IAEA
International Atomic Energy Agency
Atoms for Peace and Development

TM on Nuclear Data Retrieval, Dissemination, and Data Portals

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NAPC - Nuclear Data Section | International Atomic Energy Agency

Meeting dates

TM on Nuclear Data Retrieval, Dissemination, and Data Portals
- towards a blueprint of IAEA Nuclear Data Portal –

on **11-15 November 2024** at the IAEA Headquarter, Vienna, Austria

IAEA NDS will facilitate and support to accelerate the evolution of nuclear physics and nuclear data science. Input from member states matters.

60 years and looking ahead to the next 10 years
IAEA Nulcear Data Section

Nomination of chair and rapporteur

- Recording the meeting

- Chairperson

- Rapporteur
  - Nuclear Data Processing Tools and Codes:
  - Web Interfaces and APIs Developments:
  - Users' Feedbacks and New Demands:
  - Data Pipeline, Data Model, and Data Format:

Purpose of the meeting

"TM on Nuclear Data Retrieval, Dissemination, and Data Portals"

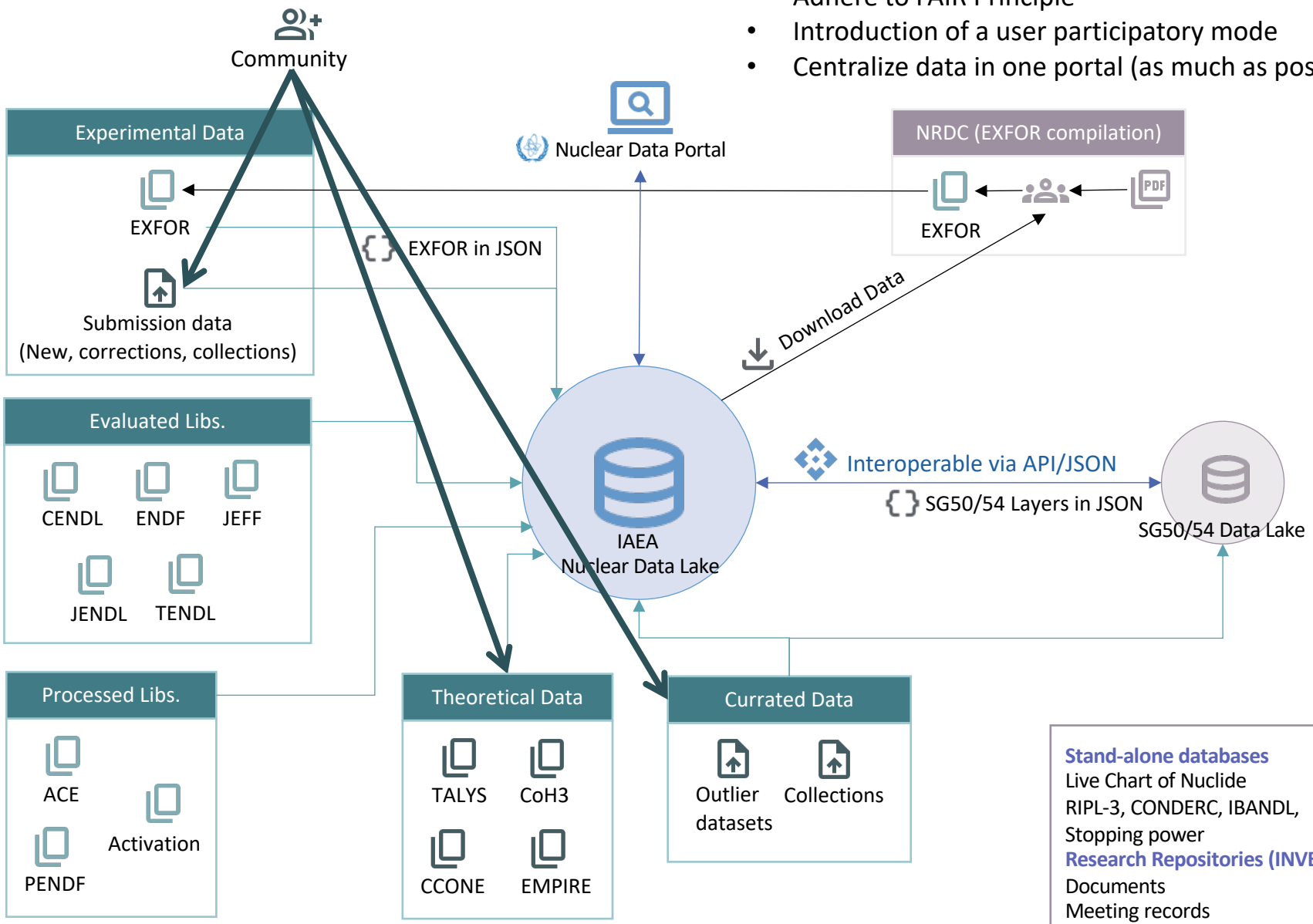
- Objective
  - Review existing nuclear data processing tools and code capabilities
  - Web Interfaces and API Developments
  - User Feedback and New Demands

- Key Discussion Points
  - Challenges in data format conversion and data store
    - Data Pipeline, Data Model, and Data Format
  - Best Practices for IAEA Nuclear Data Portal
    - Establishing efficiency and usability of data
    - Requirements (requests to the IAEA Nuclear Data Portal)

- Positive side effects
  - Facilitate information exchange
  - Networking opportunities for developers
  - Encourage more collaborations, promote inter-operativities

Goal: Centralize nuclear reaction data into “Nuclear Data Portal”

- Adhere to FAIR Principle
- Introduction of a user participatory mode
- Centralize data in one portal (as much as possible)



Stand-alone databases
Live Chart of Nuclide
RIPL-3, CONDERC, IBANDL,
Stopping power
Research Repositories (INVENIO)
Documents
Meeting records

Punch card legacy

80 Characters

This stack of 62,500 punched cards — 5 MB worth — held the control program for the giant SAGE military computer network.

- 80 characters = 1 line
  - The first 72 columns were used for the program statements.
  - The last 8 columns could be used to print a card number.

    (so that the unlucky programmer who dropped a deck of cards had some chance of reordering them properly!)
  - One card was required for each line of the program/data.
  - The early conventions of the Fortran programming language are related to the columns on a punch card.
  - Magnetic tape/floppy disc started replacing punch cards in the 1960s.
  - Today, they are rarely used or found and are considered **OBSOLETE**!
- But…!

Constraints from punch card legacy

XUNDL: Experimental Unevaluated Nuclear Data List

80 Charactors

```
10B     10B(P,P'G):XUNDL-19          2024KU19                                202409
10B  c  Compiled (unevaluated) dataset from 2024Ku19
10B  c  Phys. Rev. Lett. 133, 072502 (2024)
10B  c  Compiled by K. Setoodehnia and J. Kelley (TUNL), August 17, 2024.
10B  c  The authors performed a coincidence |g-ray spectroscopy study of {+10}B
10B 2c  and found a previously unobserved, weak M3 transition from the
10B 3c  {+10}B*(1740 keV, 0{++}, T=1) isobaric analog state (IAS) to the
10B 4c  {+10}B{-g.s.} with J{+|p}=3{++} and T=0. Earlier electron and pion
10B 5c  scattering measurements on {+10}B suggested that such a transition
10B 6c  would compete with an M1 transition from the {+10}B*(IAS) to the
10B 7c  {+10}B*(718 keV, 1{++}, T=0) level. However, this suggested M3
10B 8c  transition had remained elusive.
10B  c  The experiment was performed at the Horia Hulubei National Institute
10B 2c  for R&D in Physics and Nuclear Engineering (IFIN-HH) in Romania. A
```

XUNDL example in 2024

ENSDF: Evaluated Nuclear Structure Data File

80 Charactors

```
30F     ADOPTED LEVELS:UNOBSERVED                                    24NDS    202408
30F   H TYP=FUL$AUT=M. S. Basunia, A. Chakraborty$CIT=NDS 197, 1 (2024)$
30F 2 H CUT=31-May-2024$
30F   Q 25680     SY -740   SY                        2021WA16
30F  cQ $|DQ(|b{+-})=560, |DS(n)=730 (syst,2021Wa16)
30F  cQ $S(2n)=590 {I510}, Q(|b{+-}n)=22490 {I520} (syst,2021Wa16)
30F  c  1999Sa06: Unstable to ground state neutron emission. Reaction:
30F 2c  Ta({+40}Ar,x), E=94.1 MeV/nucleon, at RIKEN facility. Magnetic fragment
30F 3c  separator, identification by measurements of energy loss,
30F 4c  time-of-flight, magnetic rigidity for each fragment, etc. No {+30}F
30F 5c  events were identified. Similar results were reported in 2004Lu19.
30F  c  Structure calculation:
30F  c  2022Fo03: Performed large-scale shell model calculations including
30F 2c  continuum states to investigate the properties of the neutron-rich
```

^{30}F evaluation in 2024

EXFOR: Experimental Nuclear Reaction Database

```
ENTRY     C      41553   20240709                                  41553000    1
SUBENT    C   41553001   20240709                                  41553001    1
BIB                10         21                                   41553001    2
TITLE       Angular distribution gamma-rays emitted during the     41553001    3
           inelastic scattering of fast neutrons from a reactor by41553001    4
           114, 116Cd                                             41553001    5
AUTHOR     (A.M.Demidov,L.I.Govor,O.K.Zhuravlev,M.M.Komkov,       41553001    6
           I.B.Shchukalov)                                        41553001    7
REFERENCE  (J,BAS,40,(6),119,1976) Engl.translation of IZV,40,157 41553001    8
           (J,IZV,40,1241,1976) Issue 6                           41553001    9
ENDSUBENT            28          0                                4155300199999
SUBENT    C   41553002   20240709                                  41553002    1
BIB                  6         14                                   41553002    2
REACTION   ((48-CD-114(N,INL)48-CD-114,,SPC/DA,,FST)//            41553002    3
           (48-CD-114(N,INL)48-CD-114,,SPC/DA,,FST))              41553002    4
ENDBIB               14          0                                41553002   17
DATA                  8         56                                41553002   23
E-NM       E-NM-ERR   DATA       DATA-ERR   LVL-INI    LVL-INI-ER 41553002   24
LVL-FIN    MISC                                                   41553002   25
KEV        KEV        NO-DIM     NO-DIM     KEV        KEV        41553002   26
KEV        NO-DIM                                                 41553002   27
 367.7      0.6          0.62 E-2   0.06 E-2  1732.2   0.4        41553002   28
  1364.0     4.8   E-2                                            41553002   29
 448.3      0.8          0.35 E-2   0.09 E-2  1732.2   0.4        41553002   30
```

EXFOR TRANS example in 2024

Line numbers

ENDF-6: Evaluated Nuclear Data Library

```
 33        103         42          02725 1451  907
                              33         104         26          02725 1451  908
                              33         105         16          02725 1451  909
                              33         106          9          02725 1451  910
                              33         107         49          02725 1451  911
                              33         111          8          02725 1451  912
                              33         112         13          02725 1451  913
                              34           2         63          02725 1451  914
                                                                  2725 1  099999
                                                                  2725 0  0     0
 2.705900+4 5.842693+1           0          0          1          02725 2151    1
 2.705900+4 1.000000+0           0          0          1          02725 2151    2
 1.000000-5 1.000000+5           1          3          0          12725 2151    3
 3.500000+0 6.672000-1           0          0          2          32725 2151    4
 5.842690+1 6.672000-1           0          0        600        1002725 2151    5
-5.000000+3 3.000000+0 5.576800+2 9.215100+0 0.000000+0 0.000000+02725 2151    6
-5.000000+3 4.000000+0 1.898100+2 1.868200-1 0.000000+0 0.000000+02725 2151    7
-4.767000+2 4.000000+0 1.949000-2 2.148900+0 0.000000+0 0.000000+02725 2151    8
-2.258800+2 3.000000+0 8.910000+0 5.940000-2 0.000000+0 0.000000+02725 2151    9
 1.320000+2 4.000000+0 5.270100+0 4.700000-1 0.000000+0 0.000000+02725 2151   10
 4.323100+3 4.000000+0 1.041400+2 4.173700-1 0.000000+0 0.000000+02725 2151   11
 5.016000+3 3.000000+0 6.789600+2 1.332200+0 0.000000+0 0.000000+02725 2151   12
 6.389700+3 4.000000+0 1.681100+0 3.155600-1 0.000000+0 0.000000+02725 2151   13
 8.061900+3 3.000000+0 4.083300+1 4.078000-1 0.000000+0 0.000000+02725 2151   14
```

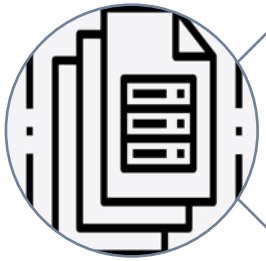
n+^{59}Co evaluation in 2024

Line numbers

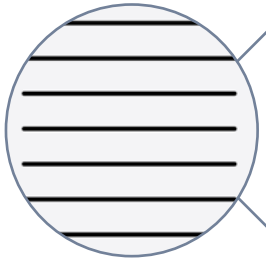
Punch card disappeared, but format constraint is still there.

Entry barriers

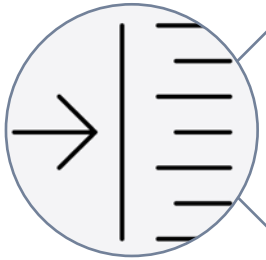
Data format is often a barrier for newcomers.



Understanding Formats: Often painful to first understand the format prior to use.



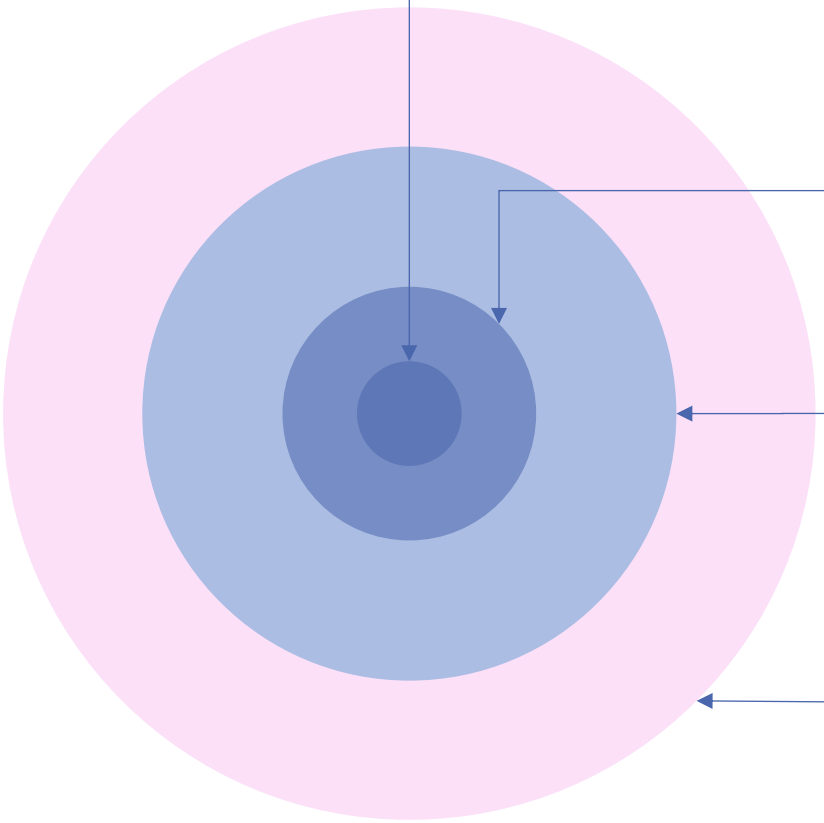
ASCII Text Files: Programmatic searching and data retrieval can be cumbersome, often requiring an additional database or pre-processing.



Fixed Width: Disrupts sentence and column alignment, limiting direct use with plotting or visualization software.

Who are the users?

Researchers and students in fields of



Nuclear data evaluations

Want to access all available experimental, evaluated, theoretical, curated data for their evaluations

Experimental/theoretical nuclear physics

Want to access the experimental, theoretical, or evaluated data for their research

Nuclear engineering

Use nuclear data natually included in the software codes, for example transport simulation (reactor simulation), shielding calculation, burn-up calculation.

Nuclear science and applications

Need to see the gamma emission lines for gamma-ray spectroscopy, decay half-life, medical isotope production cross sections..etc

Modernization efforts: Live Chart of Nuclides

https://nds.iaea.org/relnsd/vcharthtml/VChartHTML.html

2008 SINCE JAVA based, open source project

Interactive live chart of nuclides

- Nuclear structure and decay data (ENSDF) viewer
  - Levels, schema plot
  - Gammas, decay radiation
  - Nuclear moments
  - Fission yields, beta and neutrino spectra

Since 2013!

Mobile App

- Properties of over 4,000 isotopes
- No internet connection needed
- More than 180,000 downloads, 4.8 ⭐
- In 11 languages

New!

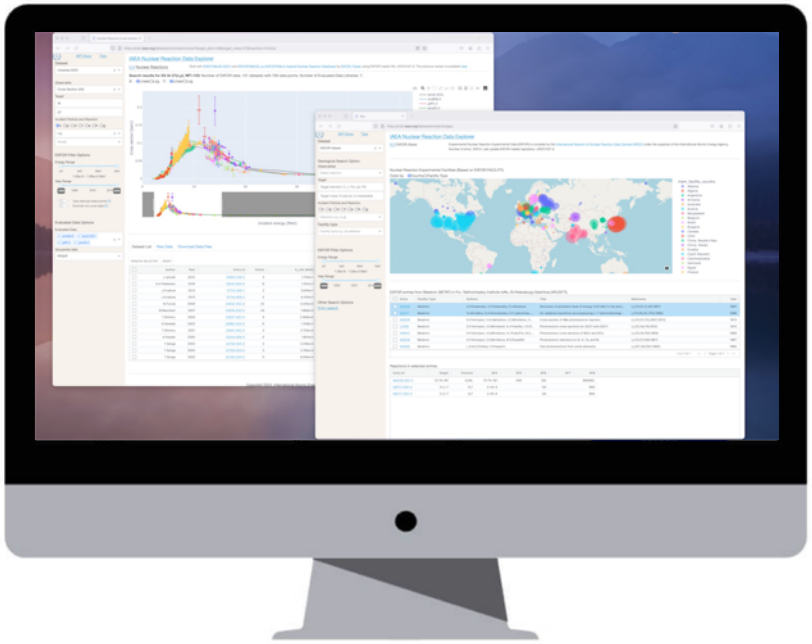
Livechart Data Download API

- Easy and direct computational access
- Downloadable in CSV

Modernization efforts: Nuclear Reaction Dataexplorer

https://nds.iaea.org/dataexplorer

Python 3 based, open source project



Reaction based data plotter

- Input target and reaction to get evaluated and experimental datasets
  - Cross section
  - Thermal neutron cross section
  - Residual production cross section
  - Fission yield

New!

EXFOR entry viewer

- Easy access without understanding of EXFOR format
  - Search by reactions
  - Entry viewer
  - Geographical analysis

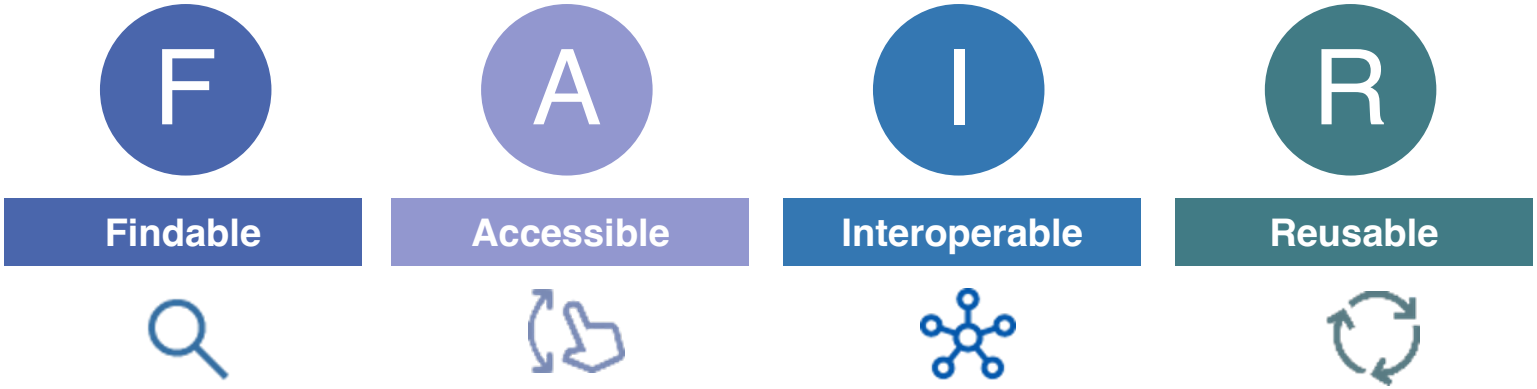
New!

RESTful APIs

- Easy computational access
  - Reaction, EXFOR entry and definition of EXFOR keywords, RIPL-3 levels

FAIR Principles

- The IAEA Nuclear Data Section aims to make nuclear data coming from research (experimental, evaluated, and theoretical) transparent and more robust by enabling users to re-use the data, following the idea of FAIR Principles.



- Adhering to the FAIR Data Principles helps ensure nuclear data:
  - Supports next-generation research in this field
  - Works well with machine learning (ML) and artificial intelligence (AI) models
  - Remains orderly and accessible at all levels of users
  - Supports data mining on prior works, saving time and resources

What should be in Nuclear Data Lake/Data Portal?

Existing nuclear data

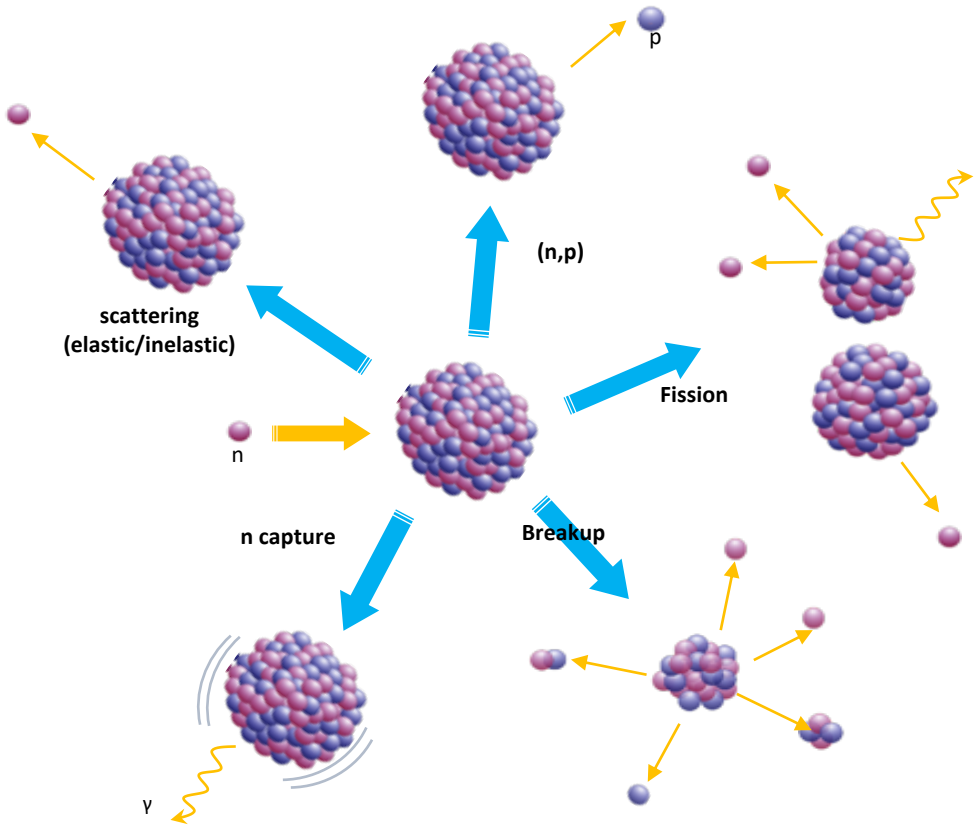
- Historical evaluated nuclear data libraries
  - Metadata and data tables converted from ENDF-6 format
- Experimental nuclear reaction data
  - Metadata and data tables converted from EXFOR entries
- Other evaluated data:
  - EGAF, RIPL-3, IBANDL, thermal neutron observables, resonance parameters, etc.

New data collections

- Theoretical Nuclear Reaction Data
  - Numerical data from theoretical studies related to scientific publications
  - Preliminary evaluation
- Users' collections
  - Users' suggestion of the correction/normalization onto experimental data
  - Users' collection
  - Users' new submission of preliminary data

- First target
  - Storing all physical quantities from the beginning is challenging
  - Start e.g. with cross-sections and fission yields

Data model



In Nuclear Physics (experiments and theories)…

Reaction cross sections
- Cumulative: total, elastic, non-elastic
- Exclusive: (n,n'), (n,2n), (n,g), (n,f), n,p),….
- Discrete level: (n,n'_1), (n,n'_2),…(n,p_0),….
- Particle production: (n,xn), (n,xp),….
- Residual production: (n,x), (p,x),….
- Resonance parameters

Angular distributions
- Elastic
- Inelastic

Single-differential emission spectra (energy)

Double-differential emission spectra (energy-angle)

Gamma-ray production cross sections

Fission yields

Fission neutron observables (average number of neutrons per fission, kinetic energy, etc.)

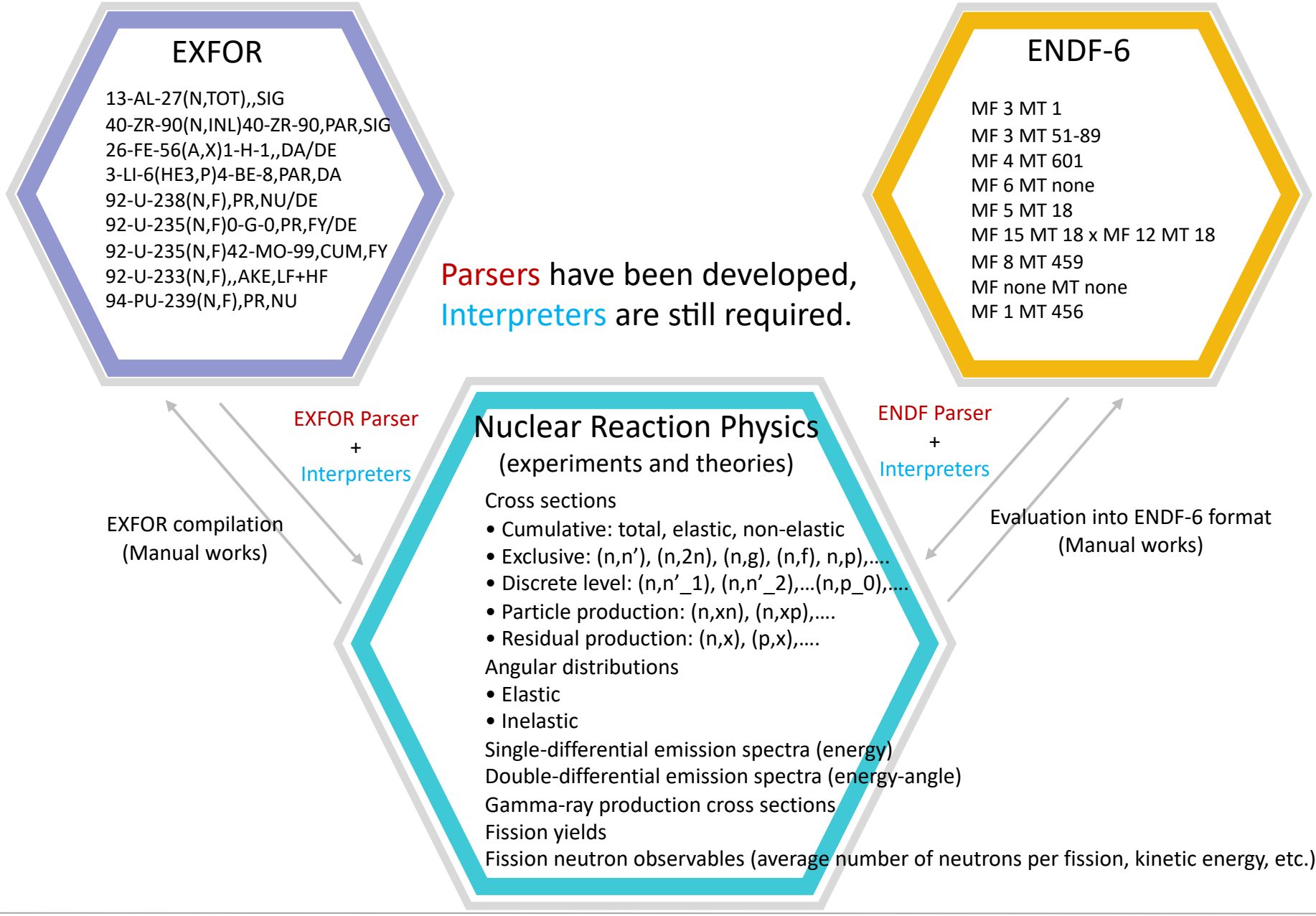
Decay
- Half-life
- Branching ratio
- Spectra

Nuclear property
- Nuclear mass
- Discrete levels, level densities

Robust and comprehensive data model development is essential.

- Metadata
- Different x-y definitions
- Not x-y data type

Nuclear reaction data in different forms



More unification?

- Metadata format
  - The DataCite Metadata Schema

Mandatory	Recommended	Optional
Identifier	Subject	Language
Creator	Contributor	Alternate ID
Title	Date	Size
Publisher	Resource Type	Format
Publication year	Related identifier	Version
	Description	Rights
	GeoLocation	

- Other data sources
  - Institutes
    - Research Organization Registry (ROR)
    - IAEA resources (Accelerator/Research reactor databases)
  - Journals, Proceedings, Books
    - ISSN/ISBN
    - DOI
    - INIS
  - Authors
    - ORCID
    - ResearcherID (Web of Science)
  - Data Unit
    - SI Unit
  - Subjects (data categories)
  - Resource Types

Current example of EXFOR dictionary

Institutes

```
1USABNL    (Brookhaven National Laboratory, Upton, NY)          9000100300071
1USABNW    (Pacific Northwest Laboratories, Richland, WA)       9000100300072
           =(previously Battelle Northwest).                    9000100300073
            Previously 1USAHAN. Compare 1USAHED                 9000100300074
```

Journals

```
PR/C       (Physical Review, Part C, Nuclear Physics)       1USA9000100500995
           vol.1 (1970) -                                       9000100500996
PR/D       (Physical Review, Part D, Particles and Fields)  1USA9000100500997
           vol.1 (1970) -                                       9000100500998
PRE        (Proceedings of the Royal Society Edinburgh)     2UK 9000100500999
```

Units

```
1/SR       per steradian                 1/A      1.E+09000102500189
B          barns                         B        1.E+09000102500190
KB         kilobarns                     B        1.E+39000102500192
MB         millibarns                    B        1.E-39000102500193
MICRO-B    microbarns                    B        1.E-69000102500194
NB         nanobarns                     B        1.E-99000102500195
```

Data model should be unified and self-explanatory

Topics covered in the meeting

- Nuclear Data Processing Tools and Code
  - Processing codes, tools, and parsers
- Web Interfaces and APIs: developments and operations
  - NNDC Portal from BNL
  - JANIS from OECD/NEA
  - Live Chart of Nuclide from IAEA/NDS
  - Dataexplorer from IAEA/NDS
- Nuclear Data Flow/Pipeline
  - Evaluated nuclear data library data flow (e.g. ENDF-B and JEFF)
  - EXFOR data compilation workflow (OECD/NEA modernization efforts)
  - Inter-exchangeable and interoperable APIs
  - Interpretations (e.g. relating EXFOR reaction codes and ENDF MT/MF to nuclear physics)
- Data Model and Data Format
  - Universal metadata
    - Tabulated, self-explanatory, ready-to-use data
  - Re-design of existing nuclear data formats
    - Generalized Nuclear Data Structure (GNDS)
    - Evaluated Nuclear Structure Data File (ENSDF) in JSON
    - Conversion of experimental nuclear reaction data (EXFOR) into JSON
  - New demands
    - Muon nuclear data (M. Niikura et al., arXiv:2403.19965)
  - Robust data model for nuclear data (primarily nuclear reaction data)
- Study from Other Fields, Users' Feedbacks and New Demands
  - Atomic and molecular data and databases from IAEA/NDS
  - High energy physics (HEPdata)
  - IAEA Data Strategy from IAEA/MTIT

Expected functions of Nuclear Data Portal (to be discussed)

- Backend
  - Pre-processing / online-processing of data
  - Handling of GNDS
  - ENDF-6 formatted data in JSON or tabulated format
  - EXFOR entries in JSON or tabulated format
  - Data flow and data strage
- Easy access to the data
  - Data model
  - (Meta)data are indexed in a searchable resource (nonSQL or SQL)
  - Enables the discovery and reuse of historical nuclear data by humans and machines
  - DOI or similar persistent URL assignment (preferably..)
  - Online plotting interface
  - Data download options with well described metadata
  - Interoperable (data retrievable) APIs between nuclear data centers
  - REST APIs endpoints for users
- User submission
  - User management in web appllications (auth by IAEA NUCLEUS?)

:

etc..

Expected outcomes (to be discussed)

- Collection of useful tools
  - Data processing, reformatting, plotting, visualizing, and storing
- Collection of use cases
  - Requests from users to developers
  - Existing AI/ML applications
  - New data idea and proposals
- Recommendations
  - Ideas for the data model blueprint
    - Idea of creating a representation of the data structures, relationships, constains
  - Ideas for user participatory model
  - Ideas for data intepretations (e.g. relating EXFOR reaction codes and ENDF MT/MF to nuclear physics)
  - Conceptual data models
- Priorities
  - Forcussing on nuclear reaction cross sections first, then?

:

etc..

Questions to be addressed

Do we understand how different types of users (e.g. researchers, students, evaluators) want to use nuclear data for their purposes?

Would the nuclear data community be willing to contribute to data collection or submission efforts?
Will it result in a rapid distribution and sharing of data?

Can (almost) all nuclear reaction data be standardized to eventually develop a Data Portal similar to those in other fields of data science?

Christmas markets in Vienna

Vienna Christmas Markets Opening Dates

- Franz-Jonas-Platz: Nov 7 - Dec 24
- Stephansplatz: Nov 8 - Dec 26
- Schönbrunn Palace: Nov 8 - Dec 24
- Maria-Theresien-Platz: Nov 13 - Dec 26
- Rathausplatz: Nov 15 - Dec 26
- Am Hof: Nov 15 - Dec 23
- Freyung: Nov 15 - Dec 23
- Karlsplatz Art Advent: Nov 15 - Dec 23
- Belvedere: Nov 15 - Dec 26
- Spittelberg: Nov 16 - Dec 23
- Prater Winter Market: Nov 16 - Jan 6, 2025
- Campus University: Nov 15 - Dec 23

Thank you for your cooperation!

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