

# The IAEA Data Centre Network : Data Evaluation Activities

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September 4-7, 2012

Joint IAEA-NFRI Technical Meeting



**IAEA**

International Atomic Energy Agency

# IAEA ATOMIC AND MOLECULAR DATA UNIT



# IAEA Atomic and Molecular Data Unit

- 5 November 1976 at Culham Laboratory, UK
  - first meeting of the Joint IFRC/INDC Subcommittee on A+M data for fusion
- Review progress and achievements of [A+M/PSI data for Fusion programme](#)
- Stimulate international cooperation in measurement, compilation and evaluation of A+M / PSI data for fusion
- IAEA A+M Unit formed Jan-Feb 1977
- Currently Two Professional Staffs and One General Staff
  - Unit Head: Bastiaan Johan Braams [b.j.braams@iaea.org](mailto:b.j.braams@iaea.org)
  - Atomic Physicist: Hyun-Kyung Chung [h.chung@iaea.org](mailto:h.chung@iaea.org)
  - Database Clerk: Khalid Sheik [k.sheikh@iaea.org](mailto:k.sheikh@iaea.org)

# International Coordination of A+M/PSI Data Research for Fusion

Consultants Meetings (CM)

Fusion Plasma Modelling

Publications (INDC, APID, Bulletin)

Measurements

Theories

*Coordinated Research Projects (CRP)*

Technical Meetings (TM)

Data Compilation

Data Evaluation

Databases (AMBDAS, GENIE, ALADDIN, Wiki...)

# Online AM/PSI Data Services:

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

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International Atomic Energy Agency

## Atomic Molecular Data Services

Provided by the Nuclear Data Section



Search  Go

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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
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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), an advisory body to the Agency's Director General.

### 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

Jun 20-22, 2012  
Consultant Meeting  
on Data Evaluation  
and the  
Establishment of a  
Standard Library of  
A+M/PMI Data for  
Fusion  
-----  
Aug 29-31, 2012  
2nd RCM of CRP on  
Spectroscopic and  
Collisional Data for  
W from 1 eV to 20  
keV  
-----  
Sep 4-7, 2012  
Joint IAEA-NFRI  
Technical Meeting on  
Data Evaluation for  
Atomic, Molecular  
and Plasma-Material  
Interaction  
Processes in Fusion  
NFRI, Daejeon, Korea  
-----  
Sep 26-28, 2012  
1st RCM of CRP on  
Data for Erosion and  
Tritium Retention in  
Beryllium Plasma

### AMO/PSI Meetings

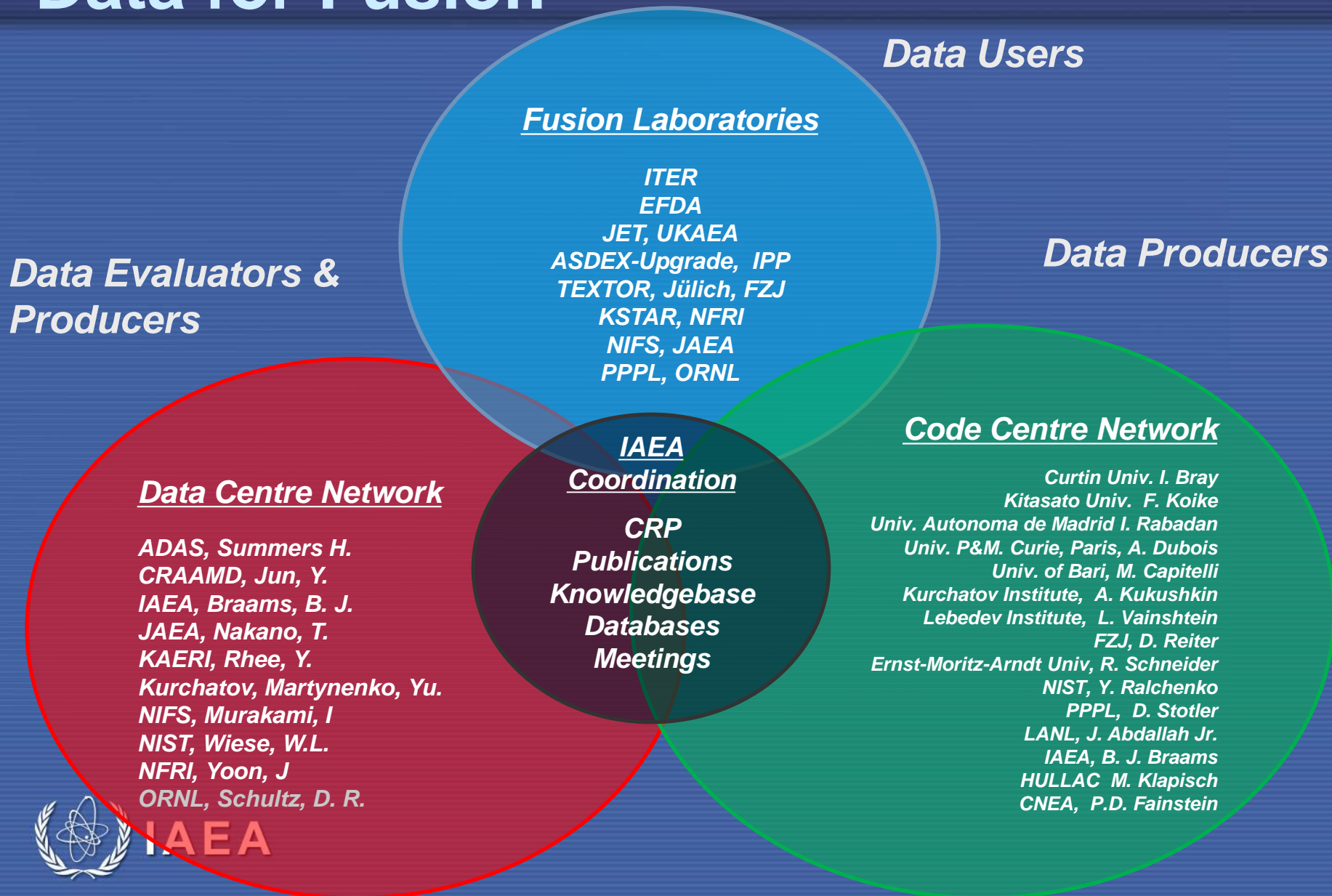
May 21-25, 2012  
20th Plasma-Surface  
Interaction  
Conference Aachen,  
Germany  
-----  
May 29-31, 2012  
11th International  
Workshop on  
Hydrogen Isotopes  
in Fusion Reactor  
Materials, Schloss  
Ringberg, Germany  
-----  
September 2-7,  
2012: 16th in a  
series of  
International  
Conferences on the  
Plasma-Fuel Interac...

Data Production, Compilation, Evaluation and Recommendation

# IAEA COLLABORATION NETWORK ACTIVITIES



# Network Collaboration for AM/PSI Data for Fusion





# IAEA Network finds the critical need of evaluated and recommended data

- Code Centre Network Meeting (October 2010)
  - Improve Online Code Capabilities to provide needed data for Data Users, particularly, Plasma Modellers
  - Generate *too many data sets without quality information*
  - Recommendation :
    - CCN workshops to improve code capabilities
    - CCN to expand as a structured network of Code Producers and Data Users, or Experimentalists (on request)
    - Code Producers need a priority list of needed data sets
    - *Data Users need **Complete sets and Recommended data***

(Data Users: D. Coster, D. Reiter, R. Schneider, D. Elder participated)
- At almost every meeting, data evaluation was an issue
  - VAMDC (Compilation & Distribution)



# Community effort towards the evaluated and recommended data

- Data Centre Network (September 2011)
  - Data Evaluation Tasks are Difficult
    - Lack-of man-power: Experts retiring or leaving the field
      - No young people get in the field (no publication, no funding)
    - Evaluation requires multiple sets : Too many or too few
    - Very few benchmark experiments for collisional data
    - Even fewer uncertainty estimates for theoretical data
  - Recommendation
    - Data should be first collected and available for evaluation
    - Evaluation activities should be organized in the community
    - Evaluation guidelines should be established in the community
    - A list of recommended data sets should be available as a final product
  - Current status
    - NFRI/KRISS: National efforts to establish standard data sets (APAN)
    - NIFS/JAEA: Evaluated data libraries, Collaboration
    - IAEA/ORNL: ALADDIN, individual consultancies

A series of meeting to organize community efforts for evaluation and recommendation of A+M/PSI Data

# IAEA ACTIVITIES ON EVALUATION AND RECOMMENDATION



# CM on Data Evaluation (Feb 12): Current status & future coordination

- 14 Participants from Korea, Japan and China (Hosted by I. Murakami at NIFS)
  - Current Data Evaluation Activities of the Data Centres
  - Data Evaluation Methods
- Discussion on Data Evaluation Methods
  - Uncertainty Approach: **Definition of Measurement and its Uncertainties (KRISS)**
  - Data Evaluation System: **Infrastructure (NFRI)**
    - Data Compilation and Evaluation Coordination with Invited Experts
  - Qualifications of Experts: **Retired or Senior scientists**
    - Breeding and Training of Young Generation – Publication Possibilities
    - Sustainable Funding Level for Experts
    - Knowledge Transfer from Experienced Experts
  - Guidelines of Data Evaluation Procedures
    - Regular meetings to review and update guidelines are needed (IAEA)
    - Uncertainty Estimates of theoretical data sets are most urgent ([IAEA-NFRI TM](#), [CCN](#))
  - Evaluation towards Recommendation
    - Recommendation should be made on the basis of applications (Close Ties with Users)
- Discussion on Data Evaluators Network



The preliminary terms of reference of Data Evaluators' Network

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# Uncertainty Approach

- Terminology in metrology

- VIM (Vocabulaire International de métrologie, Bureau Int. des Poids et Mesures) 2007
- GUM (guide to the expression of uncertainty in measurement) 2008
- Adopted by international organization for standardization (ISO) and numerous international organization including IAEA

- Measurement and uncertainty

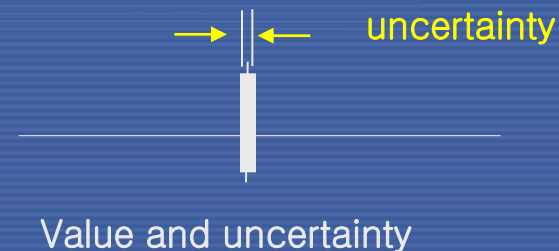
- The objective of a measurement is to determine the value of the measurand (GUM, 1993)
- In general, a measurement has imperfections that give rise to an error in its result.

- Error 1 = Measurement result – True value (**Error approach**)

True value : value consistent with the definition of a given particular quantity

- Error 2 = Measured value – Reference value (**Uncertainty approach**)

Reference value (Assigned value) : The reference quantity value can be a true quantity value of the measurand, in which case measurement error is unknowable, or an appropriate, known quantity value such as a conventional quantity value or a specified target quantity value to be realized in a production process.



# CM on Evaluation & Establishment of a Standard Library of AM/PMI Data (Jun 12)

- **Journal Editors (G. Drake, D. Schultz)**
  - D. Schultz: Data Compilation and evaluation at CFADC (ORNL)
    - Evaluation & Recommendation: compilation of annotated bibliography + data extraction + a group of experts evaluation with scaling laws, semi-empirical formulae, known asymptotic behaviours
    - Paradigm changes for finely resolved data (state resolved) from experimental data (1990s)
    - Closely integrated efforts by fusion energy researchers and AM experts are critical
  - G. Drake: Policies on uncertainty estimates for theoretical data and their implementation
    - Editorial on uncertainty estimates in 2011 [ <http://aps.org/pdf/PRA/v83/i4/e040001> ]
    - Uncertainty estimates required for papers (a) claiming high accuracy or improvements, (b) comparing with high precision experimental measurements or (c) providing interpolations or extrapolations of known experimental measurements
- **Data Users and Producers (S. Lisgo, D. Coster, J. Roth)**
  - D. Coster: Use and management of AMNS data by EFDA TF on ITM
    - Centralized source / Standard code interface
    - Emphasizes the importance of data that have been given a stamp of approval by an expert
  - S. Lisgo: ITER AM/PMI data requirement and management strategy
    - Divertor is the key area for AM/PMI data (W, Be and elements used for controlled impurity seeding)
    - Data management strategy under development: single point of entry and data tracking (origins, version, etc)
  - J. Roth: Plasma-wall interaction and associated uncertainties
    - Physical sputtering uncertainties: experimental limitations and surface conditions



# CM on Evaluation & Establishment of a Standard Library of AM/PMI Data (Jun 12)

- Standard Data Centres (J. Choi, J. Yoon)
  - J. Choi: Measurement and Uncertainties
  - J. Yoon: Standard data evaluation activities at DCPD (NFRI)
- Discussions
  - Uncertainty Estimates for AM/PMI data
    - e-atom scattering : uncertainty estimates are challenging and require expert understanding of codes: Locate model papers of careful e-scattering calculations with a credible estimate
    - Heavy particle collisions: no widely shared codes, “COLTRIMS” experimental benchmarks
    - PMI: the benchmark has to be experiment with better characterization of surface and bulk
  - Coordination of the development of a standard library
    - Document precisely which data sets are used throughout the fusion modelling community
    - Evaluation of evaluated data sets
    - Code comparison workshops on precisely defined problems
- Recommendation
  - Survey of Currently Used AM/PMI Data by Fusion Community
  - Compilation of Currently Available Evaluated Data



Meetings to Establish Uncertainty Estimates for Theoretical Data

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# Currently Used Data Survey:

## Survey on the Atomic, Molecular and Plasma–Material Interaction Data for Fusion Applications

Upon the recommendations from the consultants' meeting on "Data Evaluation and the establishment of a standard library of A+M/PMI Data for fusion", this survey is designed to collect information on A+M/PMI data sets currently used by fusion community. It will provide a list of priority data sets for evaluation and quality assessment and eventually a foundation for the internationally recommended library of A+M/PMI data sets. Accurate and detailed information on currently used data sets will be highly appreciated. Please send any questions or comments to [IAEA A+M data unit](#) regarding this survey.

Your email:

### Heavy Particle Collisions (Projectile->Target)

#### Charge Exchange

Elastic Scattering

Dissociation

Excitation

Ionization

Particle Exchange

### Photon Collisions (hv->Target)

Excitation

Ionization

Recombination

### Electron Collisions (e->Target)

Elastic Scattering

Dissociation

Excitation

Ionization

Recombination

### Plasma Surface Interaction (Projectile->Surface)

Reflection

Chemical Sputtering

Physical Sputtering

Sublimation

Mean Penetration Depth

Priority List of Critically Needed Data

Database of Available Data for Evaluation

Basis of Evaluated Data Library



# Evaluated Data Library : Prototype

## List of Currently Available Evaluated Data Sets

- [-] Heavy Particle Collisions (Projectile->Target)
  - [+] Charge Exchange
  - [+] Elastic Scattering
  - [+] Dissociation
  - [+] Excitation
  - [+] Ionization
  - [+] Particle Exchange
- [-] Photon Collisions (hv->Target)
  - [+] Excitation
  - [+] Ionization
  - [+] Recombination
- [-] **Electron Collisions (e->Target)**
  - [+] Elastic Scattering
  - [+] **Dissociation**
  - [+] Excitation
  - [+] Ionization
  - [+] Recombination
- [-] Plasma Surface Interaction (Projectile->Surface)
  - [+] Reflection
  - [+] Chemical Sputtering
  - [+] Physical Sputtering
  - [+] Sublimation
  - [+] Mean Penetration Depth

Authors	Year	Quality	Source
R.K. Janev, W.D. Langer, K. Evans Jr., D.E. Post Jr.	1987	B-C	<a href="#">ALADDIN</a>
R.K. Janev, W.D. Langer, K. Evans Jr., D.E. Post Jr.	1987	B-C	<a href="#">ALADDIN</a>
R.K. Janev, W.D. Langer, K. Evans Jr., D.E. Post Jr.	1987	B-C	<a href="#">ALADDIN</a>
R.K. Janev, W.D. Langer, K. Evans Jr., D.E. Post Jr.	1987	B-C	<a href="#">ALADDIN</a>
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R.K. Janev, W.D. Langer, K. Evans Jr., D.E. Post Jr.	1987	B-C	<a href="#">ALADDIN</a>
R.K. Janev, W.D. Langer, K. Evans Jr., D.E. Post Jr.	1987	B-C	<a href="#">ALADDIN</a>
R.K. Janev, W.D. Langer, K. Evans Jr., D.E. Post Jr.	1987	B-C	<a href="#">ALADDIN</a>
R.K. Janev, W.D. Langer, K. Evans Jr., D.E. Post Jr.	1987	B-C	<a href="#">ALADDIN</a>
R.K. Janev, W.D. Langer, K. Evans Jr., D.E. Post Jr.	1987	B-C	<a href="#">ALADDIN</a>
R.K. Janev, W.D. Langer, K. Evans Jr., D.E. Post Jr.	1987	B-C	<a href="#">ALADDIN</a>

unevaluated)data in the databases

A => '3% to 10%', B => '10% to 25%', C => '25% to

# TM on Data Evaluation (Sep 12)

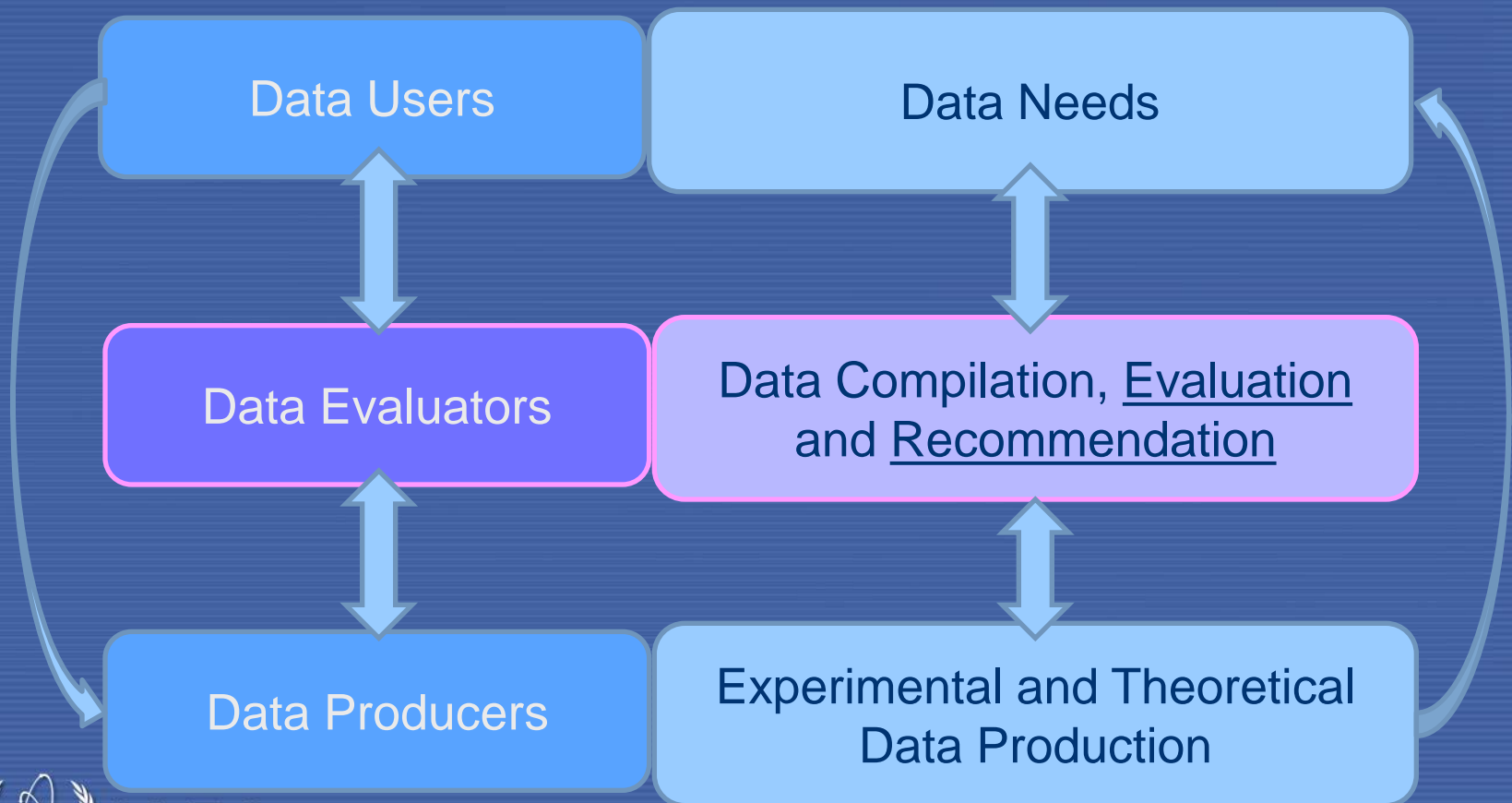
- Joint IAEA-NFRI Technical Meeting on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion
  - In conjunction with the 8th International Symposium on Standard Reference Data (sponsored by the Korea Research Institute of Standards and Science)
  - Hosted by the National Fusion Research Institute, Republic of Korea
  - 4-7 September 2012, Daejeon, Republic of Korea
- Technical Sessions (Focused on Reaction Data)
  - Evaluation Methods and Experiences (Itikawa, Kumar, Cho, Karwasz)
  - Current Evaluated Databases (Kramida, Landi, Mason, Biemont)
  - Error Propagation and Sensitivity Analysis (O'Mullane, Ballance, Reiter, Krstic)
  - Theoretical Data Evaluation (Aggarwal, Liang, Takagi, Song)
  - Experimental Data Evaluation (Nakamura, Buckman, Shevelko, Imai)
  - Data Centres Network Activities (Yoon, Murakami, Mason, Chung, Braams)

Need the community feedback and support

# FUTURE ACTIVITIES

# Long-term goal....

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



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# Data Evaluators' Network:

## Expanding existing network:

IAEA DCN, APAN (Asia-Pacific), China-Japan, SUP@VAMDC

## Membership of Data Evaluators Network

- Data centres , Collaborators of data centres, Senior (and/or retired) experts
- Code producers (of the IAEA Code Centre Network, CCN)
- Spectroscopic analysts

## Roles and Responsibilities of Data Evaluators Network

- write down the guidelines for evaluation of AM/PSI data
- evaluate/update old evaluated data according to the guidelines
- serve in a technical committee for evaluation
- serve in an advisory board to recommend evaluated data sets for the standard data library

## Meetings of Data Evaluators Network

- Hold meetings to recruit and train new evaluators, and expand the community
- Hold a technical committee meeting for data evaluation
- Hold an editorial board meeting from the technical committee for data recommendation

# Roadmap to the internationally agreed standard data library for AM/PSI data for fusion applications

## Phase 0: Inventorise the AM/PSI Data Collection used by Fusion/Plasma Community

- Priority list of critical data needs and data sets currently used by data users
  - There are a variety of A&M/PSI data sets required for fusion applications.
  - A users' network of intensive data applications should be established to provide and update the priority list of critical data needs for fusion applications.
- World Draft AM/PSI Data Collection : Absolute grand canonical list of presently used data sets
  - Questionnaires (ITM)
  - Working group formation
  - Reconcile, remediate and upgrade/expand/complete data library
- Standard Data Format: Easy Data Access

## Phase 1: Establishment of infrastructure for evaluated data library

- IAEA A+M Unit: Development of databases to host the standard data library
- Data Centers: Compilation of relevant data for evaluation
- Data Centers and Evaluators: Establishment of data evaluators' network
- Data Evaluators: Guidelines of evaluation methods
- Data Producers: Guidelines of uncertainty estimates.



Data Users: Priority list of critical data needs

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# Roadmap to the internationally agreed standard data library for AM/PSI data for fusion applications

## Phase 2: Establishment of evaluated data library

- IAEA: Establishment / maintenance of databases to host the evaluated data library
- Data Centers: Coordination of data evaluators' network activities
- Data Evaluators: Evaluation of data sets
- Data Producers: Guidelines of scaling laws / fit expressions
- Data Users: Development of data format compatible to applications

## Phase 3: Establishment and maintenance of standard data library

- IAEA: Establishment / maintenance of databases to host the standard data library
- Data Evaluators and Data Centers: Coordination of Technical Committees
- Data Producers: Feedback on data sets (production of missing data, data improvement)
- Data Users: Feedback on data sets