Using XML in the IAEA-NDS: status, feedback and proposals

Viktor Zerkin

International Atomic Energy Agency, Nuclear Data Section

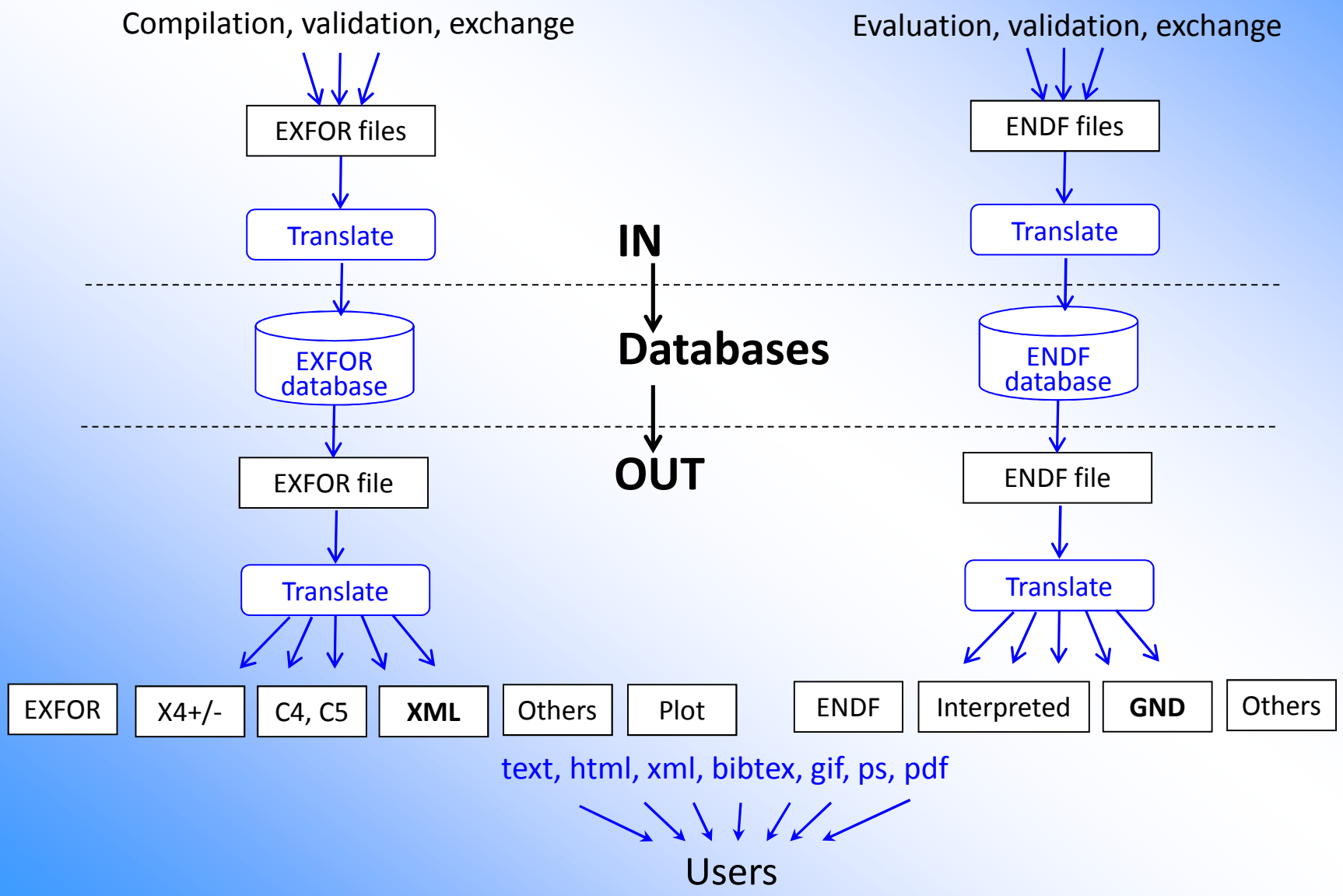
WPEC Subgroup-38 Meeting-6
OECD Nuclear Energy Agency, Issy-les-Moulineuax, France
Paris, 20-22 May 2015

Topics:

1. Data formats in EXFOR-ENDF database and Web retrieval systems
   - Data flow in EXFOR-ENDF Web system: overview
   - Web translation EXFOR to XML: tasks
   - Web translation ENDF-6 to GND, errors and feedback
2. Requirements for low level containers: EXFOR vs. ENDF
3. Proposals:
   - “Normalized” XML presentation
   - Low level I/O Fortran library for accessing XML files
   - Extensions for low level containers
4. Summary (highlights)

1. Data formats in EXFOR-ENDF systems

Data flow in EXFOR-ENDF Web system



Usage of EXFOR, ENDF-6 and XML

1. EXFOR and ENDF-6 formatted data are used as:
    1. exchange
    2. input for database population software
    3. input for data dissemination programs
2. XML in EXFOR system:
    1. output logical equivalent to original EXFOR/Dictionaries
    2. output computational formats
    3. output/input of recipe for EN-EN correlation matrices
    4. intermediate format for input to the databases (sql.xml)
3. XML in ENDF systems:
    1. output format (GND)
    2. intermediate format for input to the databases (sql.xml)

XML is mostly used only as one of output formats

Web-translation EXFOR to XML 2009-2013

Tasks

1. To translate original EXFOR files to XML from EXFOR database from Web-retrieval system
2. To translate "standardized" EXFOR output to XML
3. To translate user's EXFOR file to XML under MyEXFOR Web tool for compilers
4. To find out general problems if any
5. To study XML tools (XSL, XSD, Html-translation and validation)
6. To encourage users to use EXFOR-XML
7. To prepare background for developing EXFOR-XML as exchange format

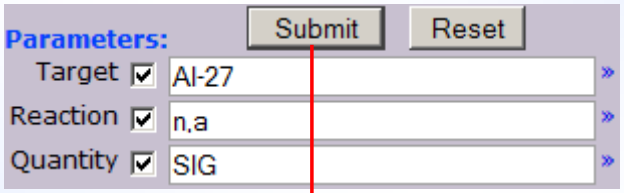
Web-translation ENDF to XML 2012-2013

Tasks

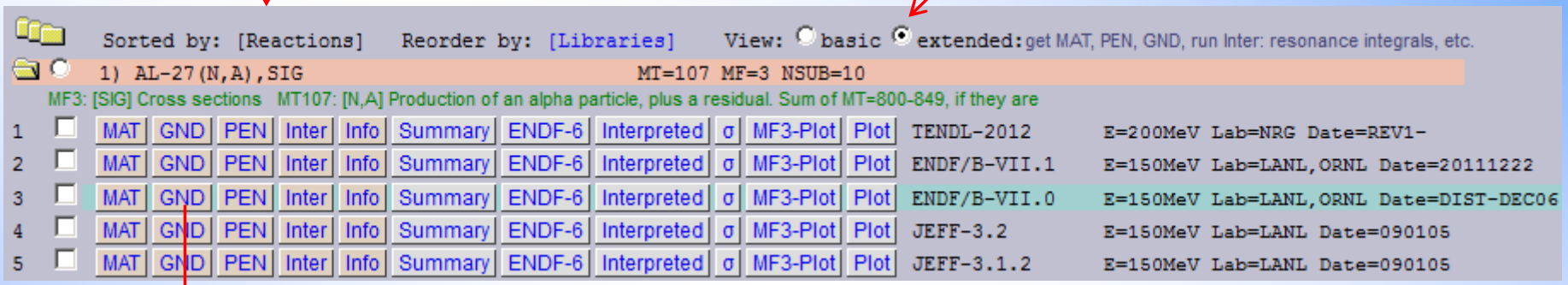
1. To translate ENDF to GND under MyENDF Web tool for evaluators (using Fudge, LLNL)
2. To translate ENDF from ENDF database to GND under ENDF Web-retrieval system (IAEA database contains 46 ENDF libraries available for all Web users)
3. To find out general problems if any
4. To find mistakes and unfinished features in translation program
5. Provide users' feedback to translation program developers (LLNL)

Translate ENDF to GND under Web retrieval system

NNDC: http://www.nndc.bnl.gov/endf
IAEA: http://www-nds.iaea.org/endf
BARC, India: http://www-nds.indcentre.org.in/endf/
CIAE, China: http://www-nds.ciae.ac.cn/endf/



Extended View



ENDF Web Retrieval System

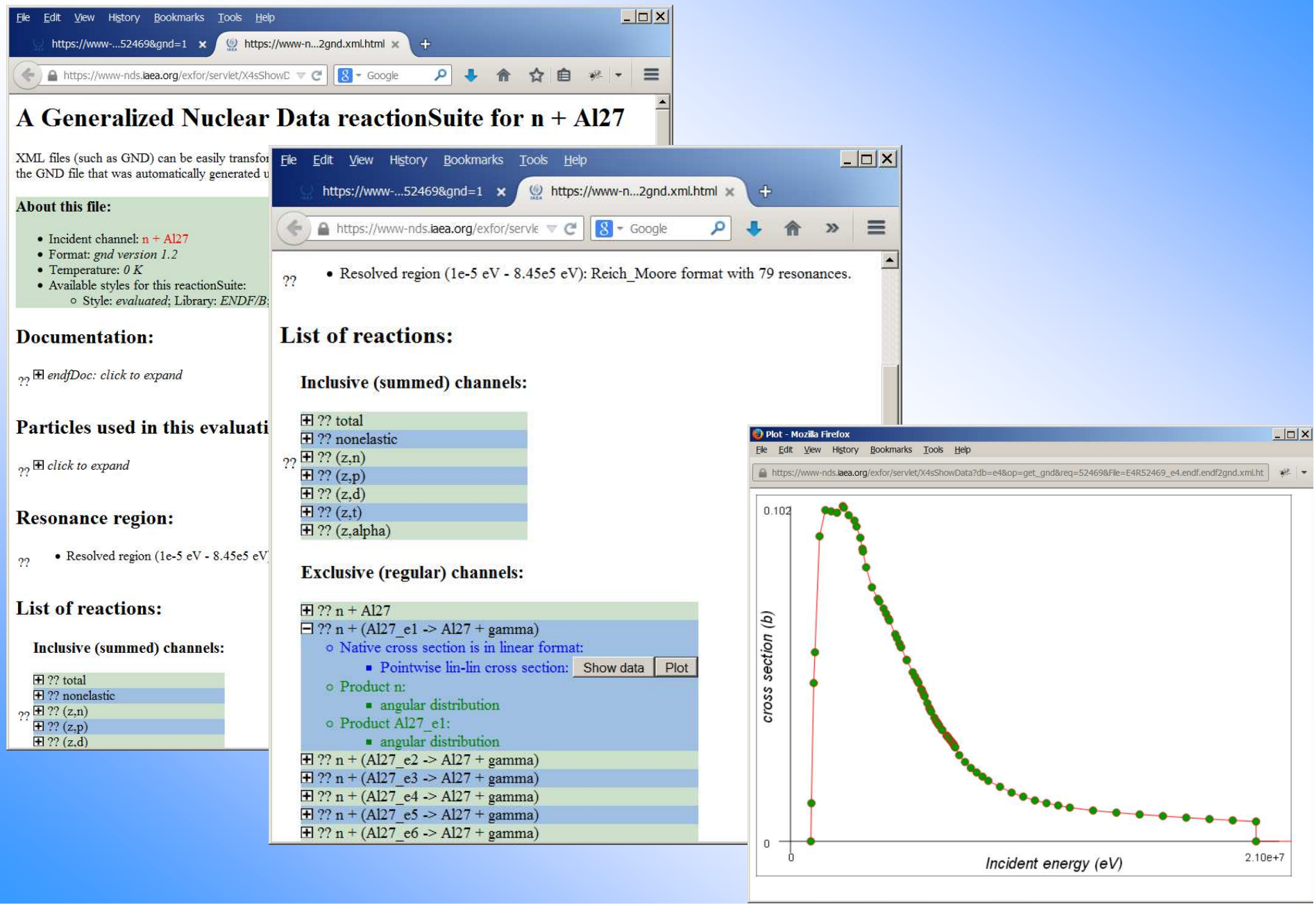
Conversion ENDF file to GND format.
Request #52469.
MAT: Library="ENDF/B-VII.1" Target="AL-27" MAT=1325 NSUB=10 (N)

#	File	Comment	Date	Length
1	gnd.endf	Input file	2014/10/28 09:32:46	2,223,045
2	gnd.xml	Main output file	2014/10/28 09:32:56	3,005,026
3	gnd.xml.html	Interpreted output file	2014/10/28 09:33:01	335,479
4	gnd.xml.txt		2014/10/28 09:32:56	3,005,026
5	gnd.covar.xml	Output covariance file	2014/10/28 09:32:56	28,239
6	gnd.noLineNumbers		2014/10/28 09:33:00	2,085,820
7	gnd.orig.noLineNumbers		2014/10/28 09:33:00	2,085,820
8	gnd.orig.noLineNumbers.cleanAndFixed		2014/10/28 09:33:00	2,085,820
9	gnd_cmd.log	Log file	2014/10/28 09:33:01	103
10	gnd_cmd.ttout	Terminal output	2014/10/28 09:33:01	38,417

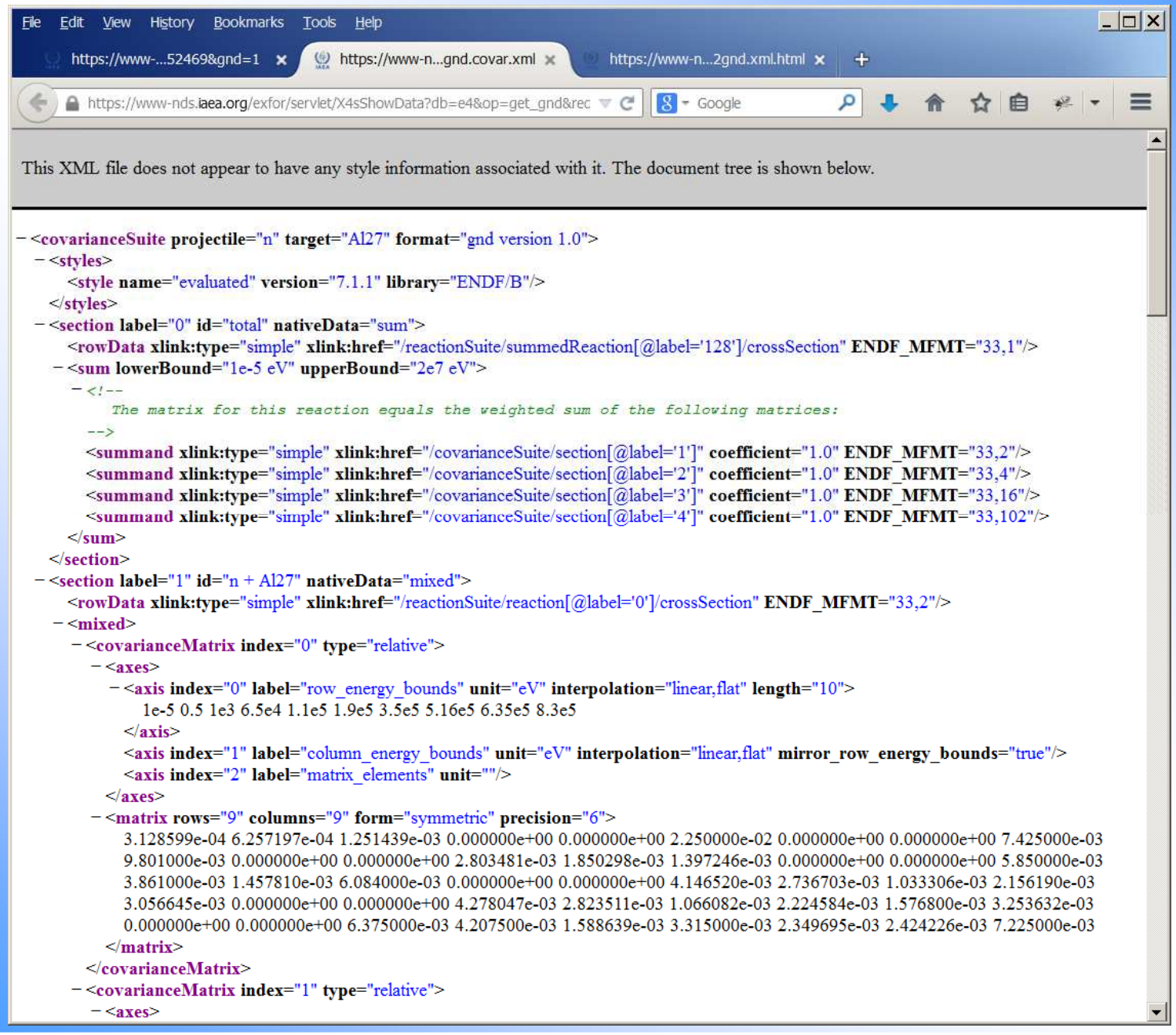
GND contacts: mattoon1@llnl.gov and beck6@llnl.gov

Translation program can be tested on 46 ENDF libraries

Display GND output via html



Display gnd.coval.xml via web browser



Errors and feedback

ENDF Web Retrieval System

Conversion ENDF file to GND format.
Request #52469.
MAT: Library="JENDL-4.0" Target="AL-27" MAT=1325 NSUB=10 (N)

#	File	Comment	Date	Length
1	gnd.endf	Input file	2014/10/28 10:27:39	582,147
2	gnd_cmd.err	Error file	2014/10/28 10:27:41	1,180
3	gnd_cmd.log	Log file	2014/10/28 10:27:41	118
4	gnd_cmd.ttout	Terminal output	2014/10/28 10:27:41	2,368

---ERROR---

GND contacts: mattoon1@llnl.gov and beck6@llnl.gov

Feedback

gnd_cmd.log

```
Running FUDGE package:
2014-10-28 10:27:39
2014-10-28 10:27:39 rePrint.py
Error running rePrint.py.......Error-code=1
```

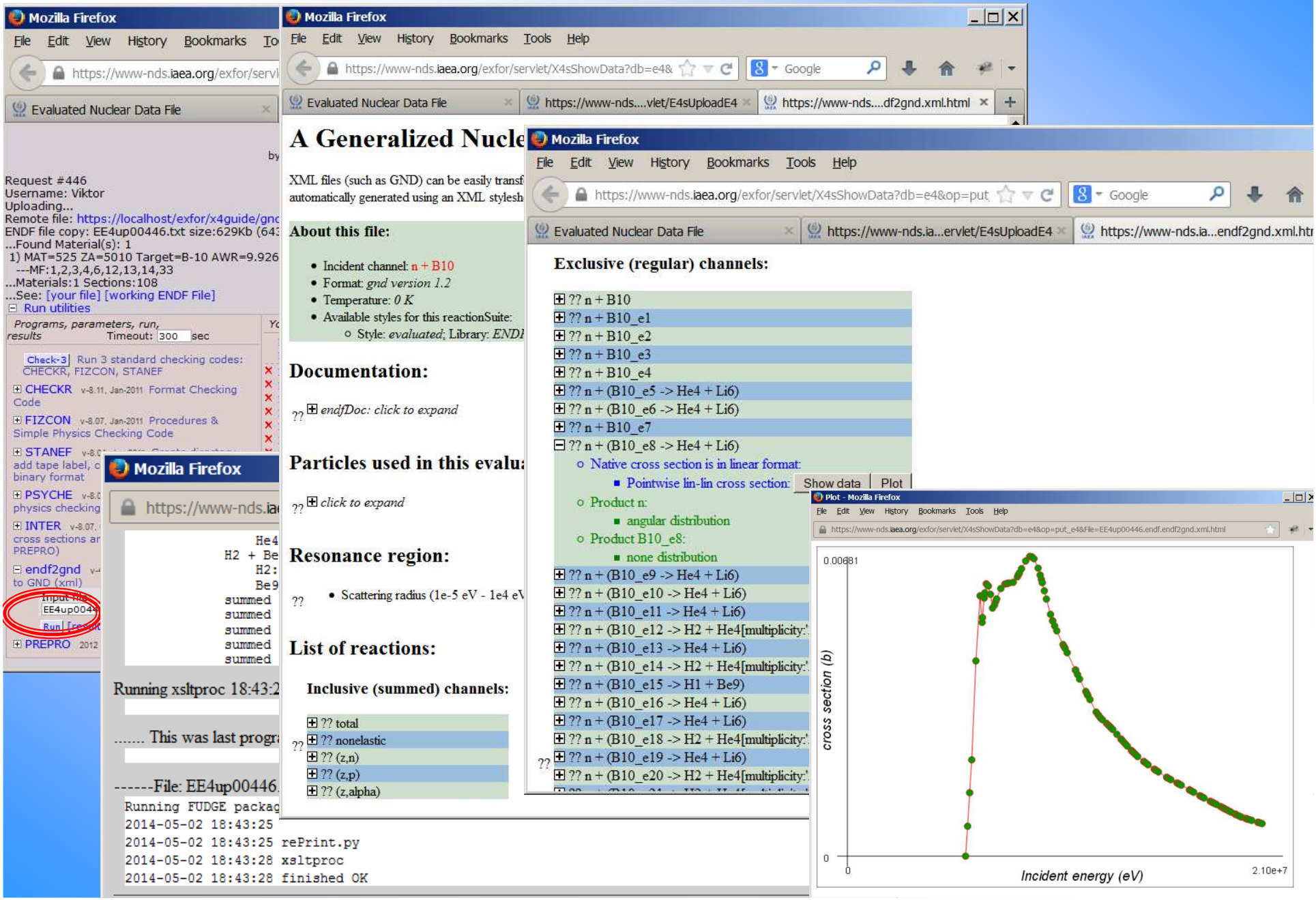
gnd_cmd.err

```
Warning from fudge2dGrouping.py: numpy not imported
Warning from endl2dmathClasses.py: numpy not imported
       WARNING: distributions for MT=3 (nonelastic) are not supported and have been ignored
Traceback (most recent call last):
  File "/usr/share/tomcat6/webapps/exfor/x4prog/./EndfUtil/gnd/fudge-4.0.0/bin/rePrint.py", line 94, in <module>
    f.write( x.toENDF6( flags, covarianceSuite=c ) )
  File "/usr/share/tomcat6/webapps/exfor/x4prog/EndfUtil/gnd/fudge-4.0.0/fudge/gnd/reactionSuite.py", line 567, in toENDF6
    channel.toENDF6( endfMFList, flags, targetInfo, verbosityIndent = verbosityIndent2 )
  File "/usr/share/tomcat6/webapps/exfor/x4prog/EndfUtil/gnd/fudge-4.0.0/fudge/gnd/reactions/reaction.py", line 399, in toENDF6
    gndToENDF6.gammasToENDF6_MF12_13( MT, 12, endfMFList, flags, targetInfo, gammas )
  File "/usr/share/tomcat6/webapps/exfor/x4prog/EndfUtil/gnd/fudge-4.0.0/fudge/legacy/converting/gndToENDF6.py", line 279, in
gammasToENDF6_MF12_13
    if( piecewise is not None ) : raise Exception( 'Only one piecewise is currently supported for MF=12 multiplicity data' )
Exception: Only one piecewise is currently supported for MF=12 multiplicity data
```

gnd_cmd.ttout

```
     WARNING: distributions for MT=3 (nonelastic) are not supported and have been ignored
    2 [3, 4] : MF=4, LTT = 1
   51 [3, 4, 12, 14] : MF=4, LTT = 2 : MF=12 LO=1 : ZAP=0 : MF=14
   52 [3, 4, 12, 14] : MF=4, LTT = 2 : MF=12 LO=1 : ZAP=0 : MF=14
   53 [3, 4, 12, 14] : MF=4, LTT = 1 : MF=12 LO=1 : ZAP=0 : MF=14
   54 [3, 4, 12, 14] : MF=4, LTT = 1 : MF=12 LO=1 : ZAP=0 : MF=14
```

Endf2gnd under MyEndf (tool for evaluators)



Google Analytics

Custom Report

Apr 1, 2015 - Apr 30, 2015

41.	ENDF	download:ENDF6-MAT	132 (0.12%)	60 (0.39%)	00:01:44	0.00	00:00:00
42.	ENDF	Search(ENDF_Explorer)	94 (0.09%)	17 (0.11%)	00:01:04	18.80	00:08:18
43.	ZVView	X4R33-Plot	90 (0.08%)	17 (0.11%)	00:00:52	0.00	00:00:00
44.	EXFOR	download:X4Out.txt	87 (0.08%)	46 (0.30%)			
45.	EXFOR	goto:X4Construct-Covar	84 (0.08%)	58 (0.38%)			
46.	EXFOR	download:R33	82 (0.08%)	20 (0.13%)			
47.	EXFOR	Search(from_CINDA)(byLink)	76 (0.07%)	11 (0.07%)			
48.	EXFOR	download:XML+XSLT	71 (0.07%)	16 (0.10%)			
49.	IBANDL	download:SaveRemoteSC33	69 (0.06%)	17 (0.11%)			
50.	EXFOR	Text-Search	57 (0.05%)	18 (0.12%)			
51.	EXFOR	goto:NSR-Keyno	53 (0.05%)	36 (0.23%)			
52.	ENDF	download:Mat2gnd	51 (0.05%)	33 (0.22%)			
53.	EXFOR	download:C5	51 (0.05%)	20 (0.13%)			
54.	ENDF	download:ENDF6-PEN	50 (0.05%)	34 (0.22%)			
55.	IBANDL	Stat	41 (0.04%)	19 (0.12%)	00:00:31	20.50	00:02:19
56.	IBANDL	Search-Ref	35 (0.03%)	15 (0.10%)	00:01:25	0.00	00:00:00
57.	ZVView	C4Plot	31 (0.03%)	11 (0.07%)	00:00:39	0.00	00:00:00
58.	IBANDL	download:ViewRemoteSC33	30 (0.03%)	20 (0.13%)	00:01:25	0.00	00:00:00
59.	IBANDL	download:ViewSC33	22 (0.02%)	13 (0.08%)	00:01:35	0.00	00:00:00
60.	EXFOR	download:X4Out.xml	21 (0.02%)	18 (0.12%)	00:00:17	0.00	00:00:00
61.	IBANDL	download:SaveSC33	21 (0.02%)	8 (0.05%)	00:03:20	21.00	00:15:49
62.	EXFOR	download:X4+(fromTextSearch)	13 (0.01%)	8 (0.05%)	00:01:14	0.00	00:00:00
63.	ENDF	download:PlottedData2	12 (0.01%)	3 (0.02%)	00:01:08	0.00	00:00:00
64.	EXFOR	download:X4CT	12 (0.01%)	7 (0.05%)	00:01:59	0.00	00:00:00
65.	EXFOR	download:XML	12 (0.01%)	11 (0.07%)	00:00:07	0.00	00:00:00

Web statistics April 2015

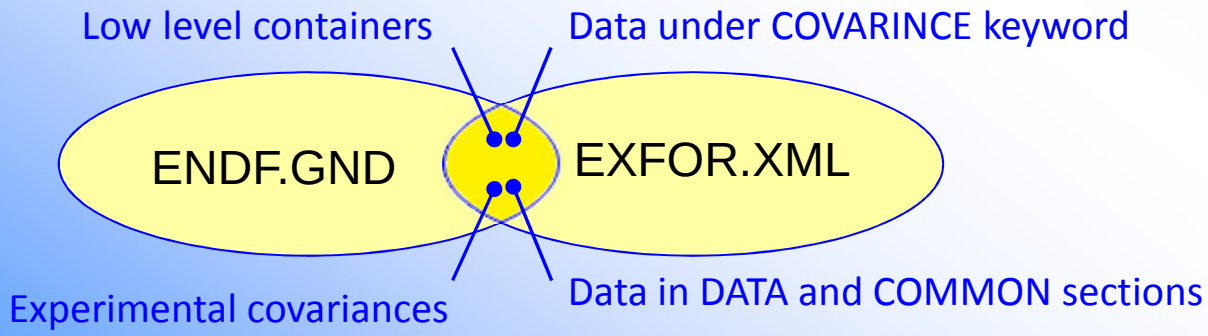
database	*data*	*downloads*	*users*
ENDF	ENDF6-MAT	132	60
EXFOR	x4out.txt	87	46
EXFOR	make-covar.	84	58
EXFOR	XML+XSLT	71	16
ENDF	Mat2gnd	51	33
ENDF	ENDF6-PEN	50	34
EXFOR	x4out.xml	21	18
EXFOR	x4.xml	12	11

Problems?

1. Now translation ENDF to GND works only for ONE material in input file. *(Legal ENDF-6 data file can contain several materials from several sub-libraries and even libraries)*
2. Translation program produces TWO output XML files: data file and covariance file. Schema and translation program should have an option to generate single GND file from one ENDF-6 file.
   (This problem might be inherited from the decision to store data in schema MAT-MT-MF as it is done in ENDL, but not MAT-MF-MT as it is done in ENDF)
3. Translation program fails on PEN file (i.e. ENDF-6 file from PREPRO chain including FIXUP)
4. Particle data properties for old evaluations: do they really to data used at that time?

2. Requirements for low level containers: EXFOR vs. ENDF

1. Large variety of Units (+translation to basic units)
2. Measured quantity is presented in vector
3. Empty values in data (<null>, “NaN”)
4. Complex descriptions of reaction/quantity
5. No curves (no need for interpolation)



3. Proposals

“Normalized” (canonical) XML file:

1) One tag in one line
2) Every tag in one line (i.e. `<tag>` and `</tag>`)
3) Every element-body text starts in new line separated from <tags>
4) 6 (or 10) numeric values in one data line (alternative: max-string-length=1024)

Fortran XML-I/O library:

1) Simplified API (~SAX) for “normalized” XML, e.g.:
```
openGndFile(fileName,iun),closeGndFile(iun)
readNextTag(iun,tag), writeNextTag(iun,tag)
readElmentBodyR8(array)
readElmentBodyText(array)
```
2) Attract ENDF programming users:
   create and offer simple examples

Proposals (cont.)

Extensions for low level containers:

1) Add possibility to <XYs> to store separately {Xs} and {Ys}
2) Allow additional arrays of dependent variables $\{Ys_j\}$ to <XYs>
3) Add possibility to generate <values> using <series>
4) Add attribute `default_value` to `<values>`

Decorative:

1) Rename manual describing low level containers from: "General-Purpose Data Containers for Science and Engineering" to: "`General-Purpose Nuclear Data Containers`"
2) Check acronyms with other networks and potential users, e.g.: `shape` vs. `dimension`; function $x_0(x_n, \ldots, x_1)$ vs. $y(x_1, \ldots, x_n)$; terminology in particle properties database with ENSDF evaluators; compatible coding of reactions in EXFOR, etc.
3) Documentation: describe allowed nesting of elements

4. Summary (highlights)

1) “Normalized” XML
2) Fortran I/O library for XML
3) Low level compatibility with EXFOR.XML
4) Translation ENDF to GND for any valid ENDF file: i.e. PEN files, files with several Materials from different sub-libraries and libraries, and for old libraries

Thank you

Citing of the materials of this presentation should be done with proper acknowledgement of the IAEA and author.