X4Lite2 and progress in EXFOR data automatic renormalization system

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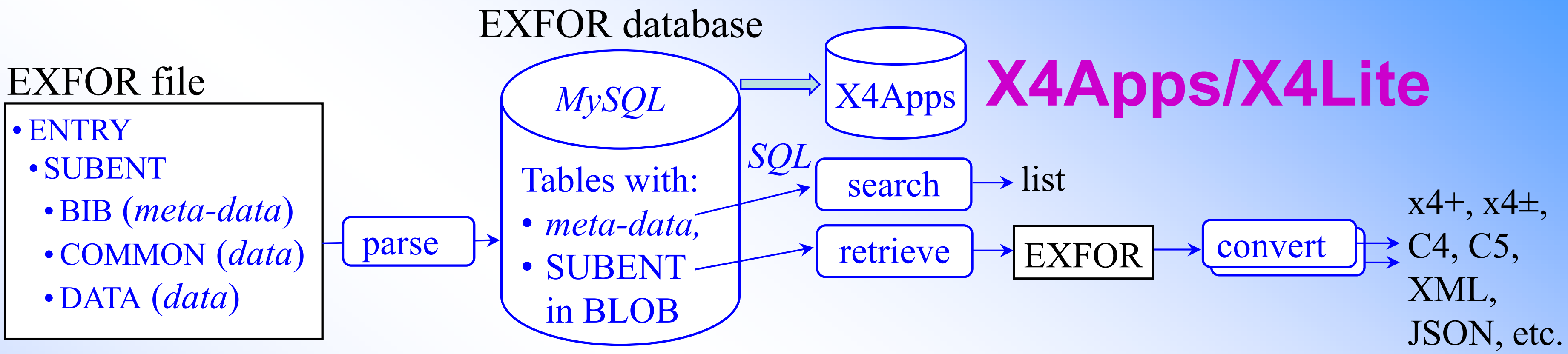
Concluding remarks

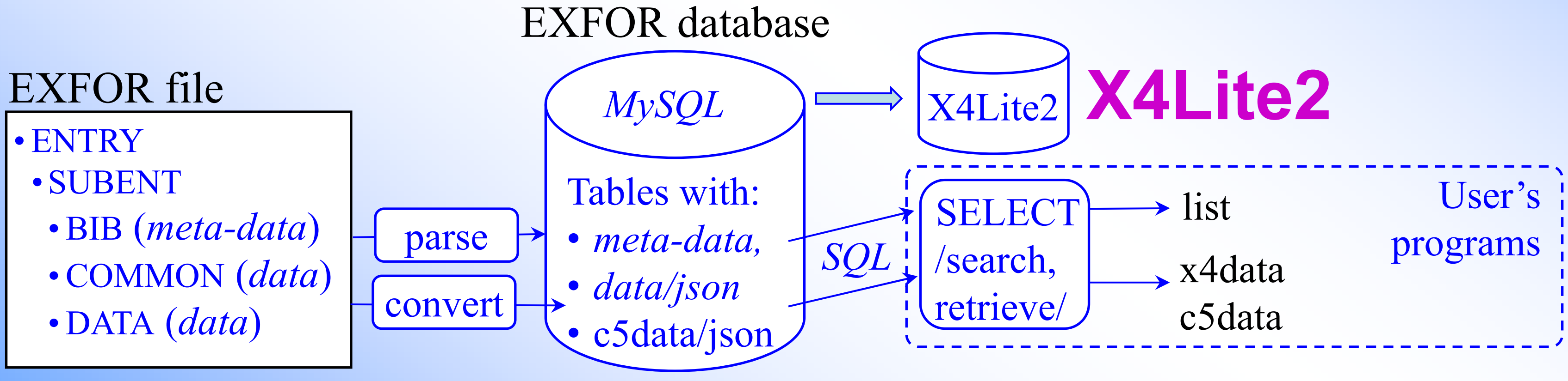
X4Lite2

1. Concept: relational database + data points in JSON fields
2. NDS-NNDC EXFOR relational database:
   1. extended by 3 tables describing datasets, headers and storing data points:
   2. original EXFOR data as they appear in DATA and COMMON sections
   3. computational data y, dy, x1, dx1, x2, dx2, etc.
   4. ported from MariaDB/MySQL to SQLite
3. Translation from MariaDB to SQLite is done automatically by a bash script working ~4 hours and producing a single 4Gb file x4sqlite1.db having 3 new tables:
   1. x4data_ds 177, 367 rows datasets
   2. x4data_hdr 1,424,906 rows header
   3. x4data_dat 18,853,364 rows data points (data columns: xdat json, cdat json)

1. Flexible solution: using single field to store one experimental data point as JSON object, e.g.: DatasetID:10045009, idat:83,
   original EXFOR data xdat:{"DATA":3.0, "DATA-ERR":10.0, "EN":2.13, "EN-RSL":0.055, "E":1465.0, "COS":0.0, "ANG-ERR":8.0, "E-NRM":846.8}
   computational data cdat:{"y":0.003, "dy":0.0003, "x1":2.13e+6, "dx1":27500.0, "x2":1.465e+6, "x3":90.0, "dx3":8.0}
2. Data from JSON field are accessible using json_extract function, and can be used also in WHERE and ORDER BY of SELECT command

X4Lite2 extension of EXFOR-relational





Main idea of X4Lite2

- No more BLOBs with zipped SUBENT - data in the databases are ready for use. Both original EXFOR data and computational data can be retrieved directly from database using only SQL commands.
- End-user does not need EXFOR converters.
- Can be used to build user's applications.

Retrieval code examples in Python #0

Connect to the database, execute SQL command

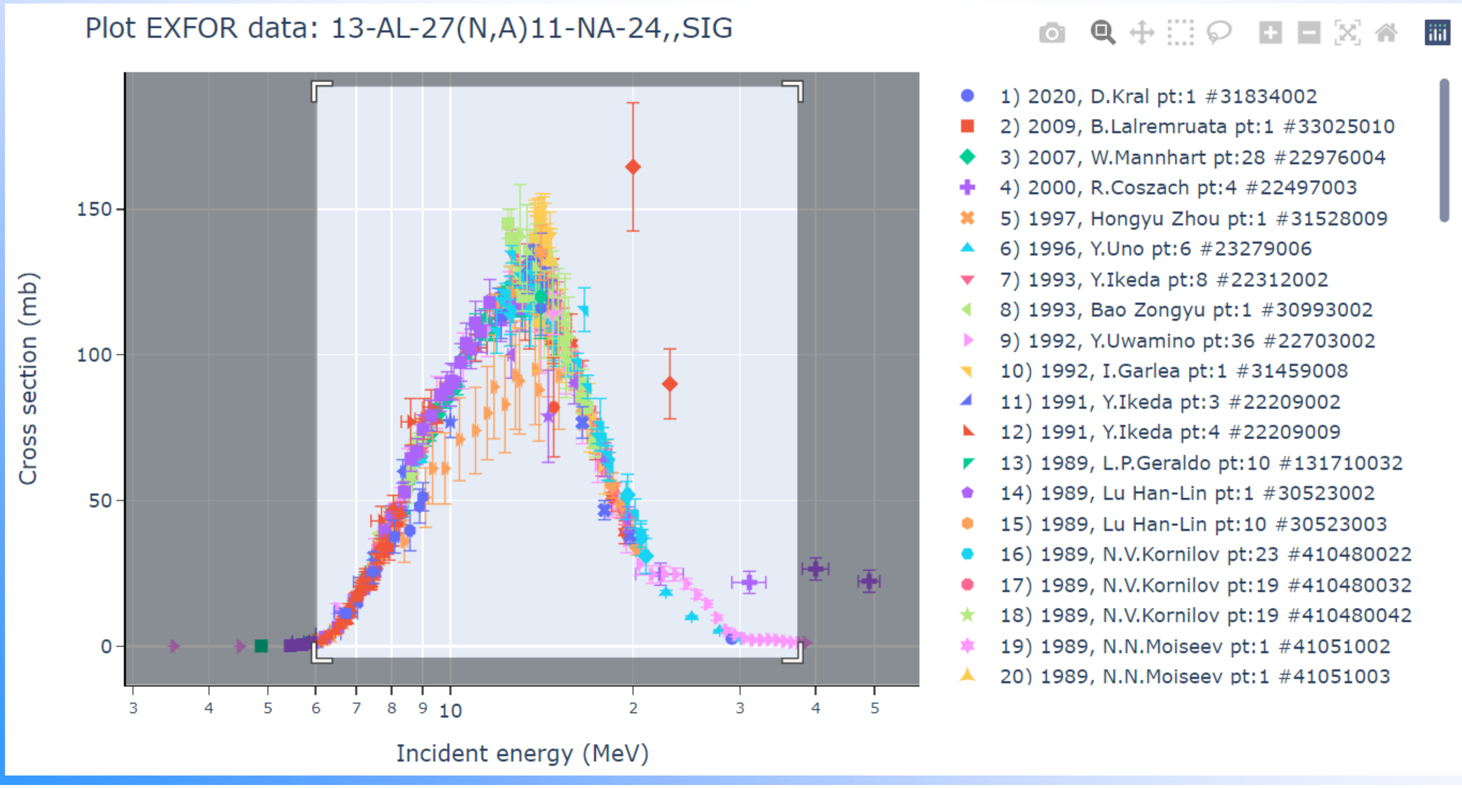
```python
import os
import sys
import sqlite3
print("---access SQLite database---")
x4db='x4sqlite1.db'
try:
    conn=sqlite3.connect('file:'+x4db+'?mode=ro',uri=True)
    conn.row_factory=sqlite3.Row
except sqlite3.Error as error:
    print("___0___sqlite3.connect.Error:\n",error)
    sys.exit(1)
cursor=conn.cursor()

sql="select Entry,YearRef1,Author1 from ENTRY where Entry like 'F%'"
try:
    rows=cursor.execute(sql)
except Exception as ex:
    print("___1___execute-SQL error: ", ex)
    rows=[]

ii=0
for row in rows:
    Entry=row['Entry']
    YearRef1=row[1]
    Author1=row[2]
    ii+=1
    print('\t'+str(ii)+') '+str(Entry)+' '+str(YearRef1)+' '+Author1)

conn.close()
```

Retrieval code examples in Python #1

Retrieve computational data from X4Lite2/MariaDB and plot using Plotly

Python:
- *code.py: 140 lines*
- *with SQL command*
- *calls interactive graphics plotly*

```
select x4data_dat.DatasetID,x4data_dat.idat as iPoint
 ,ENTRY.YearRef1,ENTRY.Author1Ini,ENTRY.Author1
 ,json_extract(x4data_dat.cdat,'$.x1')  as En
 ,json_extract(x4data_dat.cdat,'$.dx1') as dEn
 ,json_extract(x4data_dat.cdat,'$.y')   as Sig
 ,json_extract(x4data_dat.cdat,'$.dy')  as dSig
from x4data_dat
 inner join REACODE on REACODE.ReacodeID=x4data_dat.DatasetID
 inner join SUBENT on REACODE.SubentID=SUBENT.SubentID
 inner join ENTRY on ENTRY.EntryID=SUBENT.EntryID
where REACODE.fullCode='13-AL-27(N,A)11-NA-24,,SIG'
order by ENTRY.YearRef1 desc,x4data_dat.DatasetID,En,x4data_dat.idat
```

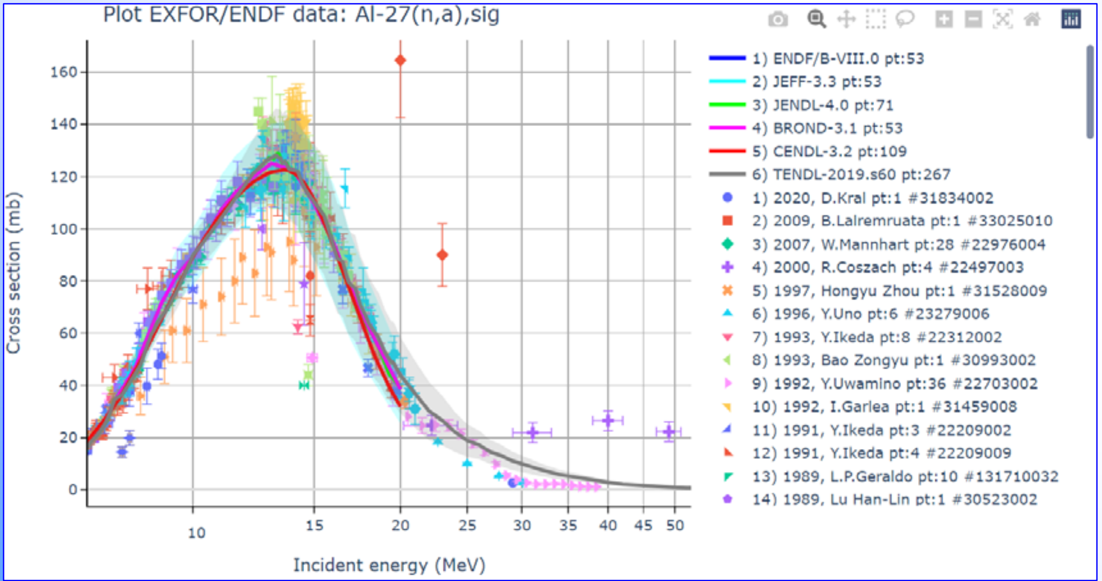


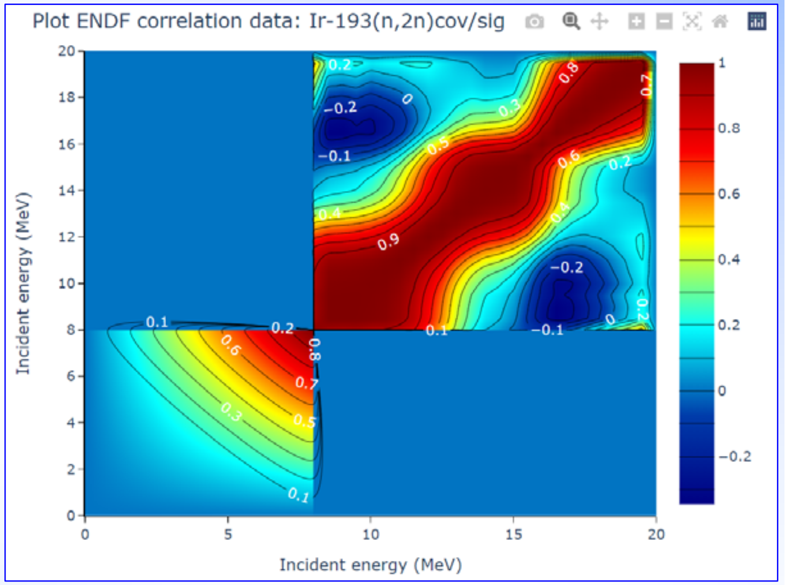
Retrieval code examples in Python #2

Retrieve data from X4Lite2 + evaluated ENDF data from Web

Python:
- *code.py: 105 lines*
- *retrieve EXFOR computational data: 70 lines*
- *retrieve ENDF data from Web for selected libraries: 112 lines*
- *calls interactive graphics plotly*

Python:
- *code.py: 130 lines: retrieve ENDF MF33 data (in JSON) from ENDF Web retrieval system, convert to correlation matrix*
- *calls interactive graphics plotly*





These python codes are trivial!

Concluding remarks

1. EXFOR relational database is extended with data points in JSON; X4Lite2 created; project continues

2. X4Lite2 database can be used as it is without EXFOR parsers

3. After discussions, tests and decision - regular distribution of X4Lite2 can be organized

Progress in EXFOR data automatic renormalization system

1. Renormalization of EXFOR data using new Decay data
   - "AR" 511 keV annihilation decay data (intensity)
   - "DR" gamma line intensity
   - EXFOR keywords: DECAY-DATA and DECAY-MON
   - Data renormalized to the current ENSDF data - thanks to M.Verpelli
2. New data types available for automatic renormalization
   - "SIG", "DA", "DE", "DAE", "FY"
3. Implementation for whole EXFOR database
   - Now automatic renormalization includes 3 types of flagged corrections: MONITOR [0], DECAY-DATA [1], DECAY-MON [2]
   - Datasets with automatic corrections: 17,025 (9.4% of total 181,398)
4. Renormalized C5 and C5M
   - x4toc5 extended by option for automatic renormalization (-ren:mon,decay)
5. Usage in Web EXFOR Web retrieval system
   - Check-box for automatic renormalization for "Monitor-xs" and "Decay-data"

Automatic vs. expert's correction

x4auto, 2021

```
$A 2021-09-21 10:01:17, x4auto, V.Zerkin
13597002  x4u:19950217  #1995,Ghorai #Pts:4
 #[0]#---Monitor xs-data
 #[0]#Reaction: 30-ZN-64(N,P)29-CU-64,,SIG
 #[0]#Monitor:  13-AL-27(N,A)11-NA-24,,SIG
 m0: [EN,MONIT,MONIT-ERR]; #[0]#old monitor(energy)
 m1: recom$al27na;         #[0]#new monitor(energy)
 dy=dy/y;                  #to rel. uncertainties
 y=y/m0*m1;                #[0]#renormalizing CS
 dy=(dy**2-dm0**2+dm1**2)**0.5; #[0]#replace monitor uncertainties
 #[1]#---Reaction decay-data
 #[1]#REACTION   (30-ZN-64(N,P)29-CU-64,,SIG)
 #[1]#DECAY-DATA (29-CU-64,12.7HR,AR,511.,0.386) #Ix_old=0.386
 a1=0.386/0.352;           #[1]#DECAY-DATA: correction to new 511 keV gamma-yield per decay Cu-64 Ix_new=0.352
 y=y*a1;                   #[1]#Renorm.factor: a1=1.0965909
 #[2]#---Monitor decay-data
 #[2]#MONITOR    (13-AL-27(N,A)11-NA-24,,SIG)
 #[2]#DECAY-MON  (11-NA-24,15.02HR,DG,1369.,1.00) #Im_old=1.0
 a2=0.999936/1.0;          #[2]#DECAY-MON: correction to new 1368.626 keV gamma-yield per decay Na-24 Im_new=0.999936
 y=y*a2;                   #[2]#Renorm.factor: a2=0.999936
 dy=dy*y;                  #to abs. uncertainties
```

K.Zolotarev, 2011

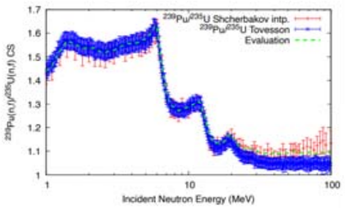
```
$C 2011-05-16, K.Zolotarev 2011, Zn64(n,p)Cu64
13597002            #1994 S.K.Ghorai+
a0=0.386/0.348;     #correction to new  511 keV gamma-yield per decay Cu-64
a1=0.999936/1.0;    #correction to new 1368 keV gamma-yield per decay Na24
a2=0.84351;         #renorm. factor to the preliminary evaluated integral of cs
                    #in the neutron energy interval 14.2-16.2 MeV.
a3=a0*a1*a2;        #total energy independent correction factor
c2=0.0115           #added error in 511 keV gamma-yield per decay Cu-64 - 1.15%
c3=0.02             #added error in remorm. factor - 2%
m0: [en, monit];    #old cs for Al27(n,a)Na24 monitor reaction
m2: [en, monit-err];#abs. error in old cs for Al27(n,a) monitor reaction
c0=m2/m0;           #rel. error in old cs for Al27(n,a) monitor reaction
m1: rrdf10 $ al27na;#new cs for Al27(n,a)Na24 monitor reaction
c1=dm1/m1;          #relative error in new cs for Al27(n,a) monitor reaction
dy=dy/y;            #relative error in original cs for Zn64(n,p)Cu64 reaction
fc=m1/m0*a3;        #total correction factor
y=y*fc;             #correction exp. cs
dy=dy^2-c0^2+c1^2+c2^2+c3^2; #determination the quadrature of new total error
dy=dy^0.5*y;        #determination the absolute value of new total error
```

Example of expert's corrections: ^{239}Pu/^{235}U(n,f)

D.Neudecker, SG50, 2021-06-21

I take ^{239}Pu/^{235}U(n,f) cross sections by Tovesson that were already highlighted as questionable by Standards.

- Tovesson et al. and Shcherbakov et al. data raised questions in the Neutron Standards evaluation -> Standards rejected Tovesson data above 13 MeV -> nice example for layer 3.
- Also some information was lost from literature when translated into EXFOR format -> nice example for layer 1.
- This is neither a criticism of experimentalists nor compilers! Both have a hard job.

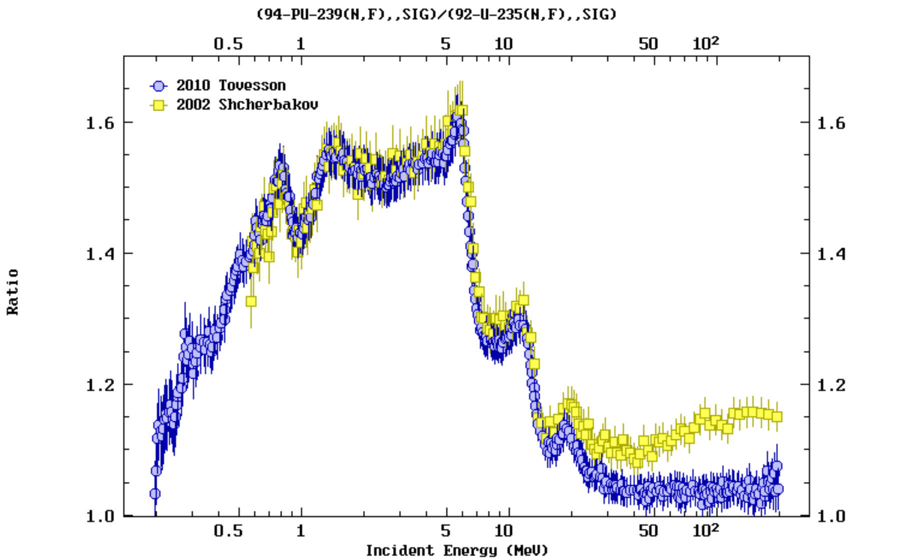


Tasks:

1. Remove Tovesson's data above 13MeV (1)
2. Renormalize Scherbakov's data and include missing uncertainties (2)
3. Store and share this information between evaluators (3)

Solution in EXFOR Retrieval system:

```
$C 2021-09-24, V.Zerkin for SG50 2021, 239Pu(n,f)sig/235U(n,f)sig

142710031  x4u:20201215  #2010,F.Tovesson
#Reaction: (94-PU-239(N,F),,SIG)/(92-U-235(N,F),,SIG)
e:13e6 *; del; #data above 13 MeV rejected in Neutron Standard evaluation (2017)

41455005  x4u:20170724  #2002,O.Shcherbakov
# REACTION    ((94-PU-239(N,F),,SIG)/(92-U-235(N,F),,SIG))
# MONITOR     ((94-PU-239(N,F),,SIG)/(92-U-235(N,F),,SIG))
# MONIT-REF   (,,3,JENDL-3.2,,1994)
# COMMENT     Of Authors.
#             The fission cross-section ratio normalization
#             has been done in the 1.75-4.0 MeV energy interval
#             using data of JENDL-3.2.
dy=dy/y;        #convert abs. uncertainty in cs-ratio to rel. uncertainty
a0=1.535;       #used ratio normalization factor (using data of JENDL-3.2), E:1.75-4.0 MeV
c0=1.668/100;   #1.535 +-1.668%  (this uncertainty is not included to error analys)
a1=1.5393;      #ratio normalization factor (using data of ENDF/B-VIII.0), E:1.75-4.0 MeV
c1=2.82/100;    #1.5393 +-2.82%  (uncertainty should be added)
fc=a0/a1;       #total correction factor
y=y*fc;         #correction exp. cs
dy=dy**2+c1**2; #calc. new quadrature of total uncertainty
dy=dy**0.5*y;   #back to absolute uncertainty
```



Before correction

```
$C 2021-09-24, V.Zerkin for SG50 2021, 239Pu(n,f)sig/235U(n,f)sig
142710031  x4u:20201215  #2010,F.Tovesson
#Reaction: (94-PU-239(N,F),,SIG)/(92-U-235(N,F),,SIG)
e:13e6 *; del; #data above 13 MeV rejected in Neutron Standard evaluation (2017)

41455005  x4u:20170724  #2002,O.Shcherbakov
# REACTION   ((94-PU-239(N,F),,SIG)/(92-U-235(N,F),,SIG))
# MONITOR    ((94-PU-239(N,F),,SIG)/(92-U-235(N,F),,SIG))
# MONIT-REF  (,,3,JENDL-3.2,,1994)
# COMMENT    Of Authors.
#            The fission cross-section ratio normalization
#            has been done in the 1.75-4.0 MeV energy interval
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c0=1.668/100;   #1.535 +-1.668%  (this uncertainty is not included to error analys)
a1=1.5393;      #ratio normalization factor (using data of ENDF/B-VIII.0), E:1.75-4.0 MeV
c1=2.82/100;    #1.5393 +-2.82%  (uncertainty should be added)
fc=a0/a1;       #total correction factor
y=y*fc;         #correction exp. cs
dy=dy**2+c1**2; #calc. new quadrature of total uncertainty
dy=dy**0.5*y;   #back to absolute uncertainty
```

Corrections protocol

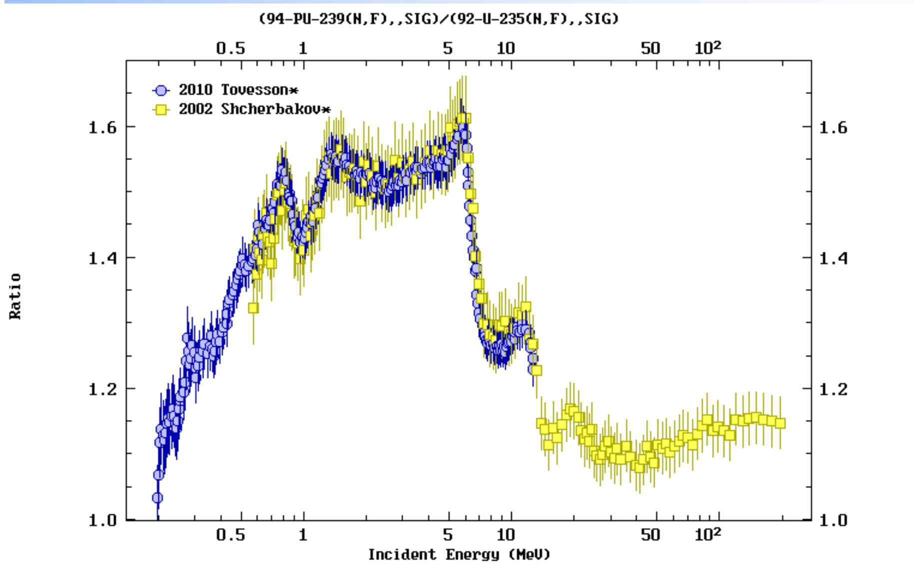
Applied corrections. Datasets: 2

1) EXFOR:#142710031 Ref:F.Tovesson, (10) Corrected_Points:0 Deleted_Points:238 Unchanged_Points:362

2) EXFOR:#41455005 Ref:O.Shcherbakov, (02) Corrected_Points:166 yFactor_Ave:0.997207 yFactor_Min:0.997206 yFactor_Max:0.997207

142710031 X4U:20201215; E:1.3e+7 *; Del;

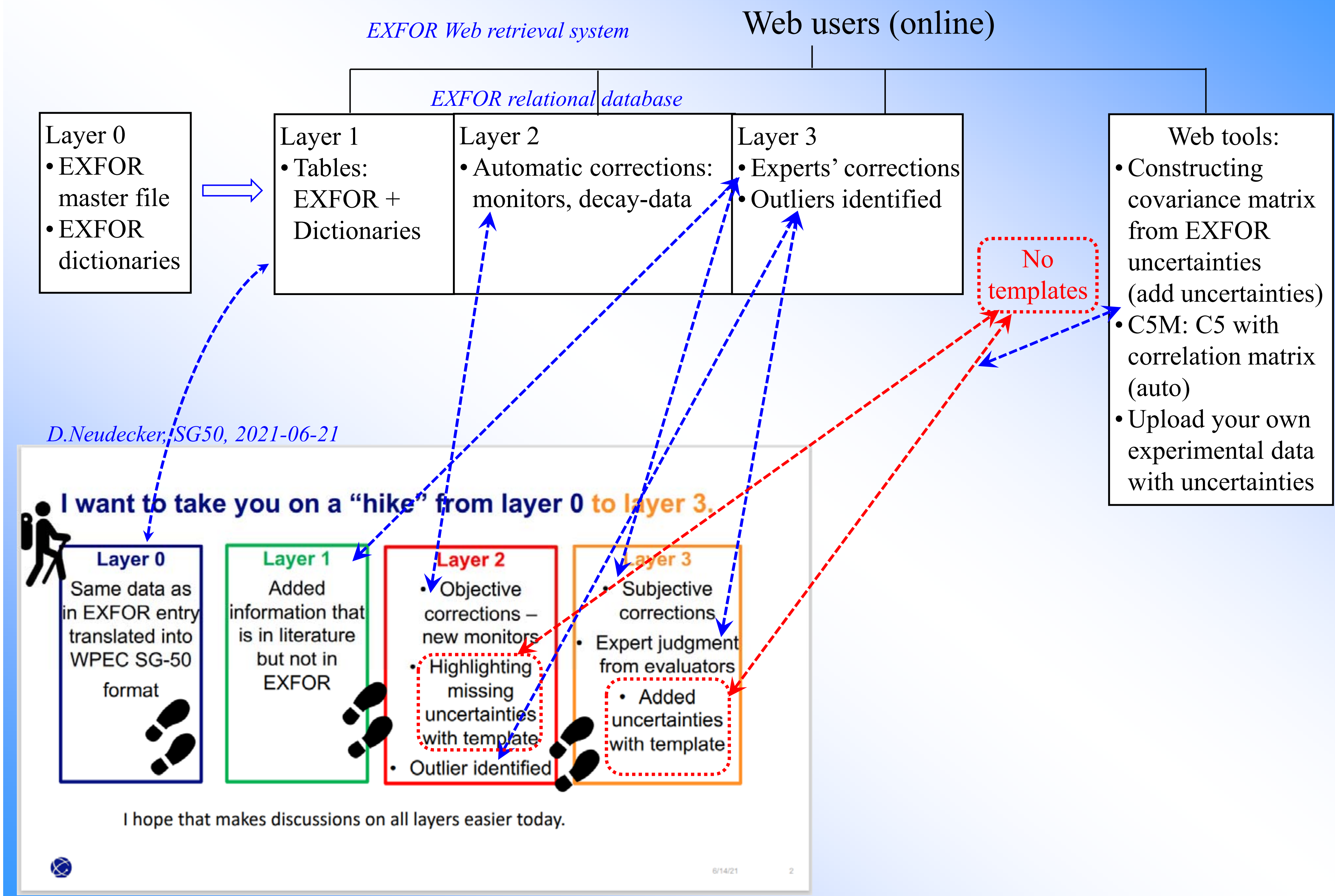
41455005 X4U:20170724; dY=dY/Y; a0=1.535; c0=1.668/100; a1=1.5393; c1=2.82/100; Fc=a0/a1; Y=Y*Fc; dY=dY^2+c1^2; dY=dY^0.5*Y;



After correction

```
Data check:
 . . . . . . . . . . .  Y(ratio*1000)
-50   En(MeV)=1.773  Y=1541       dY=40.4767  (2.63%)   41455005   O.Shcherbakov,
+50                  Y=1536.7     dY=59.221   (3.85%)   41455005   *Fc=0.997207
-51   En(MeV)=1.829  Y=1531       dY=39.9504  (2.61%)   41455005   O.Shcherbakov,
+51                  Y=1526.72    dY=58.6578  (3.84%)   41455005   *Fc=0.997206
-52   En(MeV)=1.887  Y=1491       dY=38.9867  (2.61%)   41455005   O.Shcherbakov,
+52                  Y=1486.84    dY=57.1796  (3.85%)   41455005   *Fc=0.997207
-53   En(MeV)=1.949  Y=1552       dY=40.7403  (2.63%)   41455005   O.Shcherbakov,
+53                  Y=1547.66    dY=59.6265  (3.85%)   41455005   *Fc=0.997206
 . . . . . . . . . . .
-154  En(MeV)=83.32  Y=1147       dY=23.0894  (2.01%)   41455005   O.Shcherbakov,
+154                 Y=1143.8     dY=39.63    (3.46%)   41455005   *Fc=0.997207
-155  En(MeV)=88.22  Y=1157       dY=23.2452  (2.01%)   41455005   O.Shcherbakov,
+155                 Y=1153.77    dY=39.9491  (3.46%)   41455005   *Fc=0.997206
-156  En(MeV)=93.57  Y=1139       dY=22.965   (2.02%)   41455005   O.Shcherbakov,
+156                 Y=1135.82    dY=39.3748  (3.47%)   41455005   *Fc=0.997206
-157  En(MeV)=99.46  Y=1146       dY=22.6142  (1.97%)   41455005   O.Shcherbakov,
+157                 Y=1142.8     dY=39.3335  (3.44%)   41455005   *Fc=0.997206
```

Existing EXFOR data correction system vs. SG50 plans



Concluding remarks

1. The development of existing EXFOR database and correction system continues
2. New ways of the data distribution and methods of access for new users are being worked out
3. Is there a need to coordinate our development plans?

Thank you.