IAEA
International Atomic Energy Agency
Atoms for Peace and Development

Concept for new database

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The Database Needs

The use of advanced machine learning algorithms or data mining in science is ongoing and thriving in many fields:

- Improving the throughput of experimentation
  Innovation: materials, chemical substance, and drug discovery
  Automation: automatically processable, analysable, exploitable, amenable to data mining
  Prediction: predict properties without experiments

  } worldwide

- Improving the throughput of nuclear data evaluation processes
  Innovation: unearth efficient reactions
  Automation: machine-readable format
  Prediction: model development based on nuclear physics curated experimental information

  } SG50

Unified, may be not unique, machine-readable format is strongly desired.

Other Experimental Databases; EXFOR is not the only one

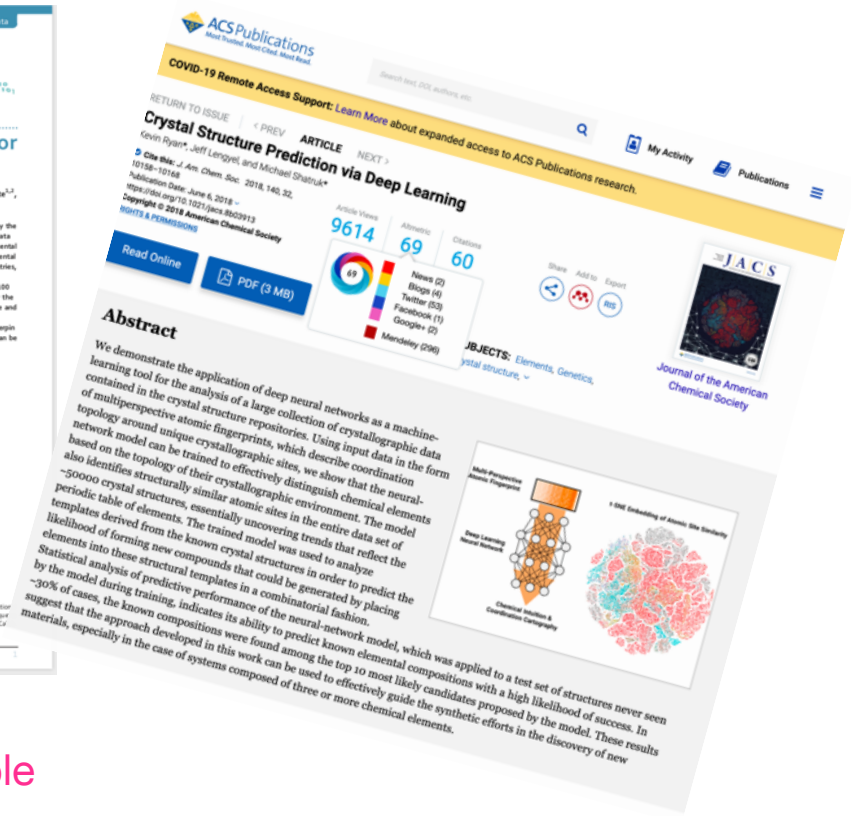
Database	Established	Number of records	User submission	Web retrival	API
Repository for publication-related High-Energy Physics data (HepData Project) https://www.hepdata.net/	(past four decades)	86,816 data tables	Yes	Yes	No
High Throughput Experimental Materials (HTEM) Database https://htem.nrel.gov/	Collected over seven years	140,000 samples	Yes (YAML format)	Yes	Yes (JSON)
Worldwide Protein Data Bank http://www.wwpdb.org/	1971	177,212 structures (2000-)	Yes	Yes	No (rsync, ftp)
The Cambridge Structural Database (CSD) https://www.ccdc.cam.ac.uk/structures/	1965	1,086,719 structures	Yes (CIF format)	Yes Limited to members	No

and more..

- Journal publishers encouraged author(s) to submit the experimental (numerical) data before manuscript submission.
- User (experimentalist) can submit the data by themselves using the unified format.
- Such unified formats can be directly used in many applications.

Machine Learning and Experimental Database

- Many attempts…e.g.
  - How to represent crystal structures for machine learning: Towards fast prediction of electronic properties [1]
  - Crystal Structure Prediction via Deep Learning [2]
  - An open experimental database for exploring inorganic materials [3]

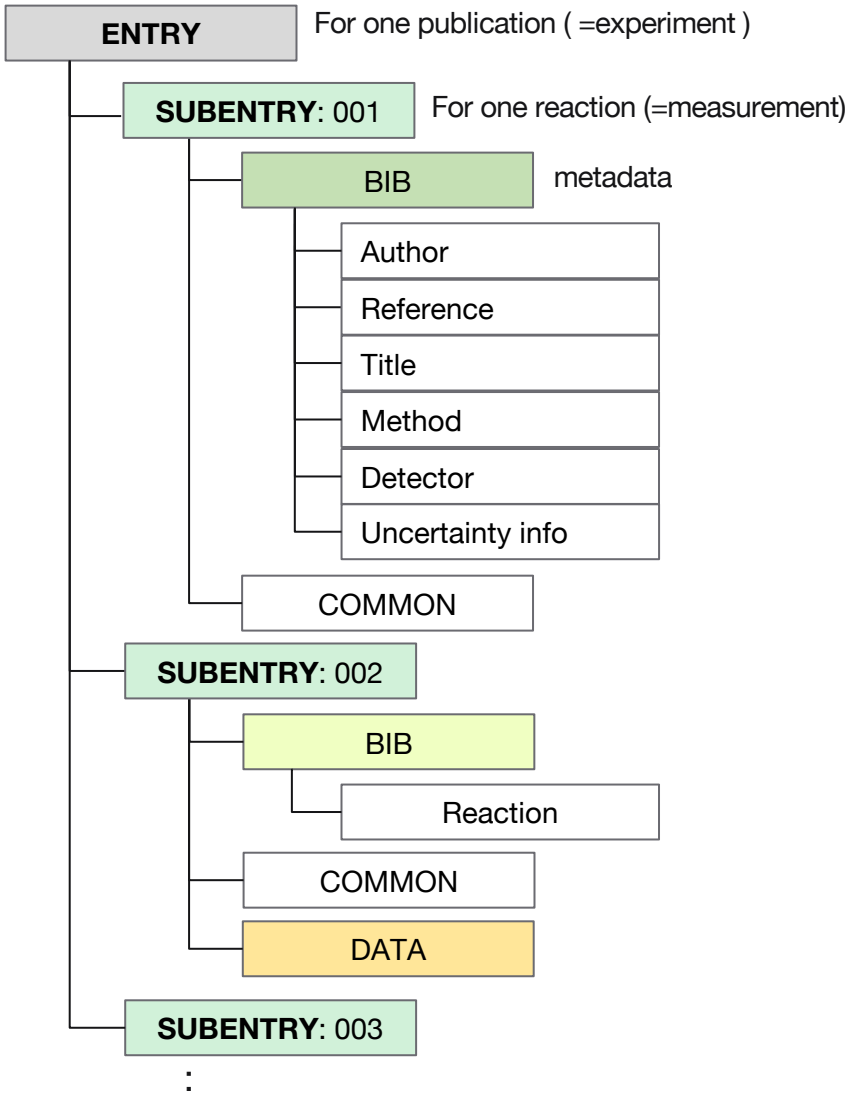


- A large data set with a unified and machine-readable data format has a good compatibility to machine learning.
- The EXFOR database covers much diverse data.

[1] K. T. Schütt, et al., Phys. Rev. B 89, 205118 (2014).
[2] K. Ryan et al., *J. Am. Chem. Soc.*, 140, 32, 10158–10168 (2018).
[3] A. Zakutayev et al., Scientific Data, 5, 180053 (2018).

EXFOR is the EXchange FORmat

```
ENTRY          13388      891220              20050926        0000
SUBENT      13388001      891220              20050926        0000
BIB                9          11
INSTITUTE  (1USALAS)
REFERENCE  (J,PR,99,730,5508)
AUTHOR     (A.C.WAHL)
TITLE      FISSION OF U-235 BY 14-MEV NEUTRONS: NUCLEAR CHARGE
            DISTRIBUTIONS AND YIELD FINE STRUCTURE
METHOD     (RCHEM)
DETECTOR   (PROPC)
ERR-ANALYS (DATA-ERR) STANDARD 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-235(N,F)42-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
```



To use DATA in subentry:001, it needs to read metadata from many places.

Fluctuations in EXFOR

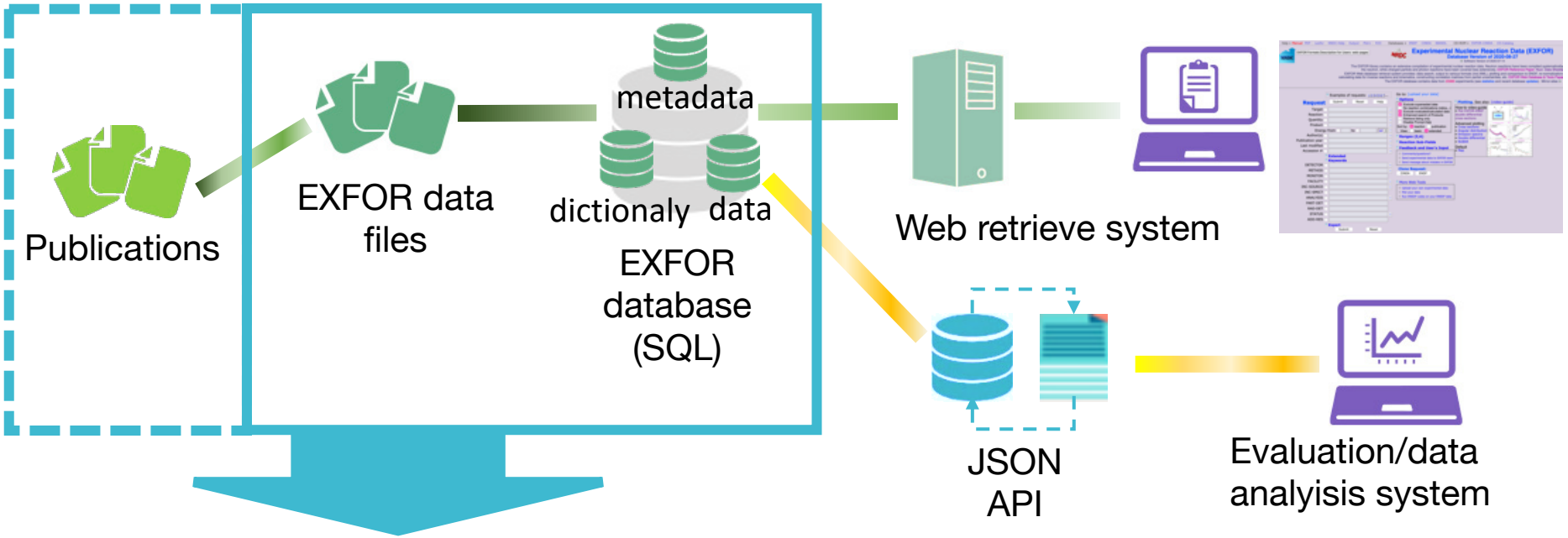
- Metadata
  - "Year" format in Reference

Case	Example	Number of data
Recommended format	J,YK,1982,(2/46),9,1982	18,033
2 digit	J,JCP,17,653,49	1,673
4digit YYMM	J,PR/C,4,723,7109	2,656
6digit not YYYYMM	J,NP/A,329,1,141,791008	56
6digit with YYYYMM	J,NSE,66,24,197804	5,798

  - Author's name
    - Augustyniak --- Augustynyak
    - Brinkmoeller --- Brinkmoller
  - Incompleteness of information as a database
    - One of the redundant information (PART-DET (G) and DETECTOR (HPGE)) are deleted during compilation.
  - Much free text
- Data
  - Uncertainty information in ERR-* fields
    - ERR-1 -- ERR-10 not always the same meaning or interpretation
  - Based on the old standards, decay data,..etc

- Some of these fluctuations are "**absorbed**" by IAEA's SQL & web retrieval system.
- However, more automatically processable and analysable format (scheme) is required.

Three Layers of Database



Layer 1

- Build the database from automatically readable format → Candidate for a novel EXFOR format

Layer 2

- Adopt objective and subjective corrections: updating standards, flagging outliers..etc

Layer 3

- Curated evaluation database

Summary

- The use of advanced machine learning algorithms require the unified and curated data.

- EXFOR, EXchange FORmat, is sufficient for compilation and data exchange but not at the level of automated use by a machine learning system or evaluation system. Such machine readability would be useful for improving the throughput of nuclear data evaluation processes.

- Layer 1 database may be implemented from the current EXFOR system which is assisted by SQL database and even by the information from original publisher or PDF.

- Layer 1 data format (scheme) would be useful for the idea of the next EXchange FORmat as well.

Thank you for your attention!

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