

Modernization and Optimization of the Evaluated Nuclear Structure Data File (ENSDF)

Elizabeth McCutchan

WANDA 2022



@BrookhavenLab

ENSDF : the ONLY comprehensive resource for

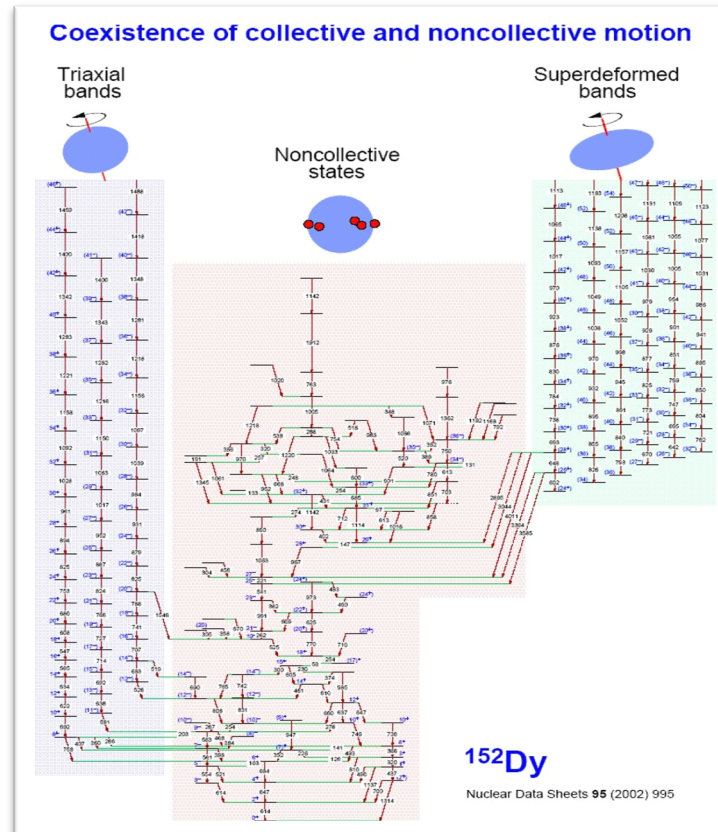
Nuclear Structure

Discrete Quantized States

- Excitation Energy
- Half-life
- Angular Momentum
- Magnetic Moment
- Configuration
- ...

Emitted Radiation

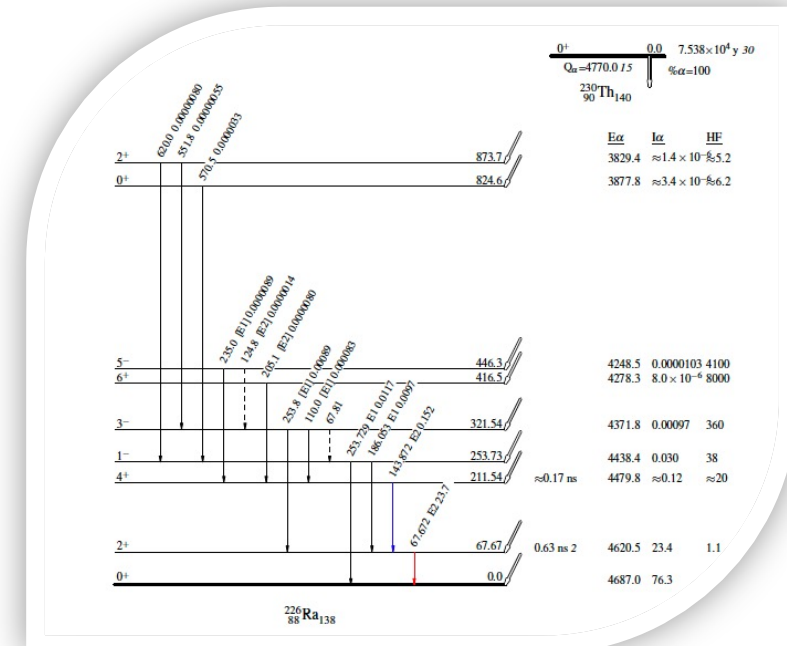
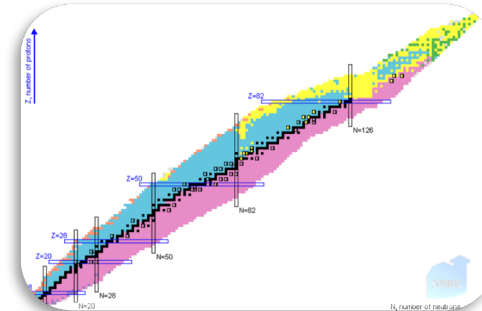
- Energy
- Intensity
- Dipole, Quadrupole, ...
- Mixing ratio
- Conversion coefficient



Nuclear Decay Data

For each decay type:

- Half-life
- Branching ratio
- Energy
- Intensity
- Coincidences
- ...



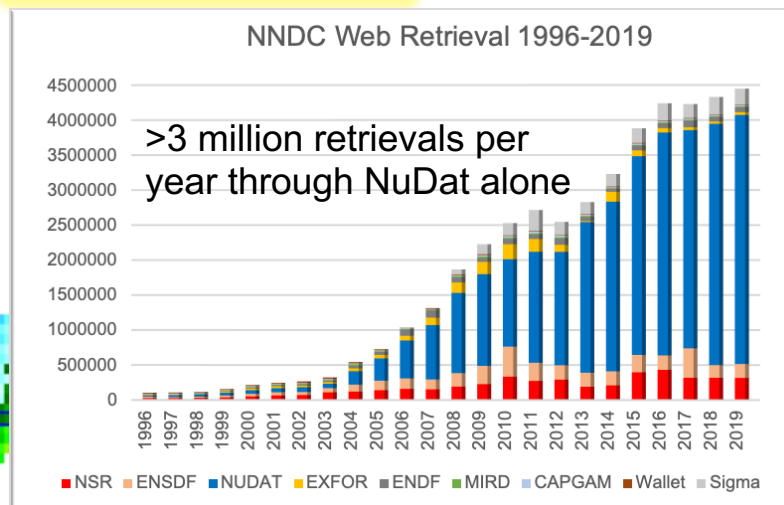
Unique :
Only database of its kind in the world

Highly used:

Z, number of protons

Authoritative:

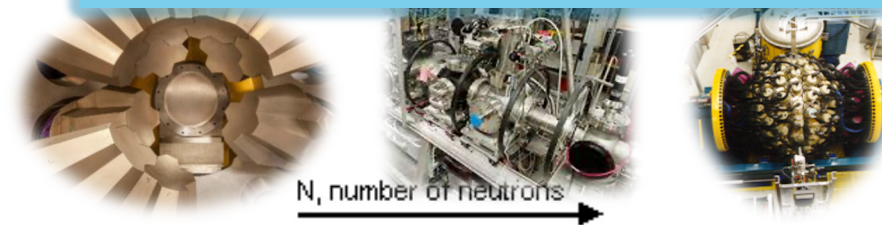
3,334 nuclides
~20,000 Reactions
~4,200 Decay



ENSDF

Evaluated Nuclear Structure Data File

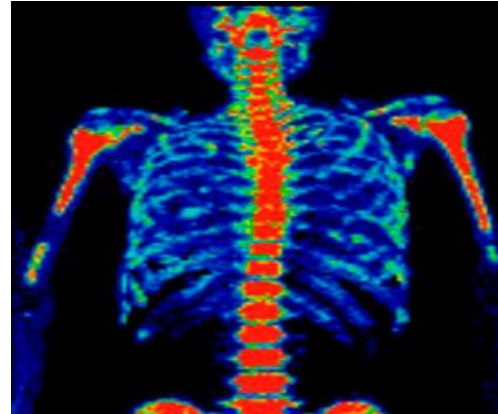
75+ years of experimental nuclear structure measurements



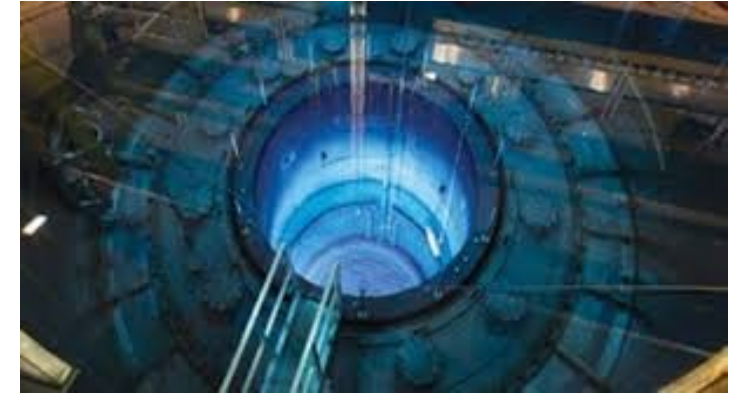
Users of ENSDF



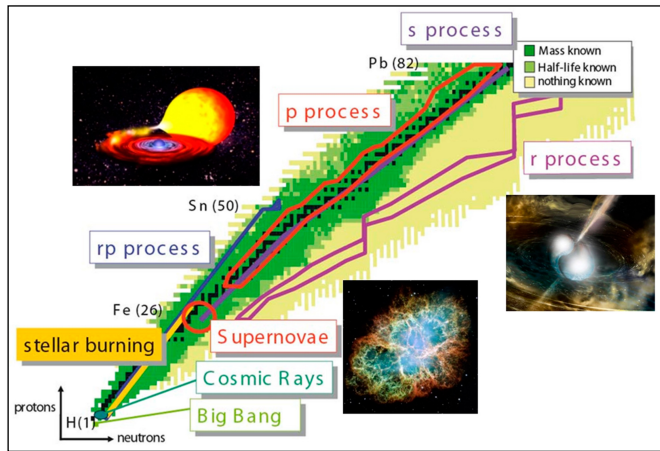
Fundamental Nuclear Science



Nuclear Medicine



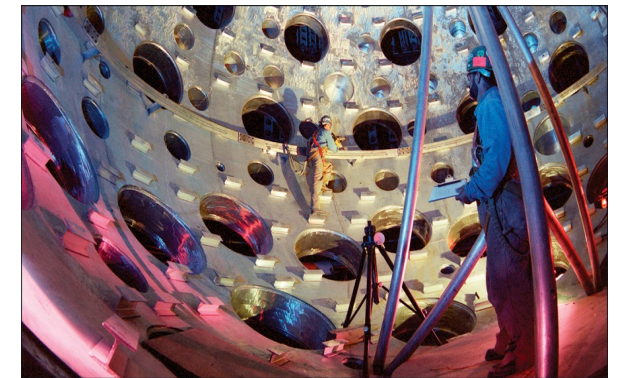
Nuclear Power



Astrophysics



Homeland Security



Stockpile Stewardship

Under the hood of ENSDF

80 Column ASCII format

SUMMARY
ENSDF STANDARD ONE-CARD FORMATS

RECORD TYPE	NUC1D	DSID	CTEXT	DSREF	PUB	DATE
IDENTIFICATION	NUC1D	DSID	CTEXT	DSREF	PUB	DATE
GENERAL COMMENT	NUC1D	SYM(FLAG)	CTEXT	DSREF	PUB	DATE
FLAGGED COMMENT	NUC1D	SYM(FLAG)	CTEXT	DSREF	PUB	DATE
NORMALIZATION	NUC1D	NR	NT	NT	BR	DBR
PARENT	NUC1D	E	DE	J	T	DT
Q-VALUE	NUC1D	Q	Q	SN	SN	SP
LEVEL	NUC1D	L	E	DE	J	T
GAMMA	NUC1D	G	E	DE	R	DR
BETA	NUC1D	B	E	DE	I	DI
EC	NUC1D	E	E	DE	I	DI
ALPHA	NUC1D	A	E	DE	I	DI
REFERENCE	AAA	R	KEYNUM	REFERENCE		
PARTICLE	NUC1D	D	E	DE	IP	DIP
XREF	NUC1D	X	DSID			

* = RTYPE
% = COLUMN 6 IS BLANK OR 1 FOR THE FIRST CARD RECORD, ANY OTHER CHARACTER FOR CONTINUATION
+ = C OR ? FOR COINCIDENCE
= PARTICLE SYMBOL
+ = "C" OR "D" OR "T"
AAA = MASS NUMBER
@ = ANY CHARACTER

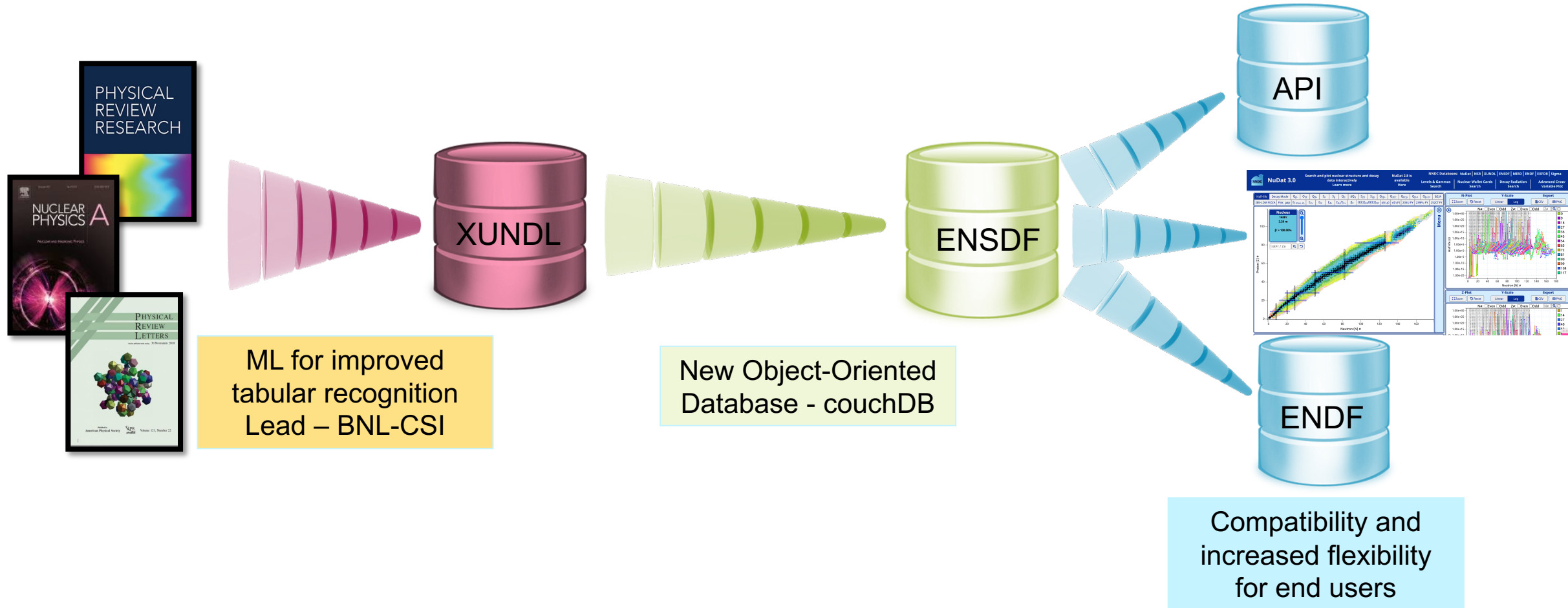
- All of nuclear physics doesn't fit in 80 columns
- No room to grow
- ML next to impossible
- Hard to engage next gen

```
137CS PN
137CS L 0.0 7/2+ 30.08 Y 9
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);
137CS9cL 10665 d {I110} (1963Ri02); 10840 d {I18} (1963Go03); 10994 d {I256}
137CSAcL (1962Fl09); 11103 d {I146} (1961Fa03);
137CSxcL 9715 d {I146} (1955Wi21). [1 y =365.242
137CS cL Other evaluated results: 30.0
137CS2cL 30.08 y {I3} (1996ChZY, 1994Ka08); 30.1
```

A LOT of data stored in comments
Non-standardized entry

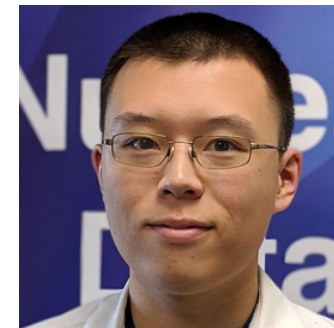
ENSDF Modernization

DOE has made significant investment to modernize and improve ENSDF
3 year project involving 3 DOE national laboratories – BNL – ANL - LLNL



Progress so far

Ben Shu



Migration from 80-column to JSON schema
Completed for “Adopted” Properties

Data is from
40-Calcium

DSID given as
non-unique text

40CA	ADOPTED LEVELS, GAMMAS	17NDS	201702
40CA	H TYP=FUL\$AUT=JUN CHEN\$CIT=NDS 140, 1 (2017)\$CUT=30-Sep-2015\$		
40CA	Q -14323.0 2815635.0 6 8328.17 2 -7039.76 3 2012WA38		
40CA	cQ \$S(2n)=28930.52 {I20}, S(2p)=14709.51 {I20} (2012Wa38)		

Record type
written here

Lines stop
at/before 80

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

JSONSchema

Official: <https://json-schema.org/>

- Defines schema & rules for a JSON document
- Can be used to validate data
- Can generate code from JSONSchema and vice-versa
- Powerful conditional rules

```
{  
  "name": "Mary",  
  "age": 25  
}
```

Incoming data

(the "document")



*Validation code
e.g. server-side*

```
{  
  "properties": {  
    "name": {  
      "type": "string"  
    },  
    "age": {  
      "type": "integer",  
      "minimum": 0  
    }  
  }  
}
```

*JSON-Schema
definition*



Testing & Validation:

Checking by eye does not work!

Batch testing found:

1 document out of 3400 where halflife was not migrated to new database correctly.

"<1." was translated to "0" because the trailing "." was not handled correctly.

Our validator asserted that halflife cannot be 0.

1 document out of 3400 where Jpi was incorrect in 80-column data.

Jpi="3/21"

Requiring integer value of 2J in JSONSchema caught this.

Tree Visualization Implemented



Donnie Mason

Tree View

JSON View

Table View

Current File:
56,144,nuclide.json

Select File:
56,144,nuclide.json

Upload File (<5MB):
Browse...

Tooltips
On Off

Collapse All

Expand All

X Size
- +

Y Size
- +

56,144,nuclide.json

- Greatly increases understanding among developers, users, evaluators
- Increases efficiency, supports group discussion

For the remainder of this year



Chris Morse

**Best Recommended Values
(Adopted Levels, Gammas)**

Decays

β^-
 $\beta^+ + \epsilon$
 α
...

Reactions

(Hl,xn)
(d,p), (p,t)
Coulomb
Ex.
(p,p')
(n, γ)
....

Schema for Decays and Reactions

- Much can be inherited from Adopted
- Synergy with other library improvement projects
 - (n,g) and (n,n'g) will be developed first to feed into GRIN
- This is where we can add new quantities - please reach out to us with needs !!

Database “schema”

Take advantage of binary data

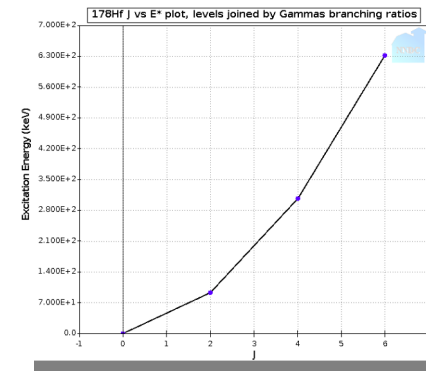
- .CouchDB handles binary objects
- .Potential to speed the workflow
- .Example: preserve valuable history of evaluator’s notes
- .Content for internal use
- .Any format → no editing needed**

```
"_id": "72,178",  
"author": {},  
"reviewDate": "1/1/1980",  
"evaluatorNotes": {↔},  
"levels": {  
  "A": {
```

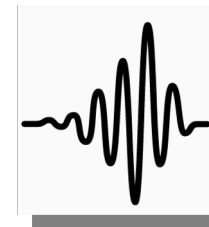
Website links

See: www.nndc...

Screenshots



Even audio



Typed notes

Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.

Scanned handwritten

E(level) [†]	L [‡]	dσ/dΩ(25°) [#]
0.0	0	266
80 1		21
264 1		12
548 1		2.1
821 2		3.7 2.9
997 2		12
1195 2		≈4.5
1217 2	0	30
1275 2		2.7
1359 3		3.0
1411		5.4
1422	0	21

Icons: thenounproject.com/indygo/

Simple API under development

Installation

Run the following to install: *(This is not yet publicly available.)*

```
$ pip install ensdfAPI
```

Usage

Output

```
from ensdfAPI import *

#Connect to ensdfServer
api = ensdfAPI(ipAddress=ensdfServerIp,port=ensdfServerPort)

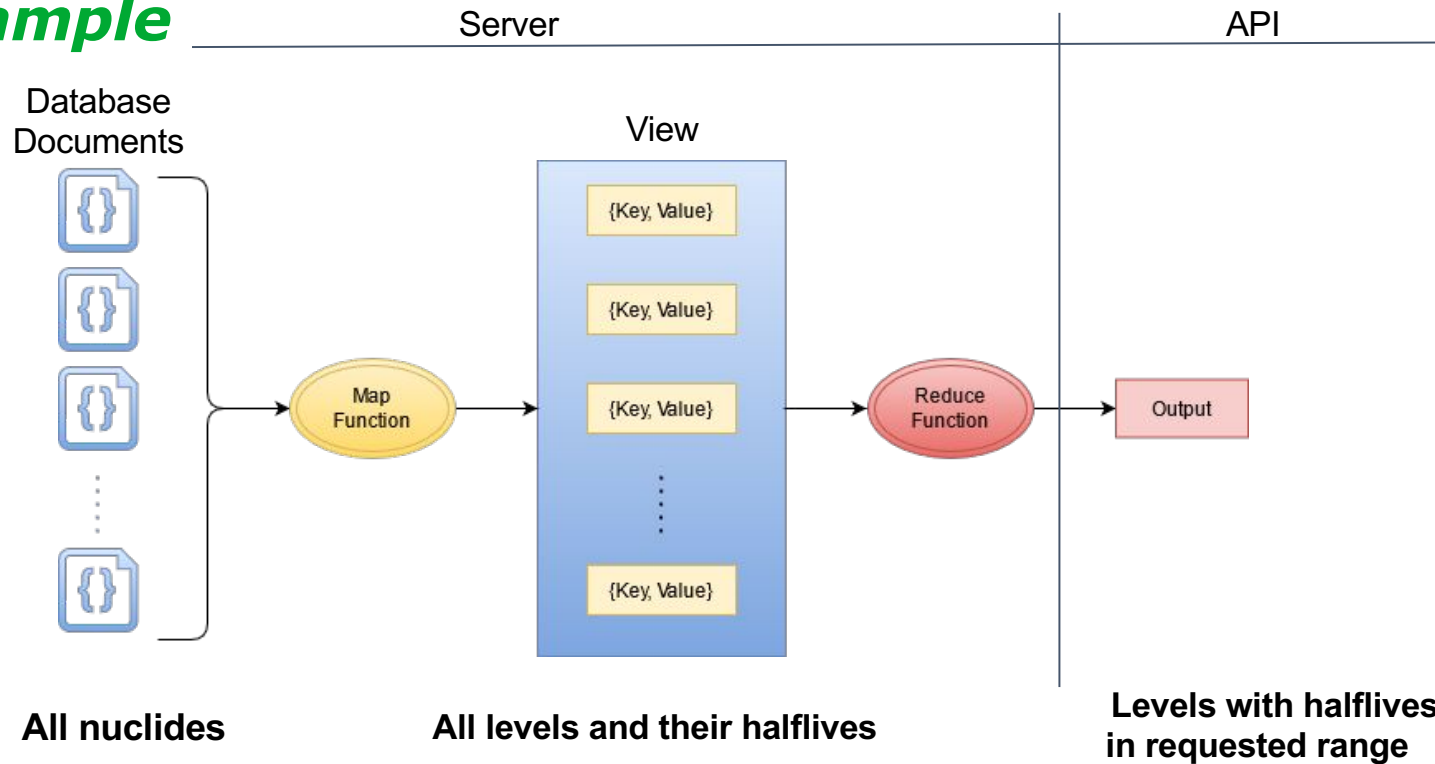
#Request the lowest levels with specified a, J, and parity
twoPlusEnergies = api.getLowestLevels(a=180, J=2, parity="+")

# Output nuclide data
print(twoPlusEnergies)
```

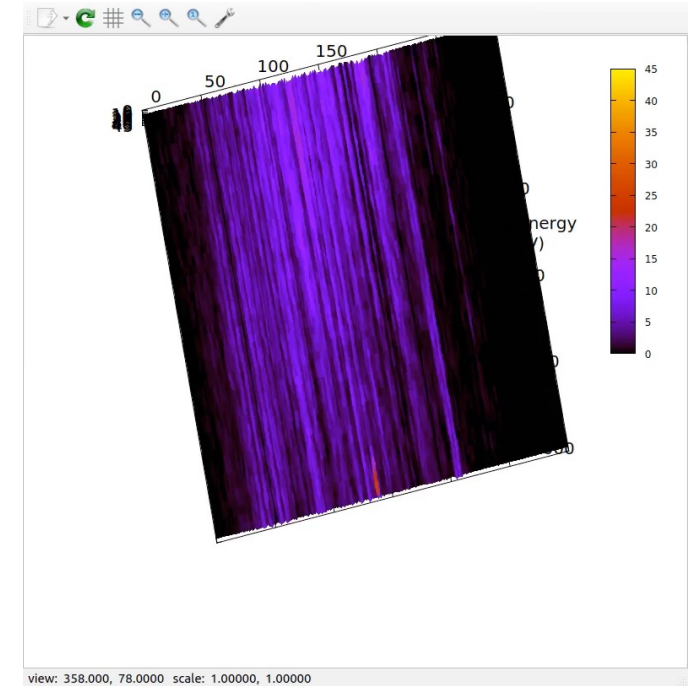
```
[
  [72,93.32],
  [74,103.56],
  [76,132.11],
  [78,153.24],
  [80,434.24],
  [82,1168]
]
```

CouchDB provides efficient search / filter with “Views”

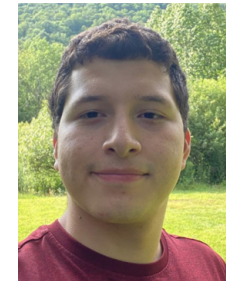
Example



**Pre-populated once
for fast result**



Coupling views with python plotting



Edwin Gomez

ENSDF upgrade status & plan

- July 2020: received funding for 3 years from Nuclear Data Interagency Working Group FOA LAB 19-2114
 - Develop new ENSDF database
 - Develop machine learning (ML) for table comprehension
 - E.A. McCutchan, S. Yoo (Co-PI's, BNL); A. Hayes, A. Mattera, S. McCorkle, C. Morse, B. Shu, A. Sonzogni, C. Soto, D. Mason (BNL); F. Kondev (ANL); C. Mattoon (LLNL) (Underlined joined project after it was funded.)
- Computer Science Initiative (CSI) at BNL leading machine learning component
- Progress in FY21:
 - Migrate numerical data from all nuclides, Adopted Levels/Gammas into new ENSDF database
 - Validate 100% of records against existing ENSDF
 - Simple Python API developed

User comments, questions, suggestions appreciated!

mccutchan@bnl.gov

cmorse@bnl.gov