



IAEA

International Atomic Energy Agency
Atoms for Peace and Development

NDS Computing Infrastructure

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



IAEA

International Atomic Energy Agency

Atoms for Peace and Development

Outline

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

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

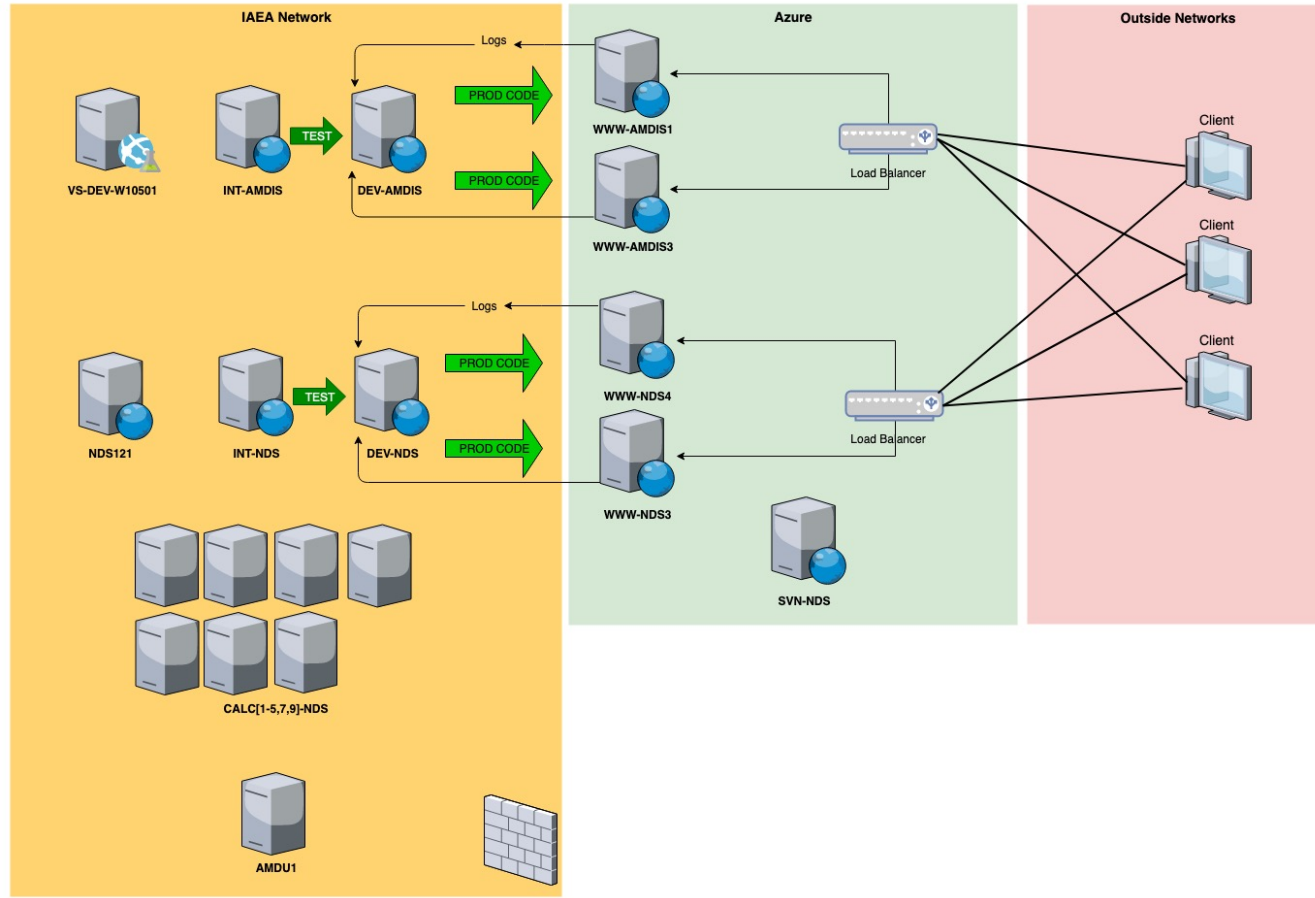


Hardware Infrastructure

Hardware Infrastructure

NDS Servers Overview

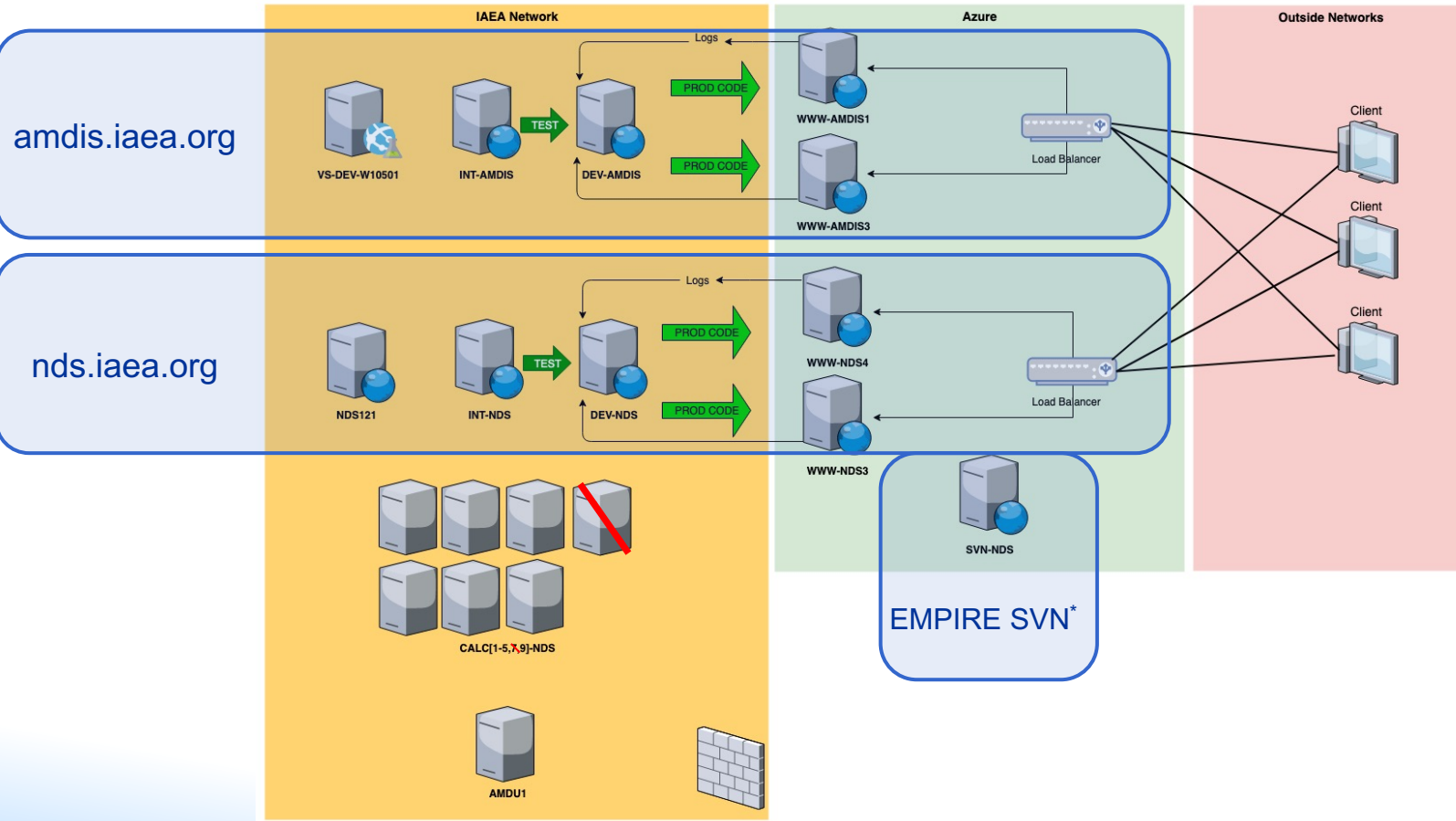
v1.0 2019-04-11



Hardware Infrastructure

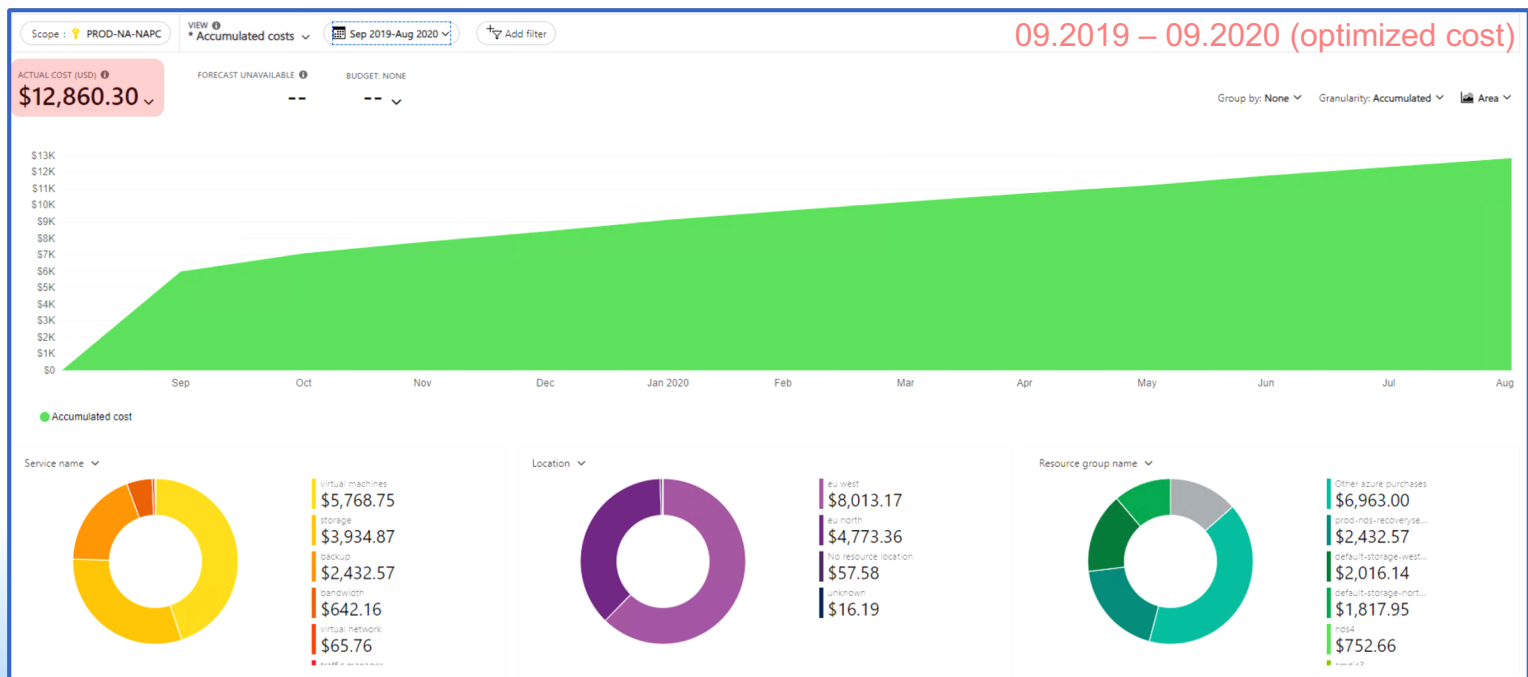
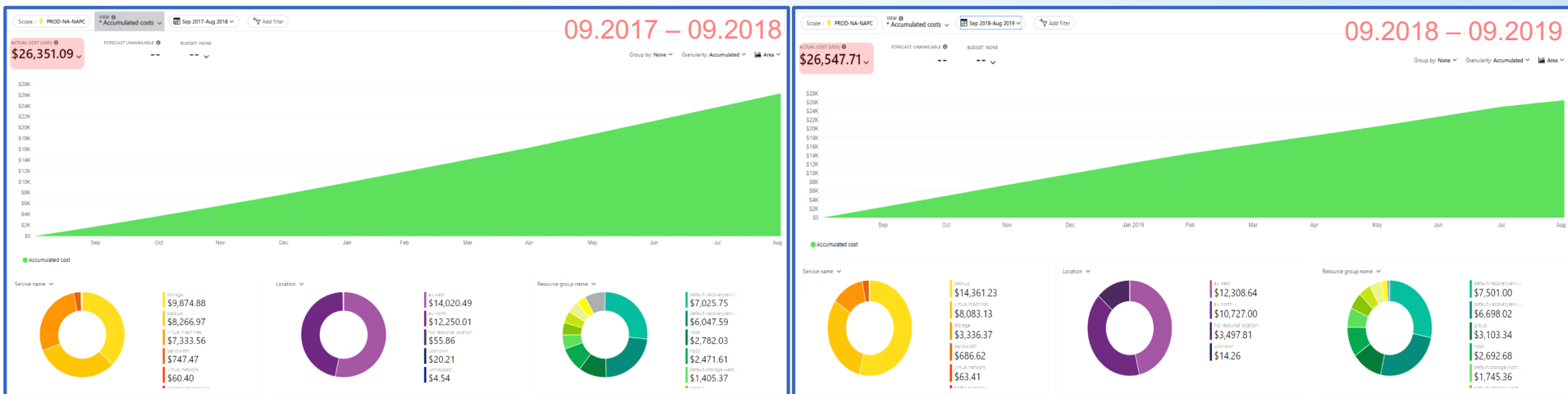
NDS Servers Overview

v1.0 2019-04-11

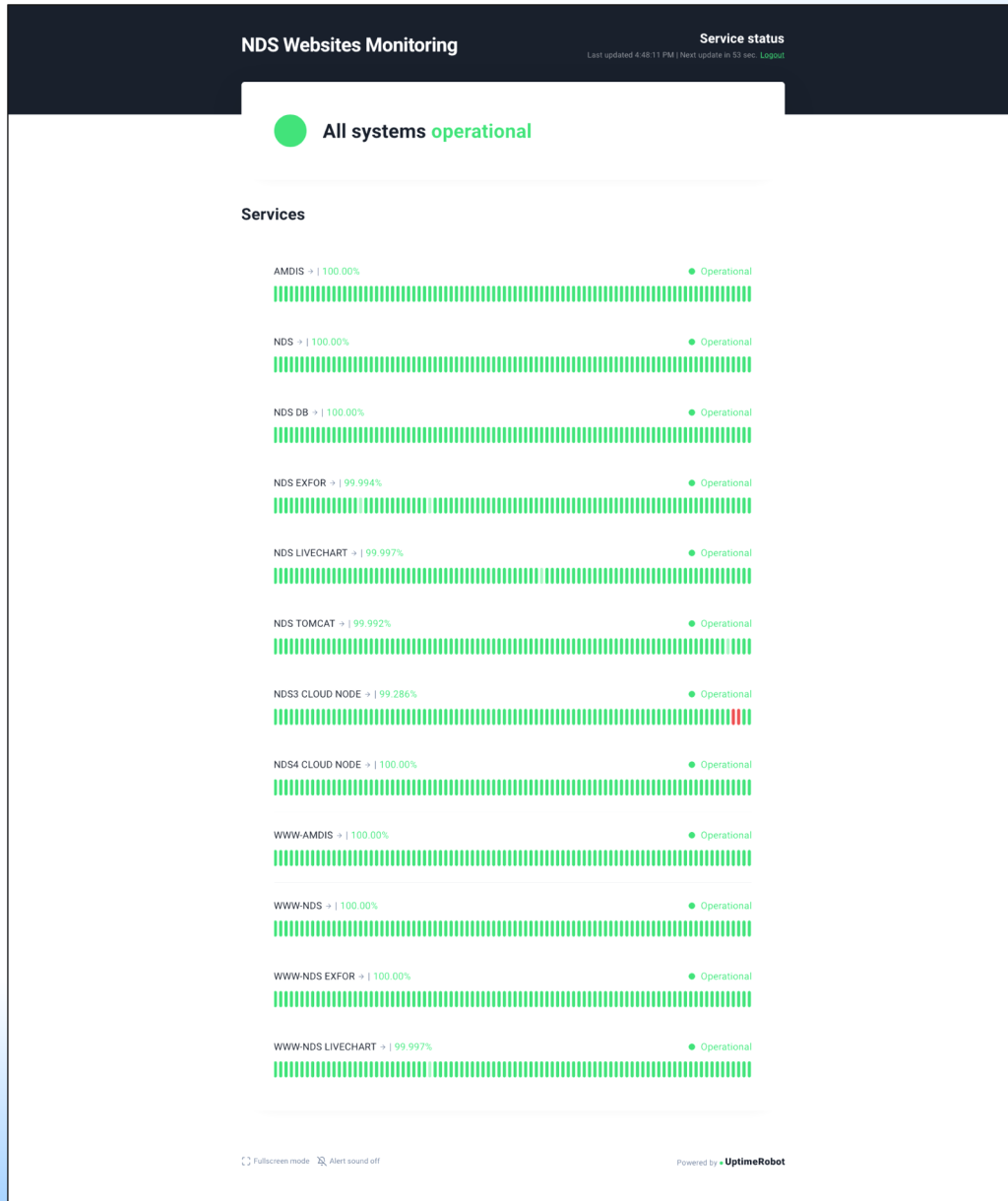


* <http://svn-nds.westeurope.cloudapp.azure.com/svnempire>

Cloud cost – 52% reduction



Availability monitoring



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

Availability monitoring



100.000%	http	AMDIS	100%
100.000%	http	amdis new	100%
100.000%	kywd	CDB	100%
100.000%	http	NDS	100%
100.000%	kywd	NDS DB	100%
100.000%	kywd	NDS ENDF REDIRECT	100%
100.000%	kywd	NDS EXFOR	100%
100.000%	kywd	NDS LIVECHART	100%
99.977%	kywd	NDS TOMCAT	100%
97.859%	http	NDS3 CLOUD NODE	100%
100.000%	http	NDS4 CLOUD NODE	100%
100.000%	http	WWW-AMDIS	100%
100.000%	http	WWW-NDS	100%
100.000%	kywd	WWW-NDS EXFOR	100%
100.000%	kywd	WWW-NDS LIVECHART	100%

Quick Stats

You are currently using 15 of your 50 monitors.

UP MONITORS

15

show "up" monitors

DOWN MONITORS

0

show "down" monitors

PAUSED MONITORS

0

show "paused" monitors

Overall Uptime

- 100.000% (last 24 hours)
- 99.382% (last 7 days)
- 99.856% (last 30 days)

Latest downtime

It was recorded (for the monitor NDS3 CLOUD NODE) on 2021-03-13 00:58:14 and the downtime lasted for 8 hrs, 54 mins.

Latest Events For All Monitors (up, down, start, pause) [Export Logs](#)

Event	Monitor	Date-Time	Reason	Duration
Up	NDS3 CLOUD NODE	2021-03-13 09:53:09	OK (200)	54 hrs, 56 mins
Down	NDS3 CLOUD NODE	2021-03-13 00:58:14	Connection Timeout	8 hrs, 54 mins
Up	NDS3 CLOUD NODE	2021-03-12 07:29:04	OK (200)	17 hrs, 29 mins
Down	NDS3 CLOUD NODE	2021-03-12 00:59:09	Connection Timeout	6 hrs, 29 mins
Up	NDS TOMCAT	2021-03-11 19:38:51	Keyword Found	93 hrs, 10 mins
Down	NDS TOMCAT	2021-03-11 19:28:59	Keyword Not Found	0 hrs, 9 mins
Up	NDS ENDF REDIRECT	2021-02-04 19:53:47	Keyword Found	932 hrs, 55 mins
Up	NDS LIVECHART	2021-02-04 19:53:27	Keyword Found	932 hrs, 56 mins
Down	NDS ENDF REDIRECT	2021-02-04 19:49:41	Keyword Not Found	0 hrs, 4 mins
Down	NDS LIVECHART	2021-02-04 19:49:29	Connection Timeout	0 hrs, 3 mins

- ### From the Blog
- [UptimeRobot March 2021 Update: New Integrations, Heartbeat & SSL Improvements](#)
 - [Latest APIv2 Updates \(CORS headers, etc.\)](#)
 - [Introducing a Completely Redesigned Mobile App!](#)
 - [Introducing Public Status Pages 2.0!](#)
 - [UptimeRobot 2020 Update: Acquisition, recent problems and future plans](#)

Security



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

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

- **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.

Software & Data Development Processes

```
if (electrons_sel.size() > 0) ...
if (muons_sel.size() > 0) ...
if (muons_sel.size() > 1) ...

// double leading_cut = (leptons[0]->PT > 20);
// double subleading_cut = (leptons[1]->PT > 10);
// if ((leptons[0]->PT > leading_cut) && (leptons[1]->PT > subleading_cut))
if (tight_lepton)
{
    countCutflowEvent("CutFlow_21_3 Tight_1", 1);
    countCutflowEvent("CutFlow_21_3 sub_1", 1);
    bool CA_3th_1 = false;
    if (leptons.size() > 2)
    {
        CA_3th_1 = leptons[2]->PT > (leptons[1]->PT);
    }
    if (taus.size() > 0)
    {
        CA_3th_1 = taus[0]->PT > 20;
    }
    if (!CA_3th_1)
    {
        countCutflowEvent("CutFlow_21_3 CA_3th_1", 1);
    }
    bool CA_low_mass = false;
}
```

Version Control



<https://github.com/IAEA-NDS>

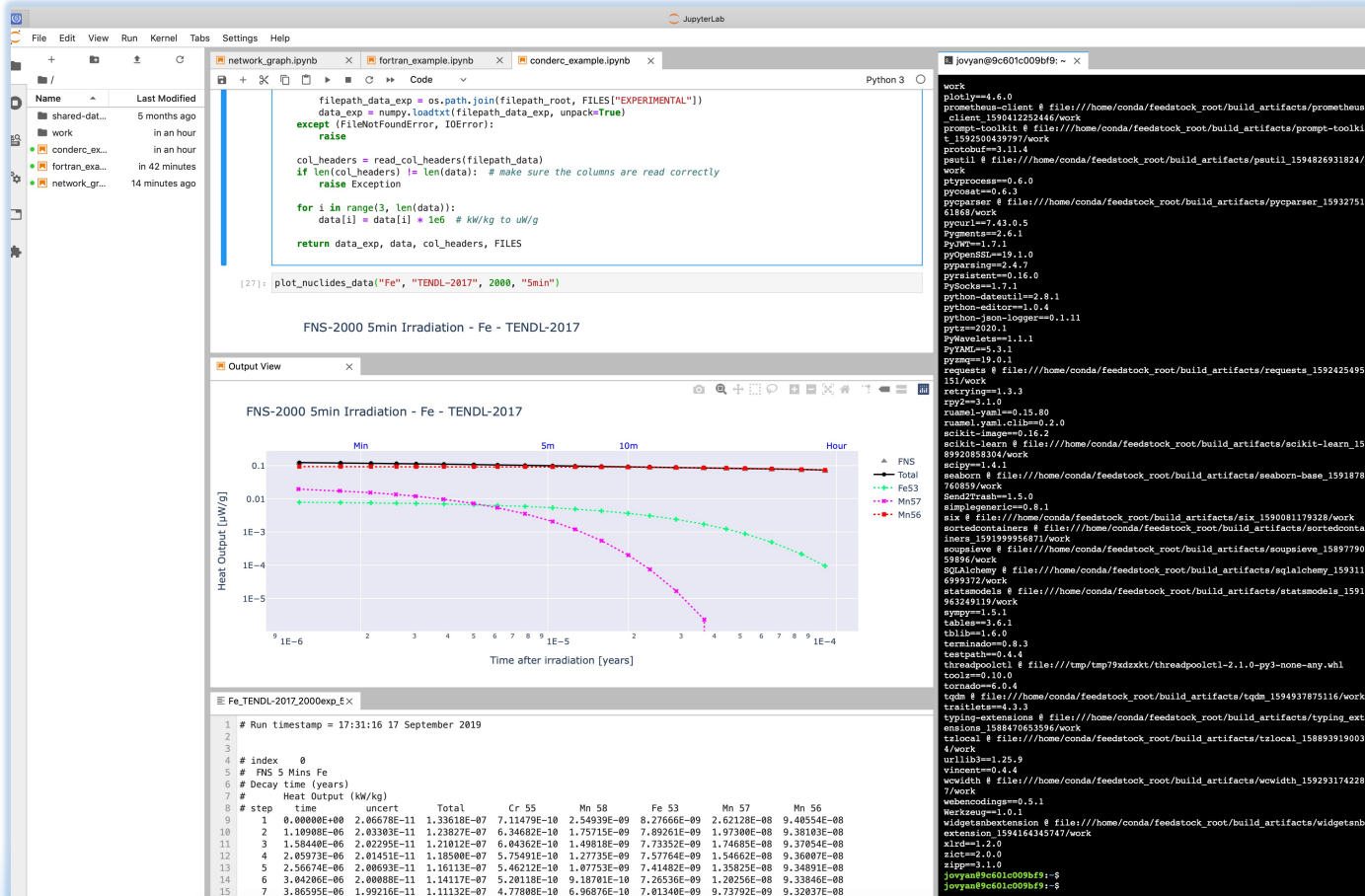
The screenshot shows the GitHub profile for the Nuclear Data Section. The profile includes a search bar, navigation links for Pull requests, Issues, Marketplace, and Explore, and a header for the Nuclear Data Section. Below the header, there are tabs for Repositories (29), Packages, People (10), Teams, Projects, and Settings. The main content area displays pinned repositories, a search bar for finding repositories, and a list of repositories with their respective languages and update dates. The repositories listed are FENDL-ENDF, stoppingPowers, conderc, cdb, TRIPOLI-dataset, and Oktavian-dataset. A sidebar on the right shows top languages (Python, Fortran, TeX, HTML, R) and a list of people.

Public Private

The screenshot shows the GitLab Projects page. The page includes a search bar, navigation links for Projects, Groups, and More, and a header for the Projects section. Below the header, there are tabs for All, Most stars, and Trending, and a filter by name search bar. The main content area displays a list of projects with their names, maintainers, star counts, and update dates. The projects listed are NDS-Website, Operations, annexed-NDS-website / annexed-NDS-subsites / 50_years_NDS, annexed-NDS-website / annexed-NDS-website, annexed-NDS-website / annexed-NDS-subsites / stopping, annexed-NDS-website, webchecks / broken-link-crawler, TALYS_webpage, CoNDERC, amdis-legacy, cdb, Amdis-New, and NDS-Website.

Internal

Jupyter Notebooks



The screenshot displays a JupyterLab environment with the following components:

- File Browser:** Shows a directory structure with files like 'network_graph.ipynb', 'fortran_example.ipynb', and 'condorc_example.ipynb'.
- Code Editor:** Contains Python code for data processing and plotting. The code includes file path handling, data loading, and a plot command: `plot_nuclides_data("Fe", "TENDL-2017", 2000, "5min")`.
- Output View:** Displays a plot titled "FNS-2000 5min Irradiation - Fe - TENDL-2017". The plot shows Heat Output [μW/g] on a logarithmic y-axis (from 1E-5 to 0.1) versus Time after irradiation [years] on a logarithmic x-axis (from 1E-6 to 1E-4). Data series include FNS (Total), Fe53, Mn57, and Mn56.
- Table:** A table titled "Fe_TENDL-2017_2000exp_5x" showing heat output data for various isotopes over time. The table has columns for step, time, uncertainty, and heat output for Total, Cr 55, Mn 58, Fe 53, Mn 57, and Mn 56.



- Python, R, Julia
- Fortran
- Fast prototyping
- Easy sharing of code
- Dependency encapsulation
- Access from browser

Internal



WORLD WIDE WEB

The WorldWideWeb (W3) is a wide-area hypermedia[1] information retrieval initiative aiming to give universal access to a large universe of documents.

Everything there is online about W3 is linked directly or indirectly to this document, including an executive summary[2] of the project, Mailing lists[3], Policy[4], November '93 newsletter, Frequently Asked Questions[5].

Modernizing Legacy Systems

What's out there?[7]Pointers to the world's online information, subjects[8], W3 servers[9], etc.

Help[10] on the browser you are using

Software Products[11] A list of W3 project components and their current state. (e.g. Line Mode[12], X11 Viola[13], NeXTStep[14], Servers[15], Tools[16], Mail robot[17], Library[18])

Technical[19] Details of protocols, formats, program internals etc

<ref.number>, Back, <RETURN> for more, or Help: █

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://amd.isiaea.org>. Existing data services at this location function as usual.

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 D₂

FC Factors & A-values of H₂ & 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 Nuclear Data Section

IAEA-NDS Mission, Staff Nuclear Data and more
 Nuclear Data Services
 Meetings Workshops
 Newsletters Research Projects
 Coordinated 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

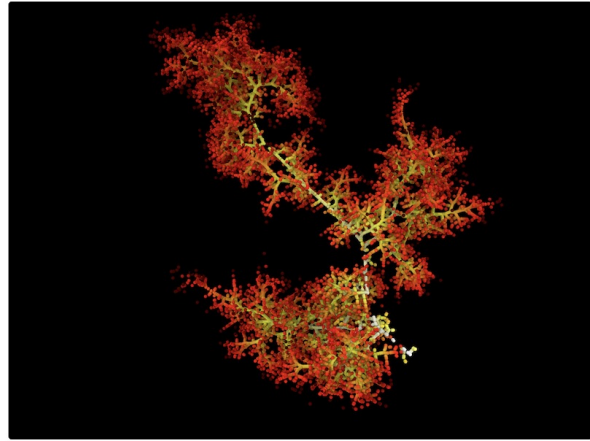
12 – 16 April 2021
 Atomic Processes in Plasmas

3 – 14 May 2021
 ICTP Workshop 2020: Radiation Damage in Nuclear Systems: from Bohr to Young

More meetings ...

Quick Links

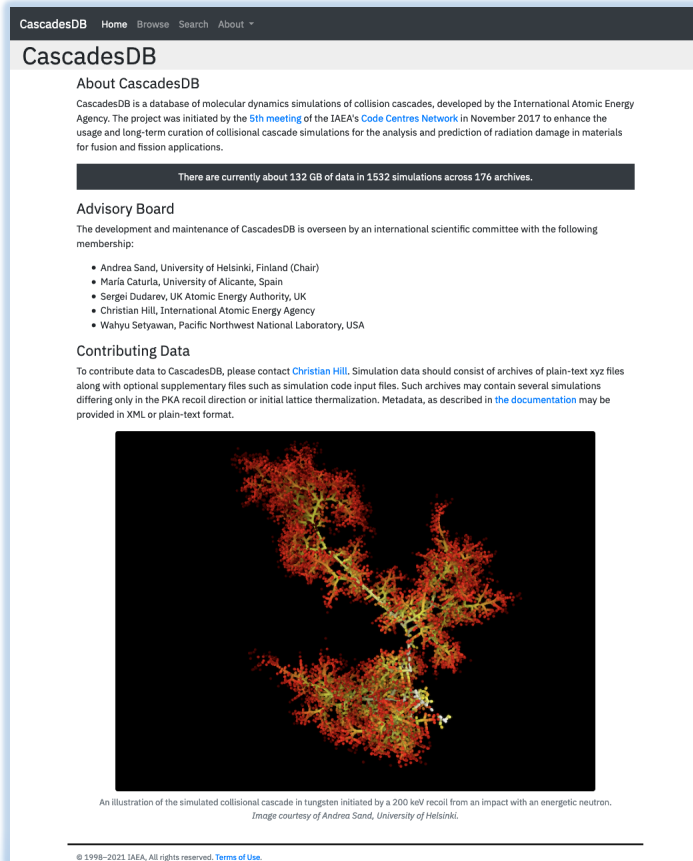
- Our CRPs
 - Hydrogen Permeation
 - Vapour Shielding
 - Neutral Beams
 - Steel Surfaces
- Our Meetings
- Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP)
- Conferences and workshops in atomic and molecular physics





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.

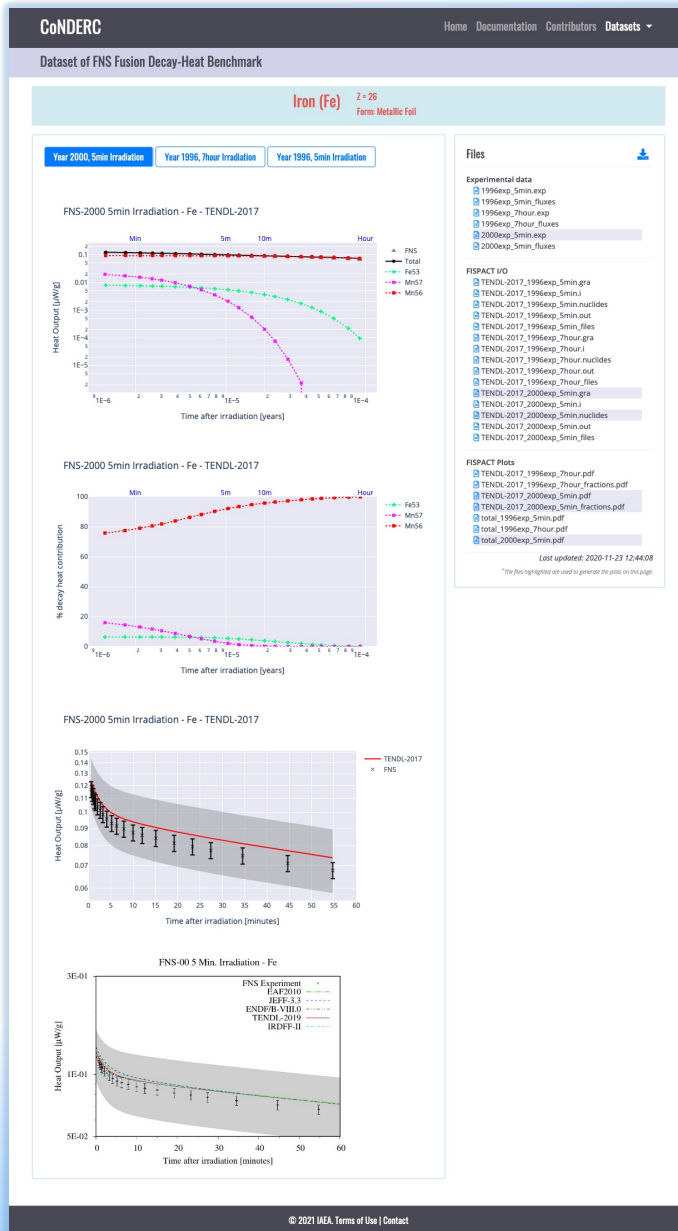
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New version, from 2020



The screenshot shows the CascadesDB website. At the top, there is a navigation bar with 'CascadesDB', 'Home', 'Browse', 'Search', and 'About'. Below this is the title 'CascadesDB' and a section 'About CascadesDB'. The text describes the database as a collection of molecular dynamics simulations of collision cascades, developed by the International Atomic Energy Agency. It mentions the project was initiated by the 5th meeting of the IAEA's Code Centres Network in November 2017. A dark bar highlights the text: 'There are currently about 132 GB of data in 1532 simulations across 176 archives.' Below this is the 'Advisory Board' section, listing members: Andrea Sand (Chair), Maria Caturla, Sergei Dudarev, Christian Hill, and Wahyu Setyawan. The 'Contributing Data' section provides instructions on how to contribute data. At the bottom, there is a large image of a simulated collisional cascade in tungsten, with a caption: 'An illustration of the simulated collisional cascade in tungsten initiated by a 200 keV recoil from an impact with an energetic neutron. Image courtesy of Andrea Sand, University of Helsinki.' The footer contains the copyright notice: '© 1998–2021 IAEA. All rights reserved. Terms of Use.'

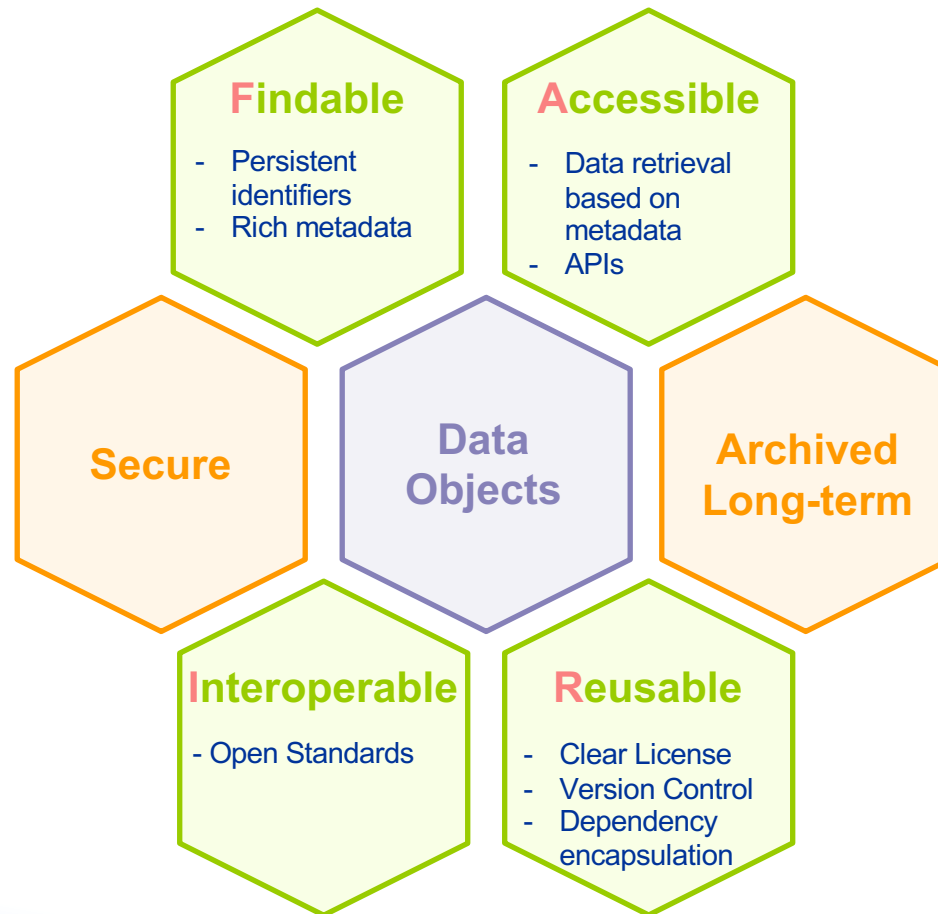
- AMDU is modernizing their legacy systems and building new ones using a new software stack (Django/Python + MySQL);
- The development is mainly done by the Unit Head, Christian Hill;
- GitHub - version control and collaborative development; 
- New applications coexist with the legacy ones on the same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



- 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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Atoms for Peace and Development

Thank you!

