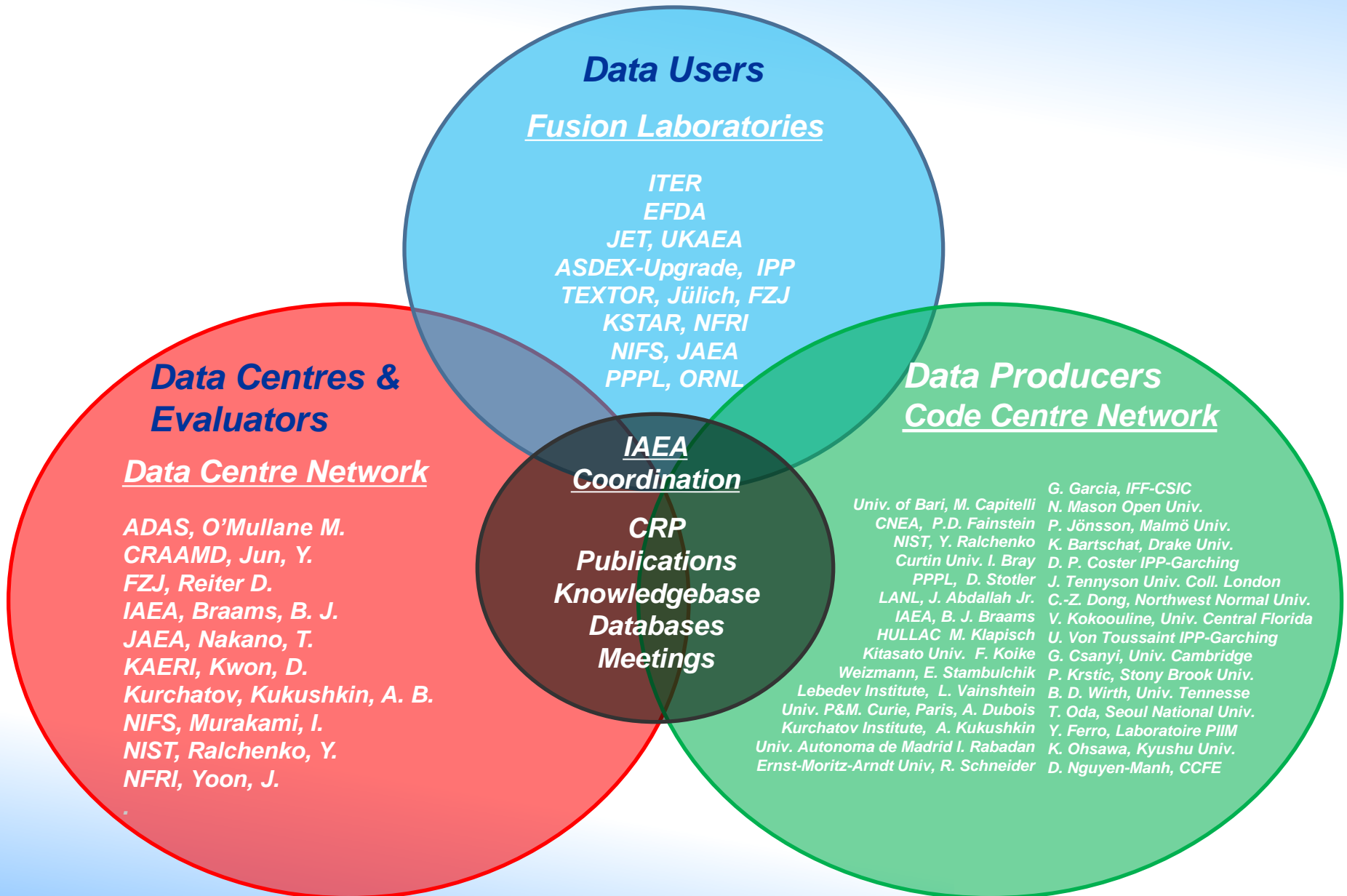
## Fusion research requires huge amounts of material data – AM/PSI data

- 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 (CRP)  
Publications  
Knowledgebase  
Databases  
Meetings**

# Collaboration Network



# A&M Data Services

<https://www-amdis.iaea.org/>

International Atomic Energy Agency  
**Atomic Molecular Data Services**  
Provided by the Nuclear Data Section

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## Atomic and Molecular Data Unit Activities

The Atomic and Molecular Data Unit operates within the Nuclear Data Section of the International Atomic Energy Agency, Vienna, Austria. The primary objective of the Atomic and Molecular Data Unit is to establish and maintain internationally recommended numerical databases on atomic and molecular collision and radiative processes, atomic and molecular structure characteristics, particle-solid surface interaction processes and physico-chemical and thermo-mechanical material properties for use in fusion energy research and other plasma science and technology applications.

### Databases on Atomic and Molecular Data for Fusion.

Atom, Molecule Plasma-Surface Data	ALADDIN Numerical Database	AMBDAS Bibliographic Database	GENIE Atomic Data Search Engine	OPEN ADAS Database Search	Rovibronic Energy levels Triplet D <sub>2</sub>	FC Factors & A-values of H <sub>2</sub> & Isotopes
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### Online Computing Capabilities

Code Centres Portal	LANL Atomic Physics	FLYCHK Non-LTE Kinetics	Heavy Particles Collisions	Averaged e- Impact Cross-section	Effective e- Ionization Rates	ATOM-AKM e- Collision Data
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### Knowledge Base for Atomic, Molecular and Plasma-Material Interaction Data for Fusion

Our Unit achieves its objectives by coordinating the activities of the **International Atomic and Molecular Data Center Network (DCN)** and **Code Center Network (CCN)**, initiation and conducting international **Coordinated Research Projects (CRP)**, organization of various types of **Expert's Meetings**, publication of **technical reports** on meetings and research activities and using other forms (research contracts, research agreements, consultancies) for stimulation of the generation, collection and critical assessment of the required atomic, molecular (A+M) and plasma-material interaction (PMI) data information.

The activity of Our Unit is supervised and biennially reviewed by the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council (IFRC A+M Subcommittee).

### IAEA Nuclear Data Section

 IAEA-NDS Mission, Staff and more	 Nuclear Data Services	 Meetings Workshops	 Newsletters	 Coordinated Research Projects	 Nuclear Reaction Data Center Network	 Nuclear Structure & Decay Data Network	 Technical Documents INDC Reports Publications	 Computer Codes
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- IAEA Meetings
  - December 19-21, 2016  
TM on Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications
  - Feb 27 - March 3, 2017  
Joint ICTP-IAEA School on Atomic Processes in Plasmas, Trieste, Italy
  - Mar 20-24, 2017  
The 4th Spectral Line Shapes in Plasma Workshop, Vienna, Austria
  - 1Q, 2017  
CM on Recommended data for hydrogen and helium in fusion plasmas
  - 2Q, 2017  
3rd RCM of CRP on Plasma-Wall

- AMO/PSI Meetings
  - Sep 11-16, 2016  
18th International Conferences on the Physics of Highly Charged Ions, Kielce, Poland
  - Sep 25-29, 2016  
10th International Conference on Atomic and Molecular data and Their Applications, Gunsan, Korea
  - Sep 29-30, 2016  
ADAS workshop 2016, Gunsan, Korea
  - Oct 10-14, 2016  
69th Annual Gaseous

# IAEA Coordinated Research Projects *60 Years* *Atoms for Peace and Development*

- **Joint research on A+M/PMI topic for fusion:**
  - Representatives from 10 to 15 institutes world-wide
  - Duration 3-4 years; 3 Research Coordination Meetings
- **Objectives:**
  - Generation, compilation and evaluation of data
  - Establishment of databases
  - Development of new techniques
- **Data and results:**
  - Journal publications
  - Final reports in “Atomic and Plasma-Material Interaction Data for Fusion” (APID)
  - Numerical data in ALADDIN
  - Looking forward to results in Knowledge Base

# Atomic and Molecular Data Unit CRPs



2009-2014: Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions.

2010-2015: Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV.

2011-2016: Data for Hydrogen and Helium and Their Isotopes in Fusion Plasma.

2012-2017: Erosion and Tritium Retention in Beryllium Plasma-facing Materials.

2013-2018: Plasma-wall Interaction with Irradiated Tungsten and Tungsten Alloys.

2015-2020: Plasma-wall Interaction with Reduced-activation Steel Surfaces.

2016-2021: Data for Atomic Processes of Neutral Beams in Fusion Plasma.

For consideration: Atomic Models and Data for Vapour Shielding in Fusion.

For consideration: Data for Plasma Interaction With Liquid Metal Surfaces.

# CRP on Neutral Beam Data

<https://www-amdis.iaea.org/CRP/NeutralBeams/>

**Objective:** Provide evaluated and recommended data for the principal atomic processes of heating and diagnostic neutral beams in fusion plasma.

- Assess the sensitivity of predictions of hydrogen beam penetration and of beam emissions (BES and MSE) to uncertainties in atomic data.
- Assess the sensitivity of predictions of charge transfer impurity spectra (CXRS or CHERS) in fusion plasma to uncertainties in atomic data.
- Based on uncertainties in the evaluated atomic data, assess associated uncertainties in representative simulations and predictions of beam penetration, beam photoemission and charge transfer spectra in fusion plasma conditions.
- Assemble, evaluate and recommend state-resolved cross sections and (where needed for fusion applications) density matrix elements for excitation and ionization in collisions between electrons and hydrogen neutrals at electron energy from about 100 eV to 100 keV.

# CRP on Neutral Beam Data (2)

- Develop, assemble, evaluate and recommend state-resolved cross sections and (where needed) density matrix elements for excitation, ionization and charge transfer in collisions between hydrogen (H, D, T) neutrals and protons or deuterons at collision energy of the neutrals from about 1 keV to 1 MeV.
- Develop, assemble, evaluate and recommend state-resolved cross sections for excitation, ionization and charge transfer in collisions between hydrogen (H, D, T) neutrals and the principal *fully* stripped impurity ions (elements He, Be, C, N, O; other light elements and Ne, Ar, Kr with lower priority) at hydrogen energy from about 1 keV to 1 MeV.
- If possible, develop recommendations for state-resolved cross sections for collisions between hydrogen neutrals and the most relevant *partially* stripped impurities (elements Ar, Fe, Kr and W) at hydrogen energy from about 1 keV to 1 MeV.
- To the extent that it matches other work in the CRP, develop and evaluate data for high energy collision processes in the hydrogen beam neutralizer and for atomic processes of neutral beams of helium and lithium in fusion plasma.



# Objectives for the First RCM

- Exchange information about ongoing work.
  - 10 participants, 10 major active research projects.
  - Modeling on neutral beam related diagnostics.
  - Fundamental data of ion-atom collisions and electron-atom collisions
- Review current status
  - Modeling codes used for neutral beam analysis
  - Atomic data required for collisional-radiative modeling
  - Uncertainty assessment of ion-atom and electron-atom collision data
- Review and coordinate work plans.
  - Each participant to review work plan for next 1-3 years in light of all the work in the CRP.
  - Make plans for cooperation; exchange of information between RCM.
  - Proposed code comparison workshops

# CRP related activities to be discussed

## Maybe code comparison workshop for beam penetration and photoemission.

- Specify a set of simple uniform plasma conditions and beam parameters.
- Contributors perform their best calculations before the workshop, put their results into a standard format, and at the meeting the results are compared in fine detail and one tries to understand the sources of all significant differences.
- Distinguish emissions from beam particles, halo neutrals, plasma impurities.
- Participants would be developers and users of the various beam codes (NUBEAM, ALCBEAM, BEAMS3D, NEMO, BBNBI, RENATE) and related atomic data sets.

## Maybe code comparison workshop for atomic collision processes.

- Principal test cases are collision of H with a highly charged ion, straight line motion at a fixed relative velocity and even a fixed impact parameter; compare results for state resolved charge transfer, ionization, and change of state of the H neutral.
- Plenty of diversity in methods: classical trajectory Monte Carlo (CTMC); Atomic Orbital Close Coupling (AOCC) using Slater-type orbitals or Gaussian orbitals; Lattice time-dependent Schrödinger equation (LTDSE) using rectangular or cylindrical, fixed or adaptive lattice; Molecular Orbital Close Coupling (MOCC).



**IAEA**

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*Thank you!*

