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IAEA
International Atomic Energy Agency
Atoms for Peace and Development

Developing a New Web Service for Experimental Nuclear Reaction Database (EXFOR) Using RESTful API and JSON Schema

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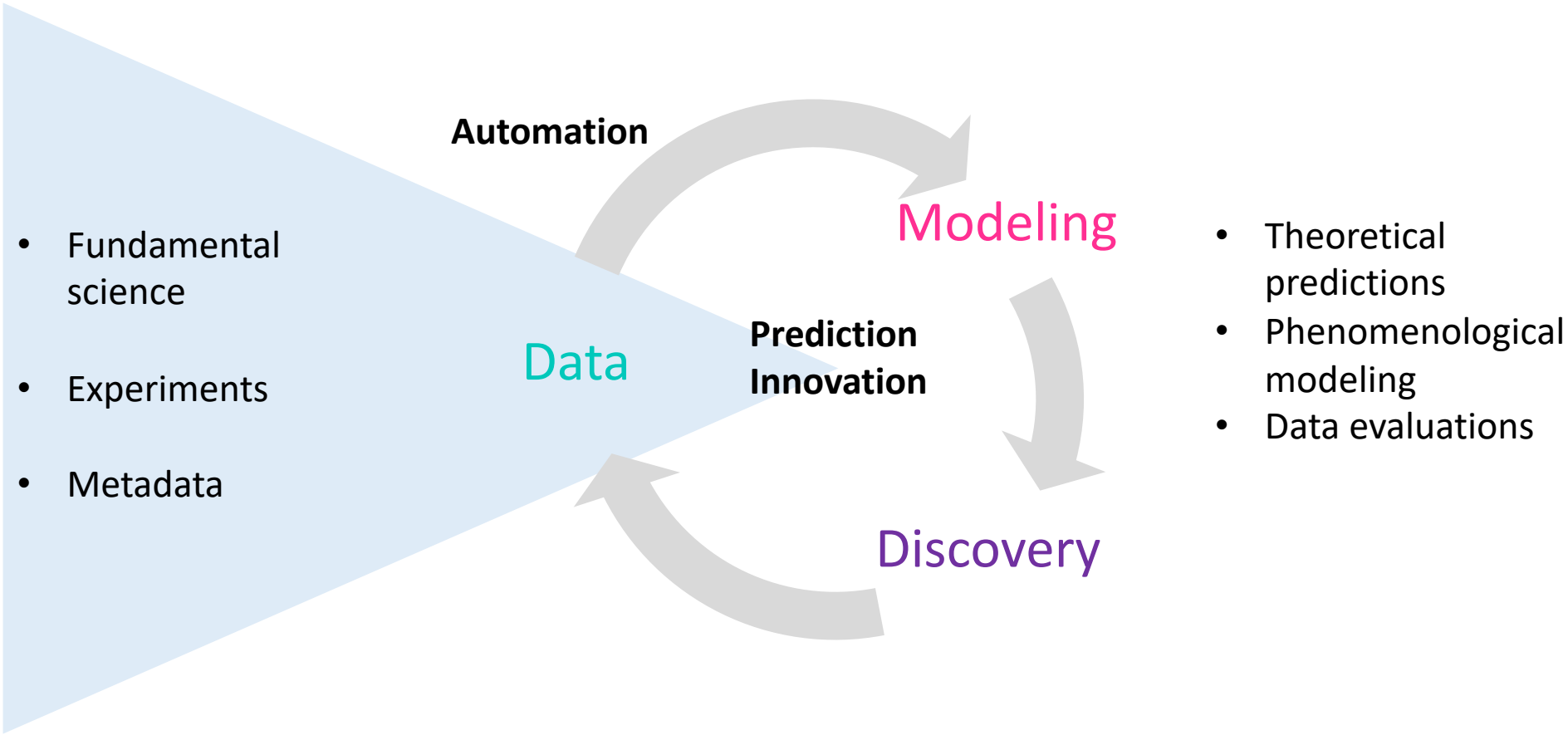
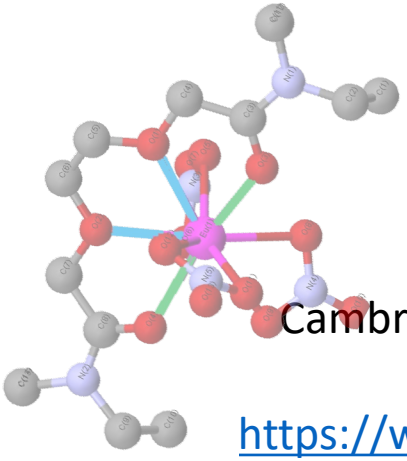
Scientific database needs

- Toward machine learning-enhanced high-throughput scientific experimentation/developments in chemistry, physics, biology.. etc
  - **Automation**: more automatic, processable, and analysable
  - **Innovation**: materials, drug, chemical substance discovery
  - **Prediction**: predict properties without experiments



Experimental databases in various fields

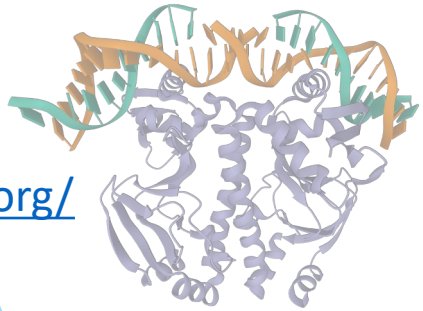


CCDC

Cambridge Crystallographic Data Centre
https://www.ccdc.cam.ac.uk/

RCSB PDB PROTEIN DATA BANK

Protein Data Bank
https://www.rcsb.org/



HEPData

High-Energy Physics data
https://www.hepdata.net/

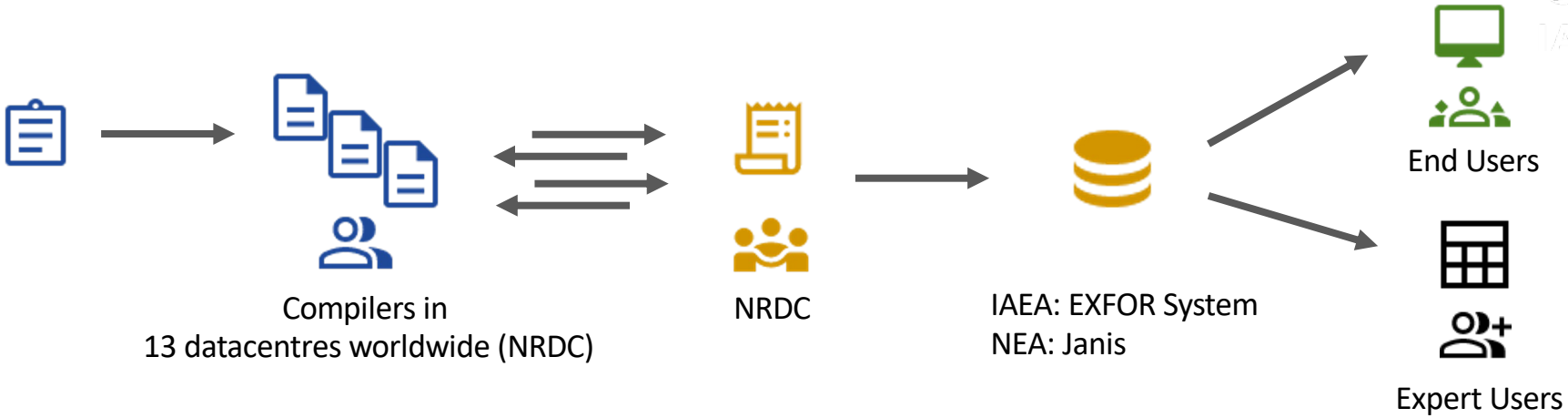
IAEA International Atomic Energy Agency

Experimental Nuclear Reaction Database (EXFOR)
https://nds.iaea.org/exfor/

HTEM

High Throughput Experimental Materials Database
https://htem.nrel.gov/

EXFOR is compiled by the international collaboration (NRDC)



1. Compile EXFOR data from publications by 13 datacentres worldwide
2. Data check done by NRDC
3. Store (create, update, or delete entries) into the IAEA system
4. Provide interface to end users via https://nds.iaea.org/exfor/
   - X4pro package, C4 or C5 (tabulated) format data for expert users

More diverse users' requirements to manipulate data in their way
- To compare and plot with model calculation or new measured experimental data,
- To analyze data for the development of a phenomenological model,
- To use data for ML/AI applications ...and so on

EXFOR: EXchange FORmat with punch-card legacy

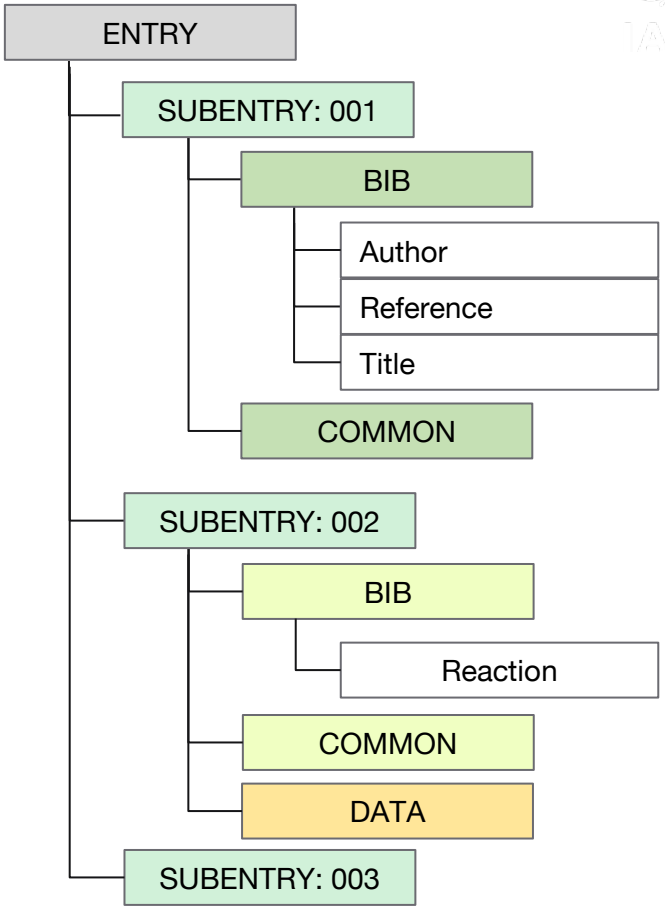
```
ENTRY          13388      891220              20050926      0000
SUBENT      13388001      891220                            0000
BIB                9          11
INSTITUTE  (1USALAS)
REFERENCE  (J,PR,99,730,
AUTHOR     (A.C.WAHL)
TITLE      FISSION OF U-235 BY 14-MEV NEUTRONS: NUCLEAR CHARGE
            DISTRIBUTIONS AND YIELD FL
METHOD     (RCHEM)
DETECTOR   (PROPC)
ERR-ANALYS (DATA-ERR) ST        DEVIATION OF THE AVERAGE OF THE
            RESULTS
STATUS     (RIDER)
HISTORY    (891212C) VM
ENDBIB            11
NOCOMMON           0           0
ENDSUBENT         14
SUBENT      13388003      891220              20050926      0000
BIB                6          12
REACTION   (92-U-235(N,F)ELEM/MASS,IND,FY)
FACILITY   (CCW)
INC-SOURCE (D-T)
MONITOR    ((MONIT1)92-U-2                 MO-99,CUM,FY)
           ((MONIT2)92-U-235(N,F)42-MO-99,CUM,FY,,SPA)
           ((MONIT3)92-U-235(N,F)ELEM/MASS,CUM,FY,,SPA)
DECAY-DATA ((1.)53-I-131,8.07D,B-)
           ((2.)53-I-132,2.3HR,B-)
           ((3.)53-I-133,20.9HR,B-)
           ((4.)53-I-134,52.5MIN,B-)
           ((5.)53-I-135,6.7HR,B-)
STATUS     (DEP,13388002)
ENDBIB            12
COMMON             4           3
EN          EN-NRM      MONIT1      MONIT2
MEV         EV          PC/FIS      PC/FIS
 14.         0.0253        5.17        6.14
ENDCOMMON          3
DATA               5           5
MASS        ELEMENT     DATA        MONIT3      DECAY-FLAG
NO-DIM      NO-DIM      PC/FIS      PC/FIS      NO-DIM
131.         53.           4.47        3.02        1.
132.         53.           5.03        4.49        2.
133.         53.           5.36        6.62        3.
134.         53.           5.20        8.00        4.
135.         53.           4.35        6.31        5.
ENDDATA            7
```

What is "(1USALAS)"?

What is "(RCHEM)"?

What is "ELEM/MASS,IND,FY"?

What is "PC/FIS"?



- EXFOR is the document-oriented database in text files
- It is difficult to use directly with plotting software such as Gnuplot
- Many jargons that the users cannot understand

Format is the big barrier for newcomers

- Understanding formats (ENDF, ENSDF, and EXFOR) is the first barrier to work in the nuclear data field.

> Modern AI/ML tools, including the development and use of Natural Language Processing (NLP) could shorten the time needed for an EXFOR compilation to be completed by automatically processing tables, graphs, and relevant in-text context. The incorporation of these tools, however, will require new skills not currently present in the EXFOR network. **Outdated formats** and compilation rules **have also substantially hindered the progress of such modern mechanisms.** This has motivated the creation of NEA SG-50, which is working to provide a modern interface to EXFOR as well as a framework for providing corrections, both simple error fixes and more complex ones discovered by evaluators in the course of their work.
>
> Second Report of the Nuclear Data Charge Subcommittee of the Nuclear Science Advisory Committee https://science.osti.gov/-/media/np/nsac/pdf/docs/2023/NSAC-ND_Report_2_031923.pdf

Being a specialist ≠ Format understandings

Large scale use cases of EXFOR outside NRDC community

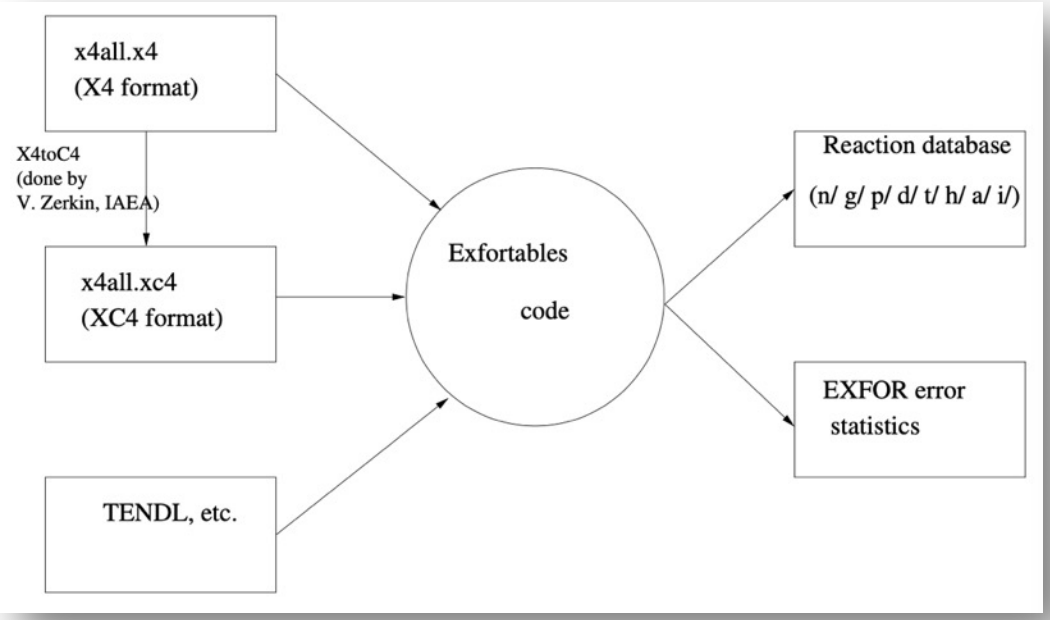
Name	Author	Purpose	Language	Data source	Source code/data
ENEL (EXFOR Nuclear Extraction Library)	**Ahmed A. Selman**	Package for MATLAB	?	C4	https://www.mathworks.com/matlabcentral/fileexchange/110930-enel-exfor-nuclear-extraction-library
EXFORTABLES	**Arjan Koning**	Developing TENDL using experimental data from EXFOR, also used in https://nds.iaea.org/dataexplorer/	Fortran	C4, C5	https://nds.iaea.org/talys/
EXFOR SQL and NucML	**Pedro Jr. Vicente-Valdez**	Modernizing the EXFOR Database using Google BigQuery and Python Pipeline for ML-based Nuclear Data Solutions	Python	C4	https://pedrojrv.github.io/projects.html
exfor-couchdb-docker	**Georg Schnabel**	EXFOR database in JSON format using CouchDB	Python	EXFOR master file	https://github.com/IAEA-NDS/exfor-couchdb-docker
x4i	**David Brown**	Parsing EXFOR: For the US evaluation (forked version: x4i3 by Anatoli Fedynitch)	Python	EXFOR master file	https://github.com/brown170/x4i
Visualization of nuclear data used in PHITS	**Naoya Furutachi**	Visualization of nuclear data with ACE format loaded in PHITS Test of a tool to convert EXFOR to PHITS "Frag data" format	Fortran	EXFOR master file	https://conference-indico.kek.jp/event/136/contributions/3032/attachments/2064/2549/P23_Furutachi.pdf
exfor-parserpy	**Georg Schnabel**	Parsing EXFOR: As a part of the developments of evaluation framework of SG-50/WPEC	Python	EXFOR master file	https://github.com/IAEA-NDS/exfor-parserpy
EXFOR_Parser	**Shin Okumura**	Parsing EXFOR: Convert EXFOR to JSON, tabulated format for the visualization	Python	EXFOR master file	https://github.com/shinokumura/exforparser

+ more local evaluation systems must exist, and data curation

Development of https://nds.iaea.org/dataexplorer/

- We developed "**dataexplorer**" in 2021 based on:
  - **EXFORTABLES** is a directory-structured database from C5 format
  - **ENDFTABLES** is a pre processed and directory-structured database

* A. Koning, iaea-nds-0235, EXFORTABLES-1.0: An experimental nuclear reaction database based on EXFOR https://nds.iaea.org/talys/
** Accessible at https://nds.iaea.org/dataexplorer/



n/Ag107/exfor/xs/102/n-Ag107-MT102-Farinaarbocco-23266106.2013.txt

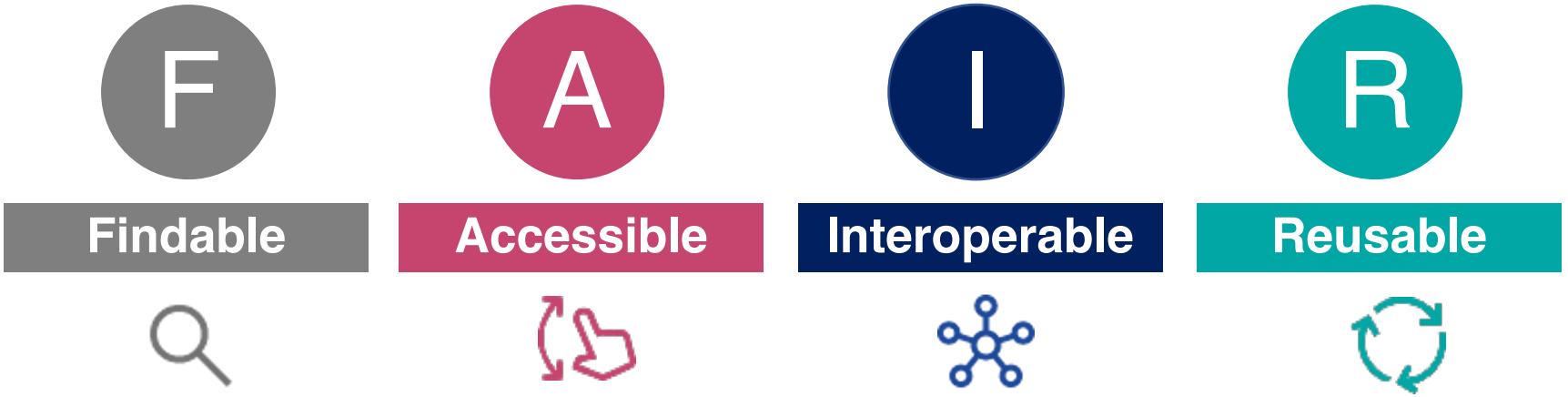
- Increase of access, but the data cannot be updated so frequently (irregularly)
- Need a processing of C4/C5 (by V. Zerkin) and EXFORTABLES production (by A. Koning)

→ Require better data pipeline to show latest EXFOR data

Experimental data and FAIR Principles[1]

Research data integrity is crucial because it ensures the transparency and trustworthiness of scientific data. Therefore,

Data should be...



- Easy to find by both human and computer with machine-readable metadata
- Retrievable by the persistent identifier (e.g. DOI)
- Easy to work from different applications, workflows, storage, or processing
- Well-described, self-explanatory

[1] Mark D. Wilkinson et al., Scientific Data, 3, 160018 (2016)

Towards FAIR for EXFOR data

Findable: Unified metadata, Query-able by SQL/ORM, graphical frontend
Accessible: RESTful API, DOI assignment
Interoperable: Open-sourced, transparent data pipeline
Reusable: Conversion of EXFOR to JSON, helper for EXFOR jargons, clear JSON schema

Primitives of EXFOR: all remain same
- EXFOR (as a format), EXFOR dictionary
- Compilation
- Data retrieval system (https:nds.iaea.org/exfor)
- Compiled data

Data model
- parsing EXFOR
- json conversion & reversion
- automation (pipeline)

RESTful API, database, data store
- data access APIs
- data management (Licence, DOI)
- data store (text, noSQL, SQL, Git repository)

UX Improvements
- Improvements of UI and API

EXFOR Parser

- A new python program to convert EXFOR text into JSON
  - Python3.x (https://github.com/shinokumura/exforparser)
  - Inspired by “x4i” by David Brown (NNDC, BNL)
  - Convert 25,000 entries into JSON in 30-40 min
- Features
  - EXFOR to JSON
    - Simplify JSON schema
    - Parse blocks (BIB, COMMON, DATA)
    - Parse identifires (TITLE, AUTHOR, REACTION, METHOD, ERR-ANALYS..etc)
    - Separate EXFOR-code and freetext
    - Separate subentries based on POINTERs
  - Outputs
    1. Pure (best effort) conversion from EXFOR to JSON (noSQL)
    2. Bib info, reaction index, and tabulated data in SQL db

Related repositories

- https://github.com/IAEA-NDS/**exfor_master**
  - Preservation of historical 24,630 EXFOR entries (= 24,630 files)
  - Recovered from more than 430 backup zip files stored in NDS since 2005
  - All updates are merged into main branch
  - Retroactive to any timestamp (commits)

- https://github.com/IAEA-NDS/**exfor_dictionary**
  - Best-effort conversion of EXFOR dictionary to JSON format

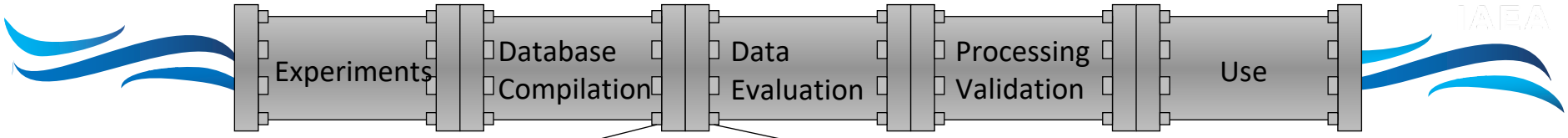
- https://github.com/IAEA-NDS/**exfor_json**
  - All entries in JSON format converted by EXFOR_parser
  - (JSON schema is not yet fixed and may will be changed)

- https://github.com/shinokumura/**exfortables_py**
  - Tabulated data files of datasets from EXFOR entry to the tabulated data like EXFORTABLES*produced by the EXFOR Parser
  - To allow user to download the data file

* A. Koning, iaea-nds-0235, EXFORTABLES-1.0: An experimental nuclear reaction database based on EXFOR

- https://github.com/shinokumura/**ripl3_json**
  - Convert RIPL3 into JSON
  - Currently, only discrete level and mass tables

Data pipeline summary



Parser

exfor_master
- https://github.com/IAEA-NDS/exfor_master
- /exforall/100/100001.x4

exfor_parser
- Conversion scripts

exfor_dictionary_parser
- Conversion scripts

ripl3_levels_parser
- Conversion scripts

Data store

exfor_json
- /json/100/10001.json
- noSQL

exfortables_py
- /exfortables/n/Ag107/n,p/xxxx.dat

exfortables_py_sql
- SQLite database

exfor_dictionary_json
- /json/trans.9127.json
- noSQL

ripl3_levels_json
- /json/levels/Ag/107Ag.json
- noSQL

Frontend

dataexplorer_api
- https://nds.iaea.org/dataexplorer/api
- Flask and Python RESTful API

dataexplorer
- https://nds.iaea.org/dataexplorer/
- Dash/Plotly modules

https://github.com/IAEA-NDS/exfor_master

- Clone/download all EXFOR files anytime

  `git clone https://github.com/IAEA-NDS/exfor_master.git`

- Easy access to change logs of entry using Git command

  `git log -p exforall/224/22449.x4`

```
commit 0dda483cd04058da0c0dbcd4b72a7b07a42c7f56 (tag: Backup-2006-06-16)
Author: shinkoo <s.okumura@iaea.org>
Date:   Sun Oct 2 00:07:10 2022 +0200

    2006-06-16

diff --git a/exforall/224/22449.x4 b/exforall/224/22449.x4
index fbc87f440..a0f5895b7 100644
--- a/exforall/224/22449.x4
+++ b/exforall/224/22449.x4
@@ -1,5 +1,5 @@
 ENTRY            22449   20000202   20010329
-SUBENT        22449001   20000202   20010329
+SUBENT        22449001   20000202   20010329   20050926       0000
 BIB                 15         38
 TITLE        .The Stellar (N,GAMMA) Cross Section of the Stable
              Iridium Isotopes
@@ -46,7 +46,7 @@ KEV        NO-DIM     NO-DIM     NO-DIM
         30.       15.7       3.67       12.2
 ENDCOMMON            3
 ENDSUBENT           45
-SUBENT        22449002   20000202   20010329
```

name of branch (=db update)

number of commits in main branch

```
{
  "entry": "22449",
  "last_updated": "2006-07-20",
  "number_of_revisions": "3",
  "histories": [
    {
      "x4_code": "(20000202C)",
      "free_txt": [
        "  Compiled by S.M."
      ]
    },
    {
      "x4_code": "(20000202U)",
      "free_txt": [
        "  Last checking has been done."
      ]
    }
  ],
```

https://github.com/IAEA-NDS/exfor_json

- Separate information by pointer
- Separate EXFOR Keyword from free text

```
FACILITY   (REAC,2UK HAR) Harwell pile at Atomic Energy Research
            Establishment.
```

```
"facilities": {
  "0": [
    {
      "x4_code": "(REAC,2UK HAR)",
      "free_txt": [
        " Harwell pile at Atomic Energy Research",
        " Establishment."
      ],
      "facility_type": "(REAC)",
      "institute": "(2UK HAR)"
    }
  ]
}
```

- Parse folded DATA block

```
EN          EN-RSL      DATA        ERR-T       ERR-S       ERR-1
ERR-2       ERR-3       ERR-4       ERR-5       ERR-6       ERR-9
ERR-10
MEV         MEV         MB          PER-CENT    PER-CENT    PER-CENT
PER-CENT    PER-CENT    PER-CENT    PER-CENT    PER-CENT    PER-CENT
PER-CENT
    1.00E-6     4.2E-9     6.38E+5        4.17        0.19        0.48
       3.81                   0.42        0.02        0.06        0.00
       0.27
    1.26E-6     5.4E-9     5.37E+5        2.62        0.26        2.03
       0.05                   0.43        0.03        0.10        0.00
       0.32
```

```
"data": {
  "heads": [
    "EN",
    "EN-RSL",
    "DATA",
    "ERR-T",
    "ERR-S",
    "ERR-1",
    "ERR-2",
    "ERR-3",
    "ERR-4",
    "ERR-5",
    "ERR-6",
    "ERR-9",
    "ERR-10"
  ],
  "units": [
    "MEV",
    "MEV",
    "MB",
    "PER-CENT",
    "PER-CENT",
    "PER-CENT",
    "PER-CENT",
    "PER-CENT",
    "PER-CENT",
    "PER-CENT",
    "PER-CENT",
    "PER-CENT",
    "PER-CENT"
  ],
  "data": [
    [
      1e-06,
      1.26e-06,
      1.58e-06,
      2e-06,
      2.51e-06,
      3.16e-06,
      3.98e-06,
      5.01e-06,
      6.31e-06,
      7.94e-06,
      1e-05,
      1.26e-05,
      1.58e-05,
      2e-05,
      2.51e-05,
      3.16e-05,
      3.98e-05,
      5.01e-05,
```

https://github.com/IAEA-NDS/exfor_dictionary

- EXFOR dictionary in JSON with EXFOR keywords as a JSON key
  - Easy to lookup programmatically from JSON friendly computer languages
- Convert abbreviations
  - e.g. ”abs.” could be "Absolute”, “Absorption” does "f." mean **f**ragment, **f**actor, **f**ission, **f**or or **f**inal?


```
"21": {
  "diction_name": "Methods",
  "codes": {
    "ACTIV": {
      "description": "Activation",
      "active": true
    },
    "AMS": {
      "description": "Accelerator mass spectrometry",
      "active": true
    },
    "ASEP": {
      "description": "Off-line mass separation of a product",
      "active": true
    },
    "ASPEC": {
      "description": "Alpha spectrometry",
      "active": true
    },
    "ASSOP": {
      "description": "Associated particle",
      "active": true
    },
    "BCINT": {
      "description": "Beam current integrated",
      "active": true
```

```
"25": {
    "EV": {
      "description": "electron-Volts",
      "additional_code": "E",
      "unit_conversion_factor": "1.E+0",
      "active": true
    },
    "GEV": {
      "description": "GeV",
      "additional_code": "E",
      "unit_conversion_factor": "1.E+9",
      "active": true
    },
    "KEV": {
      "description": "keV",
      "additional_code": "E",
      "unit_conversion_factor": "1.E+3",
      "active": true
    },
    "MEV": {
      "description": "MeV",
      "additional_code": "E",
      "unit_conversion_factor": "1.E+6",
      "active": true
    },
```

https://github.com/shinokumura/exfortables_py

- Produce-able without C4/C5
- Best effort to get smallest ”dataset” of physical observable and tabulate them

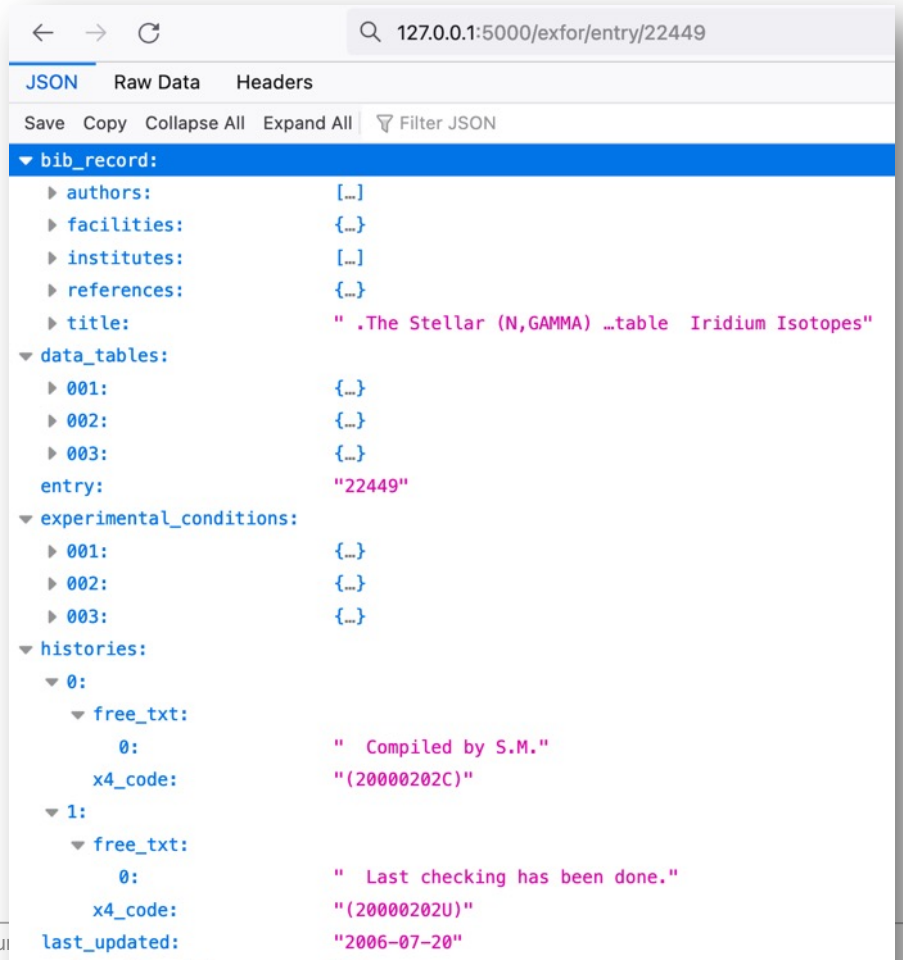
n/Fe-56/n-inl-L1/xs/Fe-56_n-inl-L1_Fe56_Almen-Ramstrom-20788-008-0-1975.txt

```
# entry-subent-pointer  : 20788-008-0
# EXFOR reaction        : ['26-FE-56', ['N,INL'], '26-FE-56,PAR,SIG']
# incident energy       : 2.02e+00 MeV - 4.50e+00 MeV
# target                : Fe-56
# product               : Fe-56
# level energy          : 8.45e-01 MeV
# MF-MT number          : 3 - ['51']
# first author          : E.Almen-Ramstrom
# institute             : (2SWDAE ): Studsvik Energiteknik AB
# reference             : (R,AE-503,197504)
# year                  : 1975
# facility              : (VDG): Van de Graaff
# git                   : https://github.com/IAEA-NDS/exfor_master/blob/main/exforall/207/20788.x4
# nds                   : https://nds.iaea.org/EXFOR/20788
#
#       E_in(MeV)       dE_in(MeV)            XS(B)           dXS(B)
      2.02000E+00      0.00000E+00      8.40000E-01      1.26000E-01
      2.27000E+00      0.00000E+00      8.85000E-01      1.33000E-01
      2.50000E+00      0.00000E+00      8.62000E-01      1.29000E-01
      2.77000E+00      0.00000E+00      7.53000E-01      1.13000E-01
      3.01000E+00      0.00000E+00      8.22000E-01      1.23000E-01
      3.29000E+00      0.00000E+00      6.12000E-01      9.20000E-02
      3.52000E+00      0.00000E+00      5.54000E-01      8.30000E-02
      3.78000E+00      0.00000E+00      4.82000E-01      7.20000E-02
      4.02000E+00      0.00000E+00      4.43000E-01      6.60000E-02
      4.26000E+00      0.00000E+00      3.52000E-01      5.30000E-02
      4.50000E+00      0.00000E+00      3.16000E-01      4.70000E-02
```

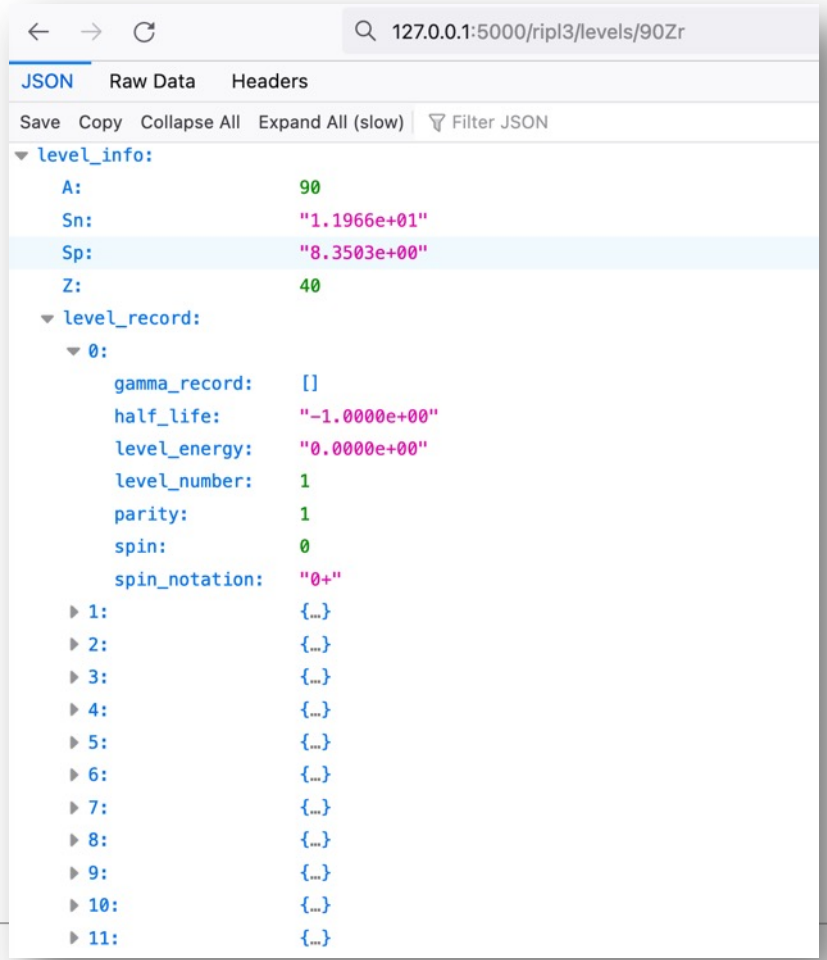
RESTful API

- An architectural style for an application program interface (API) that uses HTTP requests to access and use data - Addressability, Stateless, Uniform Interface
  - **EXFOR entry**: entry, subentry, bib, data, experimental condition, reactions
  - **EXFOR dictionary**: facilities, institutes, methods, detectors
  - **RIPL-3 descrete level**: levels, level records
- API documentation is available

/dataexplorer/api/exfor/entry/22449



/dataexplorer/api/ripl3/levels/90Zr



Decay Chain in JSON

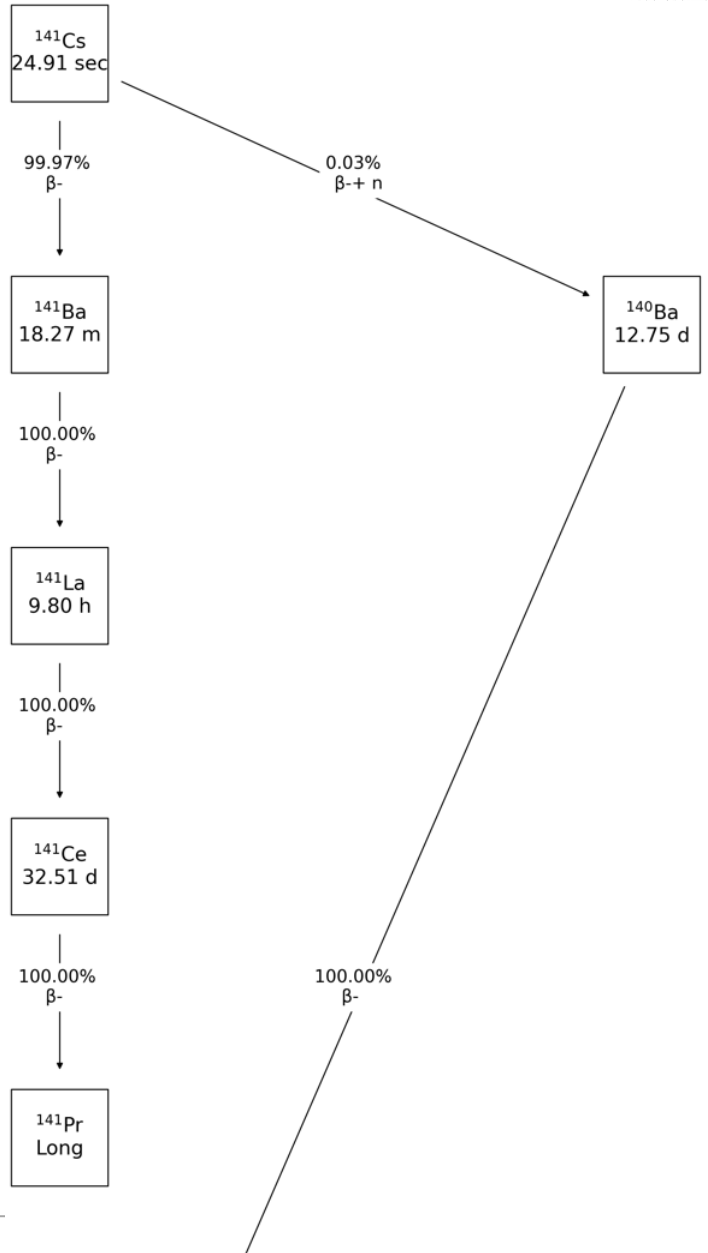
Decay data


```
"55-Cs-141-00": {
   "Z": "55",
   "ELM": "Cs",
   "MASS": "141",
   "LIS": "00",
   "HL": "2.4910000E+01",
   "LAMBDA": 0.027826,
   "En_beta": "1.5473620E+06",
   "En_gamm": "1.7248140E+06",
   "En_alpha": "7.5359650E+01",
   "DecayInfo": {
     "0": {
       "RTYP": "1.0000000E+00",
       "RFS": "0.0000000E+00",
       "Q": "5.2560000E+06",
       "BR": "9.9965800E-01",
       "DAUGHTER": "56-Ba-141-00"
     },
     "1": {
       "RTYP": "1.5000000E+00",
       "RFS": "0.0000000E+00",
       "Q": "7.2100000E+05",
       "BR": "3.4200000E-04",
       "DAUGHTER": "56-Ba-140-00"
     }
   },
   "daughters": [
     "56-Ba-141-00",
     "56-Ba-140-00"
   ]
 },
```

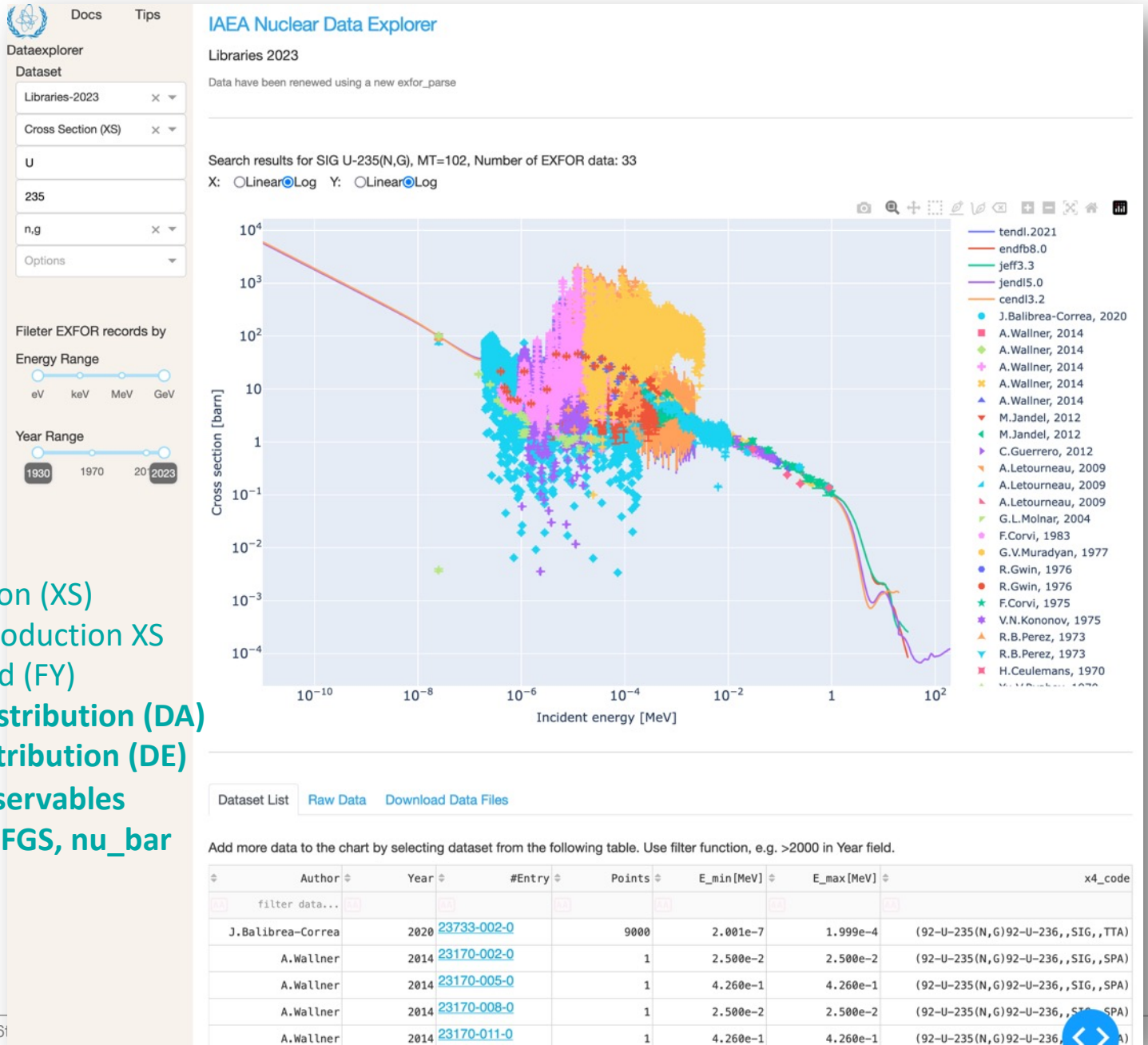

Decay chain (linearized)


```
"55-Cs-141-00": {
   "1": {
        "chain": [
        "56-Ba-141-00",
        "57-La-141-00",
        "58-Ce-141-00",
        "59-Pr-141-00"
        ],
        "branching": [
        0.999658,
        1.0,
        1.0,
        1.0
        ],
        "rtyp": [
        1.0,
        1.0,
        1.0,
        1.0
        ],
        "lmbds": [
        0.027826,
        0.00063232,
        4.9118e-05,
        2.4676e-07,
        6.9315e-51
        ],
        "en_betas": [
        "1.5473620E+06",
        "9.6628250E+05",
        "9.8713460E+05",
        "1.9438810E+05",
        0.0
        ],
        "en_gamms": [
        "1.7248140E+06",
        "9.0968270E+05",
        "2.6780420E+04",
        "7.6901970E+04",
        0.0
        ]
        },
    "2": {
        "chain": [
        "56-Ba-140-00",
        "57-La-140-00",
        "58-Ce-140-00"
        ],
```


Decay chain (network diagram plot)



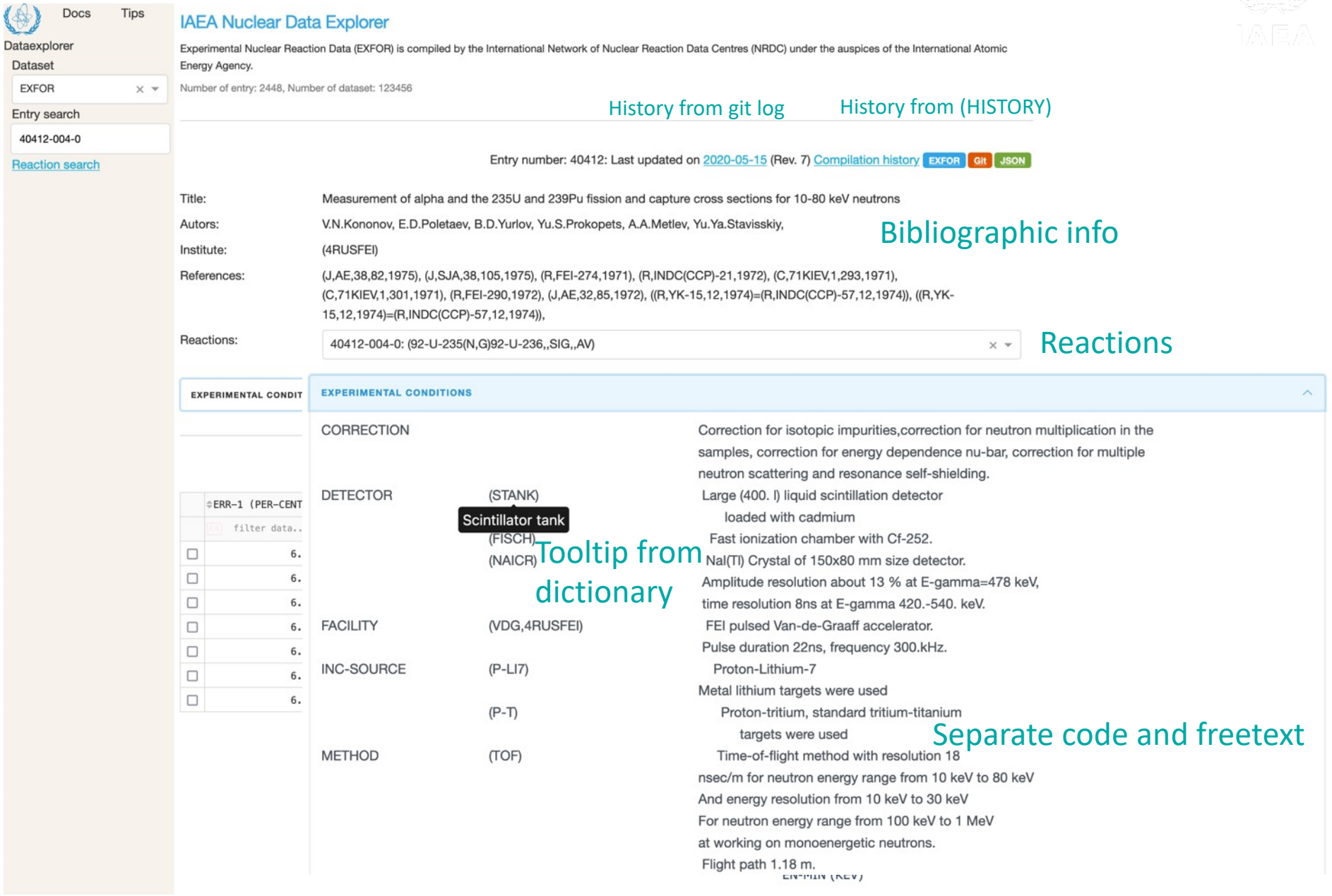
Renewed interface of https://nds.iaea.org/dataexplorer/



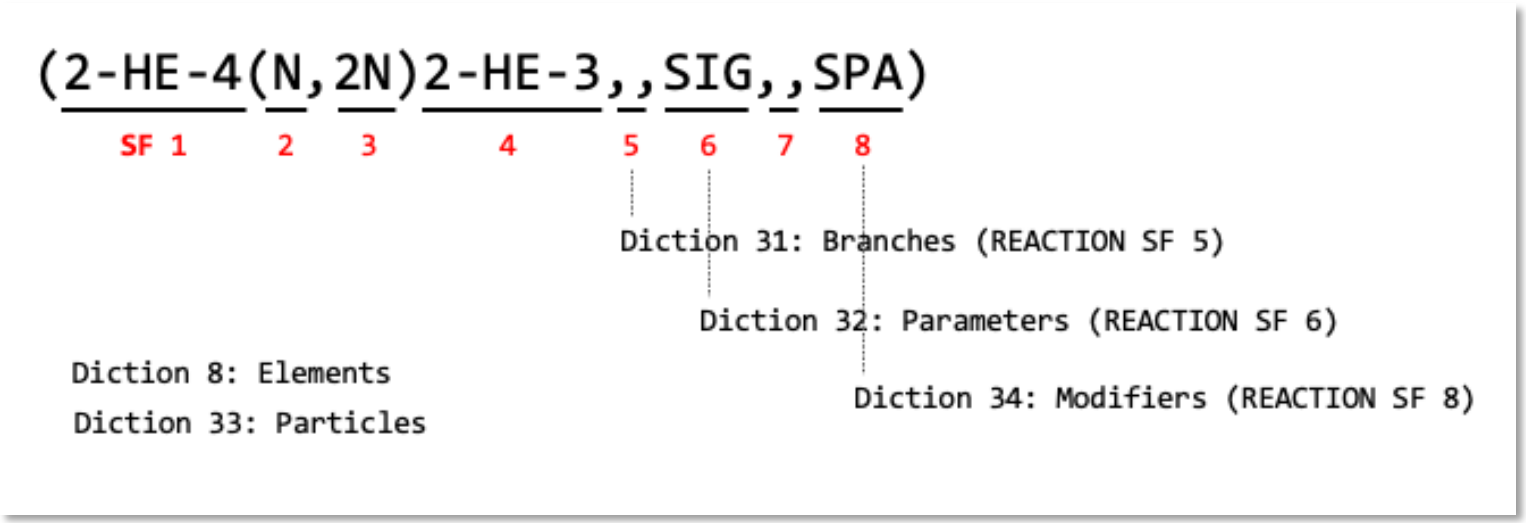
Data plots for

- Cross Section (XS)
- Residual Production XS
- Fission Yield (FY)
- **Angular Distribution (DA)**
- **Energy Distribution (DE)**
- **Fission Observables**
  - **PFNS, PFGS, nu_bar**

New UX for EXFOR entry viewer based on API



Index of all reactions



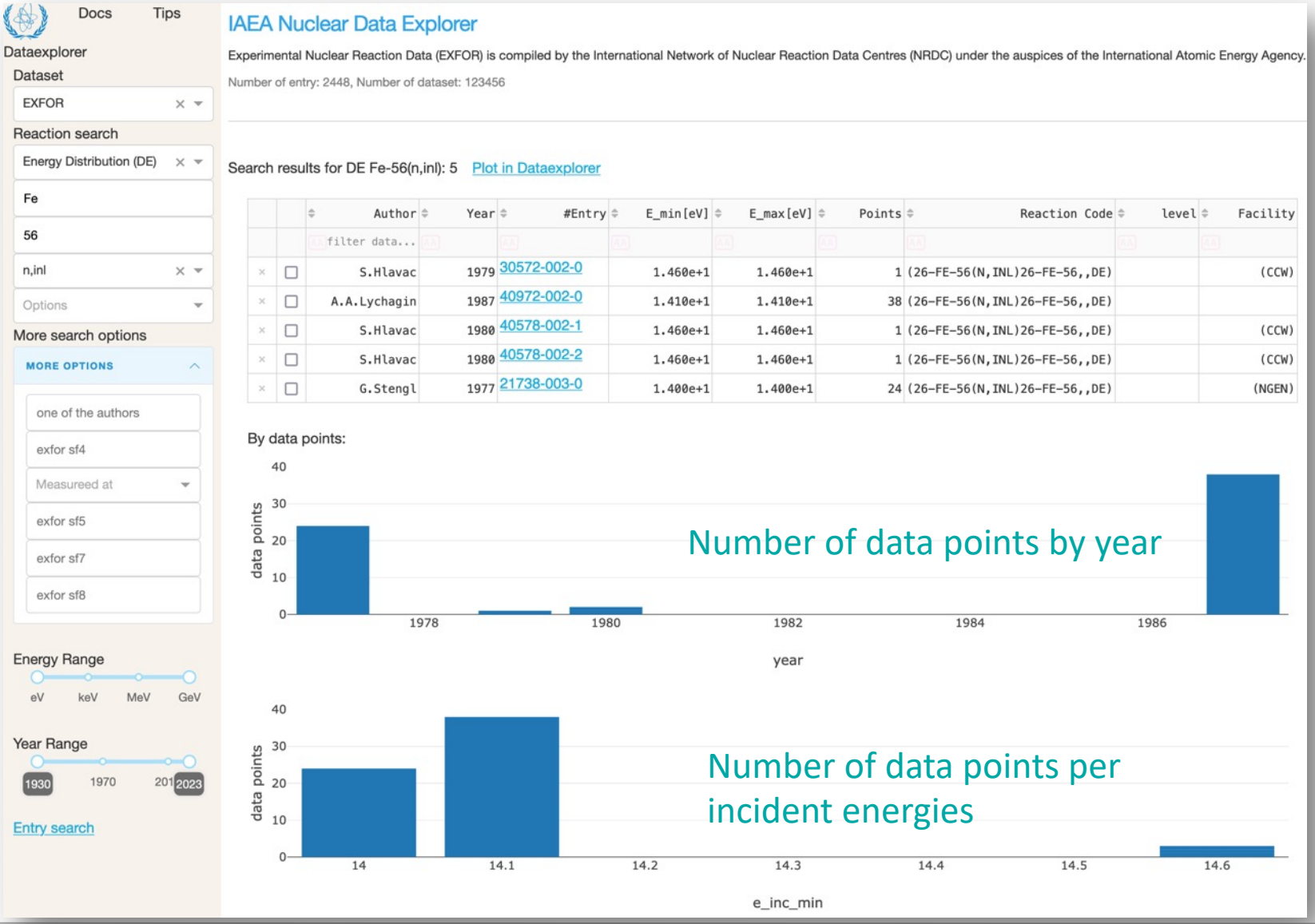
- If the PRODUCT (SF4) in REACTION is either of MASS, ELEM, or ELEM/MASS, one cannot know real products until reading DATA block

(89-AC-227(N,F)ELEM/MASS,CUM,FY,,REL/FIS)

id	year	author	min_inc_en	max_inc_en	points	target	process	sf4	residual	sf5	sf6	sf7	s
30944-002-0	1965	R.S.Iyer	1.000e+00	1.000e+00	1	89-AC-227	N,F	ELEM/MASS	35-Br-83	CUM	FY	None	REL/F
30944-002-0	1965	R.S.Iyer	1.000e+00	1.000e+00	1	89-AC-227	N,F	ELEM/MASS	38-Sr-89	CUM	FY	None	REL/F
G0074-002-0	2019	A.Chatillon	1.740e+01	1.740e+01	1	89-AC-219	G,F	ELEM	Zn	CHG	FY	None	S
G0074-002-0	2019	A.Chatillon	1.740e+01	1.740e+01	1	89-AC-219	G,F	ELEM	Ga	CHG	FY	None	S
G0074-002-0	2019	A.Chatillon	1.740e+01	1.740e+01	1	89-AC-219	G,F	ELEM	Ge	CHG	FY	None	S

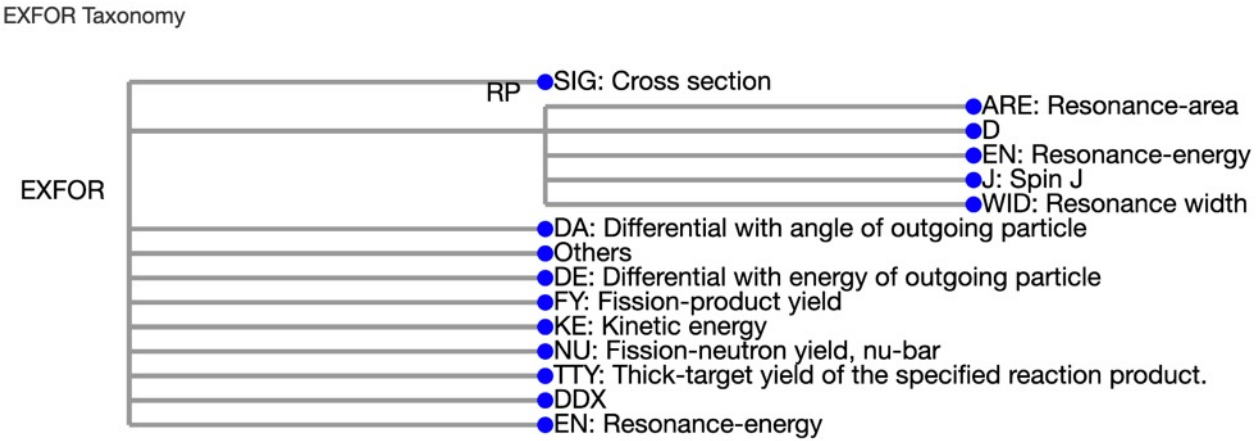
New UX to search EXFOR entry

- Search by the reaction or EXFOR subfields

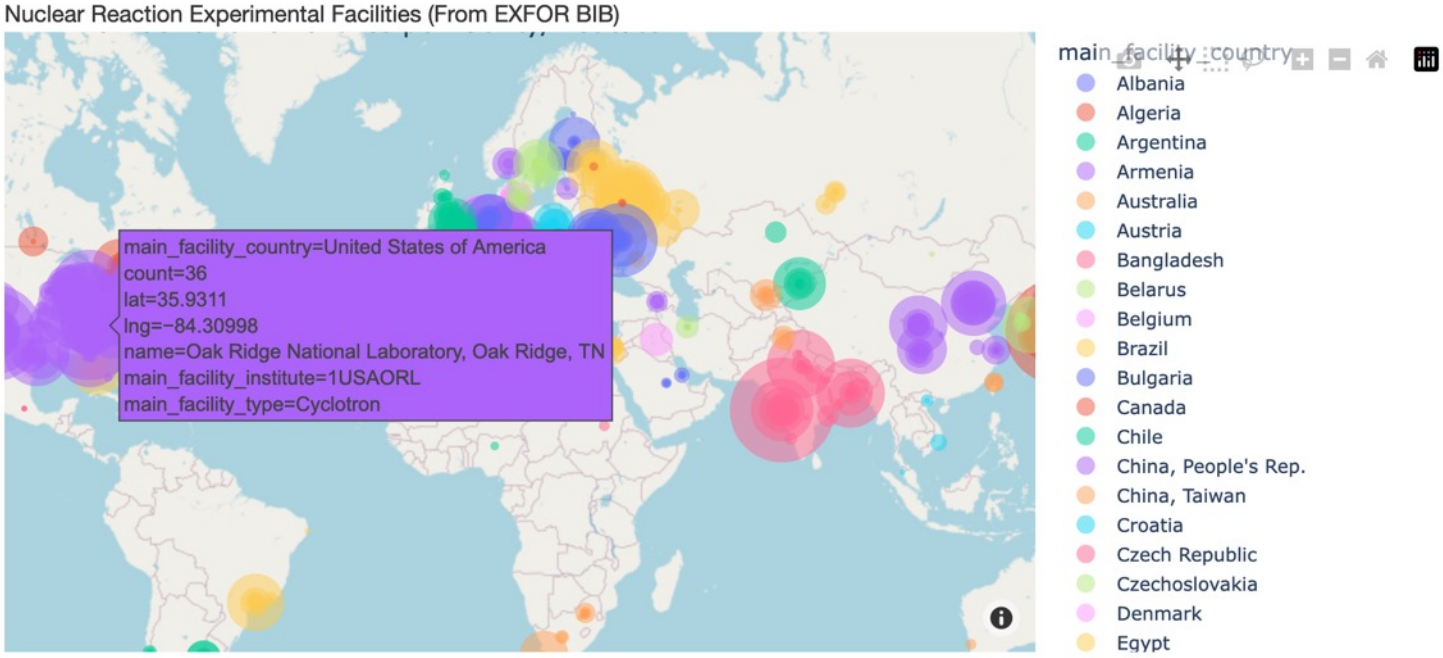


And more…

- Search by EXFOR taxonomy



- Search by geography



Summary

- We are working towards FIAR principle on EXFOR
- Open source/data on GitHub
  - EXFOR Parser: main EXFOR parsing program in Python
  - exfor_master: backup of EXFOR master files
  - exfor_json: JSON converted EXFOR files
  - exfor_dictionary: JSON converted EXFOR dictionary
  - exfortables_py: tabulated (X-Y table) reaction data
- Future work
  - Deployment, internal test, and security scan toward the production release (w/L. Marian)
  - Automatic update of data pipeline
  - Develop clear JSON schema (w/G. Schnabel)
  - Implementation of FAIR principles for EXFOR and other data stored in IAEA/NDS
    - Findable, Accessible
      - DOI assignment
      - License assignment (CC0/CC BY 4.0) is important
    - Interoperable, Reusable
      - Move on to a research repository

Thank you!

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