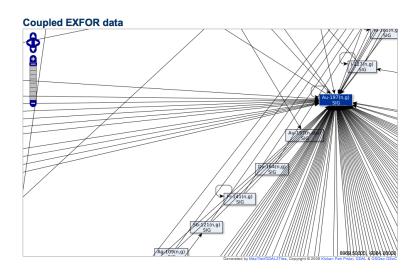
x4i, The EXFOR interface

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1 Introduction

The x4i package is an interface to the EXFOR nuclear data library. It simplifies retrieval of EXFOR entries and can automatically parse them, allowing one to extract cross-section (and other) data in a simple, plotable format. x4i also understands and can parse the entire reaction string, allowing one to build a strategy for processing the data.

EXFOR is a structured markup language for representing measured nuclear data. It is an old format, and is awkward to use for several reasons:

- It relies on data being in the correct columns in order to denote context. This is a legacy feature since EXFOR data used to be stored on FORTRAN punch cards.
- The data was often hand entered so the format rules were not always rigorously obeyed (fortunately WPEC SubGroup 30 has remedied much of this ensuring that EXFOR data can be translated into C4 format, see ref. [2]).
- The mark-up language is surprisingly complex (see refs. [3, 4, 5, 6]]). Figures 1-5 illustrate the structure of the EXFOR format.

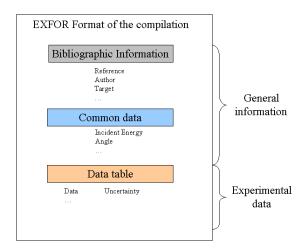


Figure 1: Structure of an EXFOR entry. The bibliographic information is always contained in the first subentry of an entry and given the index '001'. Common data is data common to all data blocks in all subentries and is found in the '001' subentry. Each dataset is given its own subentry, beginning with subentry '002.' Figure from ref. [1].

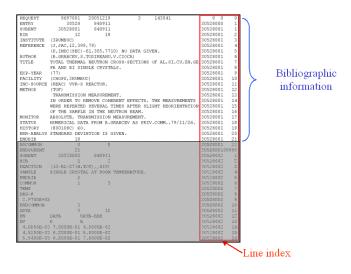


Figure 2: A close-up on the first subentry showing the bibliographic data. Figure from ref. [1].

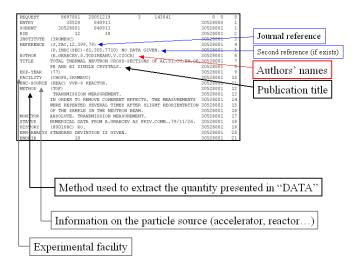


Figure 3: An even closer look at the details of the bibliographic data. Here one can see how the authors' names, institutions and publication information are specified. Figure from ref. [1].

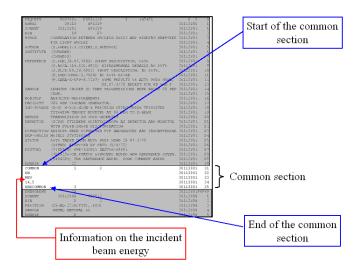


Figure 4: A sample COMMON data section. In this case, the beam energy for all data in subsequent subentries is given. Figure from ref. [1].

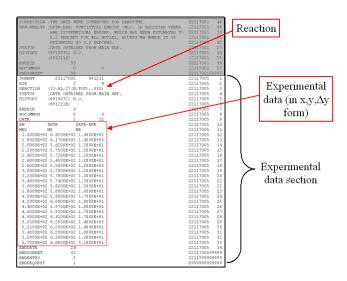


Figure 5: A sample DATA section. DATA sections contain the actual data from a measurement. This is combined with the data in COMMON data to produce an instance of the X4DataSet class detailed later in this report. Figure from ref. [1].

2 Installation

There are several ways to install x4i. They are given below in order of increasing difficulty. Please ensure your 'git' installation has large file support (see https://git-lfs.github.com).

2.1 Easiest installation: using pip and git

```
host$ pip install git+https://github.com/brown170/x4i
```

This version of the installation process automatically installs the 2021-03-08 version of the EXFOR database.

2.2 Installation from a tarball distribution

- 1. Unpack the distribution
- 2. Installation options:
 - Old-fashioned local installation: put x4i in your \$PYTHONPATH. Assuming you are in the directory containing x4i's 'setup.py' file:

```
host$ export PYTHONPATH=$PYTHONPATH:\`pwd\`
```

• Installation with pip (You can delete the x4i project once this is complete)

```
host$ pip install path/to/x4i/setup.py/directory
```

• Editable pip installation

```
host$ pip install -e path/to/x4i/setup.py/directory
```

• For site-wide installation. Assuming you are in the directory containing x4i's setup.py file (You can delete the x4i project once this is complete):

```
host$ sudo python setup.py install
```

2.3 Source installation from git

This assumes that you will be editing the project in some fashion. This installation does not automatically include the IAEA data files. You will need to download them yourself as described in step #3. below.

1. Clone the project

```
host$ git clone https://github.com/brown170/x4i.git
```

- 2. Installation options:
 - Old-fashioned local installation: put x4i in your \$PYTHONPATH. Assuming you are in the directory containing x4i's setup.py file:

```
host$ export PYTHONPATH=$PYTHONPATH:\`pwd\`
```

• Editable installation using pip:

```
host$ pip install -e path/to/x4i/setup.py/directory
```

3. To get the EXFOR library from the IAEA, run the install script. This will install the 2021-03-08 version. Assuming you are in the directory containing x4i's setup.py file, do:

```
host$ ./install.py
```

3 Upgrading

To update or change the source database, you will need a copy of the new database from the IAEA. It is available as a zipfile downloaded from the IAEA website: http://www-nds.iaea.org/x4toc4-master/. There are two sets of files there. Those with the name of the form X4-YYYY-MM-DD.zip are the ones usable by x4i. To install the IAEA library, assuming that your zip file is named X4-YYYY-MM-DD.zip:

```
$host python bin/setup-exfor-db.py --x4c4-master ~/Downloads/X4-2019-07-18.zip 13535: (1991) A.Ling, X.Aslanoglou, et al. 13564: (1970) J.Taylor, G.Spalek, et al. 13597: (1995) S.K.Ghorai, P.M.Sylva, et al. 13550: (1992) C.M.Castaneda, R.Gearhart, et al. 13501: (1991) R.R.Winters, R.F.Carlton, et al. 13511: (1991) C.M.Perey, F.G.Perey, et al. 13540: (1989) S.Nath, G.Glass, et al. 13587: (1993) R.Macklin, N.W.Hill, et al. ...
```

Please read the help message (python bin/setup-exfor-db.py -h) for more information. After you finish this step, be sure to update the information in the x4i/data/database_info.json file.

4 Basic Usage

Now we describe how to use x4i. We begin by explaining how to query the EXFOR database and how to retrieve data. All retrievals and queries are handled by the classes in the exfor manager module. The class X4DBManagerDefault defaults to the X4DBManagerPlainFS class and this is the class supported out of the box by x4i. Here is an example of its use:

```
Python 3.7.3 (default, Mar 30 2019, 03:37:43)
[Clang 10.0.0 (clang-1000.11.45.5)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> from x4i import exfor_manager
>>> db = exfor_manager.X4DBManagerDefault()
>>> help(db)
Help on X4DBManagerPlainFS in module x4i.exfor_manager object:
class X4DBManagerPlainFS(X4DBManager)
| X4DBManagerPlainFS(**kw)
   EXFOR data base manager for data stored on local filesystem in
   directory hierarchy.
Method resolution order:
       X4DBManagerPlainFS
       X4DBManager
builtins.object
   Methods defined here:
    __init__(self, **kw)
       Initialize self. See help(type(self)) for accurate signature.
   query(self, author=None, reaction=None, target=None, projectile=None,
          quantity=None, product=None, MF=None, MT=None, C=None, S=None,
          I=None, SUBENT=None, ENTRY=None, reference=None)
       Use this function to search for all (Sub)Entries matching
       criteria in query call. This function returns a dictionary
       with the following structure::
           { ENTRY: [ SUBENTOO1, SUBENTOO2, SUBENTOO3, ... ], ... }.
       Here ENTRY is the entry number whose subentries match the query.
        The SUBENTOO1 is the documentation subentry number, which is
        always included, and SUBENTOO2, ... are the subentry numbers
       matching the search criteria.
   retrieve(self, author=None, reaction=None, target=None,
             projectile=None, quantity=None, product=None, MF=None,
```

```
MT=None, C=None, S=None, I=None, SUBENT=None,
ENTRY=None, rawEntry=False, reference=None)
Execute a query, matching the criteria specified.
This function returns a dictionary with the following structure::

{ ENTRY:[SUBENTOO1, SUBENTOO2, SUBENTOO3, ...], ...}.

Here ENTRY is the entry number whose subentries match the query. The SUBENTOO1 is the documentation subentry itself, which is always included, and SUBENTOO2, ... are the subentries themselves matching the search criteria.

If the flag rawEntry is True, the raw text versions of the SUBENTS will be returned, otherwise they will be converted to X4Entry instances.
```

Once the database manager is initialized, we can run a query:

```
>>> db.query(author='Panitkin')
{'40121': ['40121001', '40121002'], '40177': ['40177001',
'40177002', '40177003'], '41335': ['41335001', '41335002'],
'41654': ['41654001', '41654002']}
```

All queries return a Python dict. The keys of the dictionary are the EXFOR entry number. The values of the dictionary are a list of subentry numbers of the EXFOR entry whose contents match the query search criteria. If a particular subentry matches the search criteria, the corresponding documentation subentry (the '001' subentry) is also returned. The complete list of search criteria are given in Table 1. A partial list of searchable observables is given in Table 2.

Retrievals also can be made using the database manager:

```
>>> r=db.retrieve(author='Panitkin')
```

The search result from a retrieval is a Python dict. The keys are the ENTRY number (as a string) and the values are X4Entry instances:

```
>>> for k in r:
... print(k)
...
40121
40177
```

Table 1: Valid search keys for queries and retrievals from the EXFOR database manager classes. One key not mentioned in this table is the recently added reference key.

Search Criteria	Details	Implemented in version 1.0	
author			
reaction	Enter in form "projectile, products," e.g. N, 2N or N, F or D, 3N+P. Wildcards may be used, e.g. *, 2N.		
target	rget Enter in form "SYM-Z," e.g. HE-3. The symbol should be in upper case.		
projectile	The standard ENDL set are supported, namely: N, P, D, T, A, G, HE-3. Additionally, the projectile may be any nucleus of form "SYM-Z" (provided such heavy-ion data exists in EXFOR).	Yes	
quantity	This defines the observable, e.g. cross-section is SIG. Table 2 lists the supported quantities.	Yes	
product	Residual nucleus (if any) of a particular reaction. Enter in form "SYM-Z," e.g. HE-3. The symbol should be in upper case.	Yes, partially	
MF	The ENDF quantity, e.g. MF=3 is cross-section data.	No	
MT	The ENDF reaction, e.g. MT=18 is fission.	No	
С	The ENDL reaction, e.g. C=12 is (n,2n).	No	
S	The ENDL reaction modifier, e.g. S=1 denotes discrete level excitations.	No	
I	The ENDL quantity, e.g. I=1 denote angular probability distributions, $P(E \mu)$.	No	
SUBENT	The EXFOR Subentry number. It is 8 characters long and the last 3 digits specify the subentry within the EXFOR entry corresponding to the first 5 characters.	Yes	
ENTRY	The EXFOR Entry number. It is 5 characters long.	Yes	

Table 2: A selection of supported quantities. The full list is given in EXFOR dictionary 30 (see ref. [4])

		Variations on quantity	Simplified translation of
Quantity	Details	supported	data available
DA	Angular distribution $d\sigma(E)/d\mu$	EVAL	Yes
DA/DE	Double differential data $d\sigma(E)/d\mu dE'$		No, high priority
DE	Energy distribution $d\sigma(E)/dE'$	EVAL	Yes
FY	Fission yields		No
NU	Average number of neutrons emitted in	EVAL, PR	Yes
	fission event $\overline{v(E)}$		
NU/DE	Fission neutron spectrum $d\overline{v}(E)/dE'$		No
POL/DA	Polarization		No, high priority
POT	Potential scattering parameter		No
RI	Resonance integral of cross-section		No
SIG	Cross-section $\sigma(E)$ or average cross-section	EVAL, MXW, SPA,	Yes
	in some variations of this observable.	FST, RTE, FIS, AV	

```
41335
41654
>>> type(r[40121])
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
KeyError: 40121
>>> type(r['40121'])
<class 'x4i.exfor_entry.X4Entry'>
```

The X4Entry class is a member of the exfor_entry module and handles all of the parsing of an EXFOR ENTRY.

In the following section, we will detail some of the things one can do with an X4Entry instance. For now, we'll just illustrate hoe to extract the cross-section data in a format we can plot:

```
>>> x=db.retrieve(target="PU-239", reaction="N,2N", quantity="SIG")
>>> x.keys()
dict_keys(['13787', '14129', '20795', '21971'])
>>> x['14129']
ENTRY
          14129
SUBENT
          14129001
                              2.0
RTR
                   12
INSTITUTE (1USALAS, 1USALRL)
REFERENCE (J,NSTS,2,(1),620,2002)
AUTHOR
          (J.A.Becker, L.A.Bernstein, W.Younes, D.P.McNabb,
           P.E.Garrett, D.E.Archer, C.A.McGrath, M.A.Stoyer, H.Chen,
>>> y=x['14129']
>>> dss=y.getSimplifiedDataSets()
>>> dss.keys()
dict_keys([('14129', '14129002', ' ')])
>>> print(dss[('14129', '14129002', ' ')])
# Authors:
             J.A.Becker, L.A.Bernstein, W.Younes, D.P.Mcnabb, ...
# Title:
             Partial Gamma-Ray Cross Sections For The Reaction ...
# Year:
             2002
# Institute: Lawrence Livermore National Laboratory, Livermore, CA
# Reference: J.Nucl.Science and Technol.Tokyo, Supplement 2, ...
# Subent:
             14129002
# Reaction: Cross section for 239Pu(n,2n)238Pu
        Energy Data d(Energy)
                                                  d(Data)
#
        MeV
                                   MeV
                                                  barns
                      barns
                                   0.2239
       6.481
                     0.1009
                                                 0.03081
```

What we've done here is extract all the datasets in our X4Entry instance using the getSimplifiedDataSets() member function. The results are stored in another Python dict, this time keyed off with a Python tuple with the following structure: (entry #, subentry #, pointer). In this case, there is no pointer so that spot is taken by a string comprising a single space character. In other cases, the pointer may be number either referring to additional data. We will explain this further in the next sections.

5 Main Classes

5.1 The X4Entry class

In this section, we provide a more detailed look into the X4Entry class and its use. A partial list of member functions is provided in Table ??.

Let us begin the discussion by picking up where we left off in the previous section's example. We return to the X4Entry in the Python variable 'y':

```
>>> y=x['14129']
>>> y.keys()
dict_keys(['14129001', '14129002'])
>>> type(y[1])
<class 'x4i.exfor_subentry.X4SubEntry'>
```

In this simple example, we have illustrated that X4Entrys are really Python dicts, with keys being the subentry accession number (in this case, abbreviated to '1') and values being instances of the X4SubEntry class. Note that the subentry accession numbers 1, '1', '001', 13883001, and '1388301' are all equivalent. Continuing:

Clearly X4Entrys and X4SubEntrys are simply nested Python dicts whose keys and values correspond to the structure of the original EXFOR (sub)entry. This example illustrates one other point: the Python str() operator returns a "pretty" version of what it acts on. In this case, the reference field of the bibliography section of subentry #1.

There are two other functions to elaborate, the getSimplifiedDataSets() and getDataSets() function. Both return dicts whose values are X4DataSets, either "plain" or "simplified." In the next section we will describe the X4DataSet and explain the difference between a "plain" X4DataSet and a "simplified" X4DataSet. Here we illustrate the use of either function:

```
>>> dss = y.getSimplifiedDataSets()
>>> dss.keys()
dict_keys([('14129', '14129002', ' ')])
```

This function returns a Python dict whose keys are a tuple: (entry #, subentry #, pointer). The EXFOR pointer here is a string consisting of a space. In many EXFOR subentries, the EXFOR compilers chose to store multiple datasets. To distinguish them (and to map the data to other fields in the EXFOR entry), the compilers gave the sets a distinct one character pointer. When x4i encounters such a case, the dict returned from getSimplifiedDataSets() will have one key per pointer.

5.2 The X4DataSet class

The X4DataSet class and its subclasses are probably the class most users of x4i will become familiar with first as instances of these classes contain the experimental data one wishes to plot and/or manipulate. In the previous section we introduced two functions in the X4Entry class that return dicts containing X4DataSets. We also introduced the concept of "plain" and "simplified" datasets. Figure 6 shows the csv output of the X4DataSet, retrieved in the previous section, in its "plain" form and its "simplified" form. As one can see, both contain the same data, but the "simplified" set is in consistent units and extraneous columns have been removed.

As one can see in Figure 6, one can think of an X4DataSet as a spreadsheet containing the dataset's values. Indeed, the Python __getitem__ operator allows us to directly access elements in this spreadsheet:

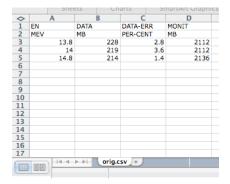
```
>>> dss.keys()
dict_keys([('14129', '14129002', ' ')])
>>> myset = dss[('14129', '14129002', ' ')]
```

Table 3: Member function reference for the X4Entry class and the X4EntryMetaData class. Functions in the X4EntryMetaData class are prefixed with the meta() call from the X4Entry class.

	Arguments	
Function	(other than self)	Description
str()		Enables Python str() function: the
		"pretty" string formatter. Recursively
		applies str() to all components of self.
repr ()		Enables Python repr() function: the
		"representation" string formatter (strings
		returned by this function are nearly
		equivalent to the original EXFOR entry).
		Recursively applies repr() to all
		components in self.
getitem (key)	key	Enables element access with the []
	-	operator (e.g. [key])Return the
		X4SubEntry instance with subentry
		number key.
deleted()		Returns True if this entry has been deleted
,,		(a skeletal version of the entry remains in
		the EXFOR database though).
getDataSets()		Returns a Python dict containing all of the
		X4DataSets contained in self. The keys
		of the dict are a tuple: (entry #,
		subentry #, pointer).
getSimplifiedDataSets	makeAllColumns	Similar to getDataSets except that data
()	= False	has been parsed (if possible), producing a
		simpler dataset that may be interpreted
		easier (and plotted!). See X4DataSet
		below.
meta()		Return an instance of the meta data derived
		from self.
meta().citation()		Returns a string containing the citation for
		the current entry. Suitable for publication.
<pre>meta().legend()</pre>		Returns a string containing information for
		the current entry. Suitable for use as a plot
		legend.
<pre>meta().xmgraceHeader(</pre>		Returns a string containing information for
)		the current entry. Use this as the header for
		a dataset you are plotting in xmgrace.

Table 4: Column names and units in simplified X4DataSets.

Column Label	Units	Comments
Data	barns, barns/ster, 1/MeV	Unit choice depends on nature of the observable.
	ptcls/fis, no-dim	Maybe dimensionless if data is ratio data.
Energy	MeV	Incident energy
E'	MeV	Outgoing energy
Angle	degrees	



51100					511101		
\rightarrow		Α		В	C		
1	Energ	у	Data		d(Data)		
2	MeV		barns		barns		
3		13.8		0.228	0.0	06384	
4		14		0.219		07884	
5		14.8		0.214	0.0	02996	
6							
7							
8							
9							
10							
11							
12							
13							
14							
15							
		▶ ▶ simp.csv +					

Figure 6: Difference between a "plain" X4DataSet (on the left) and a "simplified" X4DataSet (on the right). Note that the units for the simplified set are consistent between a data column and an uncertainty column. Also notice that cross sections are always given in barns and energies in MeV. Table 4 lists all the units supported in "simplified" X4DataSets.

```
>>> myset['LABELS', 0]
'Energy'
>>> myset['LABELS', 1]
'Data'
>>> myset['UNITS', 1]
'barns'
>>> myset[0, 1]
0.1009
```

Of course, X4DataSets also come with meta data describing the set:

```
>>> myset.legend()
'(2002) J.A.Becker, L.A.Bernstein, et al.'
>>> myset.citation()
'J.A.Becker, L.A.Bernstein, et al., J.Nucl.Science and Technol.Tokyo,
Supplement 2, (1), 620 (2002); Data taken from the EXFOR database,
file EXFOR 14129002 dated 2002, retrieved from the IAEA Nuclear Data
Services website.'
```

Next, we point out the two methods for exporting the data, the csv() and the str() functions. The csv() function exports the dataset to a comma separated value file, suitable for viewing in Microsoft Excel. The str() function returns a string that can be viewed in the xmgrace plotting package.

Table 5: Member functions reference for the X4DataSet class and subclasses.

	Arguments	
Function	(other than self)	Description
str()		Enables Python str() function: the "pretty"
		string formatter.
repr()		Enables Python repr() function: the
		"representation" string formatter (strings
		returned by this function are nearly
		equivalent to the original EXFOR).
getitem((i	i,j	Access the data element in row i column j.
,j))		<pre>If i = 'LABELS' or 'UNITS', then the</pre>
		corresponding string heading the column is
		returned.
citation()		Returns a string containing the citation for the
		current entry. Suitable for publication.
csv(f)	f	Writes data in self to file f in CSV format.
		The CSV format stands for "Comma Separated
		Value" and may be read by MS Excel.
<pre>getSimplified(</pre>	makeAllColumns =	Returns an X4DataSet that has been
)	False,	"simplified." See the main text for what that
	failIfMissingErrors = False	entitles. If the optional argument
	- raise	makeAllColumns is True, every data
		column will be accompanied by an
		uncertainty column even if one is not present
		in the original data. If the optional argument
		failIfMissingErrors is True, an
		exception will be raised if there is no
		uncertainty column accompanying one or more data columns.
logond()		
legend()		Returns a string containing information for
		the current entry. Suitable for use as a plot
		legend.

The complete list of member functions for the X4DataSet class is given in Table 5.

Finally, we want to elaborate on the implementation of "simplified" X4DataSets. When the getSimplifiedDataSets() function is called from, it in turn calls the getDataSets() function to get all of the data in an X4Entry. Then, the X4DataSet function getSimplified() is called to attempt to convert the X4DataSet into its simpler form. Currently very few quantities in EXFOR can be converted to simpler forms. The list as of version 1.0 of x4i is given in Table 4.

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