General Report on
A+M Data Unit Activities

C. Hill

23rd Meeting of the IFRC Subcommittee on
Atomic and Molecular Data for Fusion

16 – 17 June 2022

IAEA
International Atomic Energy Agency

Atomic and Molecular Data Unit Objectives

Main web page: https://amdis.iaea.org/

"Atomic and Molecular Data":

- Really A+M+PMI: atomic, molecular and plasma-material interaction data
- Data to support fusion energy development and other plasma applications

Organizational

- Part of the Nuclear Data Section (NDS): 4 out of 12 P-staff
- Division of Physical and Chemical Sciences (NAPC)
- Department of Nuclear Applications (NA)

Activities of the Unit

- Aim to support data development, data evaluation, data recommendation
- Maintain numerical and bibliographical databases
- Recommend and evaluate A+M+PMI data
- Organize coordinated research projects (CRPs)
- Organize technical meeting (TMs), consultancy meetings (CMs) and workshops

IAEA

Overview of AMD Unit Activities

Staffing

Christian Hill, Unit Head

Kalle Heinola, Atomic Physicist

***Ludmila Marian**, Scientific Data Manager*

***Marco Verpelli**, Nuclear Data Analyst / Programmer*

– shared across the Nuclear Data Section

Dipti, Special Service Agreement (SSA) Consultant since August 2021, Vienna-based for A+M data development and evaluation; database management.

New Unit contact email address: **fusion-data@iaea.org**

IAEA

Overview of AMD Unit Activities

Home-based Consultants

Martin Haničinec (60 days over June 2021 – January 2022)

Software tools for CollisionDB / ALADDIN2: pyvalem, django_valem; processing of existing ALADDIN data for ALADDIN2.

Utkarsh Bhardwaj (30 days, August – September 2021)

Implementation of CSaransh visualization software for the CascadesDB database.

Örs Asztalos (60 days over January – June 2022)

Preparation of data relating to processes in Neutral Beams for CollisionDB; processing of existing ALADDIN data for ALADDIN2.

IAEA

Overview of AMD Unit Activities

Website(s)

https://amdis.iaea.org/

https://cascadesdb.iaea.org/

https://db-amdis.org/collisiondb

https://db-amdis.org/hcdb

https://db-amdis.org/defectdb

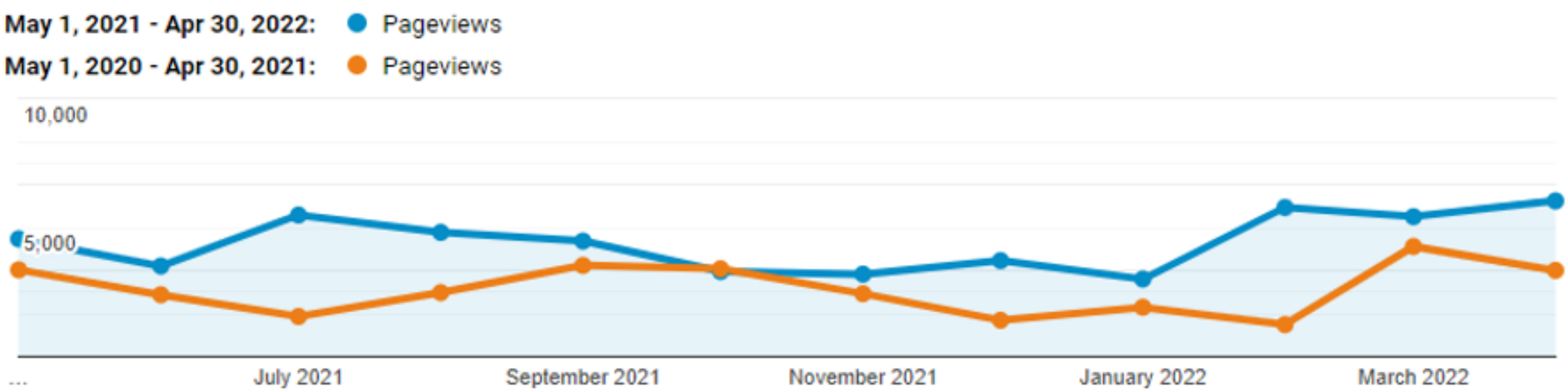
– for database development and data upload

Last 12 Months:

52 000 Page views (+49%)

19 000 Users (+58%)

IAEA



May 2021 – April 2022

Totals

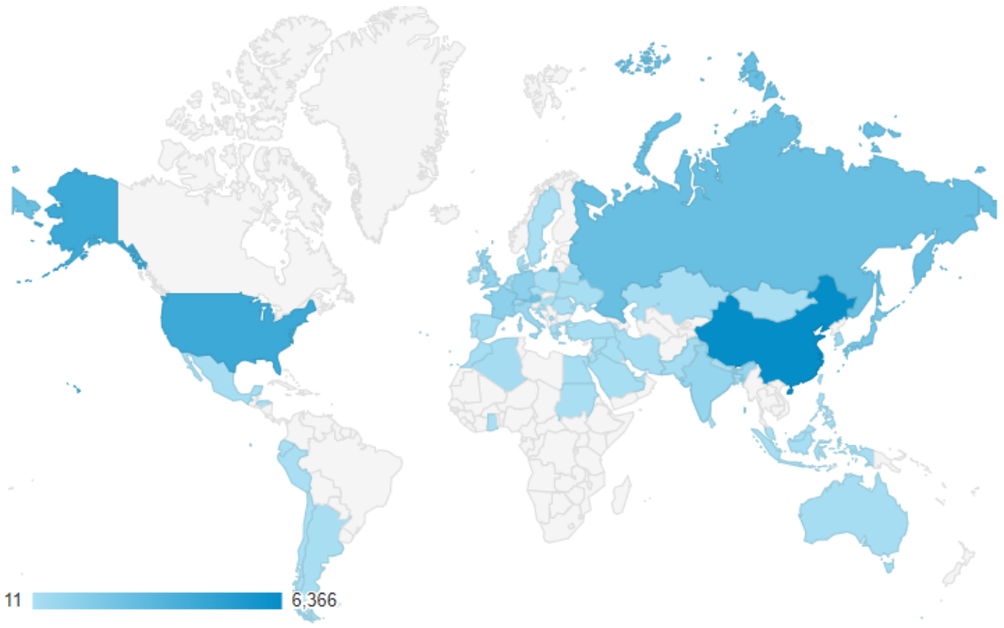
52 000 Pageviews
(35 000 previous year)

19 000 Users
(12 000 previous year)

Cascades DB

		sessions	users	pageviews
1.	/cdbmeta/	**189** (100.00%)	156 (100.00%)	2,015 (100.00%)

		sessions	users	pageviews
1.	/index.html	**5,031** (19.89%)	4,775 (18.98%)	7,168 (13.88%)
2.	/clerval/	**3,261** (12.89%)	3,194 (12.69%)	4,285 (8.30%)
3.	/FAC/	**2,560** (10.12%)	1,747 (6.94%)	4,530 (8.77%)
4.	/meetings/	**1,814** (7.17%)	1,347 (5.35%)	4,185 (8.10%)
5.	/ALADDIN/	**1,569** (6.20%)	1,324 (5.26%)	6,622 (12.82%)
6.	/workshops/	**1,536** (6.07%)	1,180 (4.69%)	2,449 (4.74%)
7.	/CRP/	**1,369** (5.41%)	1,391 (5.53%)	2,181 (4.22%)
8.	/FLYCHK/	**1,324** (5.23%)	1,102 (4.38%)	2,638 (5.11%)
9.	/AMBDAS/	**590** (2.33%)	623 (2.48%)	1,258 (2.44%)
10.	/GNAMPP/	**534** (2.11%)	612 (2.43%)	1,525 (2.95%)
11.	/GRASP2K/	**490** (1.94%)	467 (1.86%)	979 (1.90%)
12.	/GENIE/	**467** (1.85%)	534 (2.12%)	1,046 (2.03%)
13.	/CCN/	**456** (1.80%)	534 (2.12%)	545 (1.06%)
14.	/missing-resource	**445** (1.76%)	434 (1.72%)	479 (0.93%)
15.	/Workshops/	**445** (1.76%)	456 (1.81%)	590 (1.14%)
16.	/LANL/	**356** (1.41%)	434 (1.72%)	812 (1.57%)
17.	/db/	**345** (1.36%)	189 (0.75%)	968 (1.87%)
18.	/DCN/	**289** (1.14%)	423 (1.68%)	634 (1.23%)
19.	/databases.php	**256** (1.01%)	312 (1.24%)	490 (0.95%)
20.	/DATASETS/	**234** (0.93%)	367 (1.46%)	590 (1.14%)



May 2021 – April 2022

Data by country (first 20)

		users		pageviews	
1.	China	**4,931**	(25.54%)	10,874	(21.06%)
2.	United States	**3,283**	(17.00%)	7,479	(14.48%)
3.	India	**1,447**	(7.49%)	2,805	(5.43%)
4.	Netherlands	**1,247**	(6.46%)	1,558	(3.02%)
5.	Germany	**668**	(3.46%)	1,848	(3.58%)
6.	France	**657**	(3.40%)	1,892	(3.66%)
7.	United Kingdom	**657**	(3.40%)	1,714	(3.32%)
8.	Russia	**657**	(3.40%)	3,183	(6.16%)
9.	Japan	**557**	(2.88%)	2,460	(4.76%)
10.	Italy	**501**	(2.59%)	1,603	(3.10%)
11.	Austria	**467**	(2.42%)	5,832	(11.29%)
12.	South Korea	**278**	(1.44%)	590	(1.14%)
13.	Canada	**189**	(0.98%)	378	(0.73%)
14.	Indonesia	**189**	(0.98%)	223	(0.43%)
15.	Pakistan	**189**	(0.98%)	323	(0.63%)
16.	Spain	**178**	(0.92%)	467	(0.90%)
17.	Switzerland	**145**	(0.75%)	378	(0.73%)
18.	Australia	**134**	(0.69%)	301	(0.58%)
19.	Brazil	**134**	(0.69%)	323	(0.63%)
20.	Turkey	**122**	(0.63%)	256	(0.50%)

Overview of AMD Unit Activities

Completed CRPs since 2016

Steel Surfaces (2015 – 2020)

[Final report pending]

Irradiated Tungsten (2013 – 2018)

Final report: Atomic and Plasma–Material Interaction Data for Fusion **18** (2019)

Beryllium Surfaces (2011 – 2016)

Final report (Invited Review): De Temmermann et al., “Data on erosion and hydrogen fuel retention in Beryllium plasma-facing materials”, *NME* **27**, 100994 (2021).

IAEA

Overview of AMD Unit Activities

Currently Active CRPs

Neutral Beams (2018 –)

Vapour Shielding (2019 –)

Hydrogen Permeation (2020–)

Planned CRPs

Atomic Data for Injected Impurities in Fusion Plasmas

- Consultancy Meeting, (Hybrid) 7 – 8 June 2022
- First RCM in October 2022

Formation and Properties of Molecules in Edge Plasmas

- First RCM planned for 2023

IAEA

Overview of AMD Unit Activities

Networks (biennial meetings)

- Data Centres Network (DCN)
- Code Centres Network (CCN)
- Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP)

Databases and Data Services

- ALADDIN / ALADDIN2
- AMBDAS
- ~~Knowledgebase~~
- GENIE
- CascadesDB
- DefectDB
- CollisionDB
- hcdb

IAEA

Overview of AMD Unit Activities

Code Services

- HEAVY, AAEXCITE and RATES
- FLYCHK
- FAC
- ~~LANL~~
- GRASP2K

Joint ICTP-IAEA Project on DFT modelling of HEAs

- Dhanshree Pandey started at the ICTP with Nicola Seriani in December 2021
- Initial calculations on simply alloy compositions including W and Ti
- Next: DFT calculations of interactions between defects in simple alloys
- Data to be deposited with the AMD Unit's DefectDB database

IAEA

Overview of AMD Unit Activities

Technical Meetings

- Technical Meeting on Nuclear Fusion Fuel Permeation in Reactor First Wall Components (Hybrid, 4 – 6 October 2021):
  - A large (54 participants) meeting related to the Hydrogen Permeation CRP.
- 2nd Meeting of the Global Network for the Atomic and Molecular Physics of Plasmas (Virtual, 6 – 9 December 2021)
  - 68 participants;
  - Aspects of the collisional-radiative properties of tungsten and hydrogen in the edge plasma of fusion devices, follow-up to TM in spring 2021.

IAEA

Overview of AMD Unit Activities

Technical Meetings

- Technical Meeting on the Effects of Hydrogen Supersaturation and Defect Stabilization in Nuclear Fusion Reactor Materials (11 – 12 April 2022, Aix-en-Provence, France)
  - Related to conclusions drawn from the 5th International Workshop on Models and Data for Plasma-Material Interaction in Fusion Devices (MoD-PMI 2021).

- 21st Atomic Processes in Plasmas (APiP) Conference (postponed to 15 – 19 May 2023)

- IFRC Subcommittee on Atomic and Molecular Data for Fusion (this meeting!)
  - Held in virtual form, 14 – 15 June 2021
  - In-cycle, hybrid meeting, 16 – 17 May 2022

IAEA

Overview of AMD Unit Activities

Technical Meetings

- Technical Meeting on Artificial Intelligence for Nuclear Technology and Applications (**ai4atoms**), 25 – 29 October 2021 [Virtual]
  - Multi-departmental IAEA Meeting (335 participants); Working Groups on:
    - Ethics, Human Health, Food and Agriculture, **Nuclear Fusion**, Nuclear Physics, Nuclear Power, **Nuclear, Atomic and Molecular Data**, Nuclear Security, Radiation Protection, Radioisotopes and Radiation Technology, Safeguards Verification, Water and Environment
  - https://nucleus.iaea.org/sites/ai4atoms/SitePages/WG-AI4ND.aspx
  - Conclusion: the need for more accessible databases, reference data sets, licensing and validation for Machine Learning applications.

IAEA

Overview of AMD Unit Activities

ICTP Workshops

- Atomistic Modelling of Radiation Damage in Nuclear Systems (Virtual, 4 – 8 October 2021)
- Atomic Processes in Plasmas: Data-Driven Research (Virtual, 13 – 17 December 2021)
- Advanced School/Workshop on Computational Nuclear Science and Engineering (Hybrid event, 23 – 27 May 2022), with Physics Section
  - *Radiation Damage in Nuclear Systems: from Bohr to Young (to be resubmitted for 2023)*

Other Workshops

- Workshop on Computational Nuclear Science and Engineering (Virtual, 12 – 16 July 2021), with NDS-NDU and Physics Section

IAEA

Overview of AMD Unit Activities

Publications

- Meeting Reports
- CRP Reports
- Atomic and Plasma-Material Interaction Data for Fusion (the "Green Books")
- Standards Documents
- Journal Articles

IAEA

Overview of AMD Unit Activities

Co-Authored, Peer-Reviewed Publications

- V. Laporta, R. Agnello, G. Fubiani, I. Furno, C. Hill, D. Reiter, F. Taccogna, “Vibrational excitation and dissociation of deuterium molecule by electron impact”, *Plasma Physics and Controlled Fusion* **63**, 085006 (2021)
- H. Ganser, C. Hill, J. H. George, J. M. Brown, M. Jackson, “Re-investigation of the infrared spectrum of the NCN radical by laser magnetic resonance spectroscopy”, *Journal of Molecular Spectroscopy* **382**, 111547 (2021)
- I. E. Gordon et al., “The HITRAN2020 molecular spectroscopic database”, *Journal of Quantitative Spectroscopy and Radiative Transfer* **277**, 107949 (2022)
- A. Hollingsworth, M.-F. Barthe, M. Yu. Lavrentiev, P. M. Derlet, S. L. Dudarev, D. R. Mason, Z. Hu, P. Desgardin, J. Hess, S. Davies, B. Thomas, H. Salter, E. F. J. Shelton, K. Heinola, K. Mizohata, A. De Backer, A. Baron-Wiechec, I. Jepu, Y. Zayachuk, A. Widdowson, E. Meslin and A. Morellec, “Comparative study of deuterium retention and vacancy content of self-ion irradiated tungsten”, *J. Nucl. Mat.* **558**, 153373 (2022).
- O. Lindblom, T. Ahlgren, K. Heinola, “Molecular dynamics simulations of hydrogen isotope exchange in tungsten vacancies”, *Nucl. Mater. Energy* **29**, 101099 (2021).
- A. Widdowson, J. P. Coad, Y. Zayachuk, E. Alves, N. Catarino, V. Corregidor, M. Mayer, S. Krat, J. Likonen, K. Mizohata, C. Rowley, M. Zlobinski, M. Rubel, D. Douai, K. Heinola, T. Wauters, L. Dittrich, S. Moon, P. Petersson, A. Baron-Wiechec, L. Avotina, “Evaluation of tritium retention in plasma-facing components during JET tritium operations”, *Phys. Scripta* **96**, 124075 (2021).
- S. Krat, M. Mayer, J. P. Coad, C. P. Lungu, K. Heinola, A. Baron-Wiechec, I. Jepu, A. Widdowson, “Comparison of JET inner wall erosion in the first three ITER-Like Wall campaigns”, *Nucl. Mater. Energy* **29**, 101072 (2021).

IAEA

Overview of AMD Unit Activities

Duty Travel

- Saclay Nuclear Research Centre, France: to work with CEA on the population of the DefectDB database for primary radiation damage calculated by first-principles DFT methodologies (Christian Hill, 10 – 14 October 2021)
- CECAM-HQ-EPFL, Lausanne, Switzerland: to attend and present at the Workshop on Multiscale Modelling of Irradiation-Driven Processes for Emerging Technologies (Christian Hill, 15 – 19 March 2022)
- Aix-en-Provence, France: to act as Scientific Secretary to a Technical Meeting on the Effects of Hydrogen Supersaturation and Defect Stabilization in Nuclear Fusion Reactor Materials (Kalle Heinola, 10 – 13 April 2022)
- UCL, London, UK: implementation and evaluation of software for standardizing atomic and molecular data for plasma collisional processes appropriate to machine learning applications (Christian Hill, 26 April – 1 May 2022)

IAEA

Overview of AMD Unit Activities

Practical Arrangements with NFRI (now Korea Institute of Fusion Energy, KFE)

Cooperation in the area of Atomic, Molecular and Plasma-Material Interaction Data Relevant to Fusion.

- evaluation of atomic, molecular and plasma-material interaction data and their inclusion in internationally-recommended data libraries;
- exchange and dissemination of unclassified information, including publications and sharing of experiences and best practices in the area of atomic, molecular and plasma-material interaction data as well as fusion plasma physics and related technology;
- collaboration in the compilation and further development of numerical and bibliographical databases on atomic, molecular and plasma-material data relevant to fusion; and
- promotion of scientific exchange of information with regard to the production and evaluation of atomic, molecular and plasma-material interaction data as well as developments done in fusion plasma physics and related technology, in particular through the facilitation of meetings and workshops.

September 2018 – September 2021

Renewal process (September 2021 – September 2023) complete, signatures exchanged.

IAEA

Remainder of the Meeting

Monday 16 May 2022

10:30 – 11:00 Review of Vapour Shielding and Hydrogen Permeation CRPs

11:00 – 11:15 Coffee Break

11:15 – 11:45 Review of Neutral Beams and Steel Surfaces CRPs

11:45 – 12:15 Review of Edge Plasmas Technical Meeting Series

12:15 – 12:45 Activities of the DCN, CCN and GNAMPP Networks

12:45 – 14:00 Lunch

14:00 – 14:30 Database activities in the AMD Unit

14:30 – 15:00 The Women in Fusion Network

15:00 – 16:00 Discussion and Review of AMD Unit activities

Tuesday 17 May 2022

09:30 – 10:00 Future Events and Projects in the AMD Unit

10:00 – 10:30 General discussion: future CRP Proposals, Cooperations and Outreach

10:30 – 11:00 Coffee Break

11:00 – 12:00 Discussions concerning the Subcommittee Terms of Reference and membership

12:00 – 12:30 Any other business; meeting recommendations and conclusion

IAEA