Brookhaven National Laboratory

U.S. DEPARTMENT OF ENERGY

Challenges, Opportunities and Priorities for Nuclear Data

Elizabeth McCutchan

National Nuclear Data Center, Brookhaven National Laboratory

@BrookhavenLab

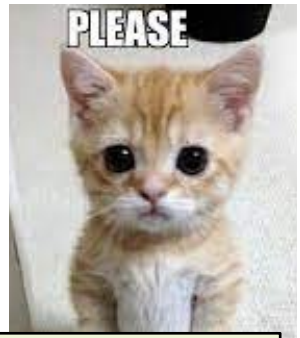
We are here to

16	92	16	73	49
S	U	S	Ta	In
Sulfur	Uranium	Sulfur	Tantalum	Indium

your research and/or
your application

We need your input on

- Priorities
- Needs
- Areas for improvement



Email us at nndc@bnl.gov

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US Nuclear Data Program

National Nuclear Data Center

U.S. DEPARTMENT OF ENERGY | Office of Science

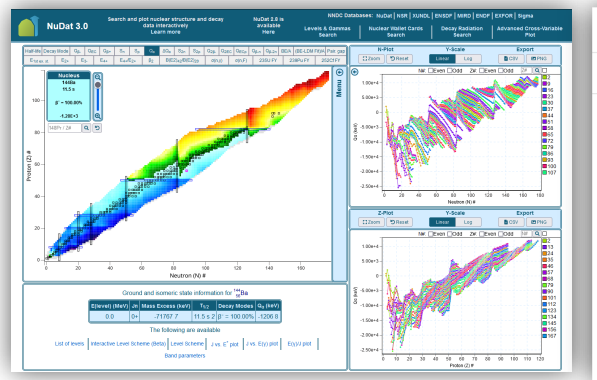
Maintaining and improving nuclear data for world-wide use

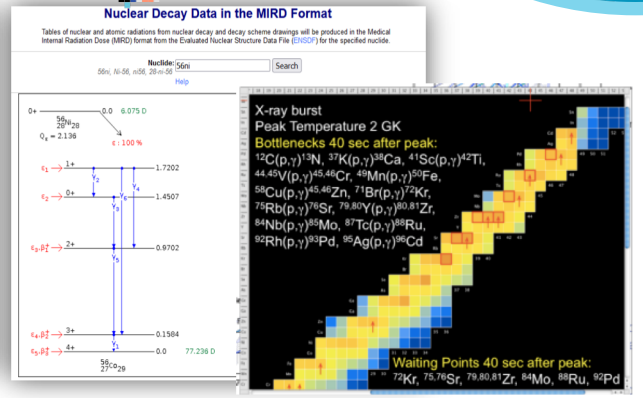
Mission

To provide current, accurate, authoritative data for workers in pure and applied areas of nuclear science through compilation, evaluation, dissemination and archiving of nuclear data. USNDP also addresses gaps in data through targeted experiments and use of theoretical models.

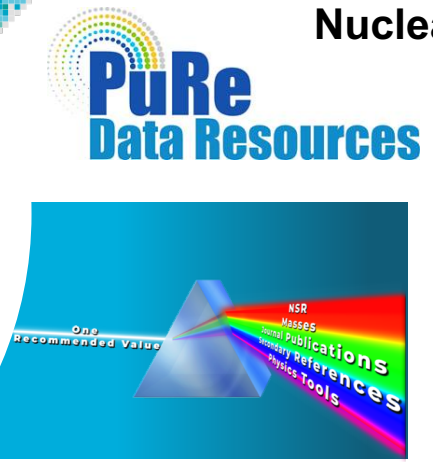
Services

Disseminate nuclear data through feature-rich web applications





Databases



PuRe Data Resources

Nuclear Structure & Decay:

- ENSDF
- XUNDL

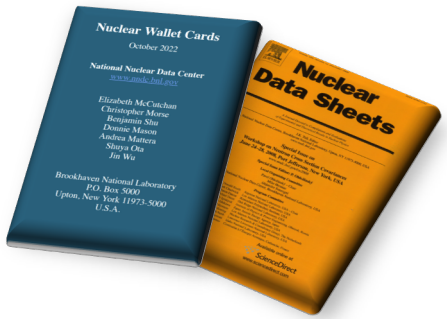
Nuclear Reaction:

- ENDF
- EXFOR

Bibliographic:

- NSR

Publications



Nuclear Data Sheets:
World leading journal on nuclear data evaluations and research

Nuclear Wallet Cards:
Ground and isomeric state nuclear properties of all-known nuclei

What progress has been made since the last LRP?

NNDC is the latest PuRe Data Resource

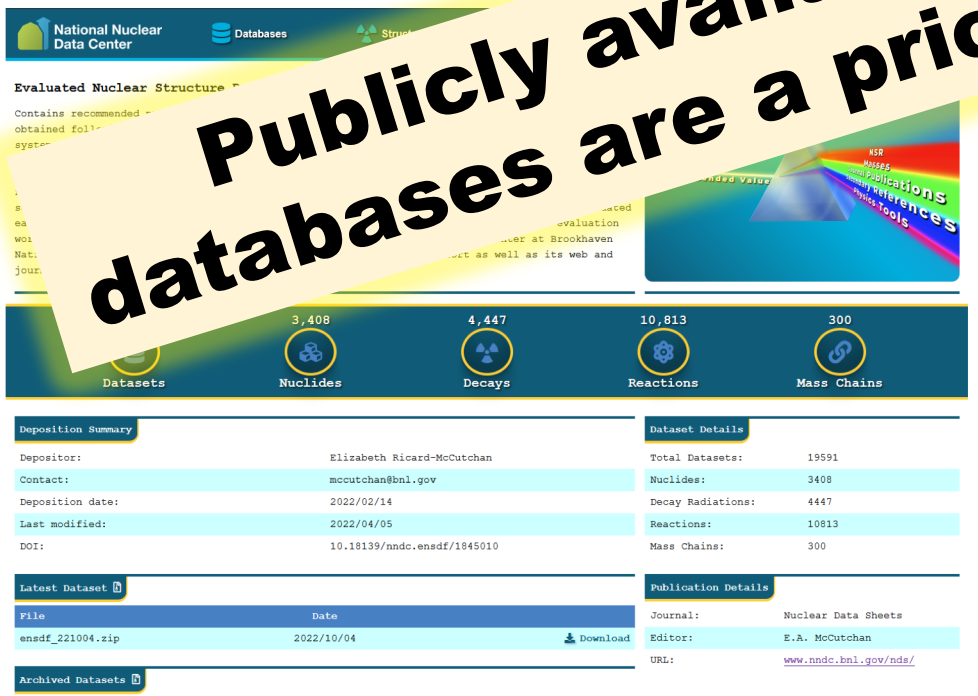
As a **Public Reusable Research (PuRe) Data Repository** the NNDC strives to make data publicly available to advance scientific knowled

Publicly available databases are a priority

3 major libraries already have library-wide DOIs:

- ENSDF
- XUNDL
- NSR

ENDF is next!



PuRe Data Resources

The Materials Project
materials • analysis • open-source code • contributed data

ARM

JGI JOINT GENOME INSTITUTE
A DOE OFFICE OF SCIENCE USER FACILITY

KBase
PREDICTIVE BIOLOGY
DOE Systems Biology Knowledgebase

PDG particle data group

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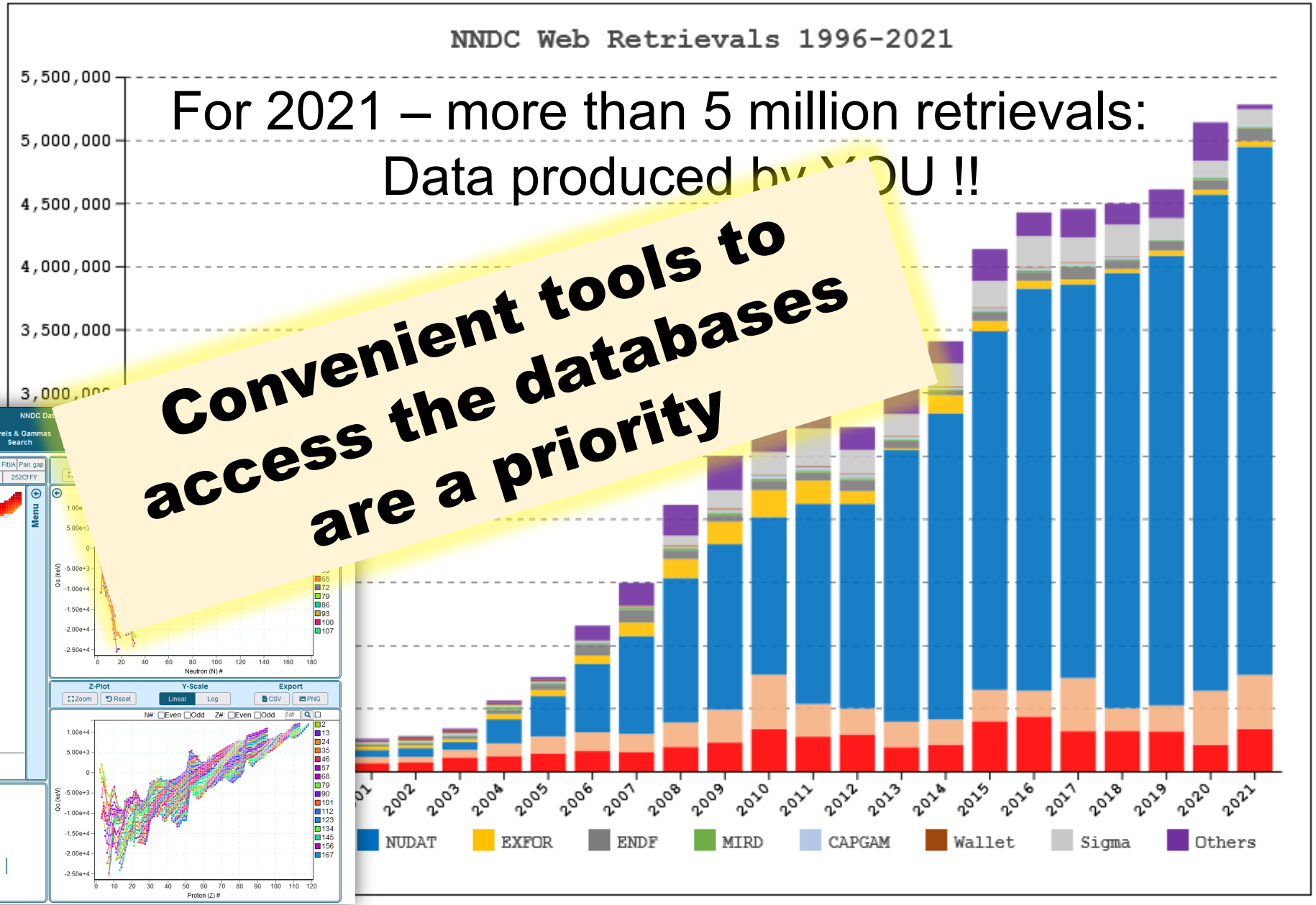
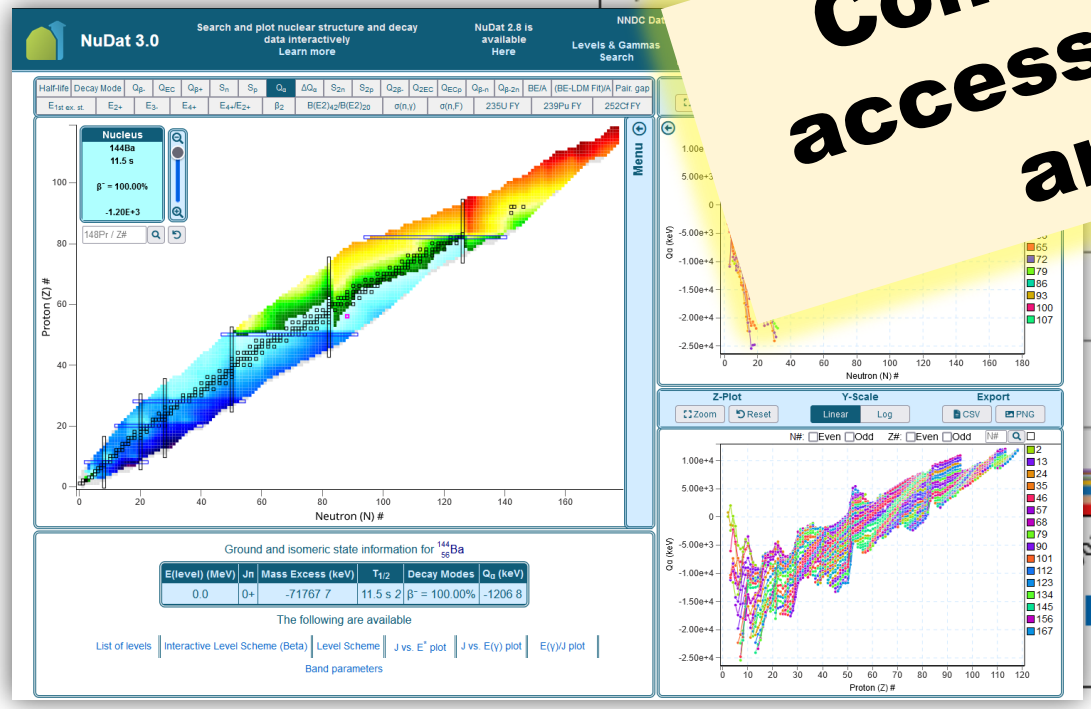
Open Data Web Downloads

The Taylor Swift of Nuclear Physics?

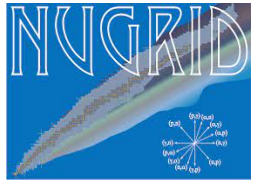




5 Million +++++

- **Many nuclear modeling packages embed ENDF/B and ENSDF data**
- **Impossible to count**

- Reactor design, simulation and licensing codes.
- Nuclear waste and repositories.
- Radiation spectroscopy, dose, detectors and shielding.
- Defense
- CTBTO
- Non-proliferation
- Space physics
- Industry



scale
Nuclear Systems Modeling & Simulation

GEANT4
A SIMULATION TOOLKIT

FLUKA

DAKOTA
Explore and predict with confidence.

MCNP6

OpenMC

ALARA
Adaptive Laplacian and Analytic Radioactivity Analysis

MESA

PHITS

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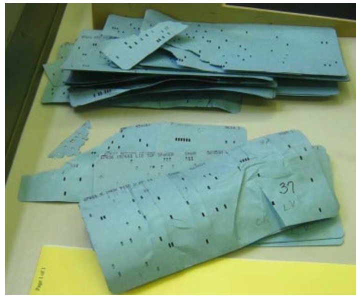
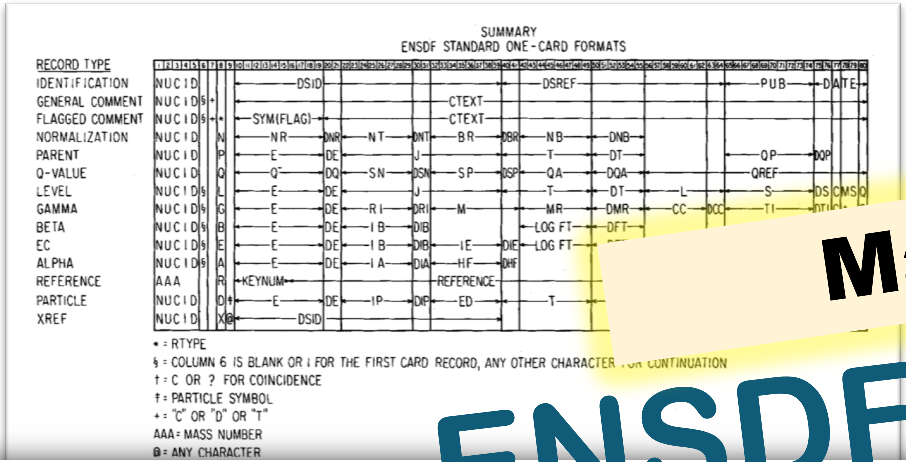
Moving Past Punch Cards



- Major databases based on 50+ year old technology
- Limitations imposed by the 80 column format
- Hard to engage next generation
- Difficult to implement ML/AI



ENSDF

```
137CS PN                                                        6
137CS  L 0.0          7/2+              30.08 Y  [illegible]        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
137C[illegible]
137C[illegible]
```

A LOT of data stored in comments
Non-standardized entry

Major Challenge

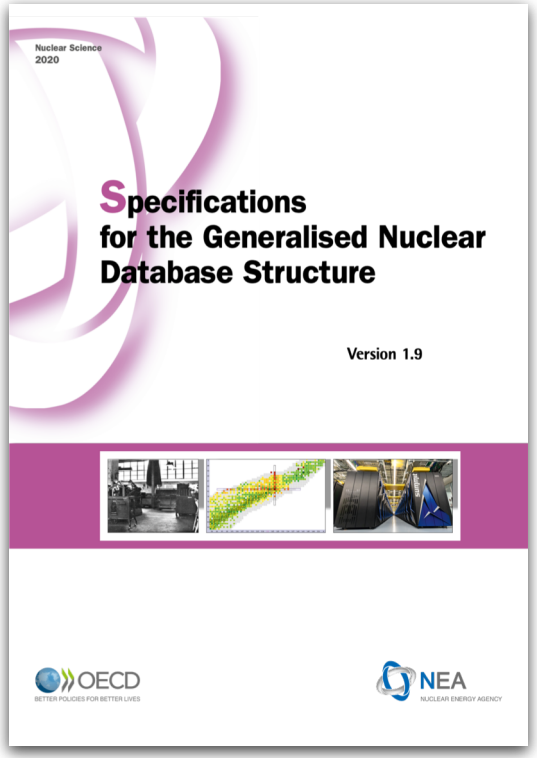
ENDF

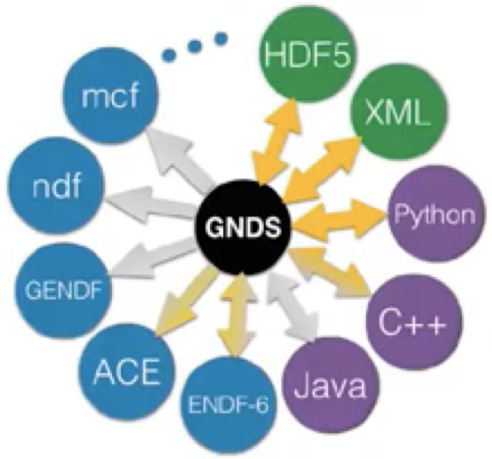
```
                               1          451         41          0 925 1451     40
                               8          457        311          0 925 1451     41
 0.000000+0 0.000000+0         0            0          0          0 925 1  099999
 0.000000+0 [illegible]                     0          0          0 925 0    0      0
 [illegible]                                0          0          5 925 8457      1
                                            0          6          0 925 8457      2
                               1.848838+5 2.040733+1 0.000000+0 925 8457      3
                              0            0         12          2 925 8457      4
 [illegible]0.000000+0 8.094836+6 6.424000+3 9.998930-1 5.000000-6 925 8457      5
 1.500000+0 0.000000+0 8.089200+5 7.770000+3 1.070000-4 5.000000-6 925 8457      6
 0.000000+0 0.000000+0          0          0          6         53 925 8457      7
 1.000000+0 0.000000+0 2.146589+6 1.848838+5 0.000000+0 0.000000+0 925 8457      8
 9.670000+4 6.000000+2          0          0          6          0 925 8457      9
 1.000000+0 0.000000+0 1.617000-3 9.601171-4 0.000000+0 0.000000+0 925 8457     10
 3.861000+5 3.000000+2          0          0         12          0 925 8457     11
 1.000000+0 0.000000+0 2.508000-3 1.007861-3 0.000000+0 0.000000+0 925 8457     12
 4.850000-3 7.000000-5 4.290000-3 5.999999-5 4.720000-4 7.000000-6 925 8457     13
 3.935000+5 1.000000+2          0          0         12          0 925 8457     14
 1.000000+0 0.000000+0 1.254000-2 4.607515-3 0.000000+0 0.000000+0 925 8457     15
 4.629999-3 7.000000-5 4.100000-3 5.999999-5 4.499999-4 7.000000-6 925 8457     16
 5.698000+5 1.000000+2          0          0         12          0 925 8457     17
 1.000000+0 0.000000+0 5.610000-2 2.066518-2 0.000000+0 0.000000+0 925 8457     18
 1.960000-3 2.999999-5 1.737000-3 2.499999-5 1.890000-4 3.000000-6 925 8457     19
 7.036000+5 3.000000+2          0          0         12          0 925 8457     20
```

Line number, so you can put your punchcards back in order if you drop them

Current Database Modernization Efforts

ENDF-6 Format is transitioning to GNDS, GNDS-2.0 almost ready





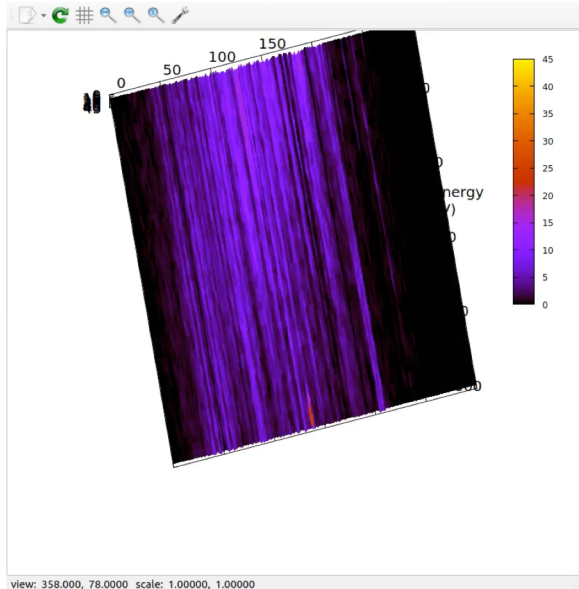
- ~10 year project
- ENDF/B-VIII.0 released in both ENDF6 and GNDS formats

ENSDF modernization project well under way

```
"header": {
    "schemaVersion": "1.0",
    "documentType": "nuclide",
    "z": 62,
    "n": 90,
    "a": 152,
    "elementName": "Samarium",
    "elementSymbol": "Sm",
    "history": [{
        "evaluationType": "full",
        "cutoffDate": "2013-08-31",
        "authors": [{
            "name": "M. J. MARTIN"
        }],
        "publication": "NDS 114, 1497 (2013)"
    }]
},
```

CouchDB

- 3 year project
- CouchDB object-oriented database
- JSON schema for validation
- ENSDF API with python plotting packages



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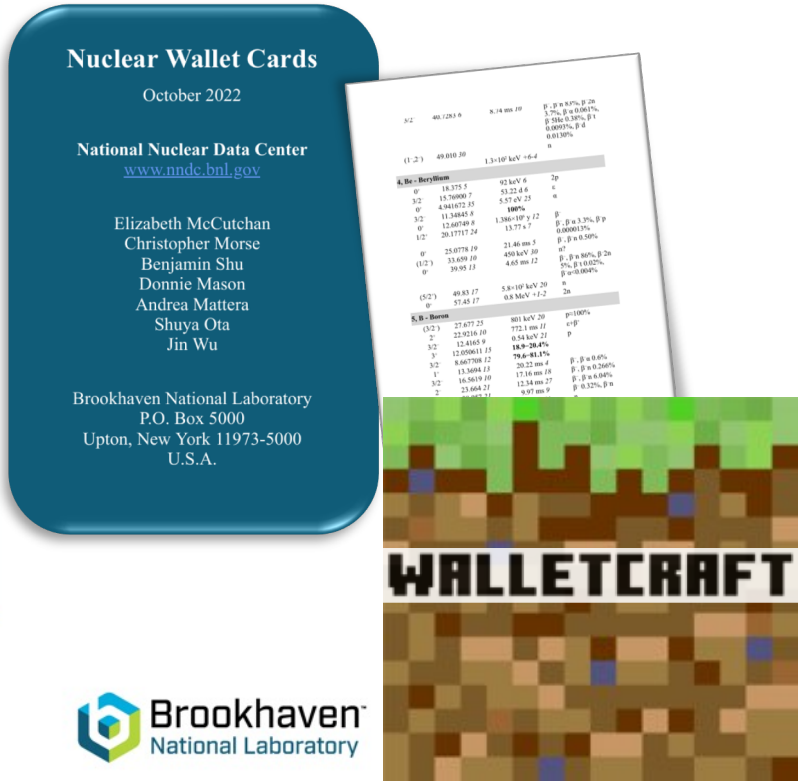
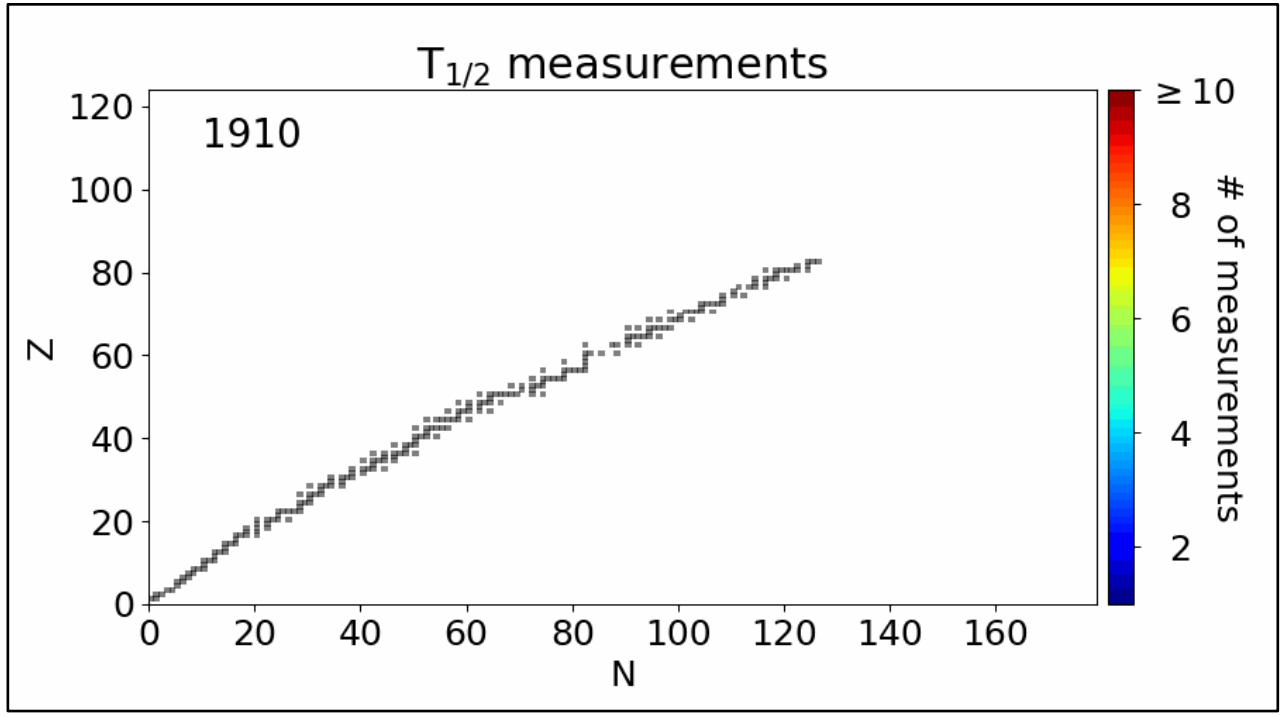
WalletCraft: a new evaluation of properties of ground-state and long-lived isomers for all known nuclei

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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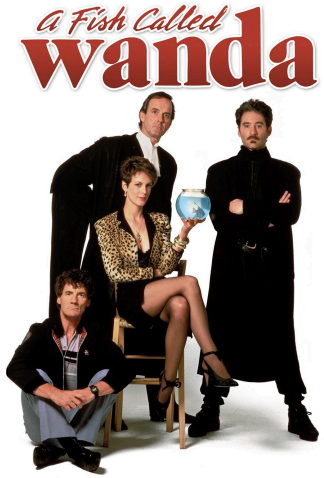
Improving Connections with Users

WANDA – Workshop for Applied Nuclear Data Activities

Yearly meeting since ~2018

Input to NDIAWG FOA's



PHYSICAL REVIEW RESEARCH 4, 021001 (2022)

Perspective

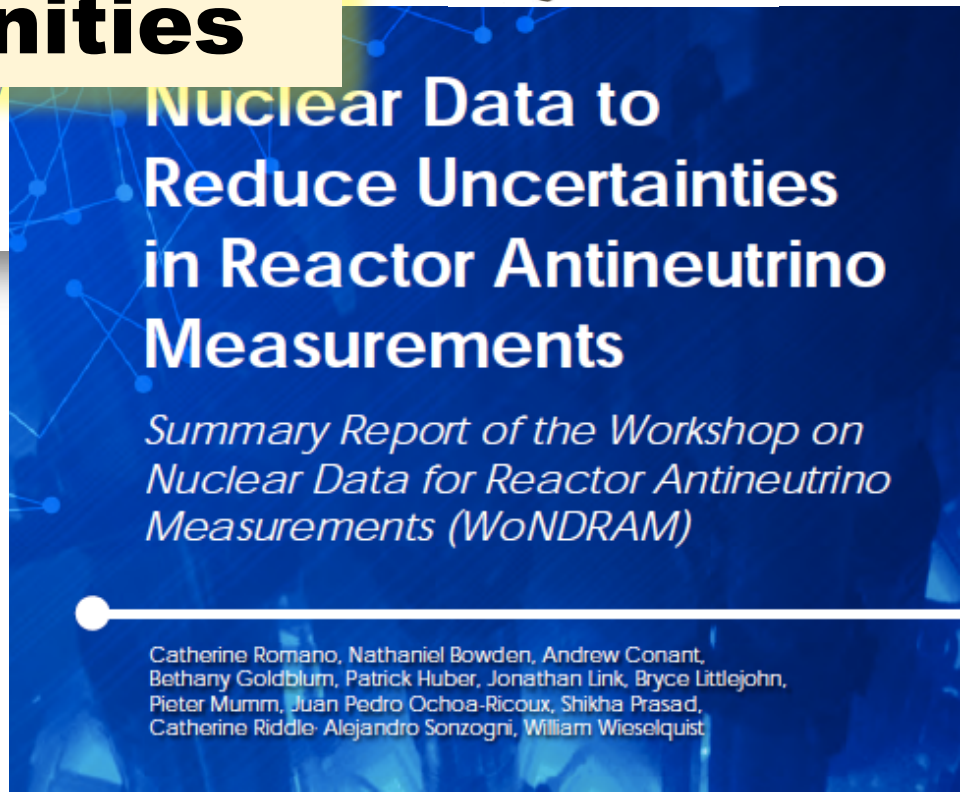
Current nuc

Karolina Kolos,[1] Vladimir Sobes,[2] Ramona Vogt,[1,3] Catherine E. Romano,[4] Michael S. Smith,[5] Lee A. Bernstein,[6,7]
David A. Brown,[8] Mary T. Burkey,[9] Yaron Danon,[10] Mohamed A. Elsawi,[11,12] Bethany L. Goldblum,[6,7]
Lawrence H. Heilbronn,[2] Susan L. Hogle,[13] Jesson Hutchinson,[14] Ben Loer,[11] Elizabeth A. McCutchan,[7]
Matthew R. Mumpower,[15] Ellen M. O'Brien,[16] Catherine Percher,[17] Patrick N. Peplowski,[18] Jennifer J. Ressler,[9]
Nicolas Schunck,[1] Nicholas W. Thompson,[14] Andrew S. Voyles,[6,7] William Wieselquist,[19] and Michael Zerkle[20]

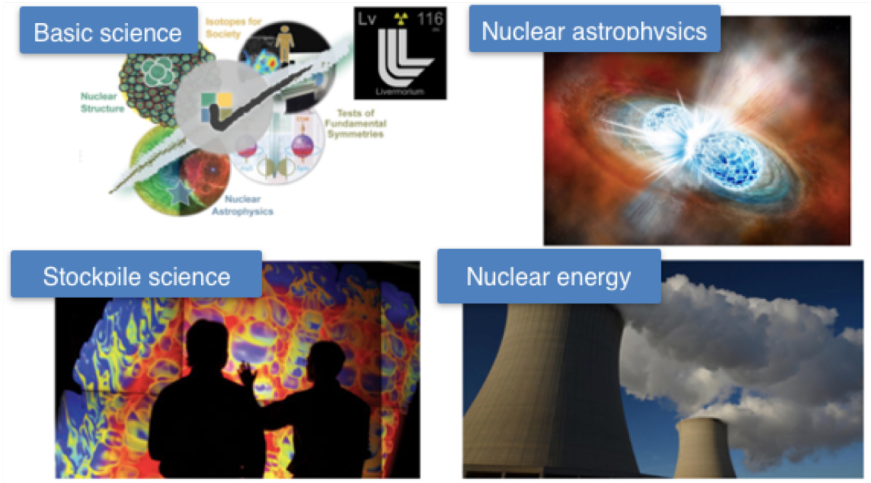
Lots of Opportunities

Topics of 2021 Meeting

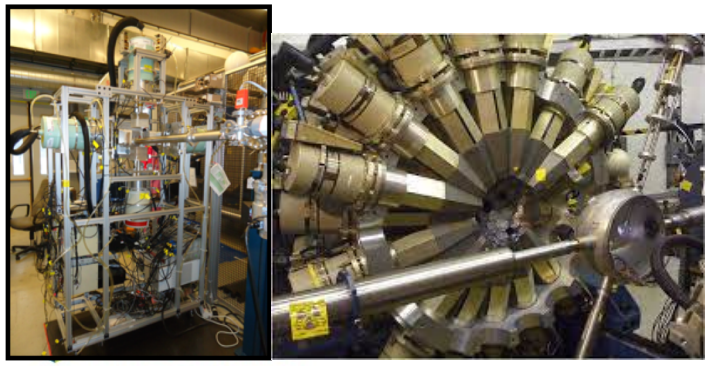
- HPC in Nuclear Data
- Predictive Codes for Isotope Production
- Benchmarks and Validation for Nuclear Data
- Nuclear Data For Space Applications
- Nuclear Data For Advanced Reactors
- Human Pipeline for Nuclear Data



Addressing Cross Cutting ND Needs



- **Isomer to ground state FY ratio** measurements
- **Decay spectroscopy** of fission products with **X-Array/Gammaspere** at **nuCARIBU**
- LLNL, ANL et al., collaboration



Courtesy of K. Kolos

See talk: K. Kolos, ND Working Group session

Nuclear Physics

How Do Neutrons Interact with Reactor Materials?

OCTOBER 27, 2022

- Inelastic neutron scattering measurements
- University of Kentucky, USNA, LLNL et al.,
- Important for reactors, space, homeland security

See talk: B. Crider, ND Working Group session

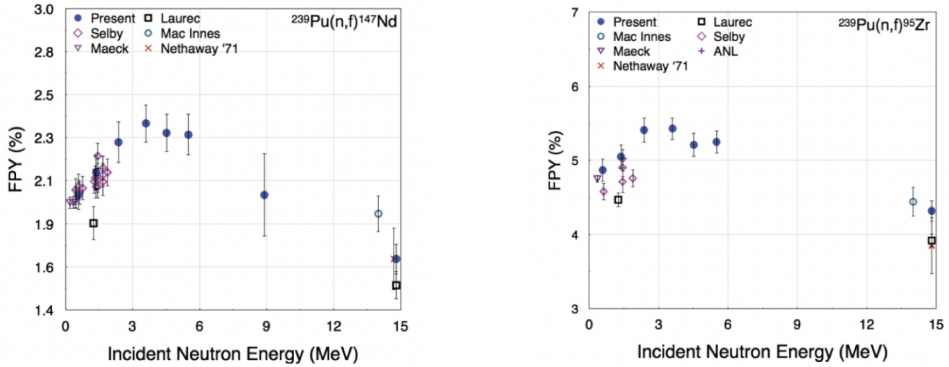
See talk: E. Chimanski, ND Working Group session

Fission product yield re-evaluation effort

A tour de force of measurement, theory and evaluation

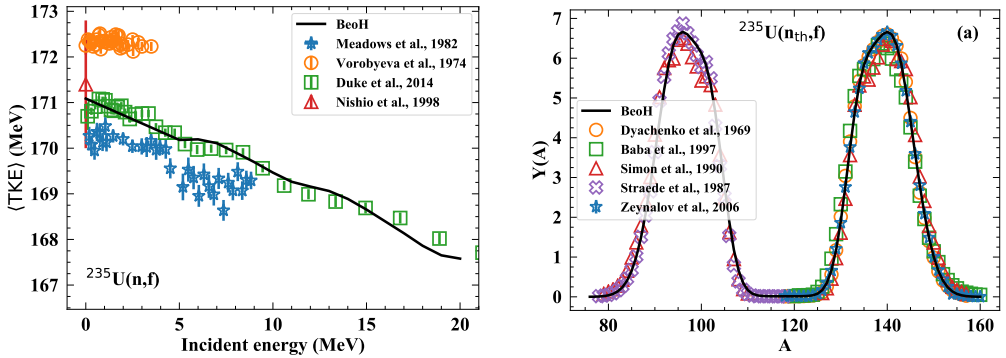
Evaluation and Compilation of Fission Product Yields
1993
T. R. England and B. F. Rider
Los Alamos National Laboratory
October, 1994

New measurements with a range of incident neutron energies (including results from LBNL, UCB, PNNL)



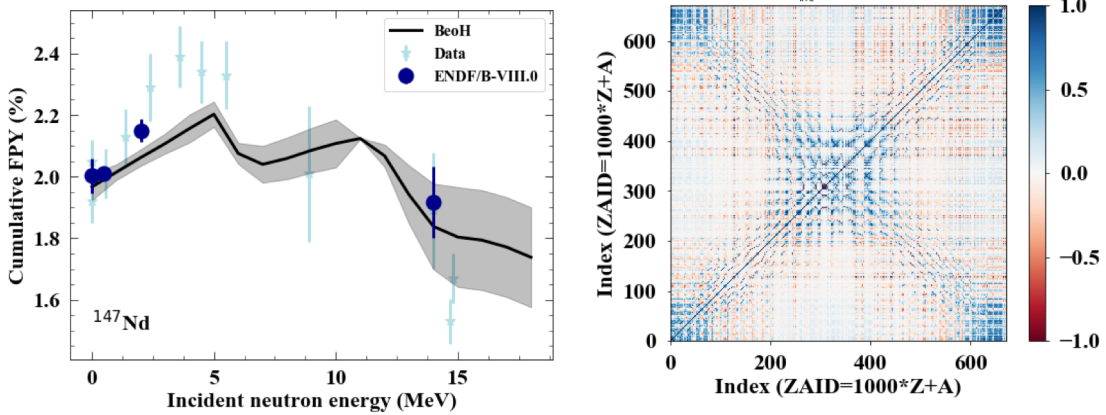
M.E. Gooden, et al., NDS 131, 319 (2016)

- Consistent fission modeling with constraints from prompt and delayed data;
- Initial conditions informed by microscopic calculations



A.E. Lovell, et al., PRC 103, 014615 (2021)

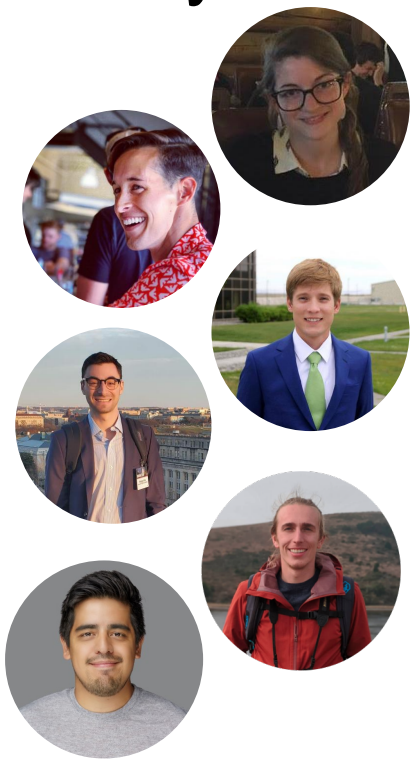
Energy-dependent fission product yields with full covariance information are being produced for inclusion into ENDF



Slide courtesy of A. Lovell

Training the next generation in Nuclear Data

Bay Area Nuclear Data – 2020-2021 PhDs



1. "Uncertainty Analysis Procedures for Neutron-Induced Cross Section Measurements and Evaluations" Amanda Marie Lewis – Spring 2020* *NNL Staff*
2. "Fission plasmas and their novel application to power producing nuclear reactors in space" Austin Troy Lo – Fall 2020 *ORNL Postdoc*
3. "Advancements in the Nuclear Data of Fission Yields"
   Eric Francis Matthews – Spring 2021 *UCB Researc*
4. "Nuclear Data Evaluation of High-Energy
   Morgan B. Fox – Spring 2021
5. "Next-Generation
   Jona
6. "Machine
   Pedro V
   ata Evaluations"
   pring 2021 -- *Industry*

Training a diverse workforce is a priority

BAND Future PhDs

BAND slide courtesy of L. Bernstein

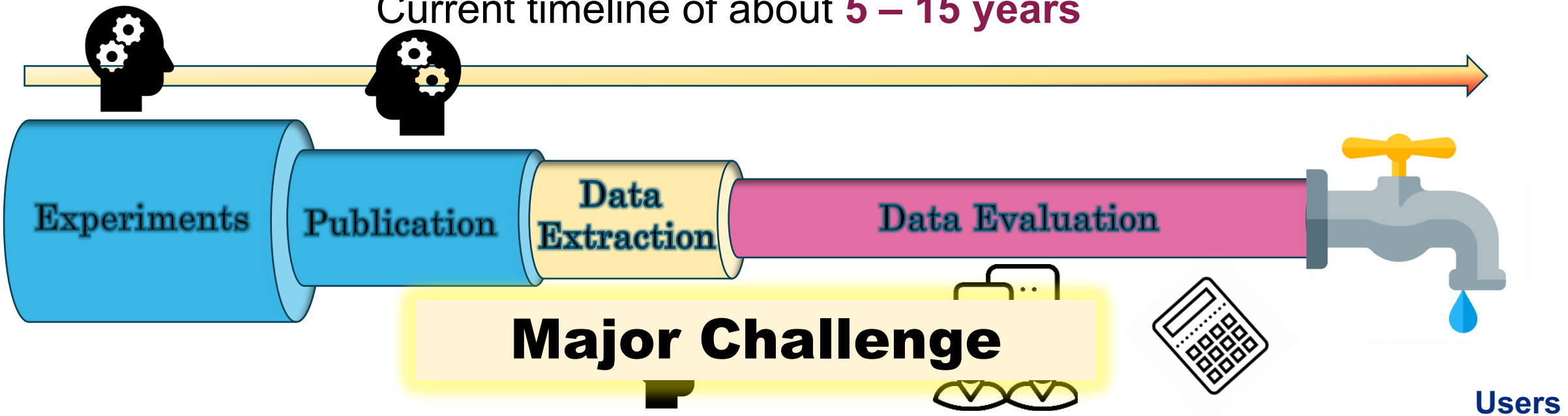
28 NNDC Summer interns in FY22!

Half of students from traditionally underserved groups

Nuclear Physics Traineeship allowing us to bring in URM students for longer term mentoring

Nuclear Data Pipeline, Now

Current timeline of about **5 – 15 years**



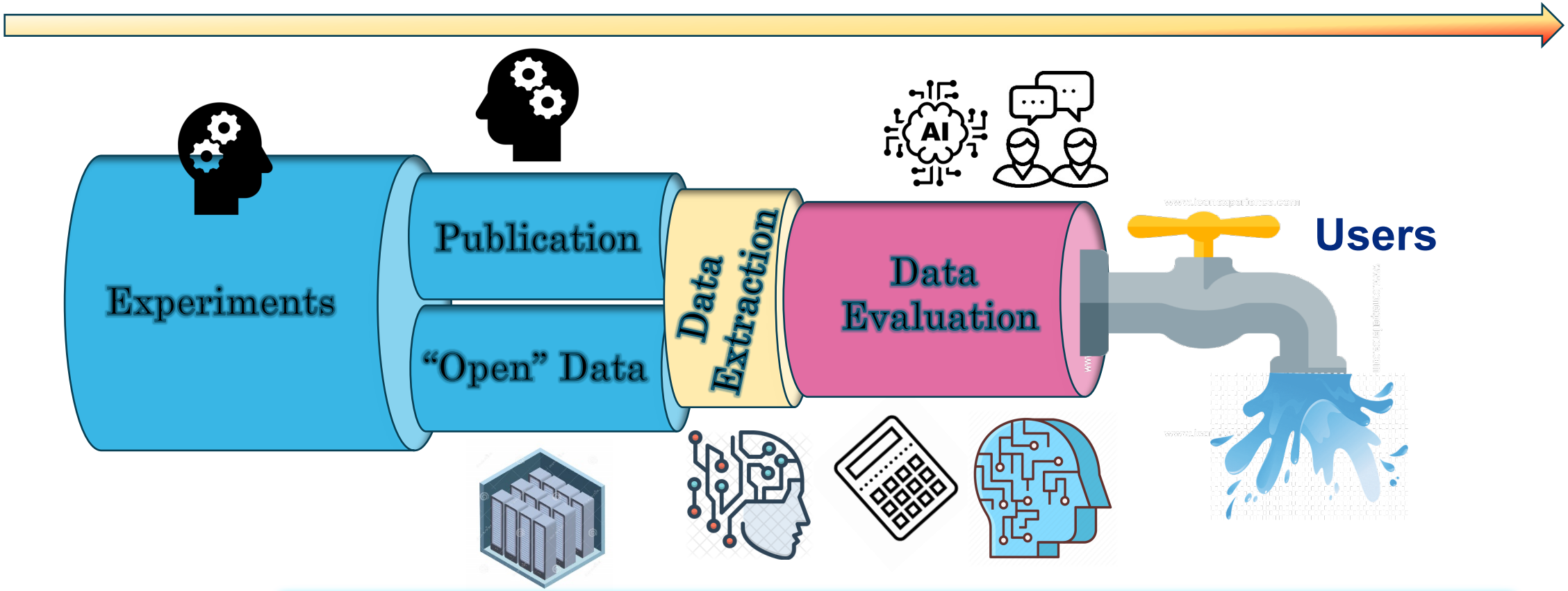
Our product's impact is limited by:

- Ancient formats
- Outdated evaluation procedures
- Lack of sufficient workforce
- Often publications only contain a portion of all data measured

Modernization of USNDP databases has started !!
Leverage this effort to fix the rest!

Nuclear Data Pipeline: Future

Proposed timeline of **1-2 years**



A new paradigm will :

- Eliminate bottlenecks
- Ensure that results of expensive experiments are properly stored
- Address stakeholders' feedback in a timely manner.

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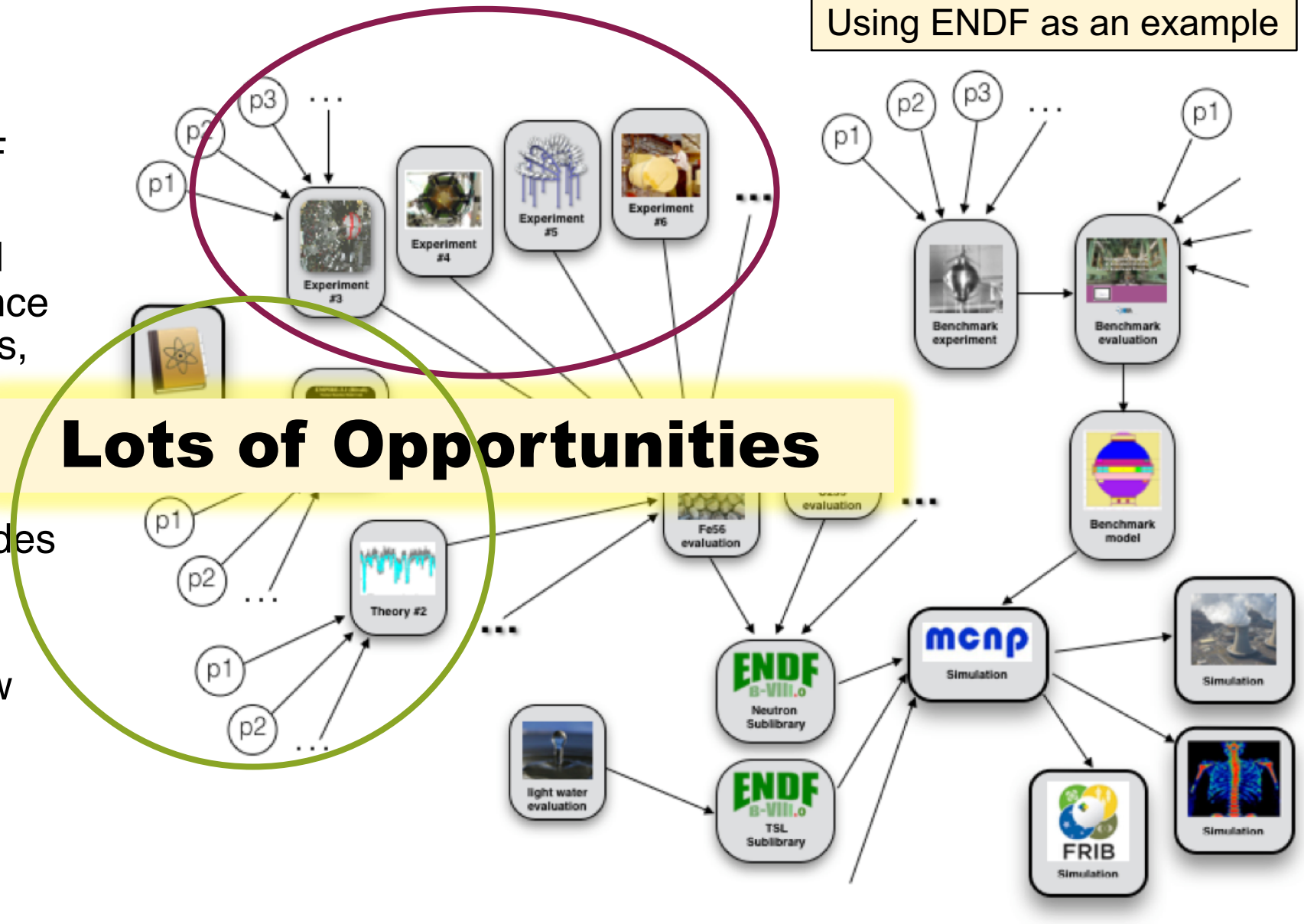
Workflows: Automatic Updates of Major Libraries

Using ENDF as an example

- Use ML + HPC + software engineering to update ENDF library
- Employ "**containers**" to hold experimental results, reference parameter sets, theory codes, benchmark experiments, evaluations of individual nuclides or reactions
- Interlink containers to be nodes in a **Bayesian network**
- Use **Gaussian Process Regression** to update a new ENDF library, when *any* NN components are updated



Lots of Opportunities

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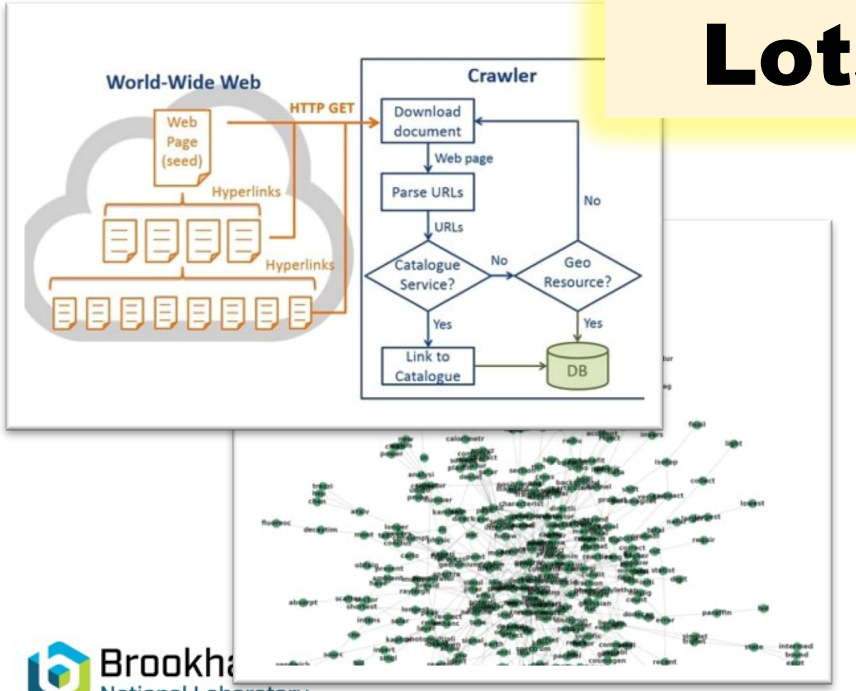
Machine Learning Throughout the Pipeline

For efficient extraction of data from publications

NuScholar for NSR

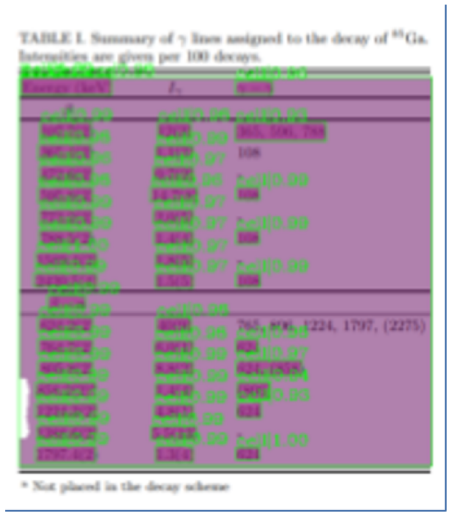
- Automated literature collection
- Automatic keyword extraction
- Natural language queries



Led by B. Goldblum, UCB

Tabular Extraction for XUNDL/EXFOR

- Modified CascadeTabNet for recognition

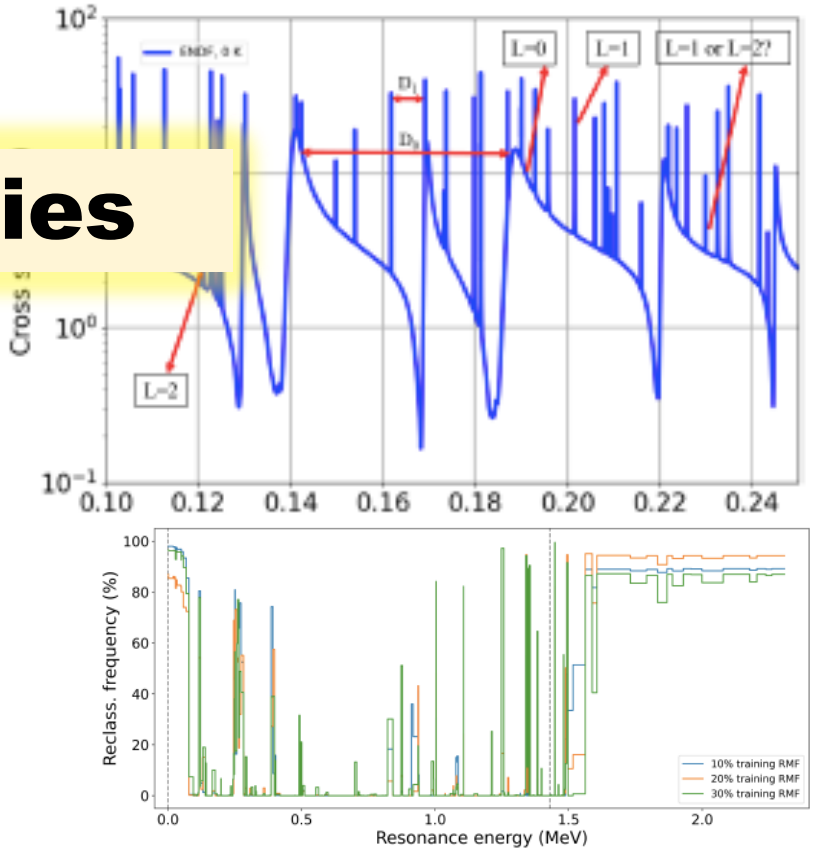


Led by C. Soto, BNL

Lots of Opportunities

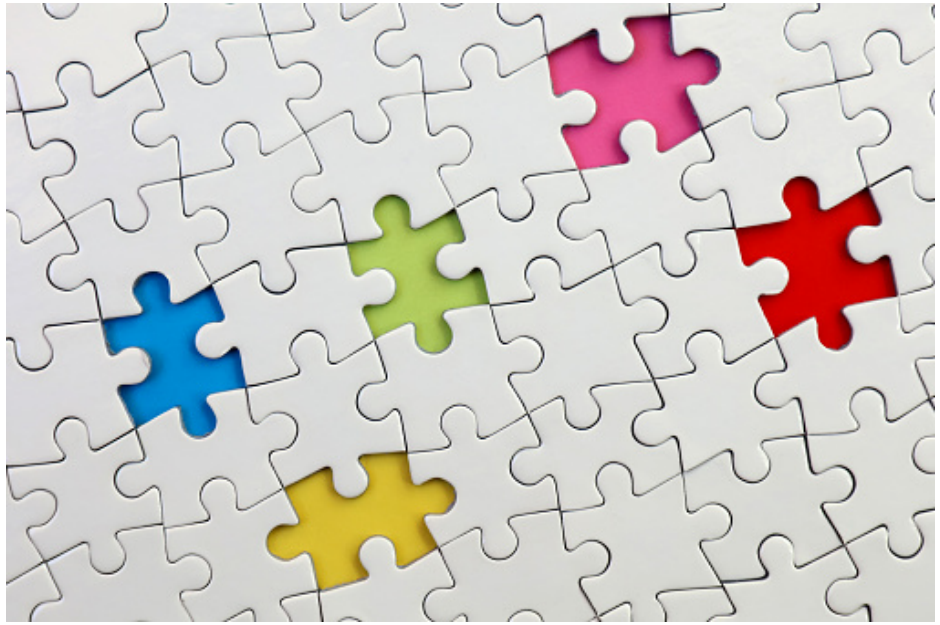
For improving evaluations

Machine Learning to Classify Quantum Numbers of Neutron Resonances

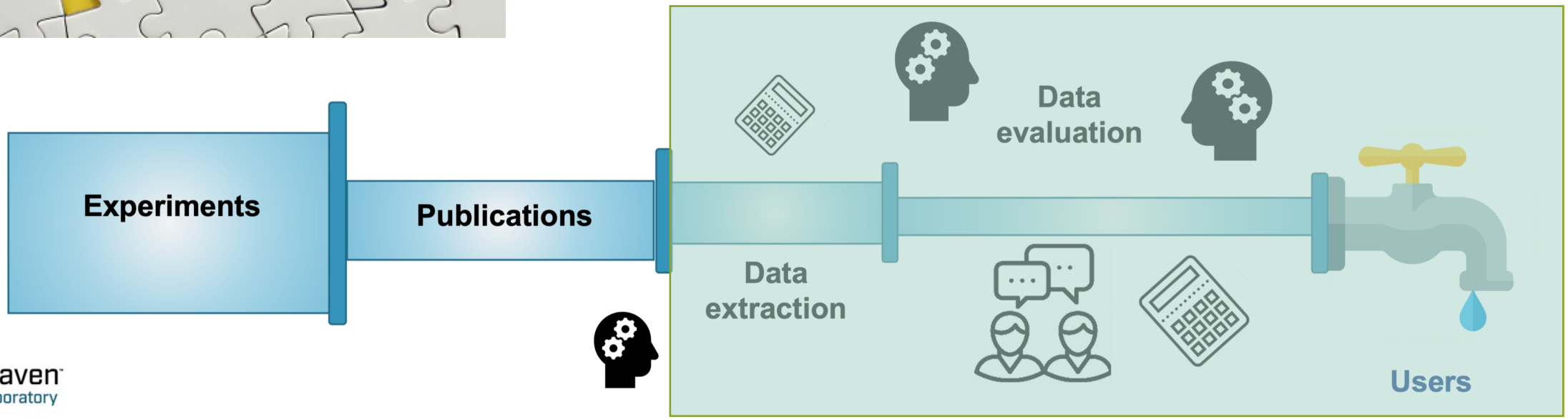


Led by G. Nobre, BNL

Still some missing pieces because …



US Nuclear Data program involved mainly after the data are published



A Step in the Right Direction:

The FRIENDS project at FRIB

FRIB Integral Experimental Nuclear Data Services

Aiming to provide seamless support for data needs to FRIB experimenters throughout all stages of an experimental work
as an integral part of the FRIB experimental support

Great Opportunity

Proposal Preparation

- Up-to-date datasets
- Consultation and discussion

- Fully customized data search

- Help on use of data tools

Publication Preparation

- Prior publication data check

researchers — FRIENDS — data evaluators

The data evaluator at FRIB leads the effort in the FRIENDS service along with the primary focus on ENSDF and XUNDL effort.

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See talk: J. Chen, ND Working Group session

Slide courtesy of J. Chen

Data Preservation

(aka Open Data, FAIR data, Data Sharing)

BRIEFING ROOM

OSTP Issues Guidance to Make Federally Funded Research Freely Available Without Delay

AUGUST 25, 2022 • PRESS RELEASES

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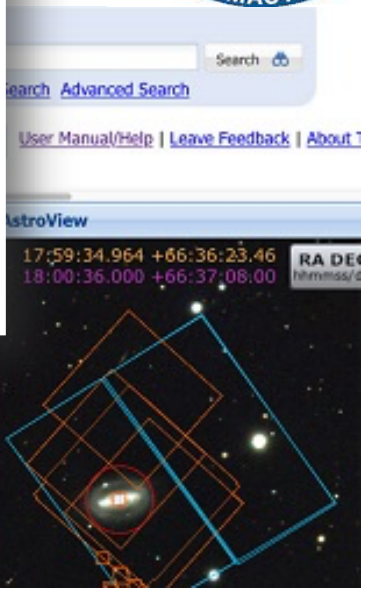

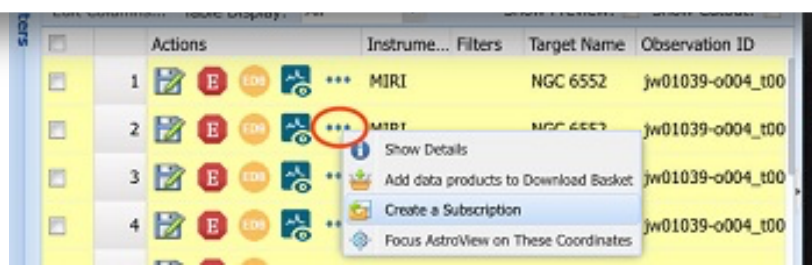

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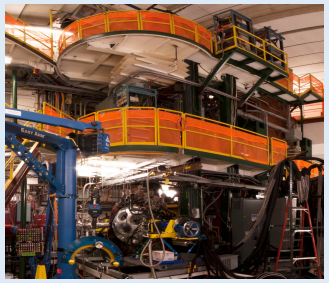
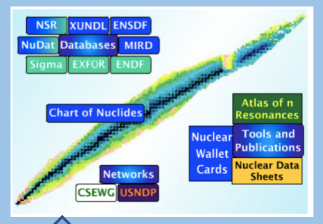
Current Low Energy Nuclear Physics Data Status

Data collection



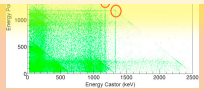
Data storage

Nuclear Databases



Data artifacts

Major Challenge



data

Analysis software

ROOT Data Analysis Framework

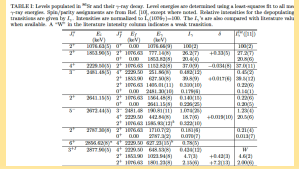
GEANT4 A SIMULATION TOOLKIT

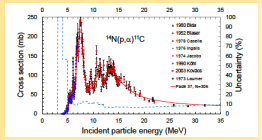
Simulation

Dissemination of Processed Results

arXiv.org

PHYSICAL REVIEW C





- Only a small fraction of experiments are fully preserved. These continue to increase in cost and complexity.
- There is **NO** centralized mechanism for data sharing, resulting in
  - Potential for repeating experiments
  - Data that goes unanalyzed
  - Less resources to plan experiments
  - No opportunity for reproducibility
- Data program parses published tables and digitizes graphs.

Average experiment costs at least $100k's
~300 experiments into XUNDL alone every year

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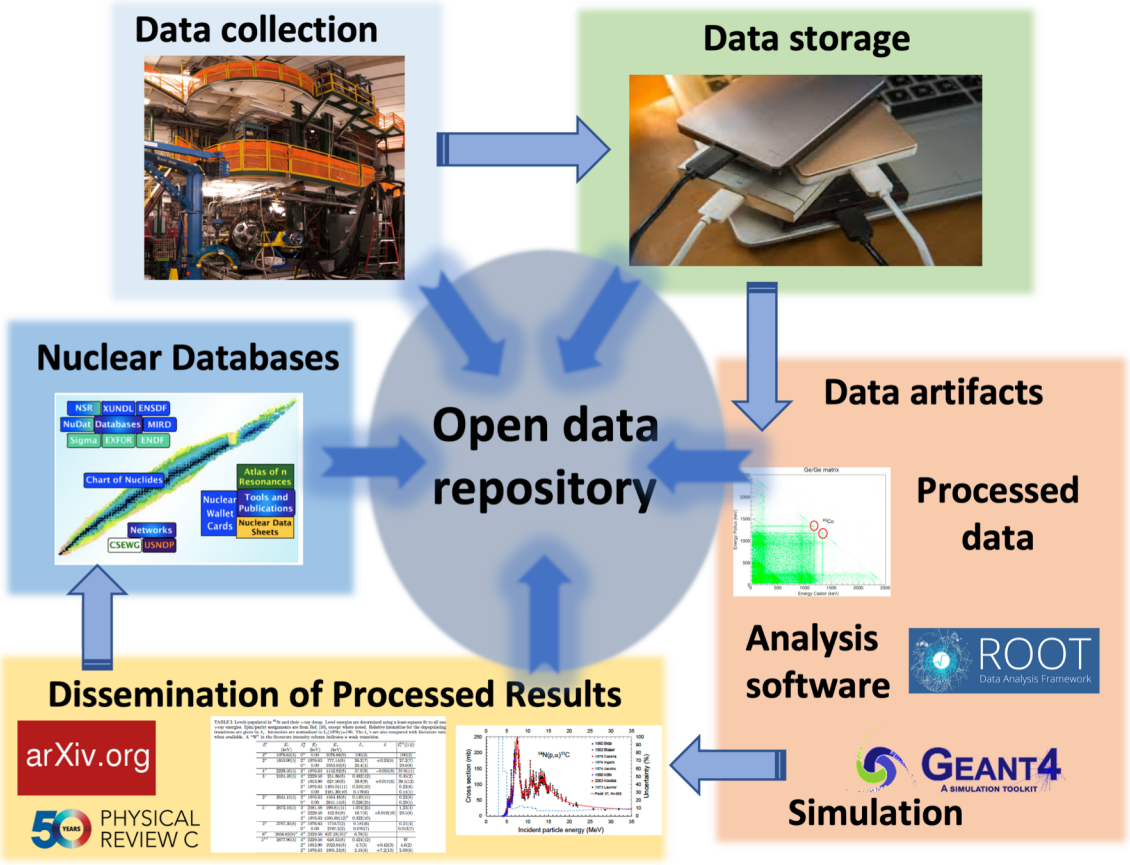
Data Preservation



Purpose is to

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

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

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See talk: J. Wu, ND Working Group session

Challenges, Opportunities and Priorities

Priorities Challenges

- Publicly available databases

  Timely and Accurate

- Tools to access the databases

  Modernization

- Training a diverse workforce

- Data Preservation

Opportunities

- Automation
- ML/AI
- Communication with Users

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