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U.S. DEPARTMENT OF ENERGY

NNDC Report to the NRDC

David Brown
National Nuclear Data Center

NRDC Meeting, IAEA, Vienna
9 May, 2023

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NNDC Vision & Mission

The National Nuclear Data Center (NNDC) vision is to be the premier global resource for nuclear data and plan to:

- ❑ Implement AI/ML algorithms to reduce the time from data publication to integration in a recommended library to less than two years.
- ❑ Establish an open data repository for low-energy nuclear physics.
- ❑ Advance dissemination efforts with modern and efficient software tools.
- ❑ Sustain a robust nuclear physics research portfolio, including the development of an experimental program to accelerate isotope production science.

The NNDC is the lead and largest unit of the U.S. Nuclear Data Program (USNDP), whose mission is to provide current, accurate, authoritative data for workers in pure and applied areas of nuclear science and engineering. This is accomplished primarily through the compilation, evaluation, dissemination, and archiving of extensive nuclear datasets. USNDP also addresses gaps in the data, through targeted experimental studies and the use of theoretical models.

US Nuclear Data Program Main Products

Nuclear Science References (NSR)
Nuclear physics articles indexed according to content

EXFOR
Compiled nuclear reaction data

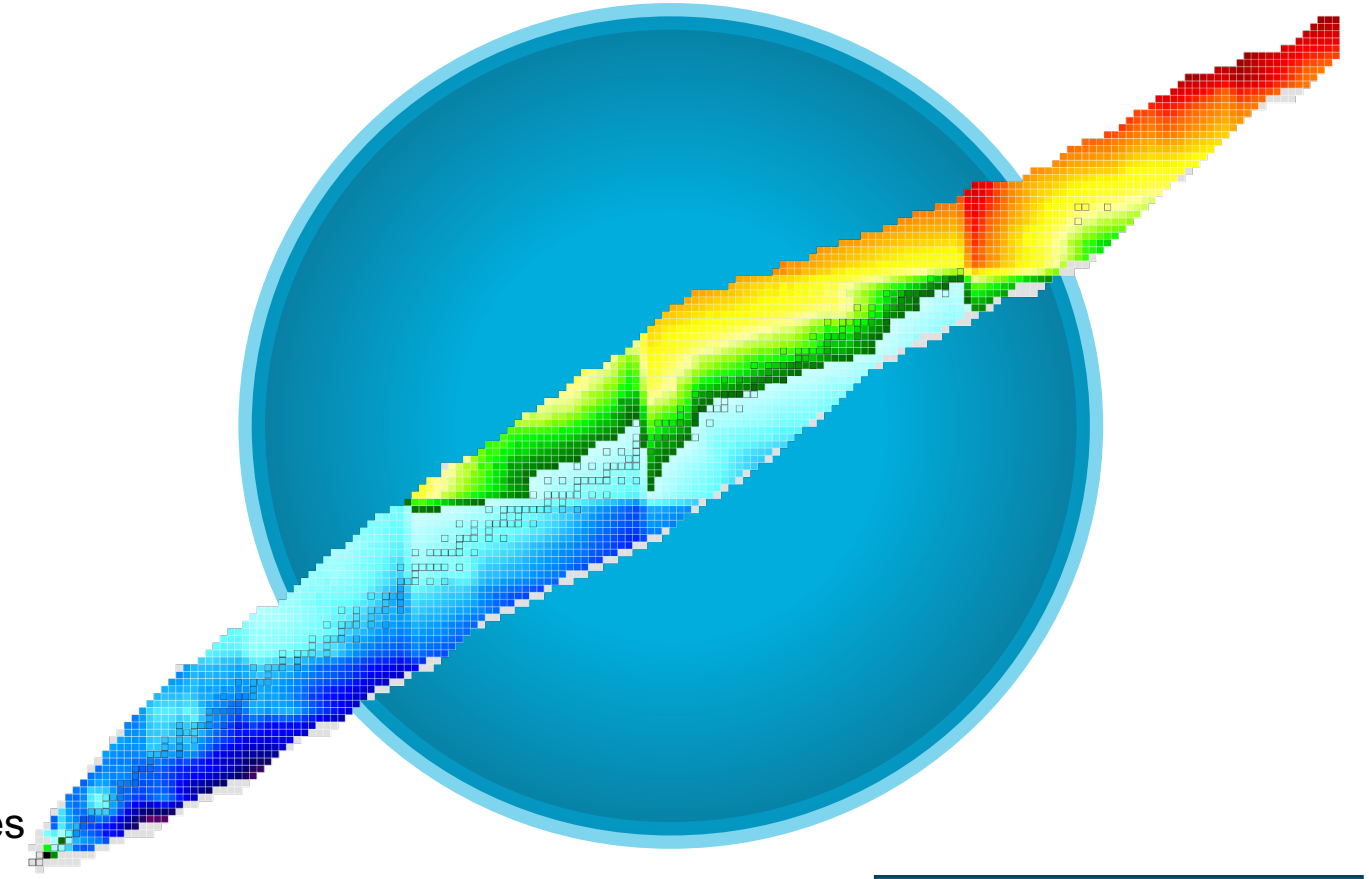
XUNDL
Compiled nuclear structure and decay data

ENSDF
Recommended nuclear structure and decay data

ENDF
Recommended particle transport and decay data, with a strong emphasis on neutron-induced reaction data

Nuclear Data Sheets
Journal devoted to the publication of nuclear data articles

Web dissemination
www.nndc.bnl.gov, nucastrodata.org



Nuclear data science capability to support the development of new reactor concepts.

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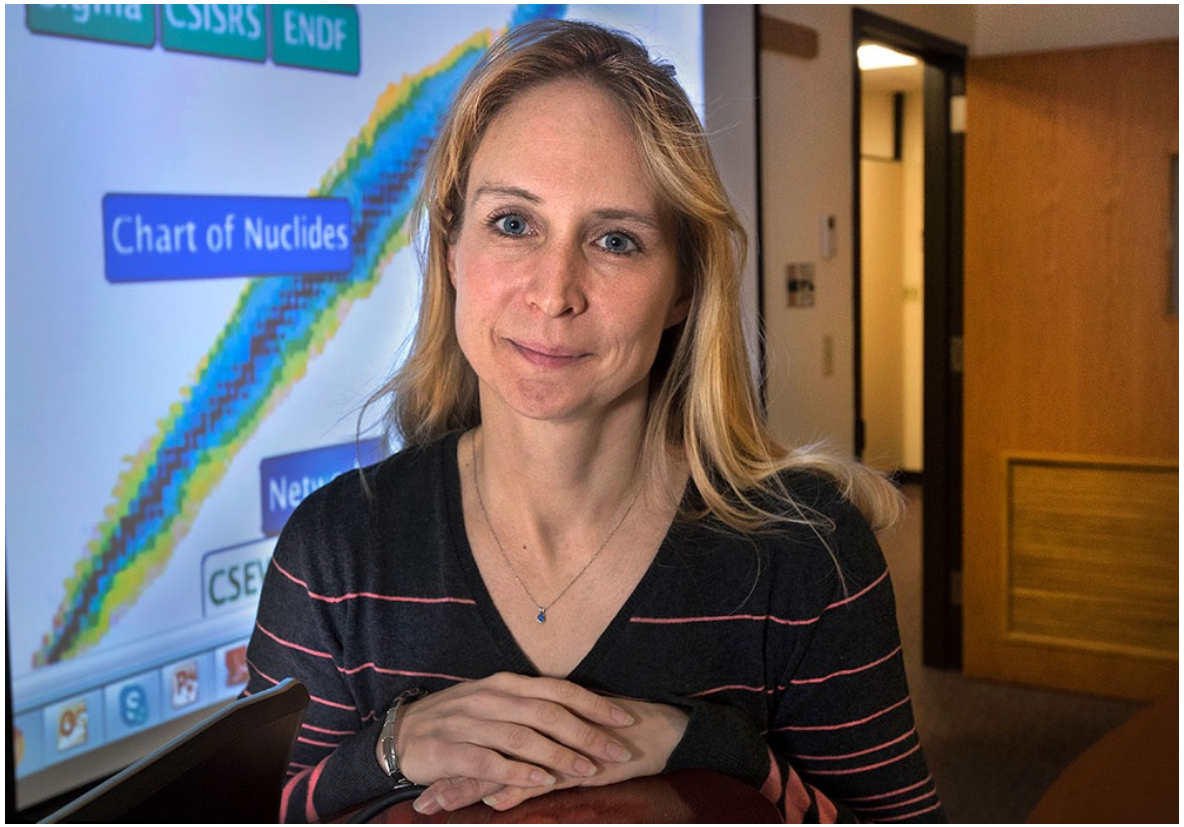
PuRe Data Resources

Personnel updates

Elizabeth (Libby) McCutchan

- APS Fellow 2022
- Citation: *"For innovative and distinguished contributions to understanding the evolution of collectivity in heavy nuclei, critical precision experiments to test ab initio methods in light nuclei, seminal analyses of antineutrino spectra, and the development of new database tools to understand nuclear data."*



https://www.bnl.gov/newsroom/news.php?a=120865

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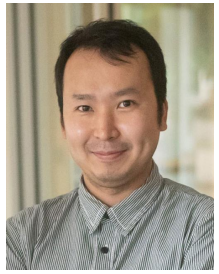
Other personnel changes at the NNDC

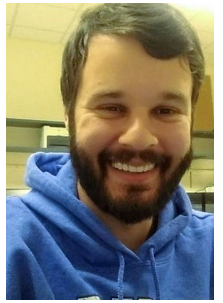


Shuya Ota joined the NNDC May 1st as a scientific staff primarily working on ENSDF and XUNDL, plus developing the NNDC decay station.

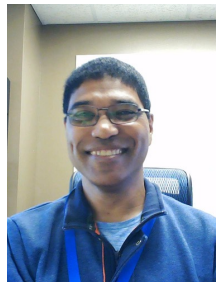
Jin Wu joined the NNDC on September 6th as a scientific staff working on ENSDF/XUNDL and gamma-ray spectroscopy.

Matteo Vorabbi left the NNDC Sep. 16th to begin a position as Lecturer at the University of Surrey, UK.

Emanuel Chimanski joined the NNDC April 11, 2022 as a post doc working on the NA-22 Gamma Rays Induced by Neutrons project. Promoted to staff in April 2023.



Sam Kim joined the NNDC as a post-doc on March 7th to analyze data that helps determine antineutrino spectra, investigate ^{69}Ga, and experiment on ^{125}Xe trapped in silicate nanostructures.



Adam Hayes left the NNDC in January 2022 to work in the private sector

The NNDC currently has 10 staff scientists, 2 post-docs, 4 professional staff and 6 contractors

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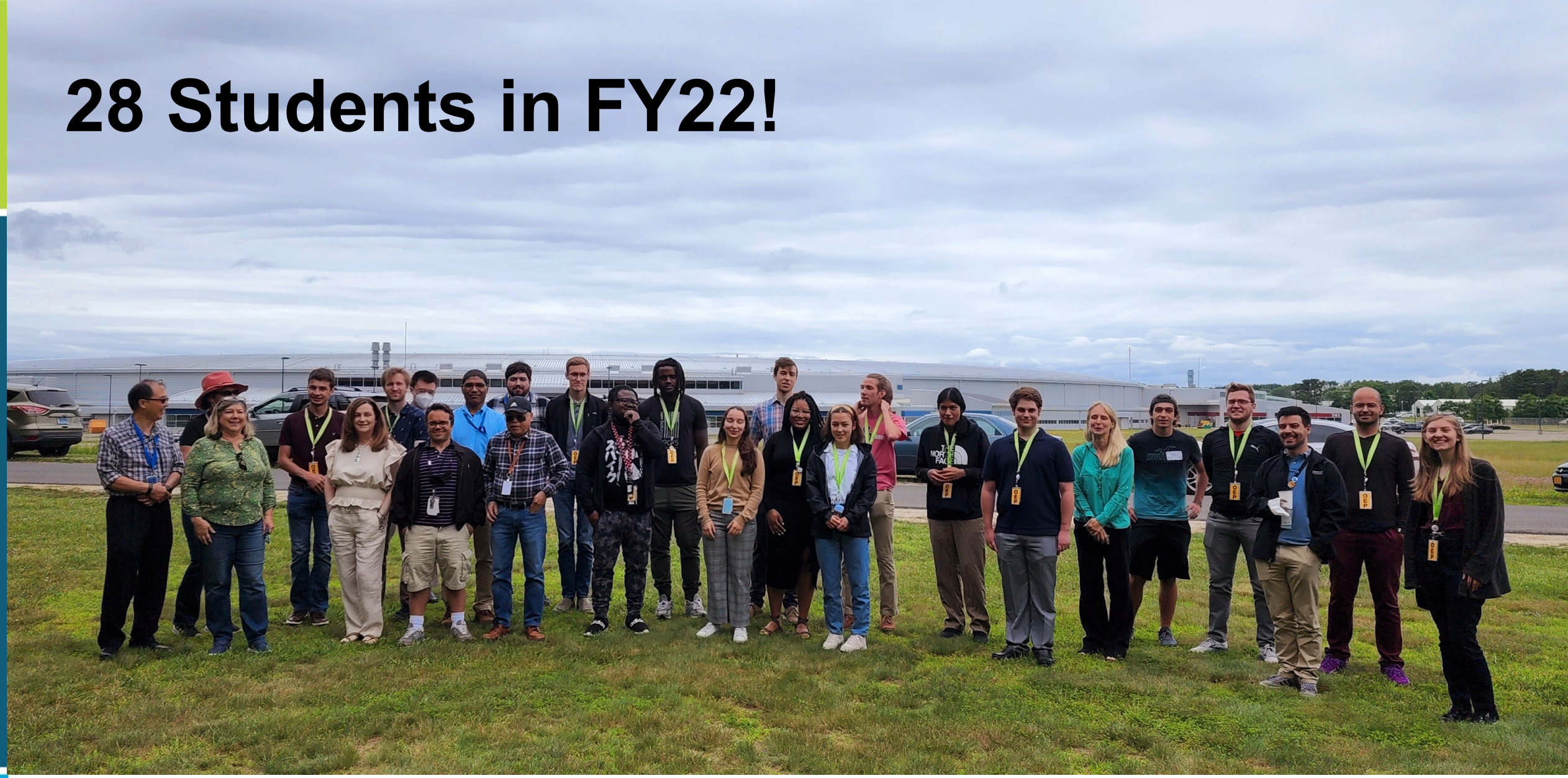
28 Students in FY22!



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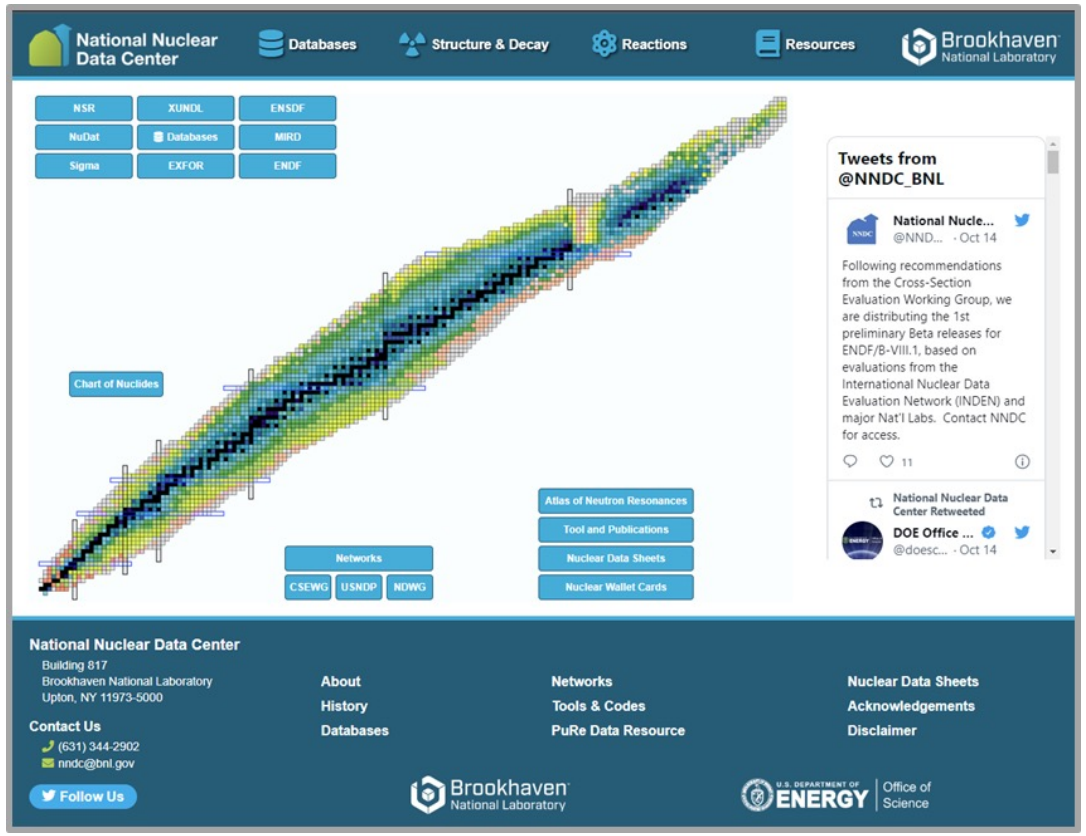
Half of students from traditionally underserved groups

NNDC Website

Website Redesign

- **New front page + header/footer**
  - Deployed in time for ND2022
  - Reduced clutter to direct users to most-trafficked websites
  - Quick access to databases
  - Use of common stylesheets for consistent design
- **Roughly 80% of site fully converted to new style; all pages have new header/footer**



Credit: Donnie Mason

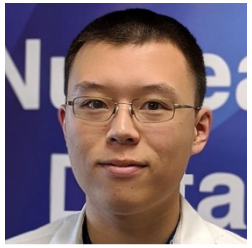
The NNDC is Proactively Addressing Cybersecurity Issues

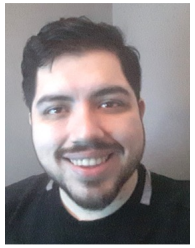
EXFOR

- Unsecured database credentials on both NNDC and IAEA mirror sites
- Solution:
  - Consulted with ITD Cyber Security Operations Manager
  - Purged **exfor/** from NNDC web servers
  - Replaced compromised database account

NSR

- Shared, unsecured passwords for article PDFs on both NNDC and IAEA mirror sites
- Solution:
  - Removed PDF access page from **nsr/**





Detected and resolved by:
Benjamin Shu + Donnie Mason

NNDC Website Modernization

Principle of least privilege

- Selective permissions for controlling access
- No one account with access to whole database
- Credentials isolated to minimize potential breaches

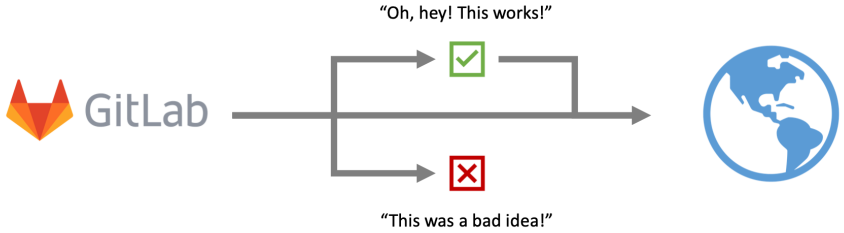
Assures a secure and reliable website consistent with modern webserver practices

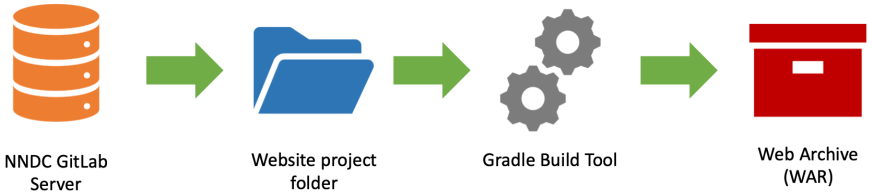
Webapp Containerization

- Use of Docker for containerized deployment
- Secure deployment with restricted credentials
- Robust, reproducible, version-controlled

podman

docker





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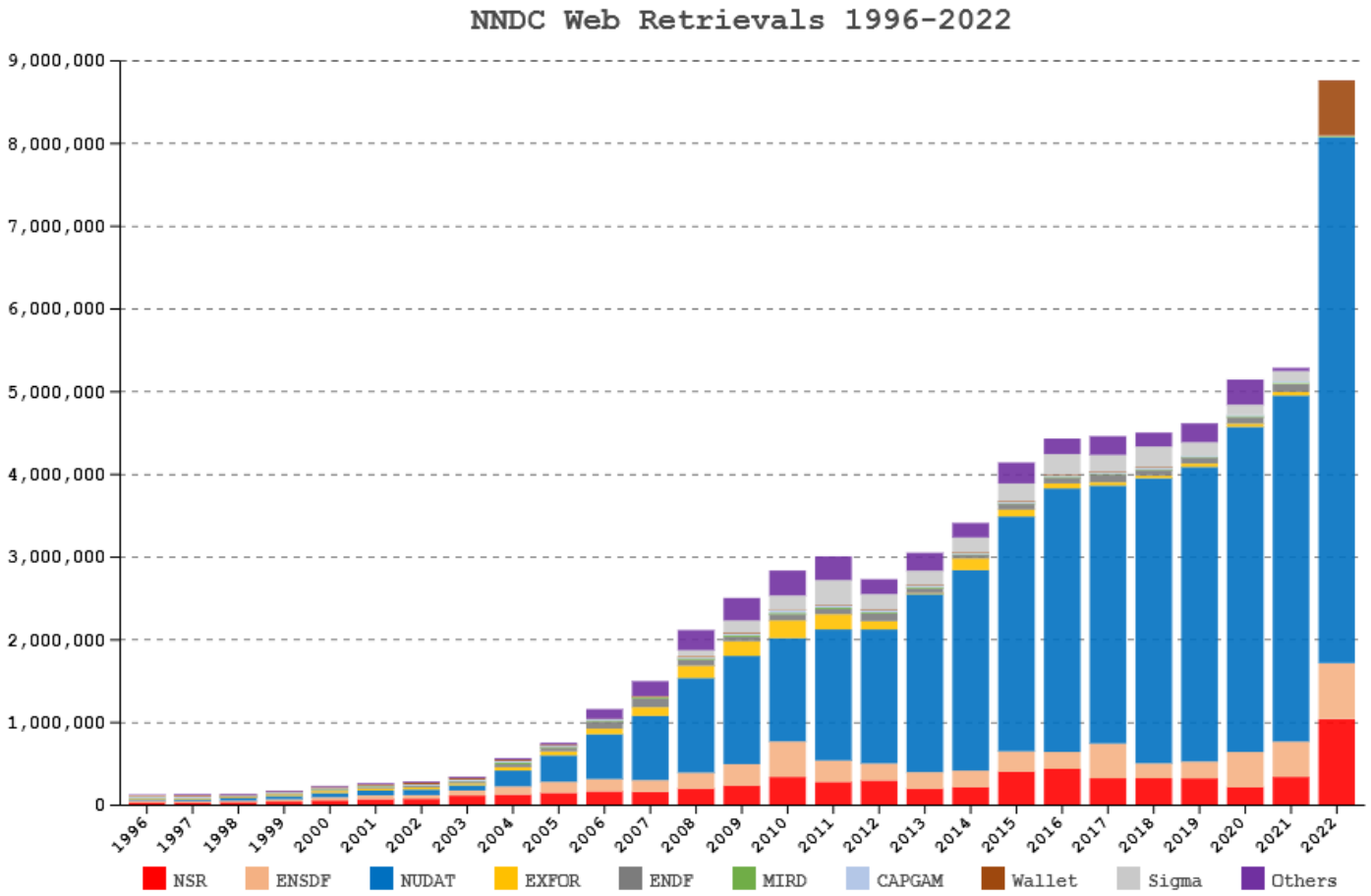
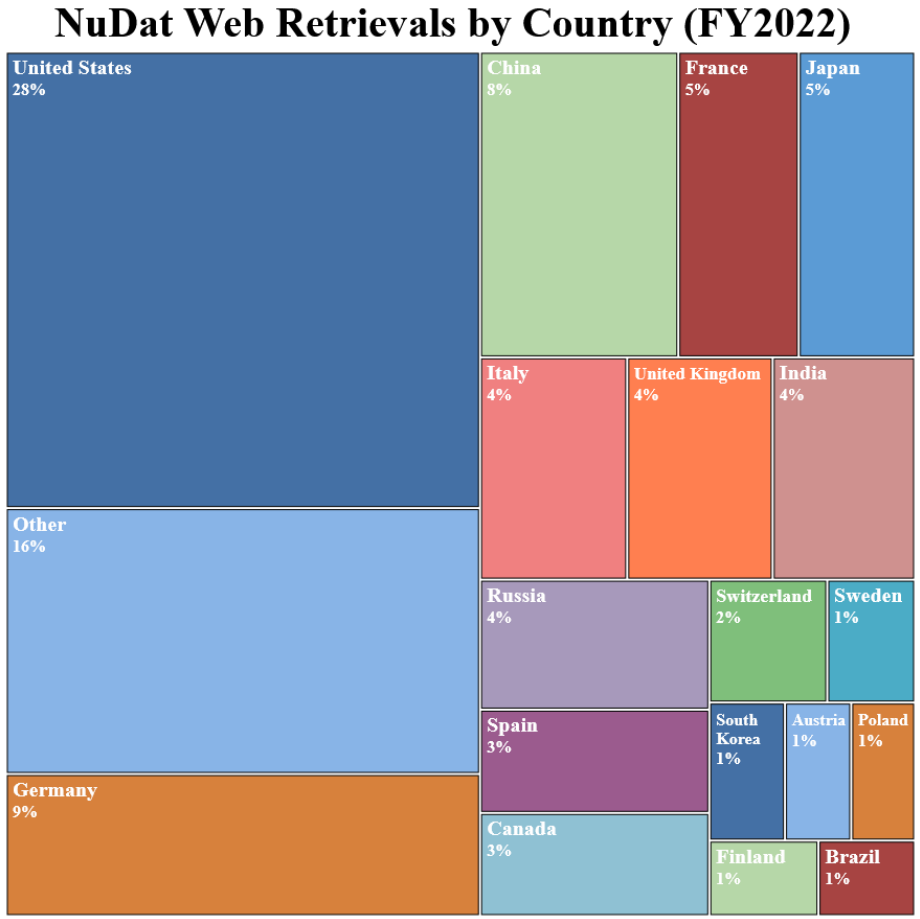
Modernization efforts paying off





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ENSDF & ENDF updates

XUNDL/ENSDF Metrics – for FY22

XUNDL

Compiler	Papers	Datasets
Shaofei	9	16
Libby	162	293
Shuya	11	17
Jin	5	10

Total of 187 papers, 336 datasets

ENSDF

Evaluator	Mass Chain	Nuclei
Chris	251	
Libby	47 (½)	30
Shuya	47(½)	

2 Mass Chains, 30 individual nuclei

NDS publications

C. Morse, "*Nuclear Data Sheets for A=267, 271, 275, 279, 283, 287, 291, 295, 299"* NDS 182, 130 (2022)

C. Morse, "*Nuclear Data Sheets for A=269, 273, 277, 281, 285, 289, and 293",* NDS 182, 167 (2022)

S. Zhu, "*Nuclear Data Sheets for A=236",* Nucl.Data Sheets 182, 2 (2022)
(reviewer comments received after Shaofei's passing)

The Cross Section Evaluation Working Group produces ENDF/B library

- **Formed 1966 & Chaired by BNL**
- **Currently ~200 members of the collaboration from 25 institutions**
  - US programs, industry and international partners
  - If you see something in the library, at some point a sponsor somewhere wanted it
- **All steps of nuclear data pipeline coordinated through CSEWG**
- **Depending on what needs done, getting required data in library can be major effort**

Preparing the next "minor" release: ENDF/B-VIII.1, due February 2024

CSEWG collaboration meeting in November 2022: our first in-person meeting since the pandemic started!

ENDF/B-VIII.1 release

Recommended particle transport and decay data

The next release of the ENDF/B library is scheduled for **February 2024!**
Although technically "minor", it will have major impact.

- Why VIII.1 and not IX?
  - There are no planned updates of the standards library for this release
  - However, many, many important and impactful changes are on the way!!
- Full release will be in both legacy **ENDF-6** format an **GNDS-2.0**
- Will have an accompanying **"Big Paper"** in Nuclear Data Sheets
- Peer reviews of (most of) new evaluations complete
- Preliminary validation testing has begun
- ***Beta2 release planned for June/July, one more beta release planned before fall***

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Modernization efforts

Digital Object Identifiers (DOIs)

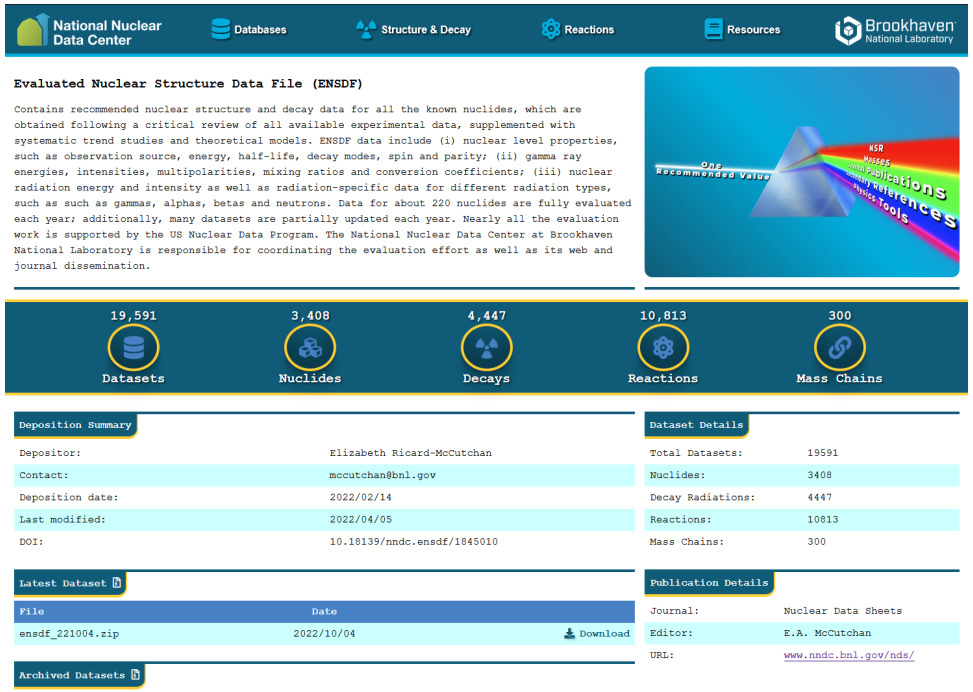
As a **Public Reusable Research (PuRe) Data Repository** the NNDC strives to make data publicly available to advance scientific knowledge

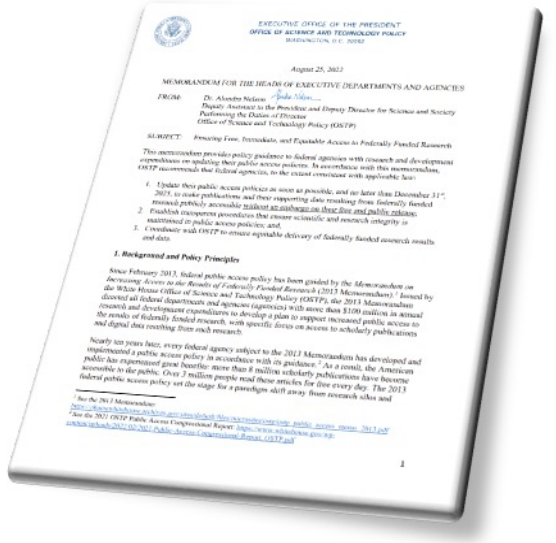
PuRe Data Resources

3 major libraries already have library-wide DOIs:

- ENSDF
- XUNDL
- NSR

ENDF & the Atlas are next!





Compliance with OSTP policy guidelines from 25 August 2022 memo

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WalletCraft

A new evaluation of properties of ground-state and long-lived isomers for all known nuclei

Evaluation for g.s. and isomers ($T^{1}/_{2}$>100ms) of:

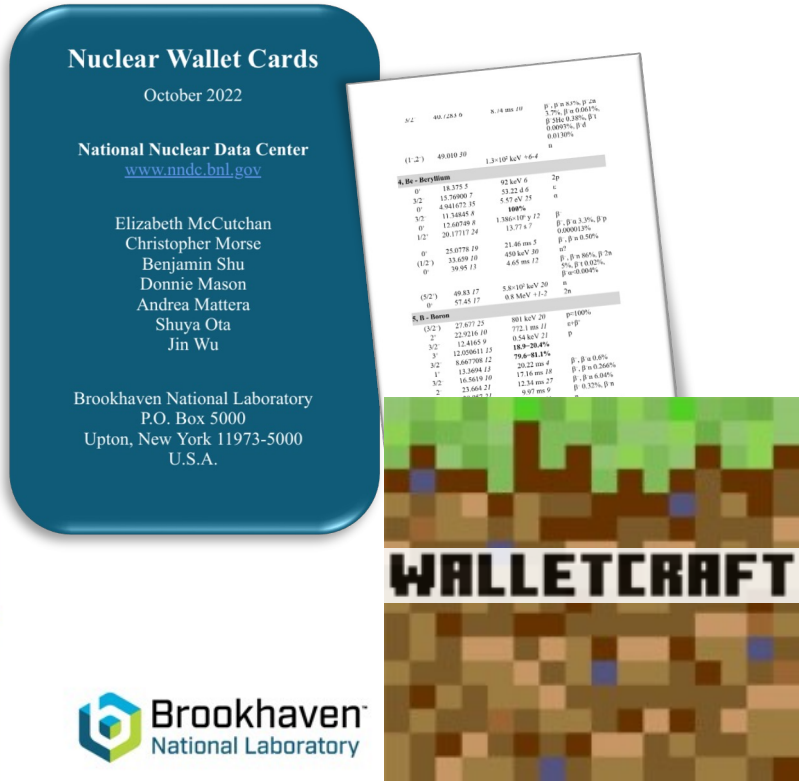
- Spin/Parity
- Mass Excess – from AME2020
- Half-life, Width or Abundance
- Decay Mode(s)

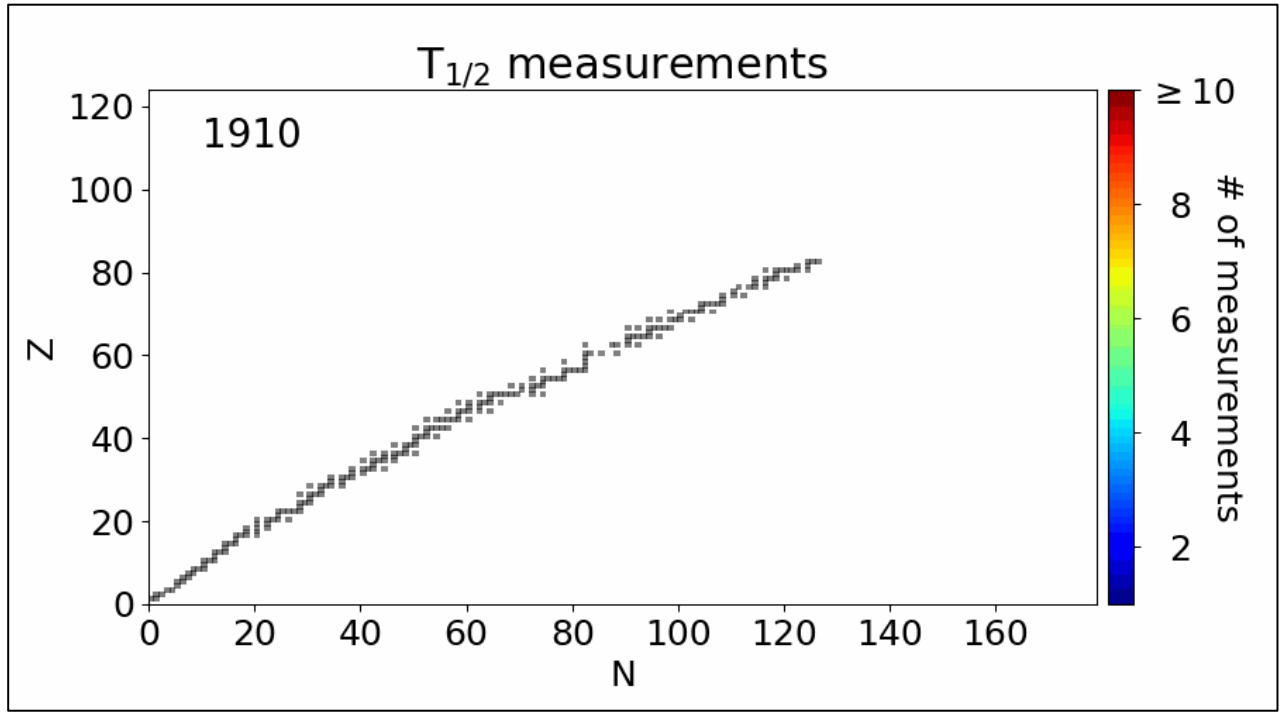
Major changes *under the hood*:

- New JSON-based OODB
- We store experimental measurements (building block of the evaluation)

Advantages:

- Transparent documentation of evaluation history
- Format can be easily read in modern codes and data plotted/analyzed
- Allows for much shorter versioning (from 5-10 yr to ~1yr)





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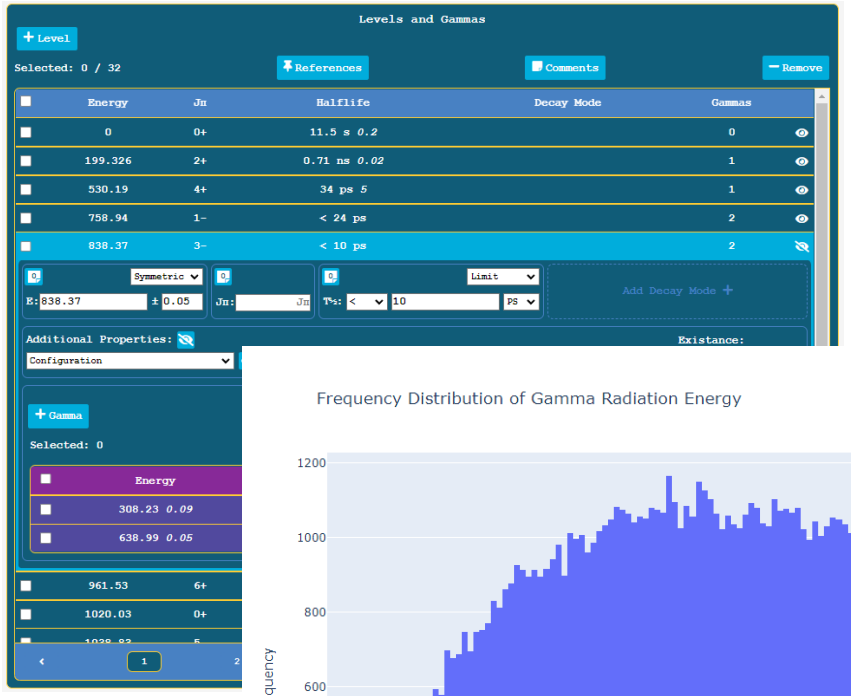
A new object-oriented database for ENSDF

We've migrated from 80 column ASCII to JSON based

```
137CS PN                                                              6
137CS  L 0.0         7/2+              30.08 Y   9                    A
137CSX L XREF=ACDEFGH
137CS2 L %B-=100$MOMM1=+2.8413 1 (1989Ra17)$MOME2=+0.051 1 (1989Ra17)
137CS cL T$Deduced by evaluators using the Limitation of Relative Statistical
137CS2cL Weights (LRSW) method for analyzing the following set of
137CS3cL discrepant (|h{+2}/|n=18.6) experimental values: 10970 d {I20}
137CS4cL (2004Sc04); 11018 d {I10} (2002Un02); 10941 d {I7} (1992Go24);
137CS5cL 10968 d {I5} (1990Ma15); 11009 d {I11} (1980Ho17); 10906 d {I33}
137CS6cL (1978Gr08); 11034 d {I29} (1973Co39); 11021 d {I5} (1973Di01); 11023 d
137CS7cL {I37} (1972Em01); 10921 d {I17} (1970Wa19); 11191 d {I157} (1970Ha32);
137CS8cL 11286 d {I256}, 10921 d {I183} (1965Fl01); 11220 d {I47} (1965Le25);
```


```
{
    "spinParityValues": [
        {
            "spin": 2,
            "isTentativeSpin": true,
            "isTentativeParity": true,
            "parity": "+",
            "parityNumber":1
        },
        {
            "spin": 3,
            "isTentativeSpin": true,
            "isTentativeParity": true,
            "parity": "-",
            "parityNumber":-1
        }
    ],
    "comments": [
        "Assignments are based on..."
    ]
}
```


Developed a new Editor for ENSDF evaluators



And (for the first time!) designed an API for

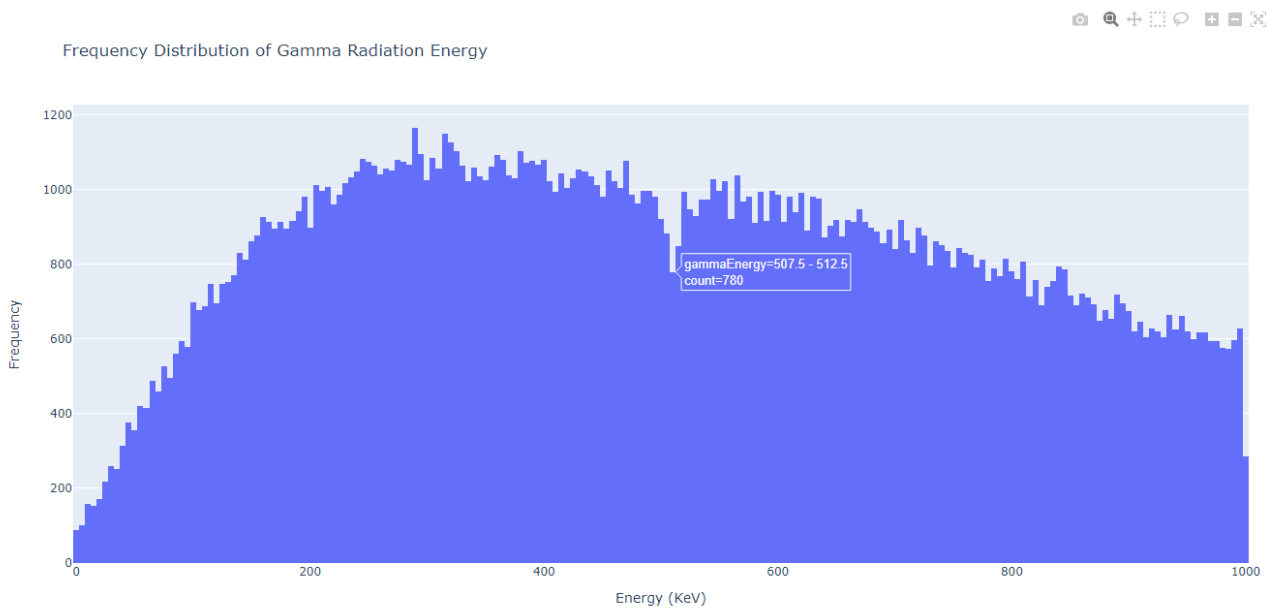
```
# Initialize API
api = ensdfAPI(ipAddress="127.0.0.1", port=5001)

# Get all gammas 0-1000 keV
values_dict=api.filterByGammas(0,1000)
dataframe = plot.createViewDataFrame(values_dict)

# Label plot
plot.configuration.setAxisTitle("x", "Energy (KeV)")
plot.configuration.setAxisTitle("y", "Frequency")
plot.configuration.setTitle("Frequency Distribution of Gamma Radiation Energy")

# Plot as a histogram
figure=plot.createHistogram(dataframe, "gammaEnergy")

plot.showFigure(figure)
```



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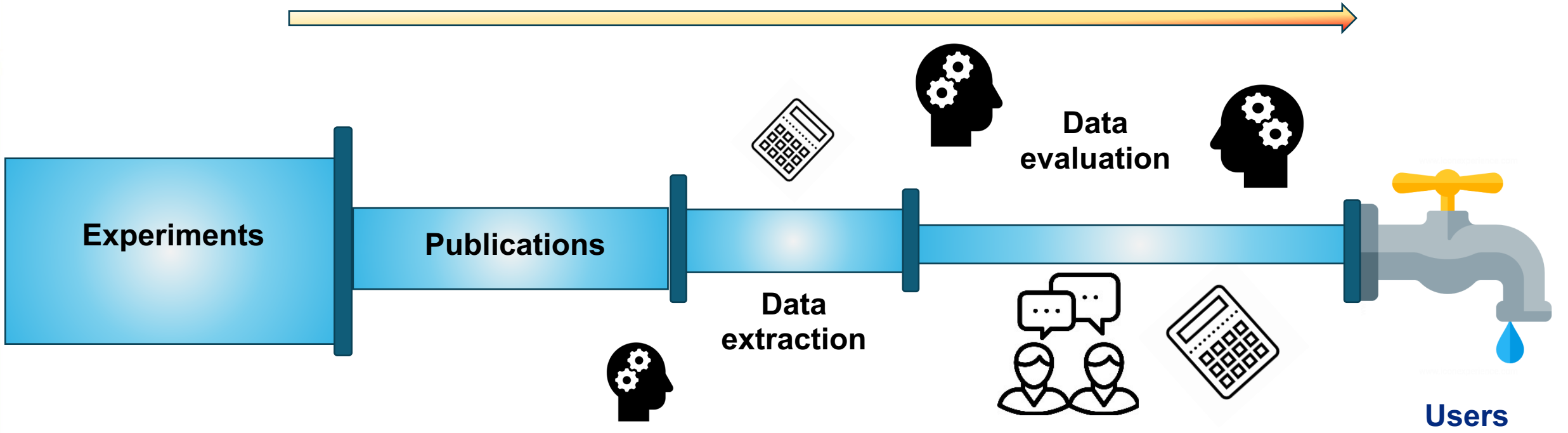
What we’re working on now

Nuclear Data Pipeline, now

Current timeline of about **5 – 10 years**



Our product's impact is limited by:

- Outdated formats
- Outdated evaluation procedures
- Often publications only contain a portion of all data measured

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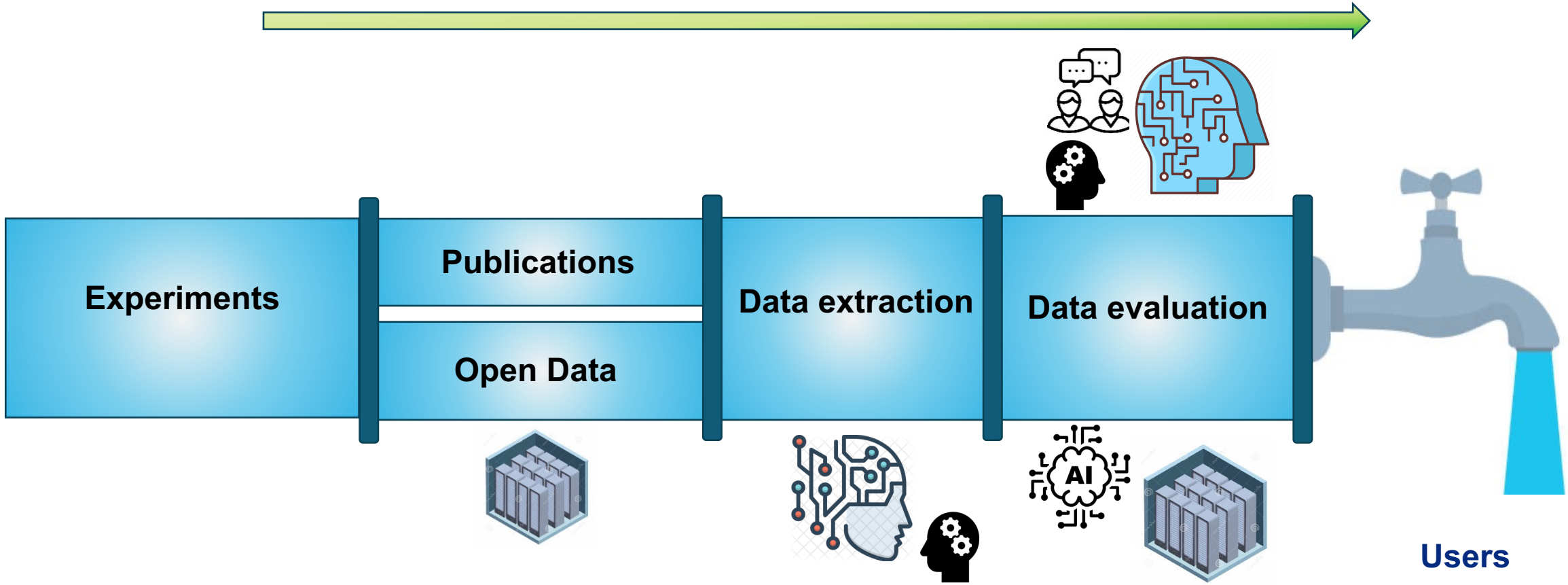
Nuclear Data Pipeline, 2028

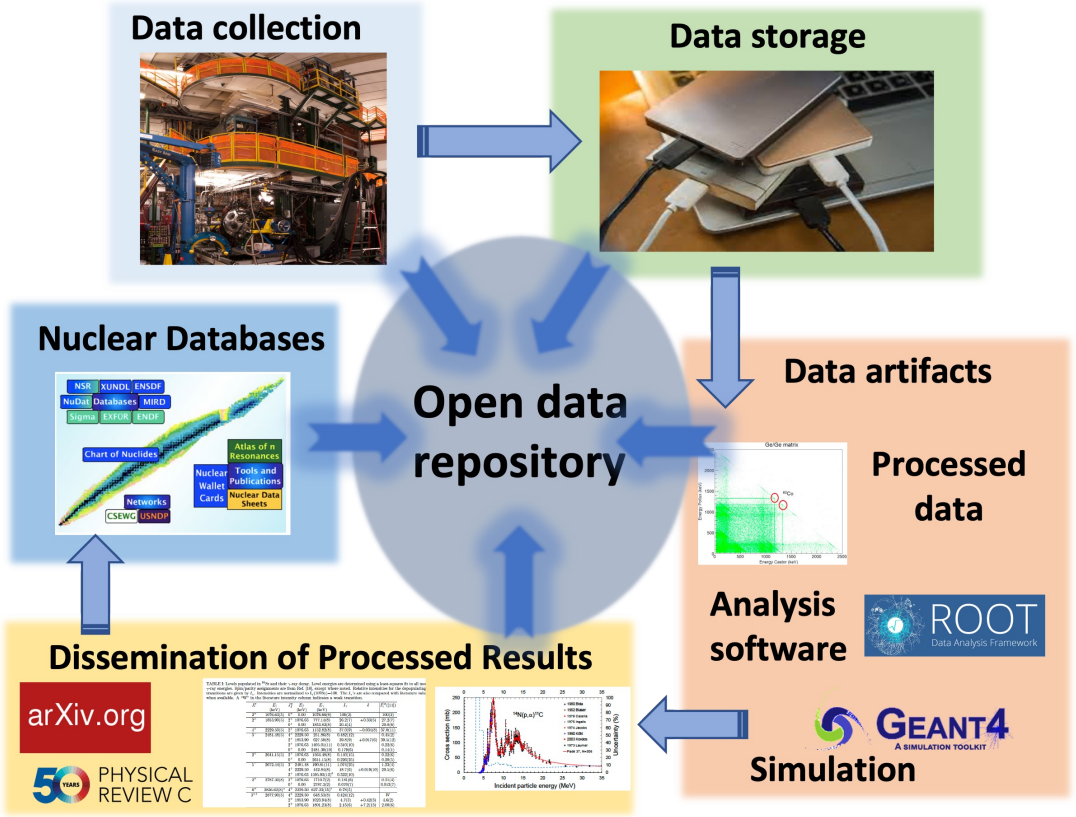
Proposed timeline of about **1 – 2 years**



This new paradigm will address bottlenecks, ensure that results of expensive experiments are properly stored, and address stakeholders' feedback in a timely manner.

Open Nuclear Data

Low Energy Nuclear Physics has strategic value and should be archived (Harriet Kung (DOE SC) at WANDA2021)



Purpose is to
ingest, **document**, and **preserve** data at each stage of an experiment

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Benefits :

– help fully realize discovery potential
– maximize return on investment
– extract more physics with advanced analysis codes
– explore additional reaction channels
– enable accurate renormalizations as “standards” change
– re-examination and validation of results
– source of critical training data for ML approaches
– useful for student training

In the US, the USNDP is the community to do this !!

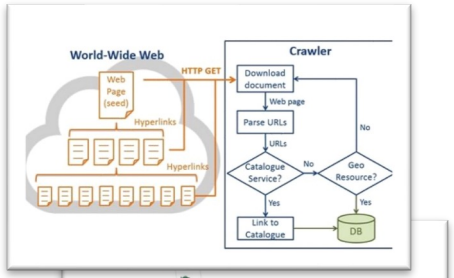
- Leverage RHIC/HP Data Computing Facility expertise
- Promote community buy in through our connections with major facilities (FRIB, ATLAS, LANCE)
- ***Integrate USNDP in Data Management Plans***

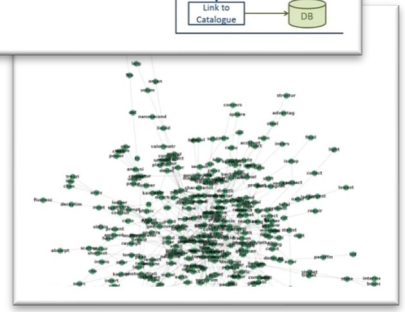
Current & Planned Modernization Efforts

Progress on more efficient extraction of data from publications

NucScholar for NSR

- Automated literature collection
- Automatic keyword extraction
- Natural language queries





Tabular Extraction for XUNDL/EXFOR

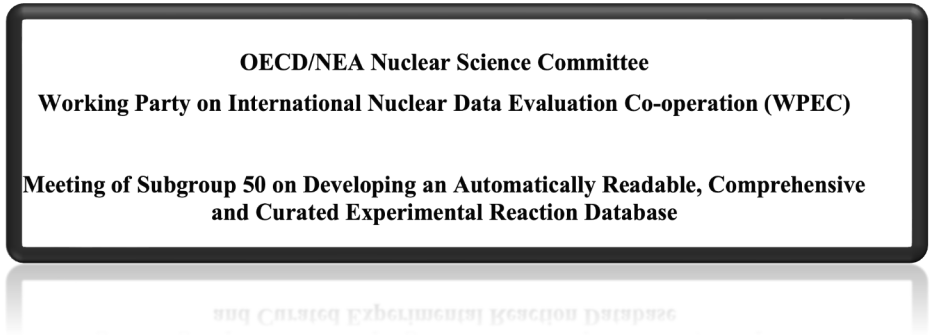
- Modified CascadeTabNet for table detection
- Im2markup for cell recognition
- To be presented at CODA 2023

EXFOR modernization is next priority

Bottlenecks:

- No descriptor on quality of data
- No record of data used in prior ENDF evaluation
- Serious gaps in non-neutron reactions

SG-50 framework is being developed by international collaboration - But no funding



Ideal ground for testing Large Language Models for :

- ✓ Remediate past coverage gaps due to budget shortfalls in 80s and 90s.
- ✓ Eliminate compilation errors caused by humans.
- ✓ Perform critical compilations by comparing to existing data and models.
- ✓ Identify outliers.
- ✓ Obtain correlations and covariances.

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