The IAEA

- Founded in 1957 to pursue the “safe, secure and peaceful uses of nuclear sciences and technology”.
- Autonomous, but reports to the UN General Assembly and Security Council. 173 Member States.
- Missions:
  - Safeguards
  - Nuclear safety
  - Peaceful uses of nuclear technology
The Atomic and Molecular Data Unit

- Founded in 1977 to “Stimulate international cooperation in measurement, compilation and evaluation of A+M / PSI data for fusion”.
- Atomic, Molecular and Plasma-Surface Interaction data.
- Five staff members:
  - Christian Hill (Unit Head)
  - Kalle Heinola (Atomic Physicist)
  - Ludmila Maria (Scientific Data Manager)
  - Marco Verpelli (Nuclear Data Analyst / Programmer)
  - Dipti (SSA Consultant: Atomic Collisional Data)

https://amdis.iaea.org
Activities: Coordinated Research Projects

- 3 – 5 Years
- 8 – 15 Laboratories
- 3 Research Coordination Meetings (RCMs)

- Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials
- Plasma-wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices
- Plasma-wall Interaction with Reduced-Activation Steel Surfaces in Fusion Devices
- Hydrogen Permeation in Nuclear Materials
Databases

- CascadesDB
  - Molecular dynamics simulations of collision cascades for modelling radiation damage …
  - This afternoon’s lectures…
  - 814 GB of data in 14382 simulations across 293 archives
  - [https://cascadesdb.iaea.org/](https://cascadesdb.iaea.org/)

Cascade in tungsten from 200 keV PKA (A. Sand)

Analysis of defect structures with CSaransh (U. Bhardwaj)
Databases

- **DefectDB**
  - DFT calculations of radiation-induced defect structures in nuclear materials
  - Under development
  - [https://db-amdis.org/defectdb/](https://db-amdis.org/defectdb/)

A periodic network of screw dislocations in bcc Fe (A. Goryaeva and M.-C. Mărinică)
This Workshop

- https://amdis.iaea.org/workshops/ictp-2021
- https://indico.ictp.it/event/9547/

Lectures and Computing Practicals:
- Molecular Dynamics (MD) simulations
- Connecting MD simulations to experiment through Kinetic Monte Carlo techniques
- Contributed talks (10’) and Posters (flash presentations: 2–3’)
- Characterising thermomechanical properties from MD simulations
- Modelling fast ion transport in nuclear materials (SDTRIM)
- Studies of microstructure evolution under high-dose irradiation
- Rate equation simulations of defects
- Q & A Session (Friday)

Contact email address: smr3573@ictp.it