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Program x4toc5

Translation of experimental data from the EXFOR format to the computation format C5

by

Viktor Zerkin

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Vienna-2024

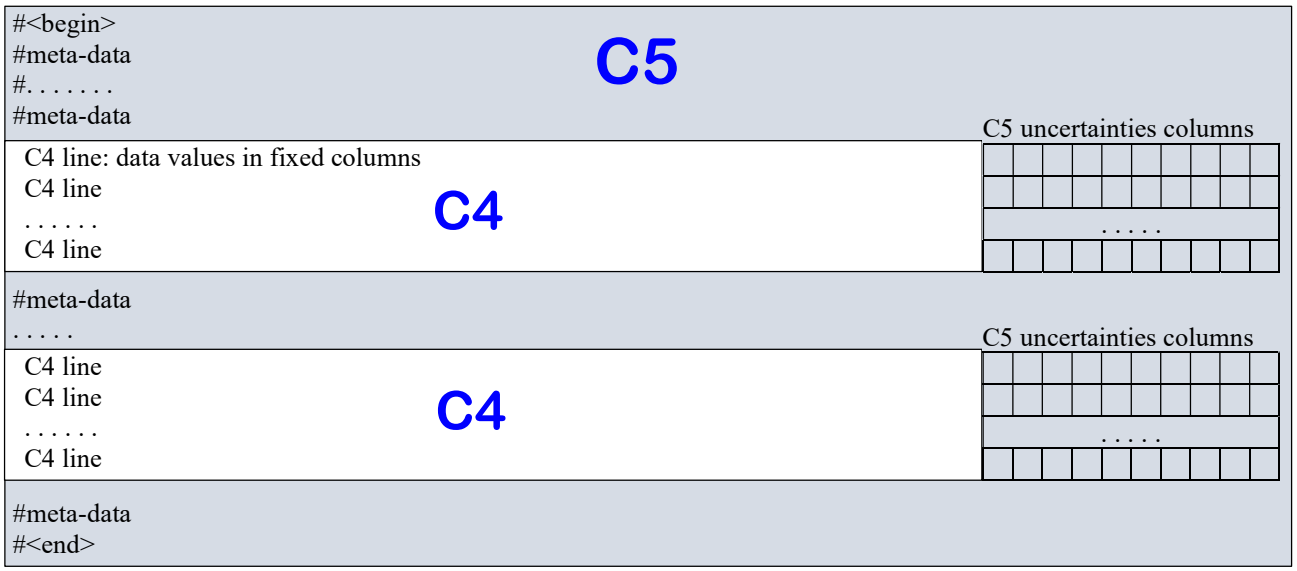
PROGRAM x4toc5

(Version 2024-06-10)

Translation of experimental data from the EXFOR format
to the computation format C5

Introduction

The x4toc5 program is designed to translate experimental data from the EXFOR format (which allows different units and flexible data order and therefore requires a lot of text analysis from a user's program) to a computation format with fixed units and numerical data columns (which is easy to read and interpret by user programs). Format C5 is built on the same basic concept as computational format C4 provided by the program X4TOC4[1][2], using the same data columns (1-132), EXFOR reaction data classification via MF.MT providing compatibility with ENDF[3] data, etc. Program x4toc5 is written on java and provides important extensions of functionality and output data in C5 format: meta data, additional data columns, extended EXFOR data coverage, interpretation of uncertainties, various data recalculations, output options, etc.



[1] Dermott E. Cullen and Andrej Trkov, Program X4TOC4, report IAEA-NDS-80, https://nds.iaea.org/publications/iaea-nds/iaea-nds-0080.pdf

[2] See also: EXFOR Formats Description for Uses, edited by Otto Schwerer, IAEA-NDS, https://www-nds.iaea.org/nrdc/nrdc_doc/iaea-nds-0206-200806.pdf#page=52

[3] ENDF-6 Formats Manual, edited by D. A. Brown, 2023, NNDC, BNL, USA, https://www.nndc.bnl.gov/endfdocs/ENDF-102-2023.pdf

C5: extensions and compatibility versus C4

Initially, program x4toc5 was created in order to provide two extensions: statistical and systematical uncertainties (in new data columns) and some "meta-data" from EXFOR, like Reaction, Method, Version, Title, Reference, etc. (new lines in the text starting with symbol #). Core structure of data line was preserved from C4 in order to provide backward compatibility for existing end-user's software.

Later, functionality of x4toc5 was extended to generate correlation matrices on the basis of EXFOR uncertainties, recalculate data for inverse reactions, etc. C5 format was extended accordingly, but until now x4toc5 has an option (flag "-c4") to generate C4 formatted output.

Converting C5 file to C4 can also be done with simple Linux command:

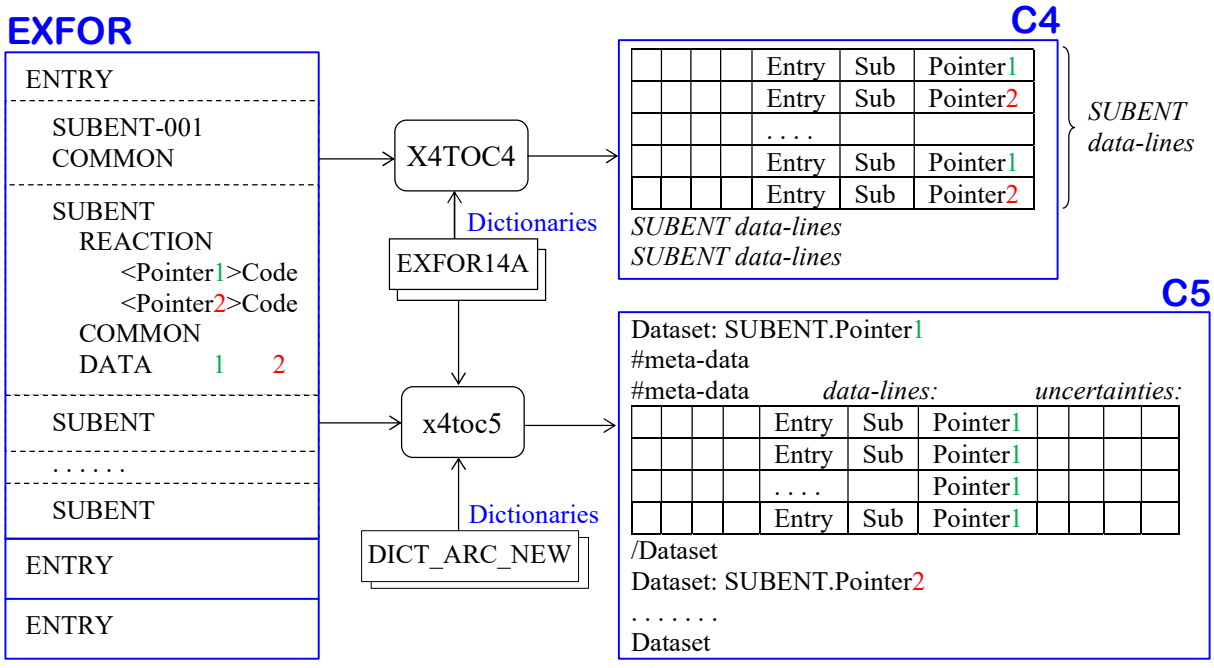
```
$ grep -v "^#" file.c5 | cut -b-131 >file.c4
```

Dictionaries

Program x4toc5 is built on general-purpose EXFOR Java package "zvv.x4" and uses EXFOR-CINDA Dictionaries (DICT_ARC_NEW.* files). In order to provide compatibility in data meaning and definitions with ENDF and X4TOC4, x4toc5 uses Dictionary EXFOR14A.DAT from X4TOC4 and extended table {EXFOR:SF*} ⇔ ENDF:MF.MT.LR created by V.Pronyaev (2007). For the cases when search in both dictionaries failed, but measured quantity can be identified on the basis of EXFOR Dictionaries, x4toc5 can generate data with known MF and MT=0 (this feature can be deactivated by using flag "-nomt0").

C5 file structure

Logically, C5 consists of Datasets. Dataset is identified by <Subentry+Pointer> presenting data-table for single Reaction-code. All information taken from Entry and Subentry is nested into Dataset. In other words, there is no nesting level for Entry and Subentry - all information is repeated in each Dataset.
Structure of EXFOR file (simplified): [ENTRY: [SUBENT: [Pointer-Reaction: data-table]]].
Structure of C4 file: [SUBENT: [data-line]].
Structure of C5 file: [Datasets: [#meta-data], [data-line]].



C5 file is text file containing Begin-line, one or many Datasets (block of lines) and End-line.

- Begin-line contains “#Format-ID”, date and time of file creation, and database time stamp.
- Dataset starts with “#DATASET” line, following with meta-data lines starting with “#”, list of data-lines and ends with “#/DATASET” line. Optionally, file can contain covariance data block (running x4toc5 with flag “-c5m”).
- End-line contains “#/Format-ID” and few numbers - summary of content.

```
#C5M.2.3        20240610    132247    20240529
#DATASET        23114002   20130924
#SUBENT         23114002   20130924
#ENTRY          23114      20170322
#TITLE          High resolution measurements of the 241Am(n,2n)
#AUTHORS        C.Sage, V.Semkova, O.Bouland, P.Dessagne, A.Fernandez,
#AUTHOR1        C.Sage+
#YEAR           2010
#METHOD         ACTIV,GSPEC
#REACTION       95-AM-241(N,2N)95-AM-240,,SIG
#C5DATA
. . . . . . . . . . . . . .
. . . . Data-lines . . . .
. . . . . . . . . . . . . .
#/C5DATA
#/DATASET       23114002
 . . . . . . . . . . . .
 . . . Datasets  . . .
 . . . . . . . . . . . .
#/C5M.2.3
```

Example of Dataset in C5M format (SUBENT 23114002)

```
#DATASET        23114002   20130924
#SUBENT         23114002   20130924
#ENTRY          23114      20170322
#TITLE          High resolution measurements of the 241Am(n,2n)
#+               reaction cross section
#AUTHORS        C.Sage, V.Semkova, O.Bouland, P.Dessagne, A.Fernandez,
#+               F.Gunsing, C.Naestren, G.Noguere, H.Ottmar,
#+               A.J.M.Plompen, P.Romain, G.Rudolf, J.Somers, F.Wastin
#AUTHOR1        C.Sage+
#YEAR           2010
#X4REF1         J,PR/C,81,064604,2010
#REFERENCE1     Jour: Physical Review, Part C, Nuclear Physics, Vol.81, p.064604 (2010)
#DATE           20130924
#INSTITUTE      2FR SAC,2ZZZGEL,2FR CAD,2FR STR,3BULBLA,1USALAS,2ZZZITU,2FR BRC
#METHOD         ACTIV,GSPEC
#REACTION       95-AM-241(N,2N)95-AM-240,,SIG
#C4Reaction     (N,2N),SIG
#ReactionType   CS
#MF             3
#MT             16
#PROJ           1
#TARG           95241
#TARGET         95241           [ ]             95-AM-241       [ ]
#REAC1          N,2N
#PRODUCT        95-AM-240
#C4ReaCode      (N,2N),SIG
#Quantity       Cross section
#DataUnits0     B
#DataUnits      ?
#D4REAC         R0#
#ReaCombi       a
#C4FOUND        1
#C4BEGIN        [    1 95241   3  16 A ]
#DATA-HDR       DATA
#VarFamily      [0 2        ]
#xVariables     1
#+              Y = Y(X1)
#ReacRatio      false
#vReacs         1
#C5EXT1         132         (4F9.0)     dSys,dStat,dOther,dTot //Absolute fully correlated, uncerrelated, partially
correlated and total uncertainties
#C5EXT2         168         (5F9.0)     dSys,dStat,dOther,dTot,dData //Relative uncertainties (dData/Data) in per-cents
#C5DATA         9
```

```
#C.M.Flag        0000
#Headers                         EN       dEN      Data     dData
#Units                           EV        EV         B         B
#Proj Targ M MF MT PXC   Energy  dEnergy     Data   dData Cos/LO/ZP dCos/LO/AP LVL/HL dLVL/HL I78 Refer (YY)             EntrySubP  dSys     dStat   dOther    dTot     dSys%    dStat%  dOther%   dTot%   dData%
#---><---->o<-><-->ooo<-------><-------><-------><-------><-------><-------><-------><-------><-><----------------------><---><->o<-------><-------><-------><-------><-------><-------><-------><-------><------->
   1 95241   3  16 A 8340000.0 150000.0.09680001 0.006292                                        C.Sage,            (10)23114  2 0.00324680.0049368 0.001862 0.006292 3.35     5.10     1.92     6.50     6.50
   1 95241   3  16 A 9150000.0 150000.0   0.16290.0092853                                        C.Sage,            (10)23114  2 0.00535340.00671850.00313340.0092853 3.29     4.12     1.92     5.70     5.70
   1 95241   3  16 A   1.333E7 150000.0   0.24180.0111228                                        C.Sage,            (10)23114  2 0.00787240.00655540.00393620.0111228 3.26     2.71     1.63     4.60     4.60
   1 95241   3  16 A    1.61E7 150000.0   0.15240.0070104                                        C.Sage,            (10)23114  2 0.00500840.00357730.00308210.0070104 3.29     2.35     2.02     4.60     4.60
   1 95241   3  16 A   1.716E7  30000.0   0.11610.0051084                                        C.Sage,            (10)23114  2 0.0038154 0.002125 0.0023480.0051084 3.29     1.83     2.02     4.40     4.40
   1 95241   3  16 A    1.79E7 100000.0   0.10570.0046508                                        C.Sage,            (10)23114  2 0.0034945 0.0015960.00234690.0046508 3.31     1.51     2.22     4.40     4.40
   1 95241   3  16 A   1.936E7 150000.0   0.0895 0.007339                                        C.Sage,            (10)23114  2 .002941270.00602980.0027875 0.007339 3.29     6.74     3.11     8.20     8.20
   1 95241   3  16 A   1.995E7  70000.0   0.10210.0059218                                        C.Sage,            (10)23114  2 0.0033553 0.0022670.00419730.0059218 3.29     2.22     4.11     5.80     5.80
   1 95241   3  16 A   2.061E7  40000.0.077900010.0068552                                        C.Sage,            (10)23114  2 0.00256010.00473980.00421310.0068552 3.29     6.08     5.41     8.80     8.80
#/C5DATA          0
#COVARIANCE      2                Generated
#COMMENT         Default2. EXFOR software ver.2020-09-24, by V.Zerkin@iaea.org (IAEA-NDS)
#+               1) If only total uncertainties are given, assume uncertainties: statistical/systematic=50/50.
#+               2) Statistical uncertainties are added to covariance matrix as uncorrelated components
#+               3) If Other uncertainties are not given (ALGORITHM=2): split total systematic uncertainties: fully/partially
correcated=50/50 (LERC/MERC)
#+                 else (ALGORITHM=3): assume total systematic uncertainties fully correlated (LERC), Other - partially correcated
(MERC)
#+               4) LERC-correlated uncertainties are added to covariance matrix as fully correlated
#+               5) MERC-correlated uncertainties are added as partially correlated using parameters:
#ALGORITHM       3           1           100.        100.        100.        0           8340000.0   2.061E7     0.5
#+               Type        Groupping   Stat.SERC   Sys.LERC    Other.MERC  Log/Lin     En-Min      En-Max      Length
#COVARDATA       1           9           9
#EnMin(eV)   EnMax(eV)    Data(b)      Std.dev.(%) Correlations(%)
#----------><----------><----------><----------><---Values: separated by space; line length: unlimited....
8340000.     8340000.     0.0968       6.4           100
9150000.     9150000.     0.1629       5.61          40 100
1.333E7      1.333E7      0.2418       4.54          40 46 100
1.61E7       1.61E7       0.1524       4.52          38 43 61 100
1.716E7      1.716E7      0.1161       4.27          40 45 62 74 100
1.79E7       1.79E7       0.1057       4.26          41 45 60 73 81 100
1.936E7      1.936E7      0.0895       8.12          21 24 29 38 43 47 100
1.995E7      1.995E7      0.1021       5.71          30 34 41 54 63 70 48 100
2.061E7      2.061E7      0.0779       8.78          20 22 27 35 42 47 34 61 100
#/COVARDATA
#/COVARIANCE
#/DATASET        23114002
```

Columns 1-131 are the same as in C4:

1-5	Proj	Projectile ZA (e.g. for neutron=1, proton=1001)
6-11	Targ	Target ZA (e.g. for 26-Fe-56=26056)
12	M	Target metastable state (e.g. 26-FE-56m=M)
3-15	MF	MF (ENDF conventions, plus additions)
16-19	MT	MT (ENDF conventions, plus additions)
20	P	Product metastable state (e.g. 26-FE-56M=M)
21	X	EXFOR status
22	C	Center-of-mass flag (C=center-of-mass, blank=lab)
23-94		8 data fields (each in Fortran E9.3 format)
1) 23-31	Energy	Projectile incident energy
2) 32-40	dEnergy	Projectile incident energy uncertainty
3) 41-49	Data	Data, e.g. cross section, angular distribution, etc.
4) 50-58	dData	Data uncertainty
5) 59- 67	Cos	Cosine or legendre order
6) 68-76	dCos	Cosine uncertainty
7) 77-85	Lvl	Identified by columns 95-97 (e.g. level E, half-life)
8) 86-94	dLvl	Identified by columns 95-97 (e.g. level E, uncertainty)
95- 97	I78	Identification of data fields 7 and 8 (LVL=level energy, LVN=level number, HL=half-life, E2=energy of outgoing particle, EXC=excitation energy, QVL=Q value, TMS=sample temperature, THS= sample thickness, etc.)
98-122	Refer	Reference (first author and year)
123-127	Entry	EXFOR Entry (accession number)
128-130	Sub	Subent (sub-accession number)
131	P	Pointer (multi-dimension table flag)

C5 extension.

C5 indicates center-of-mass flag for every data pair in C5 line "#C.M.Flag" and C4 flag C in 22nd column

Datasets	C.M.Flag	C	Ei	Data	Cos	E2
113,539	0000					
123	0001	I				C.M.
6,444	0010	E			C.M.	
38	0011	M			C.M.	C.M.
947	0100	C		C.M.		
666	0101	K		C.M.		C.M.
15,653	0110	G		C.M.	C.M.	
286	0111	O		C.M.	C.M.	C.M.
1,811	1000	B	C.M.			
105	1010	F	C.M.		C.M.	
195	1100	D	C.M.	C.M.		
159	1101	L	C.M.	C.M.		C.M.
438	1110	H	C.M.	C.M.	C.M.	
140,404	total					

#Datasets: number of Datasets with the Flag in C5 file generated from EXFOR-2024-05-29 (MT=0 excluded)

```
#Proj Targ M MF MT PXC   Energy  dEnergy     Data    dData Cos/LO/ZP dCos/LO/AP LVL/HL dLVL/HL I78 Refer (YY)              EntrySubP
#---><----><-><--><--><-------><-------><-------><-------><-------><-------><-------><-------><-><----------------------><---><->o
    1 95241   3  16 A 8340000.0 150000.0.09680001 0.006292                                          C.Sage,              (10)23114  2
    1 95241   3  16 A 9150000.0 150000.0   0.16290.0092853                                         C.Sage,              (10)23114  2
    1 95241   3  16 A   1.333E7 150000.0   0.24180.0111228                                         C.Sage,              (10)23114  2
    1 95241   3  16 A    1.61E7 150000.0   0.15240.0070104                                         C.Sage,              (10)23114  2
    1 95241   3  16 A   1.716E7  30000.0   0.11610.0051084                                         C.Sage,              (10)23114  2
    1 95241   3  16 A    1.79E7 100000.0   0.10570.0046508                                         C.Sage,              (10)23114  2
    1 95241   3  16 A   1.936E7 150000.0   0.0895 0.007339                                         C.Sage,              (10)23114  2
    1 95241   3  16 A   1.995E7  70000.0   0.10210.0059218                                         C.Sage,              (10)23114  2
    1 95241   3  16 A   2.061E7  40000.0.077900010.0068552                                         C.Sage,              (10)23114  2
```

Columns 132-212 contain detailed information about uncertainties:

132-140	dSys	fully correlated uncertainties (abs.)
141-149	dStat	uncorrelated uncertainties (abs.)
150-158	dOther	partially correlated uncertainties (abs.)
159-167	dTot	total uncertainties (abs.)
168-176	dSys%	fully correlated uncertainties (%)
177-185	dStat%	uncorrelated uncertainties (%)
186-194	dOther%	partially correlated uncertainties (%)
195-203	dTot%	total uncertainties (%)
204-212	dData%	data uncertainties (%)

Example: EXFOR 23114002.x4

```
ERR-ANALYS (ERR-T,,,P) Total uncertainty
           (MONIT-ERR,,,P) 27Al(n,a) standard x-section (1.6-5.4%)
           (ERR-1,,,U) Counting of 240Am activity       (1.4-6.3%)
           (ERR-2,,,U) Counting of 24Na activity        (0.7-2.0%)
           (ERR-3,,,F) Intensity of 240Am gamma line        (1.2%)
           (ERR-4,,,U) Number of 27Al in sample             (0.1%)
           (ERR-5,,,P) Number of 241Am in sample            (0.3%)
           (ERR-6,,,F) 24Na/240Am efficiency ratio          (3.0%)
           (ERR-7,,,F) Correction for decay of 240Am    (0.4-0.9%)
           (ERR-8,,,U) Correction for secondary neutron    (<1.4%)
```

Example: 23114002.c5, columns 132-221

dSys	dStat	dOther	dTot	dSys%	dStat%	dOther%	dTot%	dData%
0.0032468	0.0049368	0.001862	0.006292	3.35	5.10	1.92	6.50	6.50
0.0053534	0.0067185	0.0031334	0.0092853	3.29	4.12	1.92	5.70	5.70
0.0078724	0.0065554	0.0039362	0.0111228	3.26	2.71	1.63	4.60	4.60
0.0050084	0.0035773	0.0030821	0.0070104	3.29	2.35	2.02	4.60	4.60
0.0038154	0.002125	0.002348	0.0051084	3.29	1.83	2.02	4.40	4.40
0.0034945	0.0015960	0.0023469	0.0046508	3.31	1.51	2.22	4.40	4.40
.0029412	7 0.0060298	0.0027875	0.007339	3.29	6.74	3.11	8.20	8.20
0.0033553	0.002267	0.0041973	0.0059218	3.29	2.22	4.11	5.80	5.80
0.0025601	0.0047398	0.0042131	0.0068552	3.29	6.08	5.41	8.80	8.80

Program x4toc5

Translation of experimental data from the EXFOR format
to the computation format C5

User's Guide

by

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Last modified: 13 June 2024

Vienna-2024

System environment and requirements

1) Operating systems: Windows, Linux, MacOS
2) JDK/JRE version-1.5 and higher (Java Development Kit/Java Runtime Environment)
3) Disk space ~100 MiB

Package distribution

The package distribution includes

1. Source codes in Java
2. Make files (bat and bash) for Windows/Linux/MacOS
3. Dictionaries in the format DICT_ARC_NEW
4. Test EXFOR files
5. Test scripts (bat and sh)
6. Plotting examples (Python + Plotly + scripts to run)
7. Test-results for checking/comparison by end-user

```
x4toc5
    |   help.txt
    |   LICENSE.TXT
    |   make1.bat
    |   make1.sh
    |   README.md
    |   README.md
    ├──bin
    |       x4toc5.jar
    ├──doc
    |       x4toc5.pdf
    ├──src
    |   |   *.java
    |   |   package-info.java
    |   └──x4dict
    |           DICT_ARC.TOP
    |           DICT_ARC_NEW.*
    ├──tests
    |       *.x4
    |       c5file.py
    |       c5line.py
    |       c5plot1sig.py
    |       c5subr.py
    |       levels.zip
    |       plot1.bat
    |       plot1.sh
    |       test1.bat
    |       test1.sh
    |       x4toc5.jar
    └──tests-result
            *.c5
            *.c5m
            *.html
            *.png
            test1.tto
            ....
```

1. Preparation steps

1.1. Install Java

Example for Linux-Ubuntu:

```
$ sudo apt-get install openjdk-8-jdk
```

-or-

```
$ sudo apt-get install default-jdk
```

1.2. Check and install Python3 and Plotly (optional)

Example for Linux-Ubuntu:

```
$ python3 --version
$ sudo apt-get install python3-pip
$ pip3 install plotly
```

1.3. Download and check package

Example for Linux-Ubuntu:

```
$ cd ~/x4toc5
$ du -hc --time --max-depth=1
   1008K  2024-06-10 11:40 ./bin
   83M    2024-06-10 11:58 ./tests-result
   5.6M   2024-06-10 12:25 ./src
   8.8M   2024-06-10 11:47 ./tests
   99M    2024-06-10 12:25 .
   99M    2024-06-10 12:25 total
```

1.4. Prepare RIPL-Levels for tests (optional, to be used with flag “-mt51”)

Example for Linux-Ubuntu:

```
$ cd tests
$ unzip levels.zip
```

1.5. Recompile source codes and prepare new JAR archive (optional)

Linux/MacOS:

```
$ bash make1.sh
```

Windows:

```
$ make1.bat
```

2. Run program

The code and Dictionaries are distributed as source and binary (JAR archive) files ready to run in any Java Virtual Machine. The program can run from JAR file or compiled and run from class files:

```
$ java -jar x4toc5.jar myexfor.x4
```

```
$ javac -d . *.java
$ java zvv.x4.x4toc5 myexfor.x4
```

2.1. Display help (running x4toc5 without input file)

```
$ java -jar x4toc5.jar
 Translate EXFOR to C5 computational format
 Program x4toc5, ver. 2024-06-10
 V.Zerkin, IAEA, Vienna, 2010-2024

 Run:  $ java [flags] x4toc5 file.x4 [options]

 Options:
   -o:file     output file, default: file.x4.c5
   -dict:dir   directory with EXFOR Dictionaries, default: -dict:x4dict/
   -dlvl:dir   directory with levels,             default: -dlvl:levels/
   -split:dir  output C5 file for every Entry to a file in directory:
                  1/123/12345.c5
   -c5         output format: C5 (default)
   -c5m        output format: C5M (C5+correlation matrix)
   -c4         output format: C4
   -i          recalculate data to inverse reactions, e.g.:
                  6-C-13(A,N)8-O-16,,SIG --> 8-O-16(N,A)6-C-13,,SIG
                  2-HE-4(P,D)2-HE-3,,DA  --> 2-HE-3(D,P)2-HE-4,,DA
   -i:file     inverse data for the reactions listed in the file
   -cm2lab     convert EN-CM, ANG-CM, DATA-CM from C.M. to Lab. (MF4 only)
   -norr       do not convert DATA: Rutherford-Ratio to B/SR
   -noqe       do not replace Q-Value by E-Level for partial XS
   -mt51       replace MT by MT+iLevel (for MT:51,601,651,701,751,801)
   -nomt0      do not process Datasets with unknown MT
   -sort       sort data by independent variables (EN, AN, E2)
   -h[elp]     print this text
   -ps         show process
   -debug      set debug mode
 Java flags:
   -Xmx<size>  set maximum Java heap size
   -cp <paths> list of directories, JAR archives to search for class files
   -jar <path> file with binaries (archive of classes - compiled java codes)

 Examples:
   $ java x4toc5 myfile.x4
   $ java x4toc5 x4.x4 -dict:x4dict/
   $ java -Xmx400M -jar x4toc5.jar x4.x4 -i -o:x4.x4.c5i
```

3. Run tests

3.1. Tests

1) *Display help-info*
2) *Convert x4 to c5 with default options*
3) *Convert x4 to c5, split output by Entry*
4) *Convert x4 to c4*
5) *Inverse reaction data*
6) *Generate correlation matrix*
7) *Replace MT by MT+iLevel from RIPL-Levels for partial reactions*
8) *Keep Q-Value, i.e. do not replace by Energy-Level*
9) *Inverse reaction data for selected reaction*
10) *Convert C.M. to Lab system*
11) *Plotting Cross Sections*

3.2.a) Linux/MacOS

```
$ cd ~/x4toc5/tests
$ bash test1.sh
    . . . Confirm next test: Press <ENTER> ...
$ bash plot1.sh
    . . . opens window in your Web-Browser ...
```

3.2.b) MS-Windows

Press <Win/R>, type cmd *..., press <ENTER>. You should get Terminal-window.*

```
$ cd C:\x4toc5\tests
$ test1.bat
    . . . Confirm next test: Press <ENTER> ...
$ plot1.bat
    . . . opens window in your Web-Browser ...
```

3.3. Test results

Running test script, user should get new files in the "tests" directory with extensions .c5*.

Examples of output if provided in the directory "tests-result" for comparison and checking.

File *test1.tto* contains terminal output which shows what user should normally see on the terminal when test script is running correctly.

3.4. Plot results

If you have Python3 and Plotly installed, program *c5plot1sig.py* will open two tabs in your browser – see Fig.1, 2.

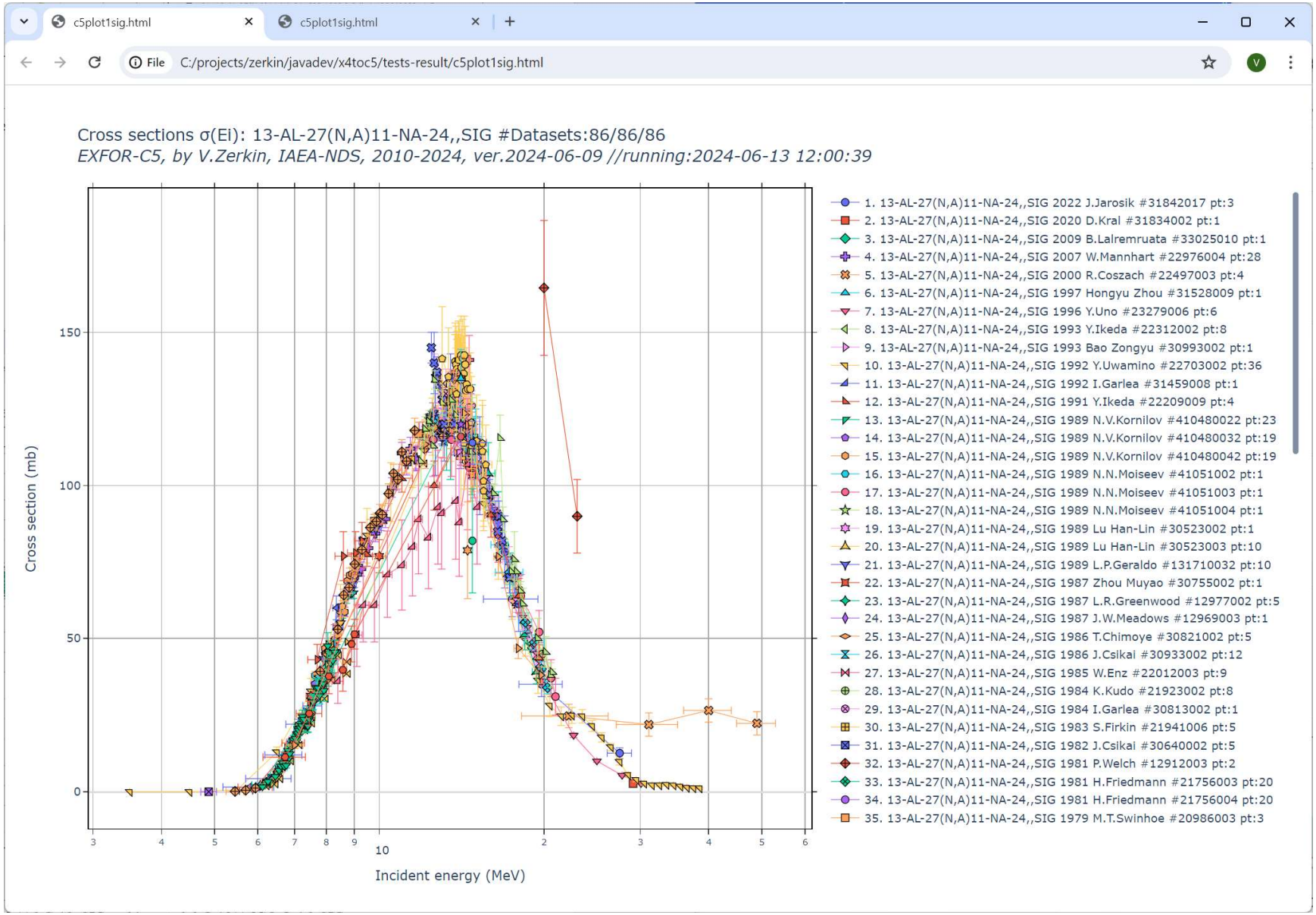

Fig.1. Data for reaction: 13-AL-27(N,A)11-NA-24,,SIG

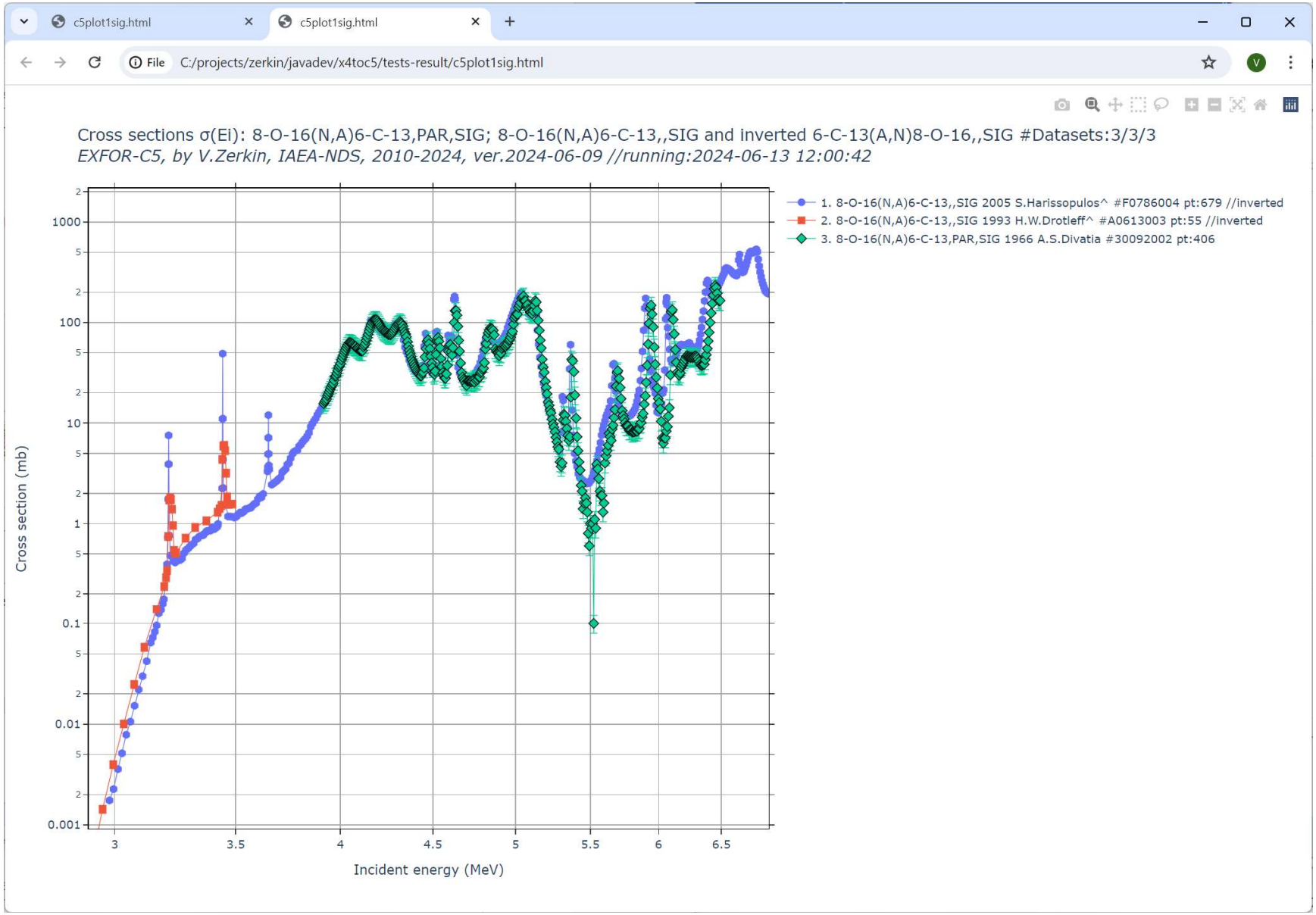

Fig.2. Data for reaction: 8-O-16(N,A)6-C-13,,SIG and inverted 6-C-13(A,N)8-O-16,,SIG