

X5 - Enriched EXFOR in JSON

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~ independent software developer ~

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Part I.

Introduction. Purpose. Concept.

Before any development

Steps to go.

1. Understand/formulate problem and possibly task(s)
2. Three questions to answer:
 - a) What already exists and can be used?
 - b) What is wrong now?
 - c) What do we want to achieve? (define ideal goal)
3. Preparations:
 - a) discuss/define main ideas, concept and possible technologies
 - b) study and test technologies, select technology
4. Plan: split problem to tasks/sub-tasks, define dates
5. Implementation: development loop

Problem and tasks

NRDC: exchange experimental data. Forms and methods of data distribution are not regulated by NRDC (no wide/deep cooperation).

1. Task: to provide EXFOR data in computational form to make available entire library in uniformed way
 - existing systems: XC4, C5, relational-DB: X4App/X4Lite/X4Pro/JANIS
2. Task: to make accessible **full power** of EXFOR hidden in meta data via providing information from EXFOR Dictionaries allowing various computations
 - existing systems: EXFOR + Dictionaries + Manual (needs a lot of expertise and programming)
3. Task: to provide related to EXFOR nuclear data: old monitor data and new standards, RIPL and decay data from ENSDF allowing data modernization and various data transformations
 - existing systems: EXFOR + Manual + RIPL + ENSDF + Literature (needs a lot of expertise and programming)
4. Task: to provide all above in a form convenient for programming in modern languages for the new generation new technologies (e.g. ML)
 - existing systems: **partially** solved in X4Pro and XML output from Web/X4Lite

What already exists and can be used?

What is wrong now?

1. NDS Web database retrieval system providing data search, retrievals, plotting, comparison with evaluated data, data presentation in various forms, methods and formats: X4+, X4±, C4, C5, C5M, two JSON's, two XML's, StdOut, CompOut
2. Web data archives with full EXFOR in XC4, C5, EXFOR, Dictionaries: download from dedicated servers and GitHub
3. Standalone retrieval systems including (relational) databases: “EXFOR for Applications”, X4Lite, X4Pro (NDS), JANIS (NEA)

1. Data provided by pieces in systems and data listed above, partially covering many tasks/needs but not consolidated: for example, (a) XML presents all keywords and information from Dictionaries, but not from external monitor files, RIPL and relevant ENSDF decay data, (b) C5 presents renormalized computational uniformed data, but no information from all keywords/codes, (c) EXFOR-Relational DB/X4Apps/X4Lite contain all keywords/codes in Tables, but also no external monitors and standards, and ENSDF decay data
2. A lot of needed data and information already generated and provided, and simply need to be consolidated in proper way in most popular form nowadays – JSON for building systems on new technologies suitable and familiar to new generation of users and new tasks (Python, R, NoSQL, ML).

What is X5json design?

1. X5json file includes
 - A. Part-I. Original EXFOR: ENTRY → SUBENT → (BIB/KW/Codes), COMMON, DATA
 - 1) structured meta-data (keywords/codes/free text) with dictionary-information
 - + REACTION: split to Strings and further to SF1..SF9 with dictionary-info
 - + REFERENCE: interpreted parameters (volume, report number, page, etc.)
 - + COVARIANCE: data extracted from free-text to arrays
 - 2) original EXFOR data from COMMON and DATA sections: 2-D array
 - + Header and Units given with interpretation and classification (form dictionaries)
 - B. Part-II. Computational data: SUBENT → Datasets: <Subent+Pointer>
 - 1) computational EXFOR data values: 1-D arrays in (a) original and (b) basic units
 - + only data relevant to Dataset (Pointer=' ' or Pointer=Dataset.Pointer)
 - + sorted and classified according to dictionaries
 - 2) computational data ~C5: {y, Δy, Δy_{stat}, Δy_{sys}, x1, Δx1, x2, Δx2, etc.}
 - 3) MF, MT for data compatible with ENDF evaluated data
 - 4) data for renormalization: monitor cross sections and standards
 - 5) decay data for renormalization from ENSDF
2. X5json distributed within X4Pro, generated online on ENFOR Web retrieval system
3. Full EXFOR translated to X5json is available on GitHub by Entries; it includes also Python scripts creating data indices, import data to “pandas”, and producing plots with and without renormalization (compared with data from full EXFOR in C5)

Part II.

X5json. Structure. Data presentation.

X5json structure

```

X5json {7}
├── format: x5json.0.1.4
├── now: 2024-01-29T10:17:34.782Z
├── program: exfor2x5z, by V.Zerkin, IAEA-NDS, 2019-2023, ver.2023-08-28
├── input {1}
├── output {1}
├── x4dbVersion: 2023-11-18
├── x4entries {3}

```

1

```

x4entries {3}
├── x4entries[0] {11} Entry:10828:20171126 1978,T.C.Chapman+
├── x4entries[1] {11} Entry:13597:20140415 1995,S.K.Ghorai+
├── x4entries[2] {12} Entry:23114:20170322 2010,C.Sage+

```

2

```

x4entries[2] {12} Entry:23114:20170322 2010,C.Sage+
├── ENTRY: 23114
├── updated: 20170322
├── x4dbVersion: 2023-11-18
├── TransID: 2258
├── TransDate: 20170512
├── y1: 2010
├── a1: C.Sage+
├── r1: J,PR/C,81,064604,2010
├── doi: 10.1103/PhysRevC.81.064604
├── ref: Jour: Physical Review, Part C, Nuclear Physics
├── title: High resolution measurements of the 241Am(
├── x4subents {2}
├── x4subents[0] {7} Subent:23114001
├── x4subents[1] {10} Subent:23114002

```

3

```

x4subents[1] {10} Subent:23114002
├── SUBENT: 23114002
├── isub: 2
├── compiled: 20130924
├── TransID: 2236
├── TransDate: 20140110
├── x4dbVersion: 2023-11-18
├── BIB {10} Bibliographic and descriptive information
├── COMMON {5} Common data
├── DATA {5} Data section
├── datasets {1} Datasets

```

4

```

BIB {10} Bibliographic and descriptive information
├── REACTION [1] Quantity given
├── DECAY-DATA [1] Decay data
├── REL-REF [6] Related reference
├── CORRECTION [1] Corrections
├── MISC-COL [4] Miscellaneous columns
├── ADD-RES [1] Additional results
├── ERR-ANALYS [10] Error analysis
├── COVARIANCE [1] Covariance
├── STATUS [1] Status
├── HISTORY [1] History of Entry/Subentry
├── COMMON {5} Common data
├── DATA {5} Data section
├── datasets [1] Datasets

```

5

```

DATA {5} Data section
├── ncols: 13
├── nrows: 9
├── x4headers {13}
├── datacols {3} Headers, Units, Pointers
├── data {9}

```

5

```

x4headers {13}
├── x4headers[0] {10} EN(MEV)
├── x4headers[1] {10} EN-ERR(MEV)
├── x4headers[2] {10} DATA(MB)
├── x4headers[3] {10} ERR-1(PER-CENT)
├── x4headers[4] {10} MONIT-ERR(PER-CENT)
├── x4headers[5] {10} ERR-1(PER-CENT)
├── x4headers[6] {10} ERR-2(PER-CENT)

```

6

```

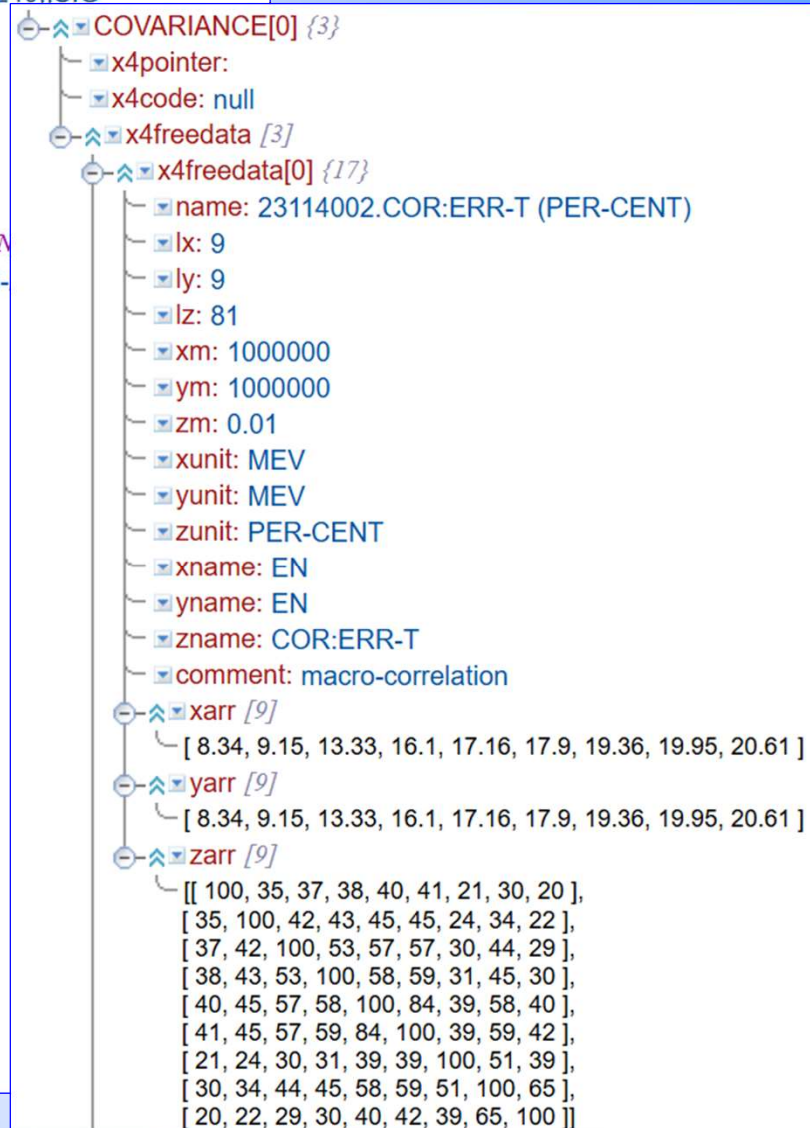
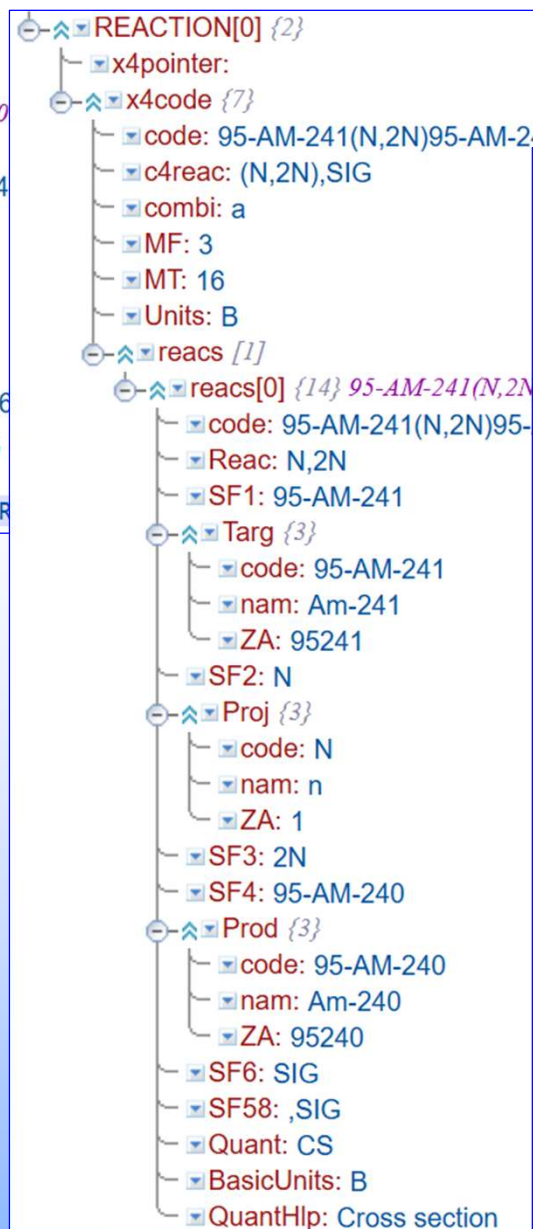
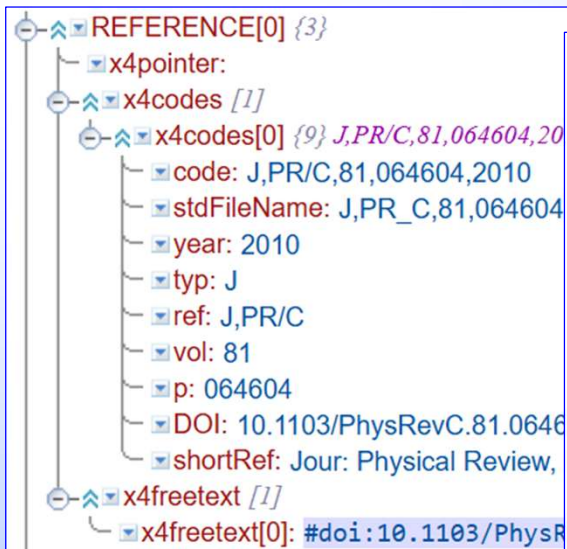
data {9}
[[ 8.34, 0.15, 96.8, 6.5, 1.9, 5, 1, 0.9, null, 0.9974, 0.9925, 1, 1 ],
[ 9.15, 0.15, 162.9, 5.7, 1.9, 4, 1, 0.6, null, 1.0731, 1.3117, 1, 1 ],
[ 13.33, 0.15, 241.8, 4.6, 1.6, 2.5, 1, 0.4, 0.3, 0.9168, 0.8288, 1, 1 ],
[ 16.1, 0.15, 152.4, 4.6, 2, 2.1, 1, 0.6, 0.3, 1.0749, 1.2335, 1, 1 ],
[ 17.16, 0.03, 116.1, 4.4, 2, 1.5, 1, 0.6, 0.3, 0.9987, 0.9878, 0.998, 0.997 ],
[ 17.9, 0.1, 105.7, 4.4, 2.2, 1.3, 0.7, 0.7, 0.3, 0.969, 0.933, 0.998, 0.997 ],
[ 19.36, 0.15, 89.5, 8.2, 3.1, 6.3, 2, 0.6, 1.3, 1.0061, 1.0157, 0.941, 0.926 ],
[ 19.95, 0.07, 102.1, 5.8, 4.1, 1.4, 1, 0.6, 1.4, 0.9822, 0.9433, 0.922, 0.891 ],
[ 20.61, 0.04, 77.9, 8.8, 5.4, 5.7, 1.6, 0.6, 1.4, 0.9938, 0.982, 0.885, 0.832 ]]

```

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X5json hierarchy reproduces structure of an EXFOR file with extensions for ease processing.
 Part-1: exactly EXFOR + information from Dictionaries
 Part-2: Datasets for computational purposes

Part-1. REFERENCE, REACTION, COVARIANCE



Part-2. Dataset: <Subent, Pointer>

```

- datasets [1] Datasets
  - datasets[0] {31} Dataset: 23114002
    - iDataset: 0
    - DatasetID: 23114002
    - Pointer:
    - Subent: 23114002
    - compiled: 20130924
    - x4dbVersion: 2023-11-18
    - year1: 2010
    - author1ini: C.
    - author1: Sage
    - zTarg1: 95
    - targ1: Am-241
    - proj1: n
    - emis1: 2N
    - MF: 3
    - MT: 16
    - nExpectedArgs: 1
    - IndepVarFamilyCode: 0 2
    - getYFormulaStr: y=DATA(EN)
    - ReactionType: CS
    - quant: CS
    - quantExpan: Cross section
    - reacode: 95-AM-241(N,2N)95-AM-240,,SIG
    + compNotes []
    + autoCorrNotes [10]
      - wx4data: 17
      - lx4data: 9
    + x4data [17]
      - wc5data: 2
      - lc5data: 9
    + c5data {2}
    + c5mon {8}
  
```

```

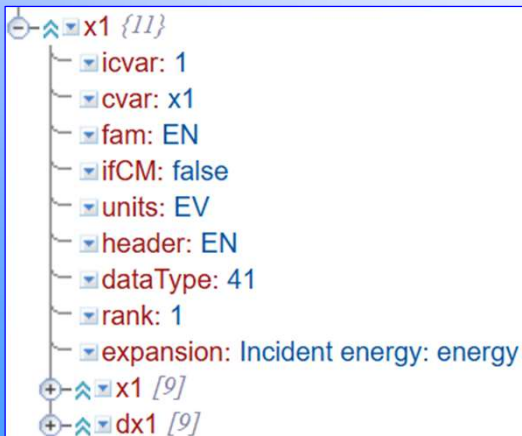
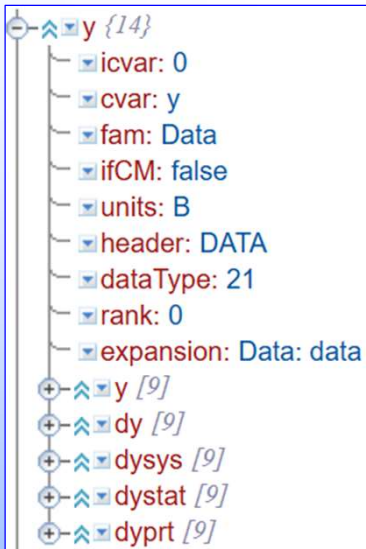
- x4data [17]
  + x4data[0] {14} DATA(MB)
  + x4data[1] {14} ERR-1(PER-CENT)
  + x4data[2] {14} ERR-1(PER-CENT)
  + x4data[3] {14} ERR-2(PER-CENT)
  + x4data[4] {14} ERR-4(PER-CENT)
  + x4data[5] {14} ERR-8(PER-CENT)
  + x4data[6] {14} ERR-3(PER-CENT)
  + x4data[7] {14} ERR-6(PER-CENT)
  + x4data[8] {14} ERR-7(PER-CENT)
  + x4data[9] {14} ERR-5(PER-CENT)
  + x4data[10] {14} MONIT-ERR(PER-CENT)
  + x4data[11] {14} EN(MEV)
  + x4data[12] {14} EN-ERR(MEV)
  + x4data[13] {14} MISC1(NO-DIM)
  + x4data[14] {14} MISC2(NO-DIM)
  + x4data[15] {14} MISC3(NO-DIM)
  + x4data[16] {14} MISC4(NO-DIM)
  
```

“dataset[]”: Dataset information
 + Bib-info
 + info from Dictionaries
 + MF.MT
 “x4data“: data from DATA and
 COMMON relevant to the
 Dataset by columns.
 Data columns are sorted.
 Data are presented in 1-D array:
 “dat0” – in original units,
 “dat1” – in basic units

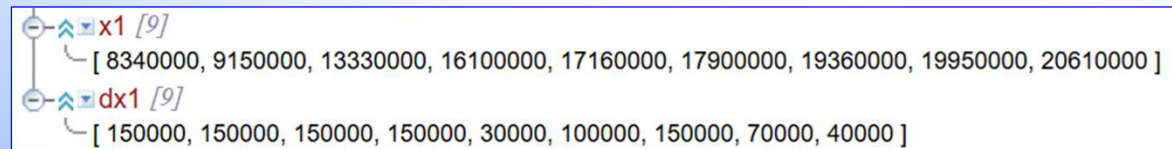
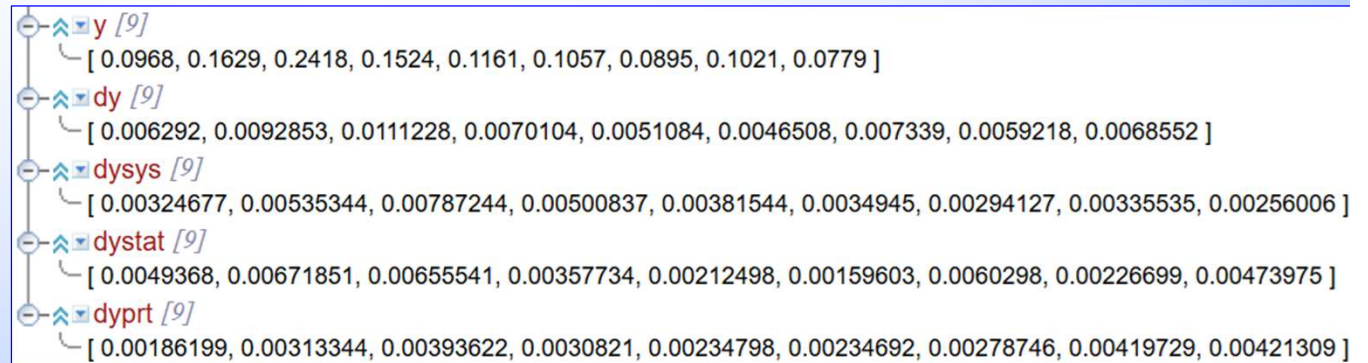
```

- x4data[0] {14} DATA(MB)
  - ivar: 0
  - cvar: y
  - fam: Data
  - ifComm: false
  - ifCM: false
  - header: DATA
  - units: MB
  - basicUnits: B
  - what: Y.Value
  - dataType: 21
  - rank: 0.1
  - expansion: Data: data
  - dat0 [9] Data in units MB
    [ 96.8, 162.9, 241.8, 152.4, 116.1, 105.7, 89.5, 102.1, 77.9 ]
  - dat1 [9] Computational data in basic units B
    [ 0.0968, 0.1629, 0.2418, 0.1524, 0.1161, 0.1057, 0.0895, 0.1021, 0.0779 ]
  
```

Part-2. Dataset: c5data



“c5data”: all values given in basic units (like in C5)
Number of independent variables (x1) is defined in
“nExpectedArgs” of dataset[0]
“dysys”: generalized fully correlated uncertainties
“dystat”: generalized uncorrelated uncertainties
“dyprt”: generalized partially correlated uncertainties



Part-2. Data for automatic renormalization

```

datasets[0] {32} Dataset: 13597002
├── iDataset: 0
├── DatasetID: 13597002
├── Pointer:
├── Subent: 13597002
├── compiled: 19950217
├── x4dbVersion: 2023-11-18
├── year1: 1995
├── author1ini: S.K.
├── author1: Ghorai
├── zTarg1: 30
├── targ1: Zn-64
├── proj1: n
├── emis1: P
├── MF: 3
├── MT: 103
├── nExpectedArgs: 1
├── IndepVarFamilyCo
├── getYFormulaStr: y
├── ReactionType: CS
├── quant: CS
├── quantExpan: Cross
├── reacode: 30-ZN-64
├── compNotes [1]
├── DECAy-DATA {10}
├── autoCorrNotes [14]
├── wx4data: 6
├── lx4data: 4
├── x4data [6]
├── wc5data: 2
├── lc5data: 4
├── c5data {2}
├── c5mon {8}

```

“compNotes”: show whether Monit-Err recalculated
 “DECAy-DATA” present old and new decay data if any
 “autoCorrNotes”: show how corrections can be done
 “c5mon” present monitor data: normalization energy,
 “m0”, “dm0” – old monitor data and uncertainties
 “m1”, “dm1” – new monitor data
 “Fc0” – factor to be applied for data value

```

reacode: 30-ZN-64(N,P)29-CU-64,,SIG
├── compNotes [1]
│   └── compNotes[0]: RECALCULATED COLUMN:MONIT-ERR,B TO:PER-CENT:L=4
├── DECAy-DATA {10} Decay data
│   ├── Nuclide: 29-CU-64
│   ├── HalfLife: 12.7HR
│   ├── HalfLife1:
│   ├── RadiationType: AR
│   ├── Ene: 511
│   ├── Ene1: 511
│   ├── Abu: 0.386
│   ├── Abu1: 0.352
│   ├── FcCorrDECAy_DATA: 1.0965909
│   └── reaction: 30-ZN-64(N,P)29-CU-64,,SIG
├── autoCorrNotes [14]
│   ├── autoCorrNotes[0]: #[0]#---Monitor xs-data
│   ├── autoCorrNotes[1]: #[0]#Reaction: 30-ZN-64(N,P)29-CU-64,,SIG
│   ├── autoCorrNotes[2]: #[0]#Monitor: 13-AL-27(N,A)11-NA-24,,SIG
│   ├── autoCorrNotes[3]: m0: [EN,MONIT,MONIT-ERR]; #[0]#old monitor(energy)
│   ├── autoCorrNotes[4]: m1: recom$al27na; #[0]#new monitor(energy)
│   ├── autoCorrNotes[5]: dy=dy/y; #to rel. uncertainties
│   ├── autoCorrNotes[6]: y=y/m0*m1; #[0]#renormalizing CS
│   ├── autoCorrNotes[7]: dy=(dy**2-dm0**2+dm1**2)**0.5; #[0]#replace monitor uncertainties
│   ├── autoCorrNotes[8]: #[1]#---Reaction decay-data
│   ├── autoCorrNotes[9]: #[1]#REACTION (30-ZN-64(N,P)29-CU-64,,SIG)
│   ├── autoCorrNotes[10]: #[1]#DECAy-DATA (29-CU-64,12.7HR,AR,511.,0.386) #lx_old=0.386
│   ├── autoCorrNotes[11]: a1=0.386/0.352; #[1]#DECAy-DATA: correction to new 511 keV gamma-yield per decay Cu-64 lx_new=0.3!
│   ├── autoCorrNotes[12]: y=y*a1; #[1]#Renorm.factor: a1=1.0965909
│   └── autoCorrNotes[13]: dy=dy*y; #to abs. uncertainties

```

```

c5mon {8}
├── m0ref: [EN,MONIT,MONIT-ERR]/al27na
├── m1ref: recom/al27na
├── enNorm [4]
│   └── [ 14200000, 15200000, 16200000, 17200000 ]
├── m0 [4]
│   └── [ 0.122, 0.108, 0.09, 0.072 ]
├── m1 [4]
│   └── [ 0.11962, 0.105011, 0.089254, 0.0731812 ]
├── dm0 [4]
│   └── [ 0.00065, 0.00196, 0.00175, 0.00141 ]
├── dm1 [4]
│   └── [ 0.000527832, 0.000531218, 0.0006517, 0.000614784 ]
├── Fc0 [4]
│   └── [ 0.980492, 0.972325, 0.991711, 1.01641 ]

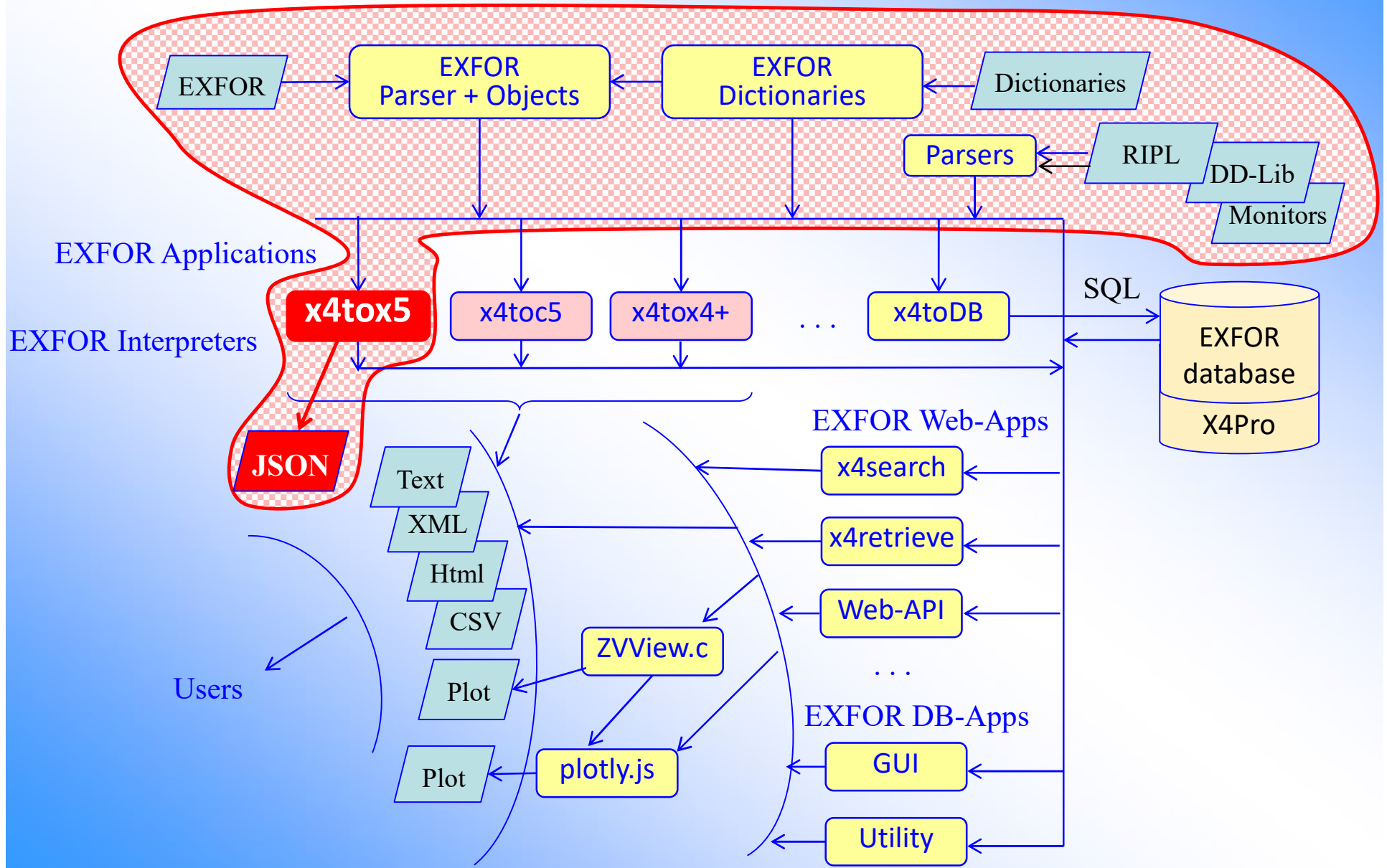
```

Part III.

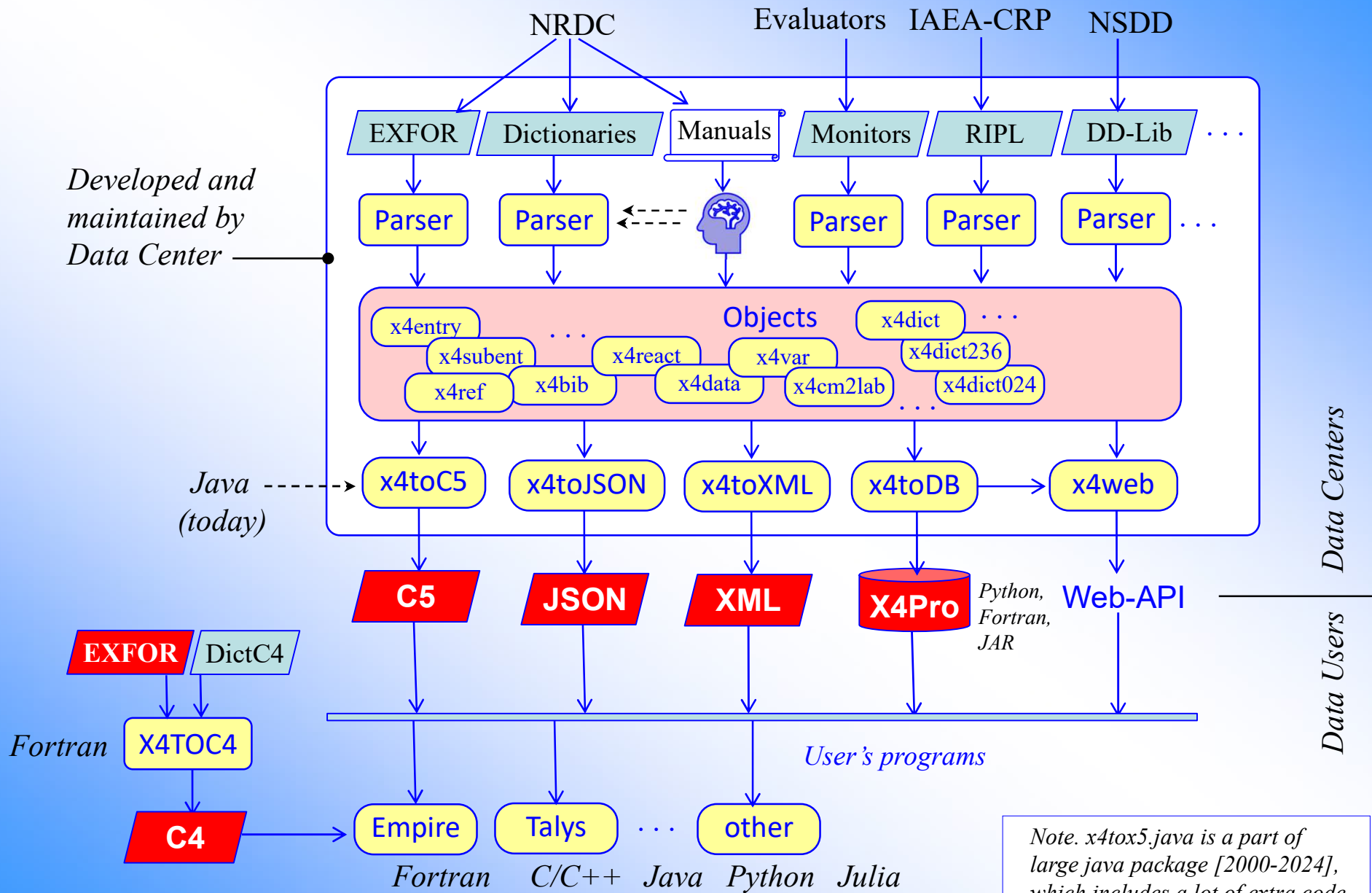
Data distribution paradigm.
System design.

X5json in EXFOR Java codes and data flows

Initially x4tox5.java was created as an extension of EXFOR database retrieval system to produce additional JSON output.



Paradigm of data distribution



Overview: EXFOR codes and systems

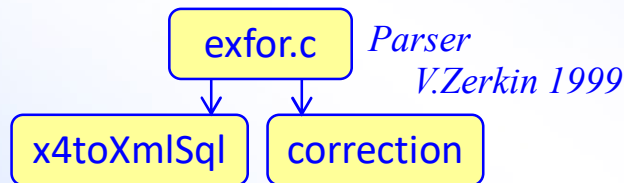
Fortran

Built-in parsers

1986 **X4TOC4** **ZCHEX** 1998

D.Cullen, A.Trkov, V.McLane, V.Zerkin

C



Java

JANIS

N.Soperra et.al. 2004

x4parsers/classes, x4toc5
/x4+/x5/xml/csv/web/db,... *V.Zerkin 2005-2024*

Python

x4i *GPLv2*

D.Brown 2011

x4i3 *GPLv2*

A.Fedynitch 2020

exfor-parserpy

G.Schnabel 2019

exforparser,
exfor_dict.,
exfor_json,...

S.Okumura 2022(?)

ForEX:
X4TOJ4,
J4TOX4,
DICA2J,...

N.Otsuka 2024

x4d, x4py,...

V.Zerkin 2024

Fortran, C, Java codes:

1. *Functioning many years (10~30)*
2. *Proven quality*
3. *Powerful (a lot of functionality)*
4. *Produce useful results already now*
5. *Needs intermediate step to deliver data to other languages (C5/XML/CSV/JSON/X4Pro/Web-API)*
6. *Large, need professional maintenance*

READY

Python codes:

1. *Can be used as is in Python codes (good for young generation using Python)*
2. *Easier to read and understand*
3. *Unknown quality (debug)*
4. *Needs JSON/XML/text to feed other languages*
5. *Require deep study of EXFOR, time and efforts to implement full functionality existing in Java*

NOT READY

Concluding remarks

1. X5 provides enriched EXFOR in JSON
 - 1) X5 gives comprehensive presentation of EXFOR content
 - 2) X5 structure reproduces data **hierarchy** of EXFOR file
 - 3) X5 presents **original data** values and data in **computational** form
 - 4) X5 includes interpretation of meta-data from EXFOR-Dictionaries
 - 5) X5 presents EXFOR data given as extension of free-text in coded way
 - 6) X5 is enriched by data from **external** data sources: monitor and standard cross sections data, decay data from ENSDF
 - 7) X5 allows to perform automatic data **renormalization** on monitor cross sections, decay and monitor-decay data
2. X5 is available via Web retrieval system (including **Web-API**). Full EXFOR translated to X5 is available on **GitHub** and on NDS download area
3. x4tox5 is implemented on **Java** as part of NDS EXFOR package

Thank you.