IAEA
International Atomic Energy Agency
Atoms for Peace and Development

NDS Computing Infrastructure

Ludmila Marian
Scientific Data Manager

33rd Meeting of International Nuclear Data Committee
March 29th – April 1st 2021

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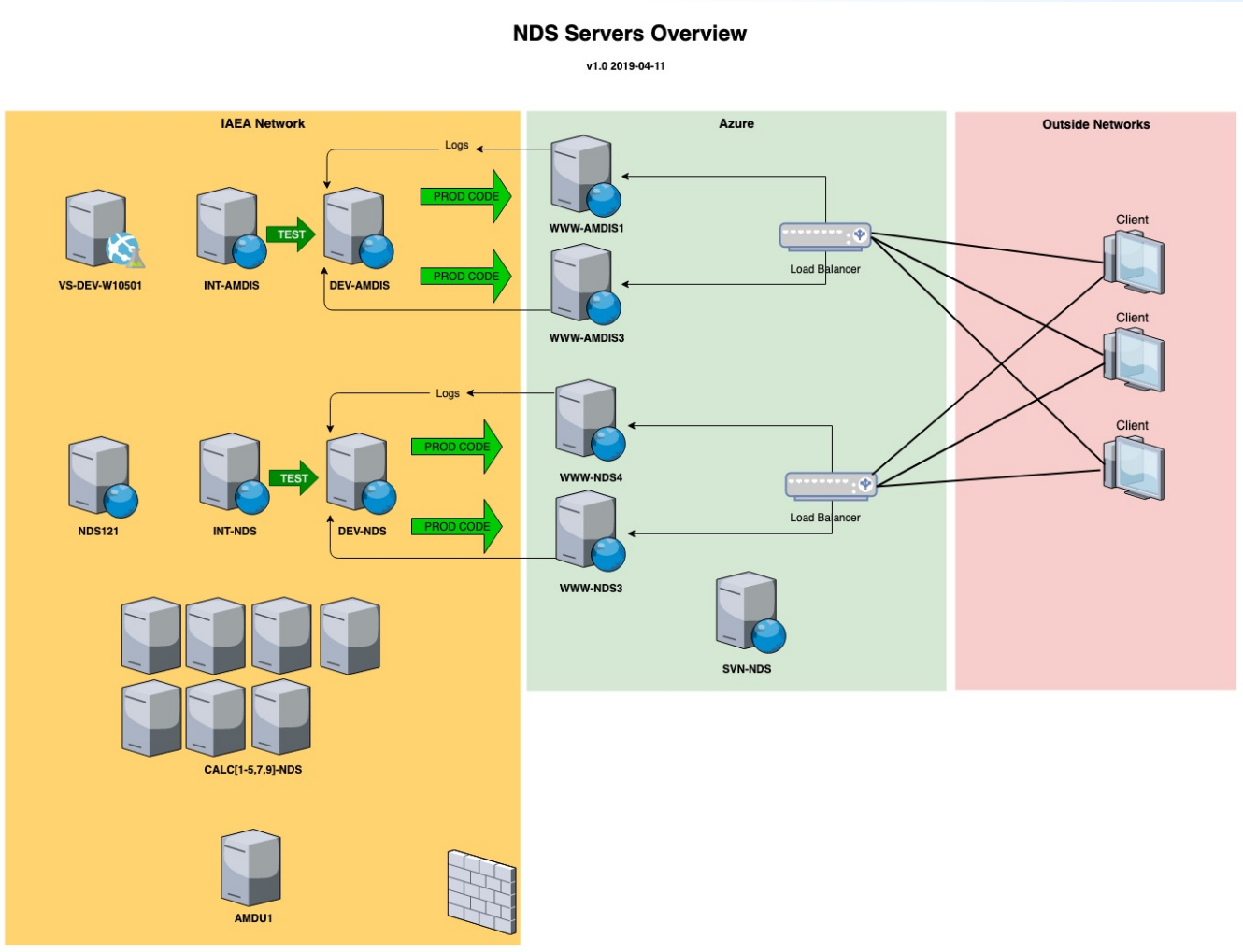
Outline

- **Hardware Infrastructure**
- **Software & Data Development Processes**
- **Modernizing Legacy Systems**

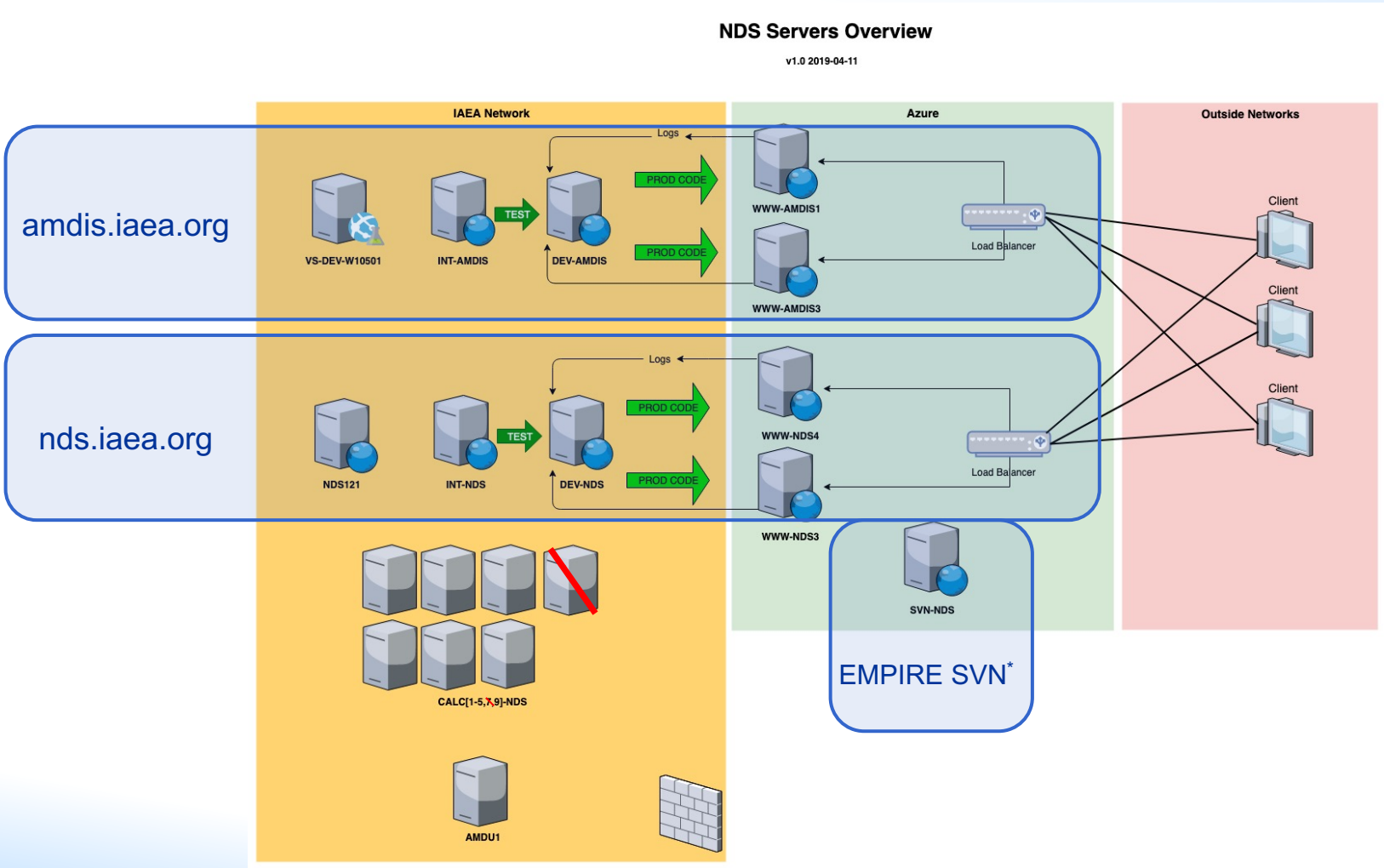
- ***Long-term Objective: Infrastructure for FAIR Data***

Hardware Infrastructure

Hardware Infrastructure

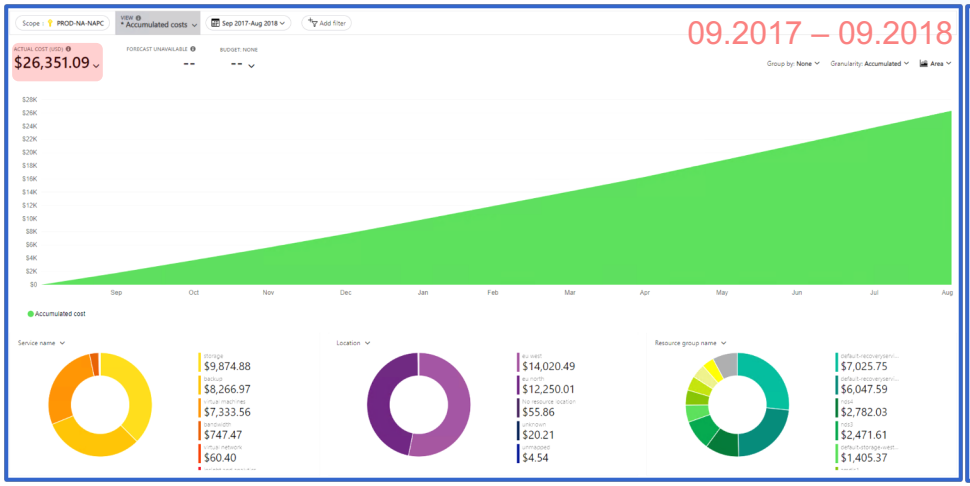


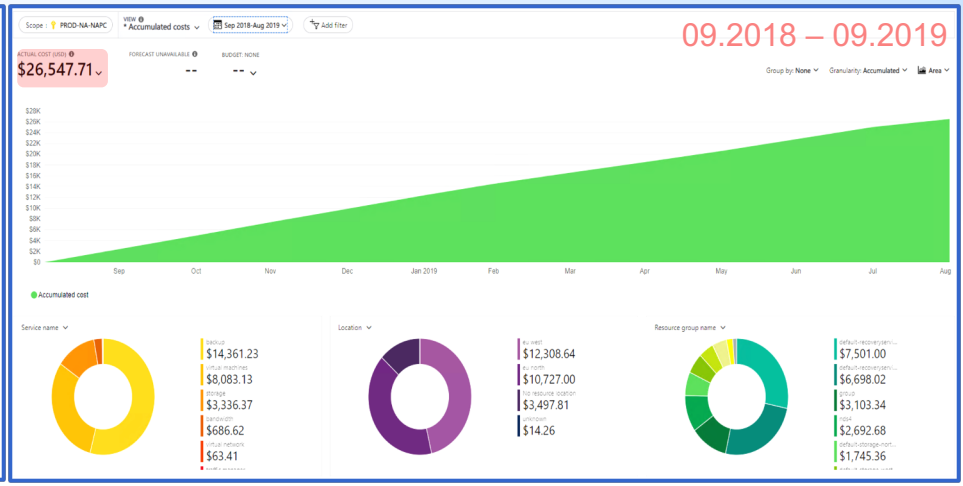
Hardware Infrastructure

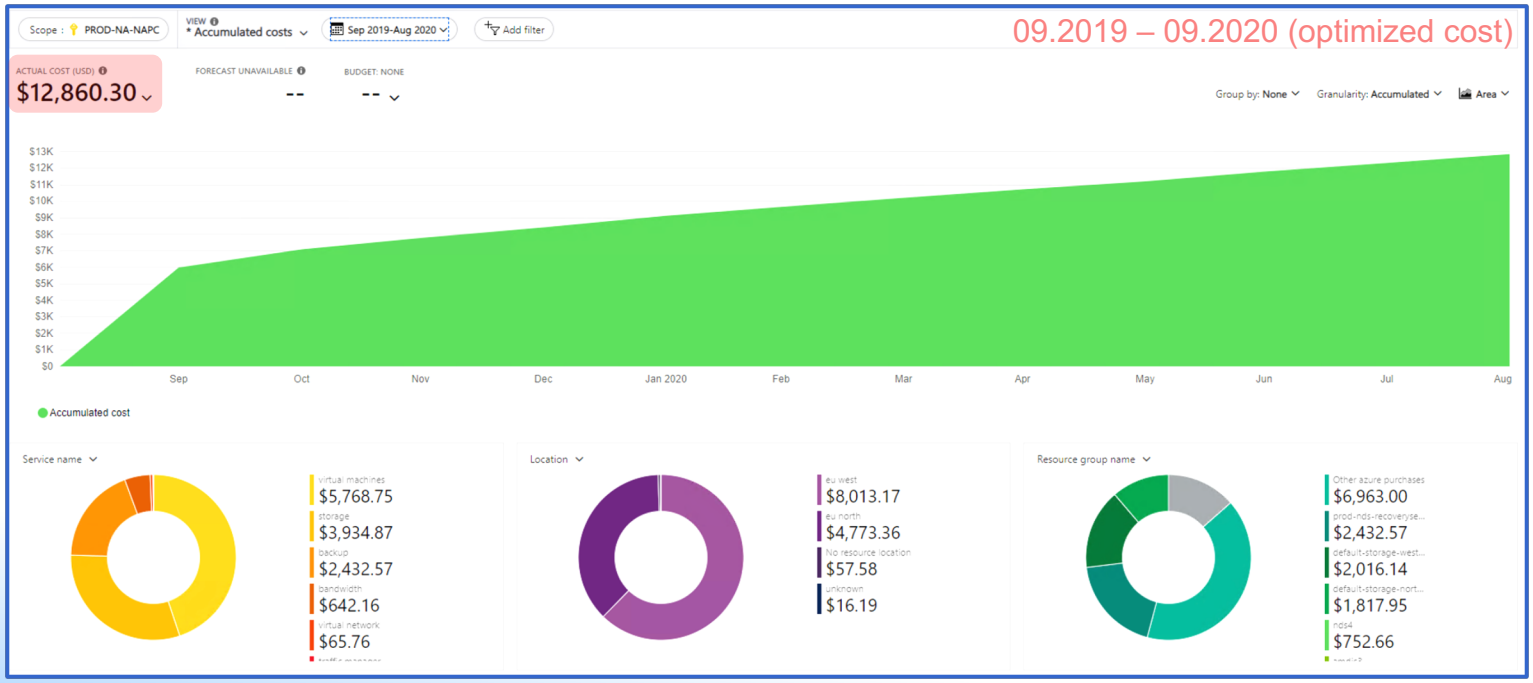


* *http://svn-nds.westeurope.cloudapp.azure.com/svnempire*

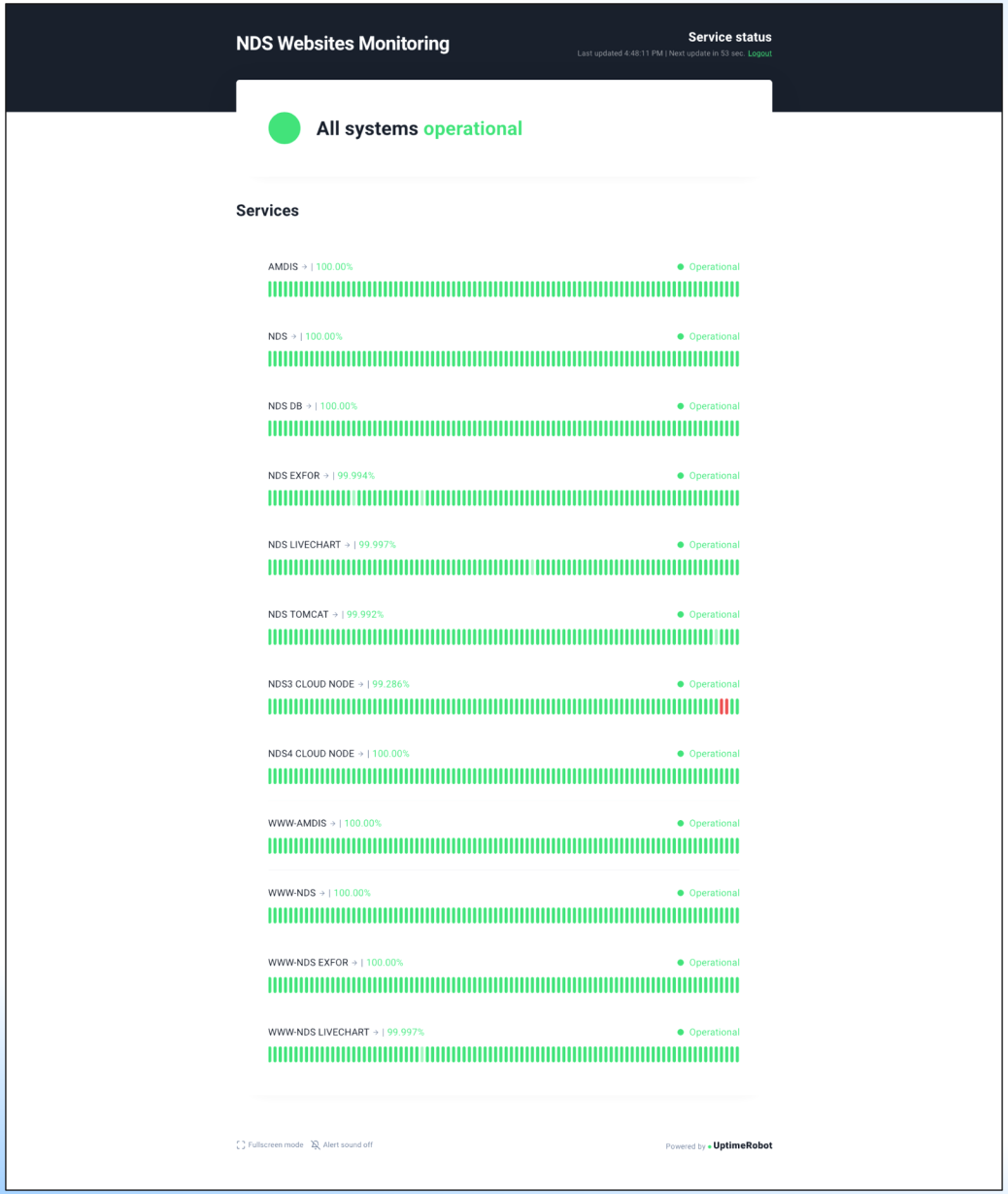
Cloud cost – 52% reduction







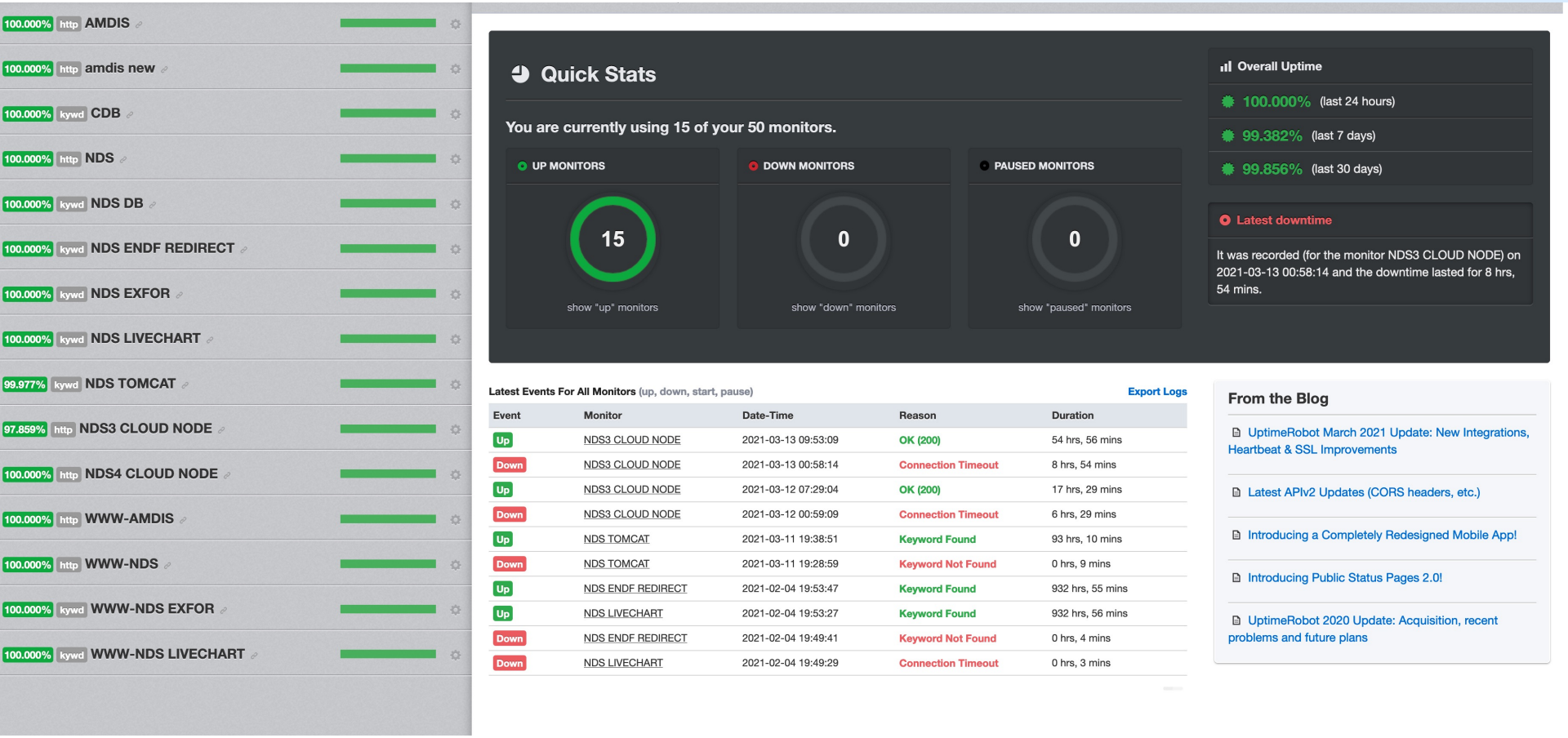
Availability monitoring



UptimeRobot

- Monitoring across the globe
- Free service
- Notifications each 5 min

Availability monitoring



Security

* Image source: https://www.netsparker.com

** NDS Dashboard was not used due to the sensitivity of the data

Security

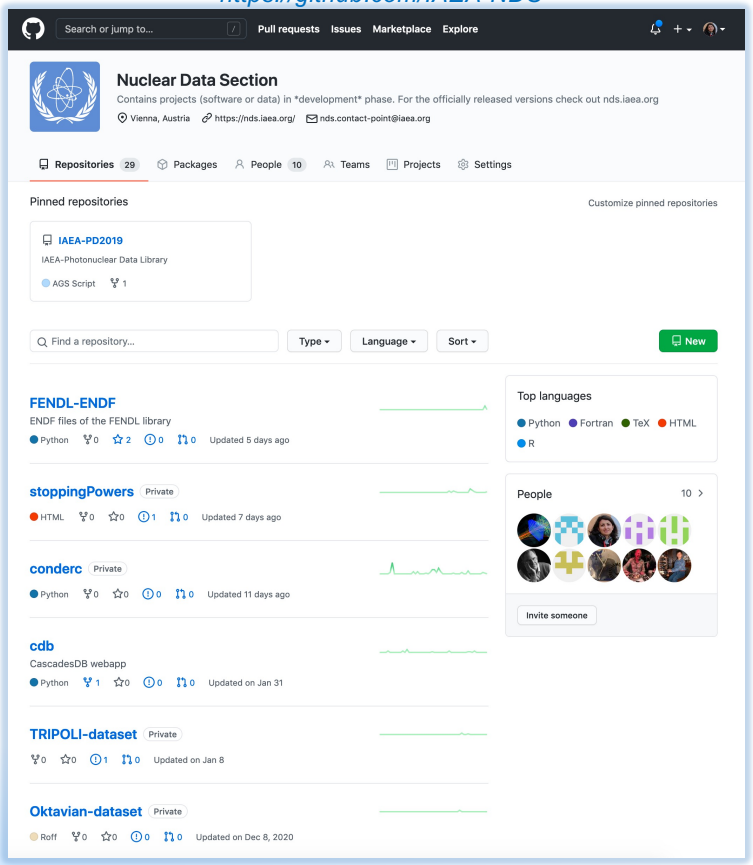
- **Dynamic Application Security Testing**
  - Netsparker - provided by IT, performed by NDS
- **System scanning**
  - Nessus - performed by IT
- **Static code analysis**
  - Developer's choice, performed by each developer
- Previous local solution (Acunetix) has been decommissioned.

© CERN

Version Control

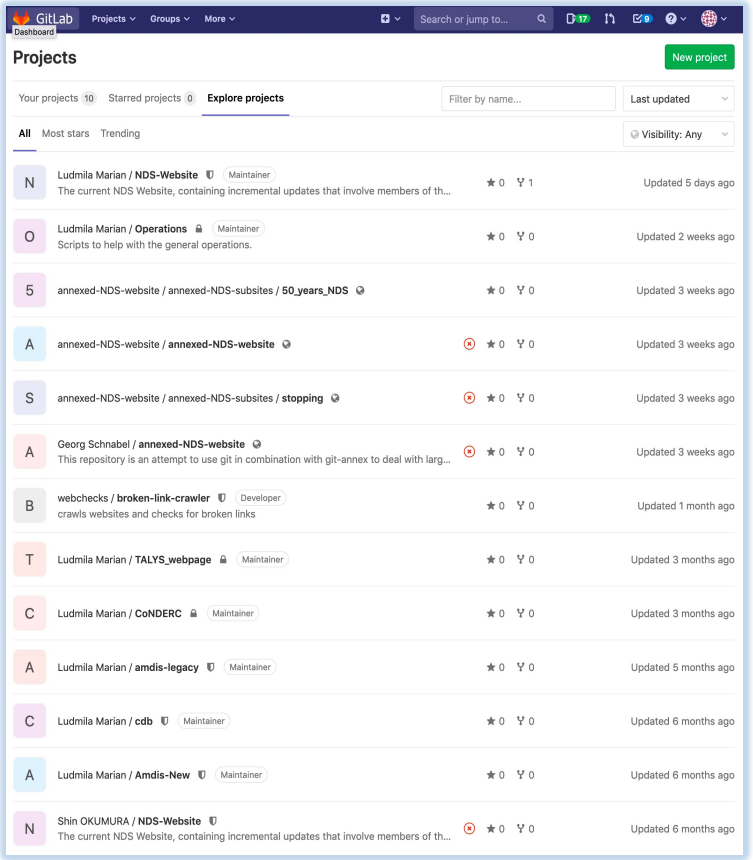
GitHub

https://github.com/IAEA-NDS



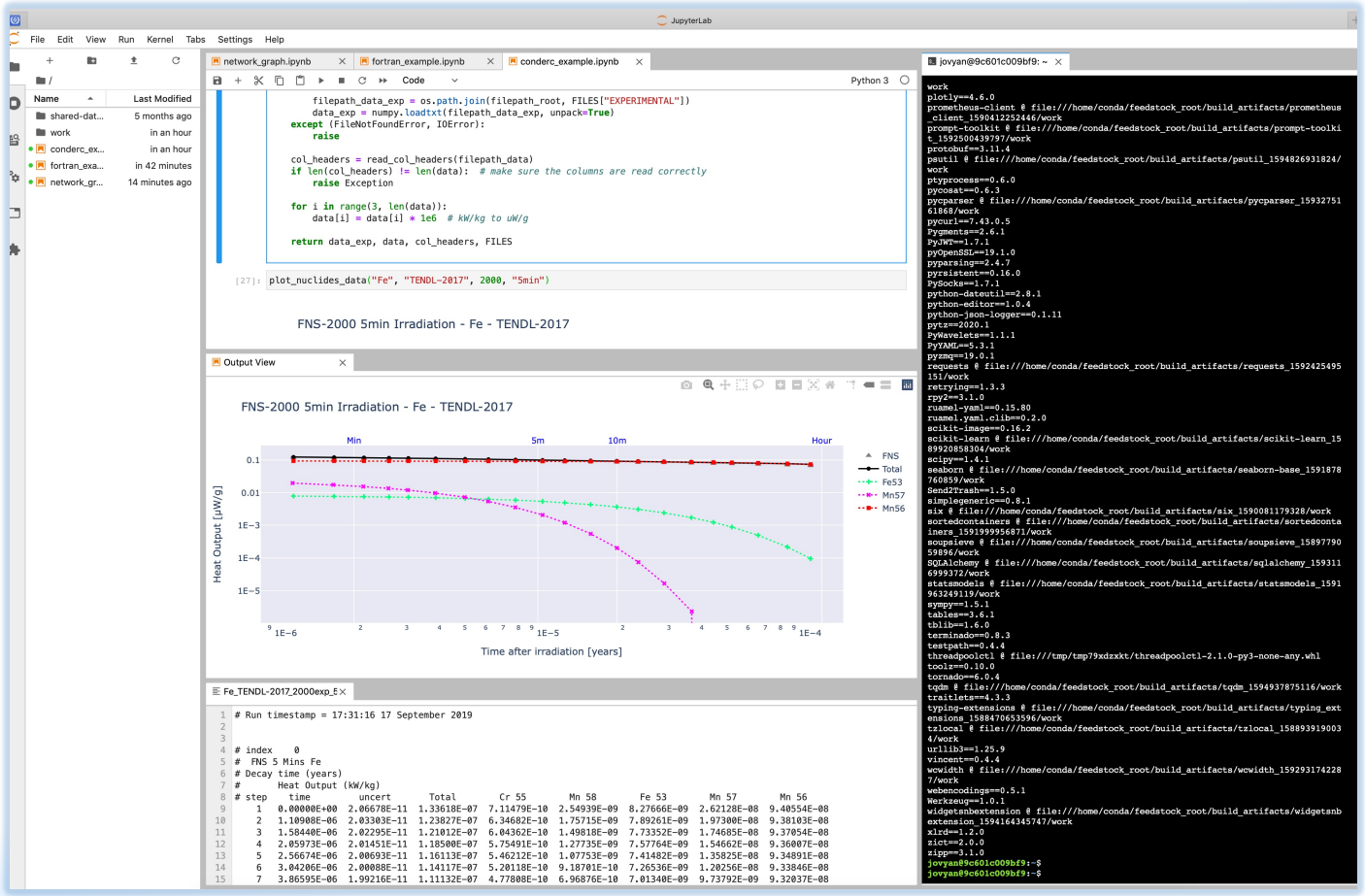
Public Private

GitLab



Internal

Jupyter Notebooks



jupyterhub

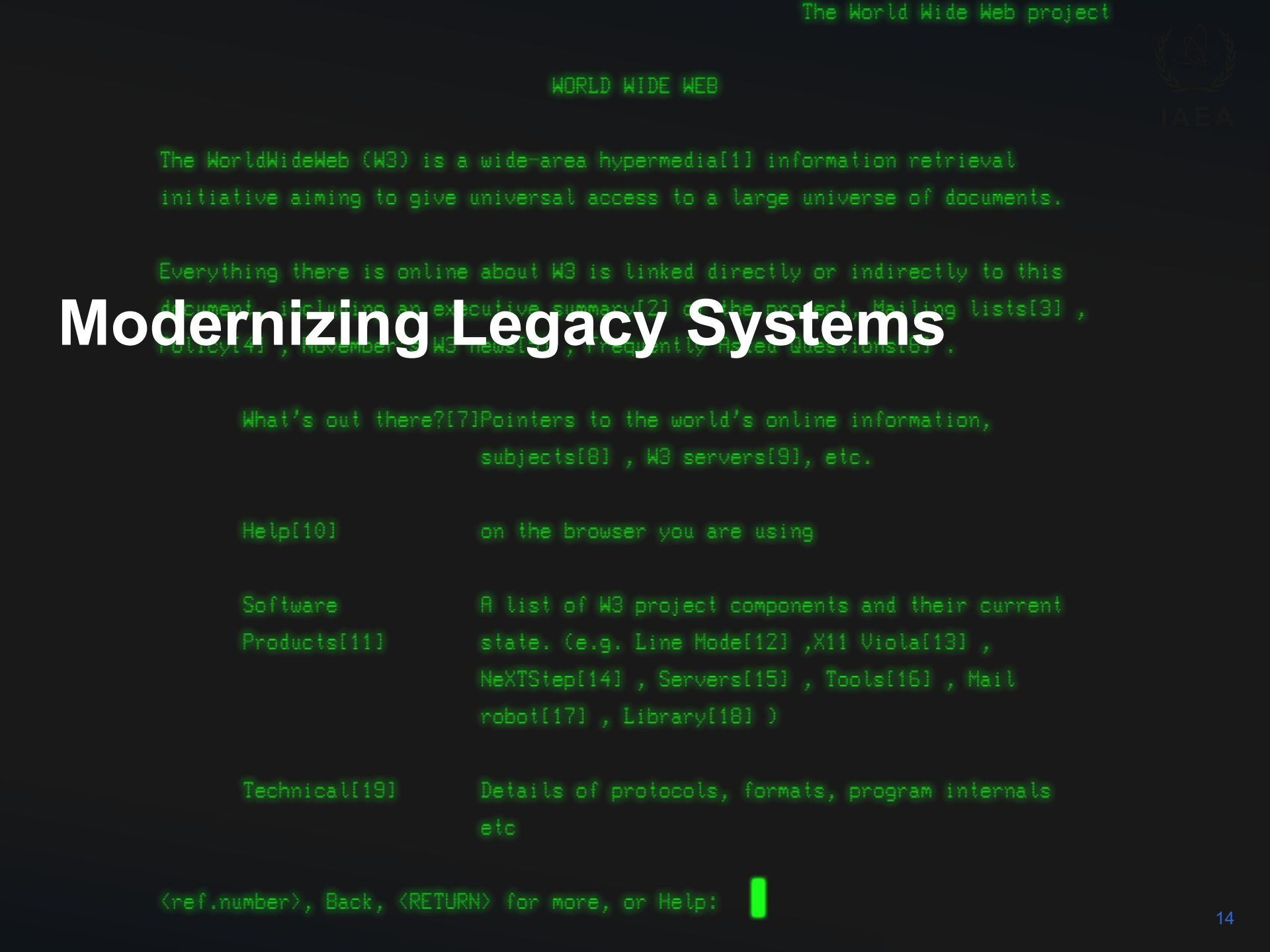
docker

- Python, R, Julia
- Fortran

- Fast prototyping
- Easy sharing of code
- Dependency encapsulation
- Access from browser

Internal

Modernizing Legacy Systems



Atomic & Molecular Data Unit

This is the legacy website for the Atomic and Molecular Data Unit.
The latest information about our activities can be found at **https://amdis.iaea.org**.
Existing data services at this location function as usual.

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

IAEA.org | NDS Mission

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_2 | FC Factors & A-values of H_2 & Isotopes

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

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 Meetings

November 16-17, 2017
TM of the Code Centre Network on Molecular Dynamics Data of Collisional Cascades after Irradiation

April 16-20, 2018
Joint ICTP-IAEA School and Workshop on Fundamental Methods for Atomic Molecular and Materials Properties in Plasma Environments

AMO/PSI Meetings

25 – 28 Jan 2018: Pacific Conference on Spectroscopy and Dynamics (PCSD 2018)

28 Jan – 2 Feb 2018: 38th International Workshop on High Energy Density Physics with Intense Ion and Laser Beams

30 Jan – 2 Feb 2018: 25th ITPA Scrape-Off-Layer and Divertor Topical Group Meeting

18 – 23 Feb 2018: Gordon Research Conference on Photoionization and Photodetachment: From Attoseconds to Nanoseconds: The Chemistry and Physics of Electrons, Atoms, Molecules, and Light

18 – 23 Feb 2018: 39th Extreme Atomic

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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Last Updated: 01-February-2021

Legacy version, 2007 – 2020
(some applications are still available)

AMD Unit | About Activities Databases Online Computing

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The Atomic and Molecular Data Unit establishes and maintains numerical databases of fundamental data for fusion energy research, and facilitates collaborative international research in the production and evaluation of such data. Read more.

Joint ICTP-IAEA Virtual Workshop on Atomistic Modelling of Radiation Damage in Nuclear Systems 3 March 2021

A Virtual Workshop, for early-stage career researchers, on the atomistic modelling of radiation damage will be held from 4 – 8 October 2021, by the International Centre for Theoretical Physics (ICTP), in cooperation with the IAEA. Click here for more details.

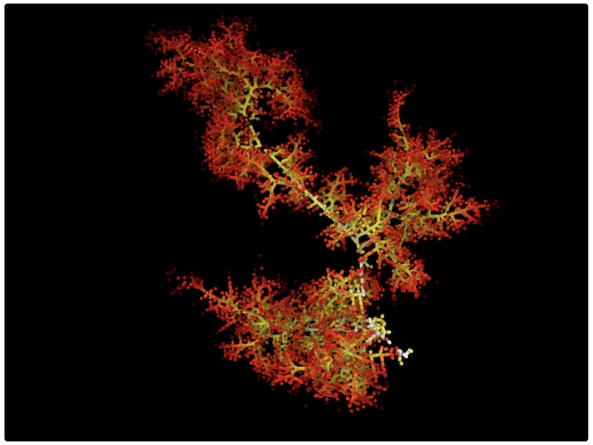
Upcoming Meetings

29 March – 1 April 2021	Technical Meeting on the Collisional-Radiative Properties of Tungsten and Hydrogen in Edge Plasma of Fusion Devices
12 – 16 April 2021	Atomic Processes in Plasmas
3 – 14 May 2021	ICTP Workshop 2020: Radiation Damage in Nuclear Systems: from Bohr to Young

More meetings ...

Quick Links

- Our CRPs
  - Hydrogen Permeation
  - Vapour Shielding
  - Neutral Beams
  - Steel Surfaces
- Our Meetings
- Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP)
- Conferences and workshops in atomic and molecular physics



An illustration of the simulated collisional cascade in tungsten caused by the impact of a 200 keV neutron.
Image courtesy of Andrea Sand, University of Helsinki.

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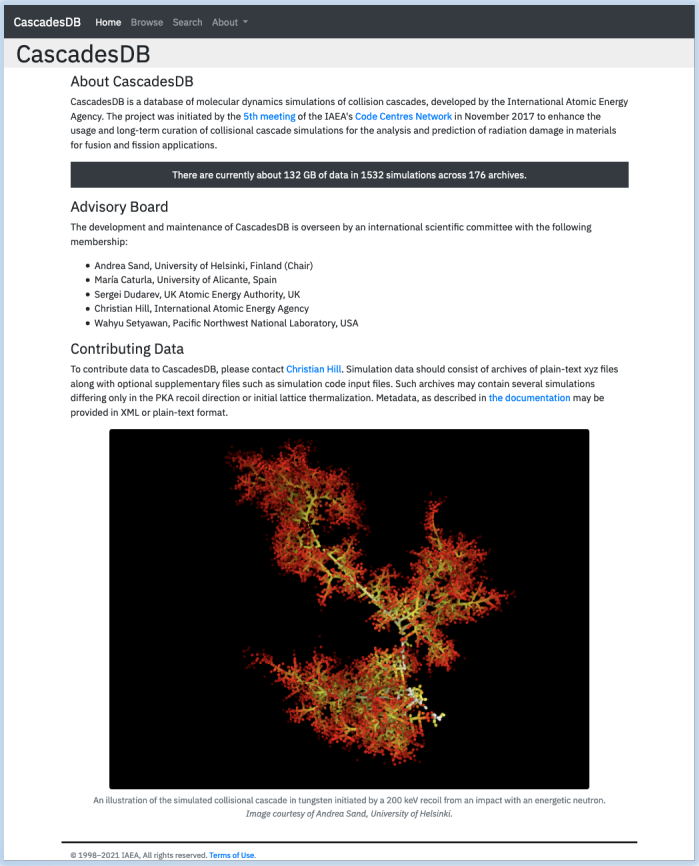
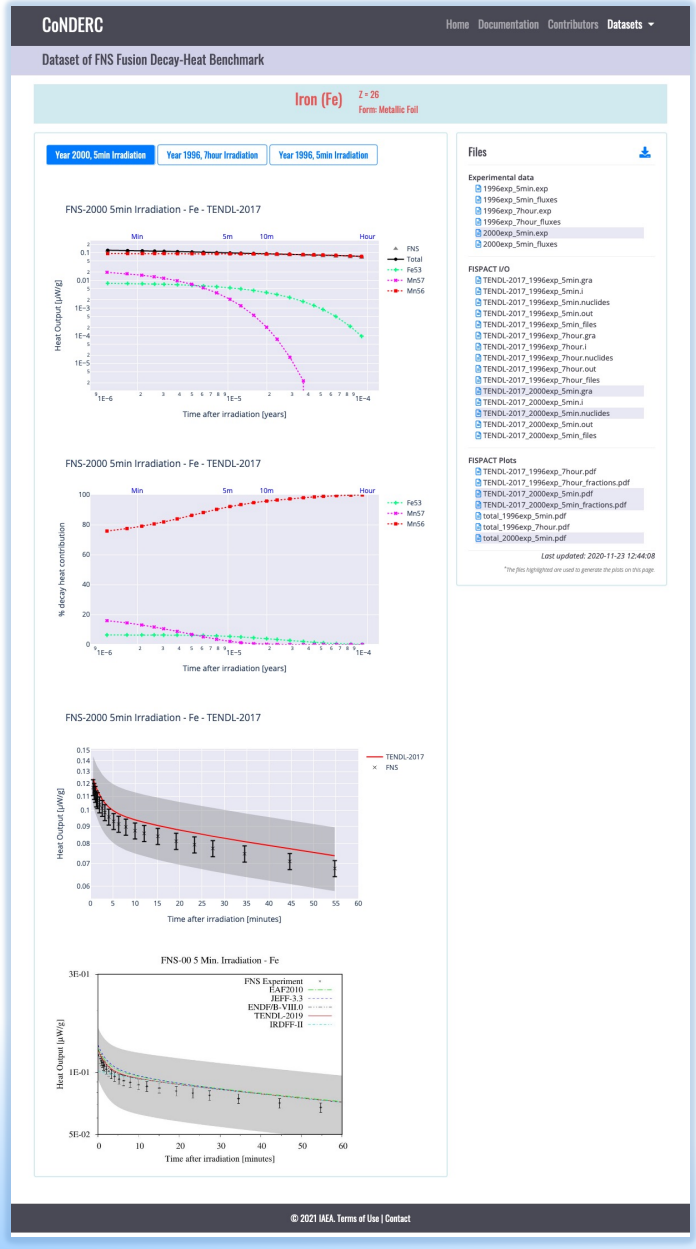
New version, from 2020

Atomic & Molecular Data Unit



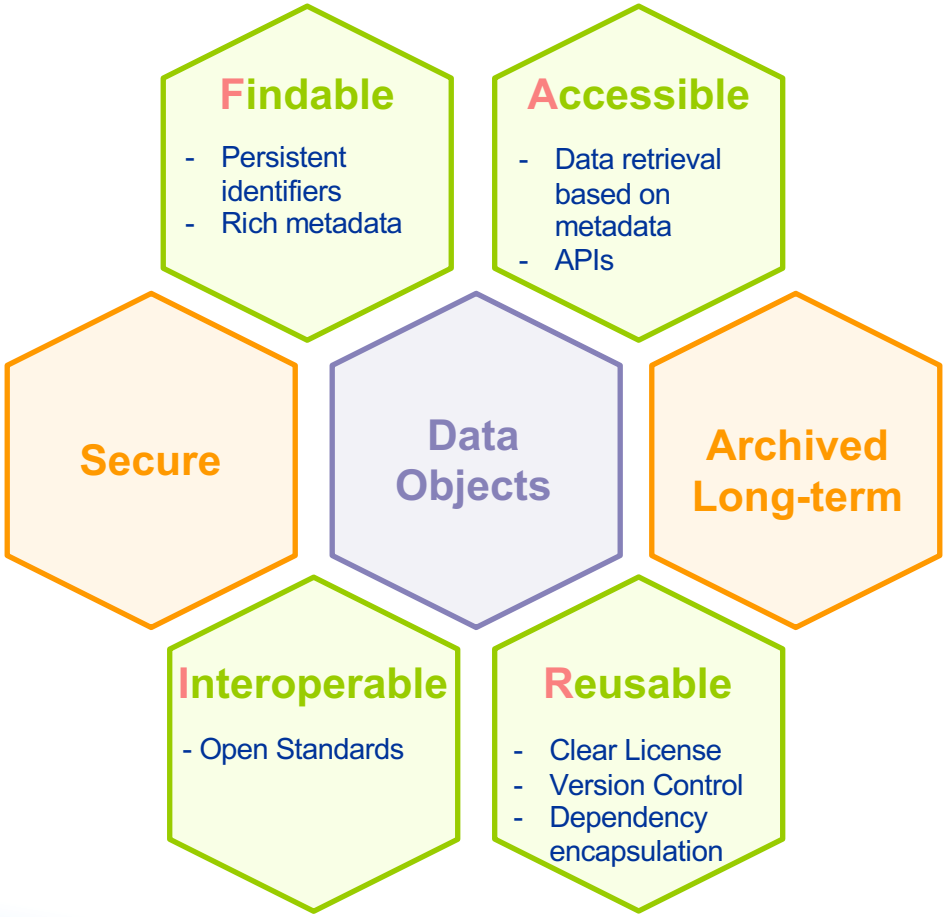
- AMDU is modernizing their legacy systems and building new ones using a new software stack (Django/Python + MySQL);
- The development is mainly done by the Unit Head, Christian Hill;
- GitHub - version control and collaborative development;
- New applications coexist with the legacy ones on the same computing infrastructure;
- Anaconda – requirements management and dependency encapsulation.

CoNDERC



- New application using a Python software stack;
- GitHub - version control, issue tracking and collaborative development;
- Coexists with the existing software applications on the same computing infrastructure;
- Anaconda – requirements management and dependency encapsulation.

Long-term Objective: Infrastructure for FAIR Data



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Thank you!