

Remote Web server calculations for EXFOR, ENDF, EMPIRE, GND

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Nuclear Data Section

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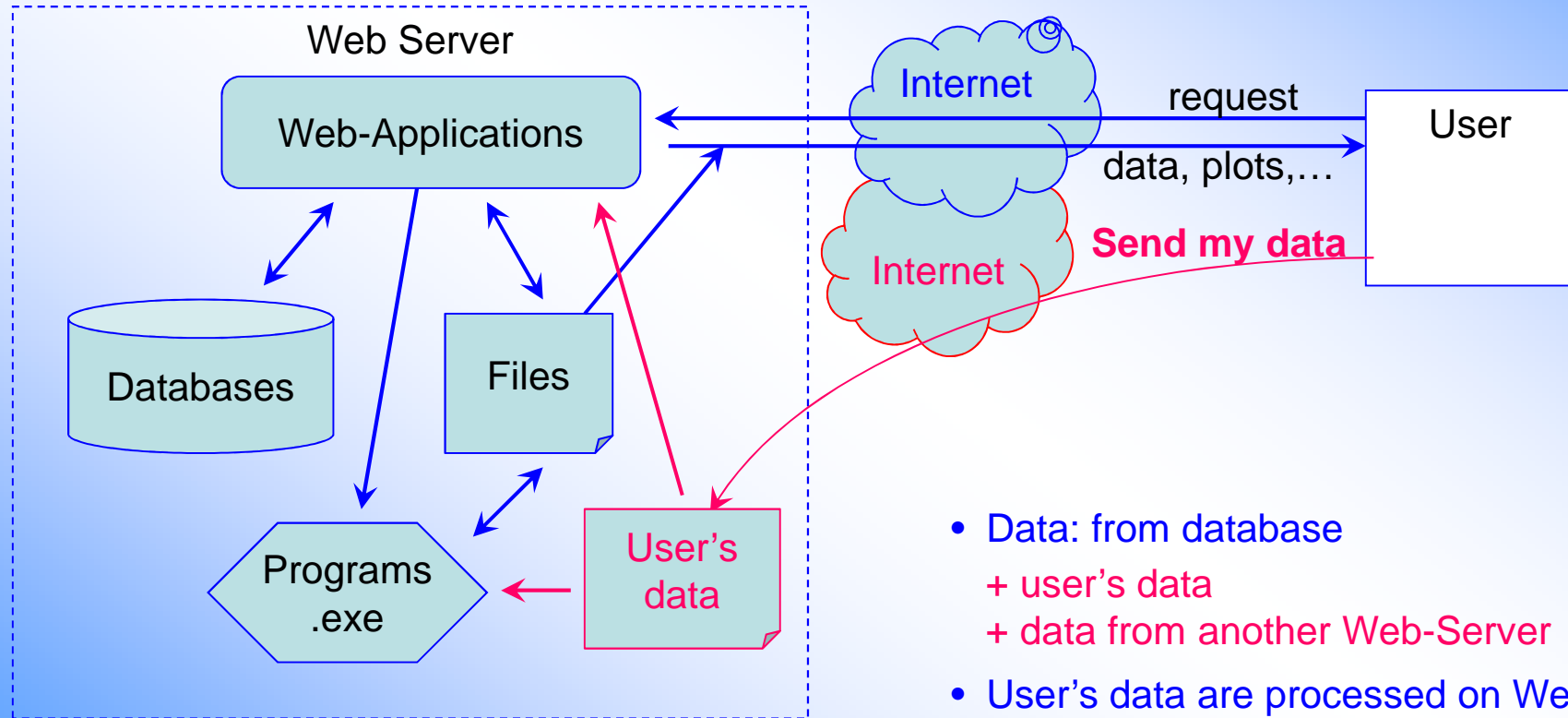
Topics:

1. Processing user's data on Web-Server
2. NDS Web server applications
3. Integrating Web Empire to Web system
4. Web interface to EMPIRE-3.1
5. Using results of Empire calculation into:
 1. ENDF Uploading system: calling ENDF utilities, Prepro, ENDF-GND software (LLNL) on-line
 2. EXFOR-ENDF database retrieval system

Processing user's data on Web-Server

▶ New type of service (for professionals)

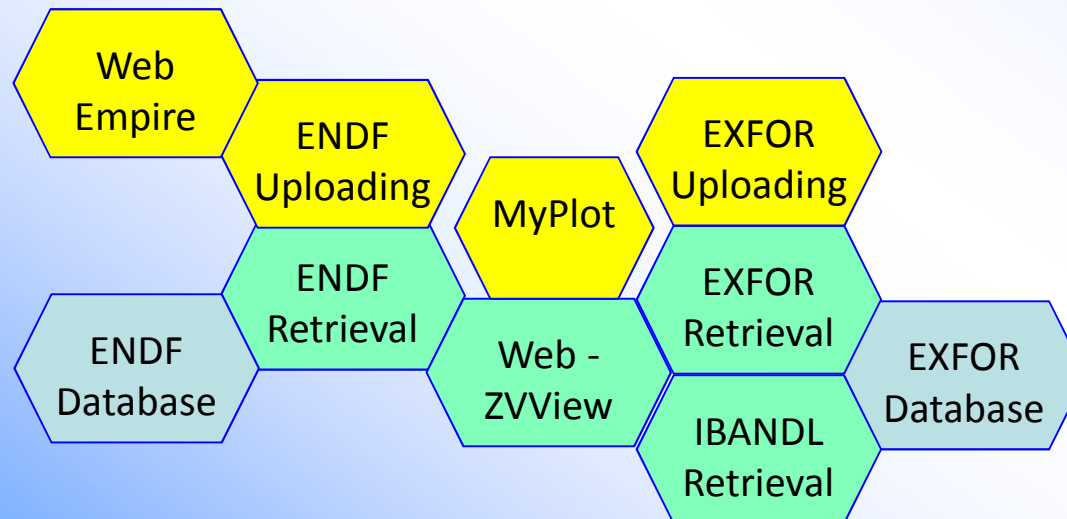
Structure and basic ideas



- Data: from database
+ user's data
+ data from another Web-Server
- User's data are processed on Web-Server
- User's data can be plotted and compared with data from databases

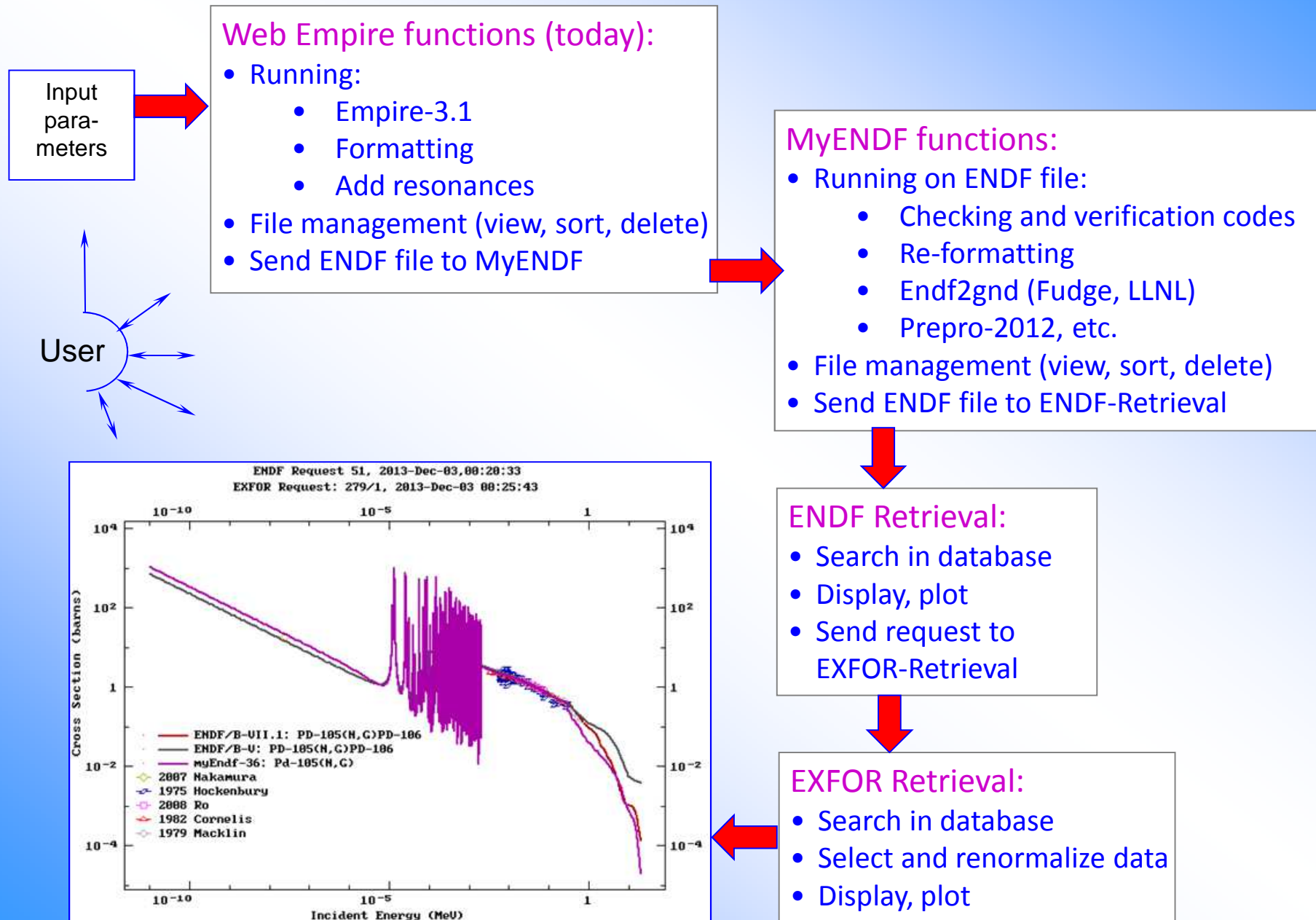
NDS Web server applications

MyPlot	Plotting with Web-ZVView (2009)
MyEXFOR	Uploading System (2010) ZCHEX, ZORDER, XTRACT, X4TOC4; Web-EXFOR
MyENDF	Uploading System (2010-2011) CHECKR, FIZCON, STANEF, PSYCHE, INTER, PREPRO, ENDVER, FUDGE, Web-EXFOR-ENDF
MyENSDF	Uploading System (2011) FMTCHK, GTOL, LOGFT, PANDORA, NDSPUB, RADLST
EMPIRE-3.1	Web Interface to Empire /under development/ (2013)



Web-Empire can be built-in to Web system easy, because many functions of Empire package are implemented in Web Applications

Integrating Web Empire to Web system



Web interface to EMPIRE-3.1

Empire-3.1 - Mozilla Firefox

File Edit View History Bookmarks Tools Help

zlinux2.iaea.org:8080/exfor3/servlet/X4sSearch5

Web-interface to EMPIRE-3.1.

by V.Zerkin, IAEA-NDS, September 2013

Submit Reset Submit in new Window

Session: 2
Your name: Viktor
Project: Pd105

Upload your input file (*.inp): Browse... No file selected.

or enter your input file to the text area below

Examples: Pd105

```
0.001 ;INCIDENT ENERGY (IN LAB)
105. 46. ;TARGET A , Z
1. 0. ;PROJECTILE A, Z
2 ;NUMBER OF NEUTRONS TO BE EMITTED
1 ;NUMBER OF PROTONS TO BE EMITTED
1 ;NUMBER OF ALPHAS TO BE EMITTED
1 ;NUMBER OF DEUTERONS TO BE EMITTED
0 ;NUMBER OF TRITONS TO BE EMITTED
0 ;NUMBER OF He-3 TO BE EMITTED
0 0. 0. ; reserved
*****
* Optional input starts here, FIXED FORMAT, (lines starting with *,#,! are comments)
*-----!-----!-----!
@ Pd105: Example input file EMPIRE-3.1
IOUT 3.
LEV DEN 0. EMPIRE NLD (EGSM RIPL-3) as default
NEX 080. Number of points in the outgoing energy grid
HRTW 3. Width fluctuations considered up to 3 MeV (for neutron induced)
```

Web and Database Programming: Viktor Zerkin, NDS, International Atomic Energy Agency (V.Zerkin@iaea.org)
Last updated: 11/05/2013 18:03:33

Find: start Next Previous Highlight all Match case

Web interface to EMPIRE-3.1

Request #24
Username: Viktor Area: EM4up00024 Project: Pd105
Input file copy: Pd105.inp size:19Kb (18492 bytes)

Projectile	Target	To be emitted: number of
n → A:1 Z:0	¹⁰⁵ Pd A:105 Z:46	→ Neutrons: 2 → Protons: 1 → Alphas: 1 → Deuterons: 1

...See copy of your input file: [\[text\]](#)

Run utilities

Programs, parameters, run, results Timeout: 3600 sec Files Refresh sorting by [\[name\]](#) [\[extension\]](#) [\[length\]](#) [\[time\]](#)

EMPIRE Empire-3.1. calculations /v-3.1, 12-Dec-2012/

Input File: Pd105

Run EMPIRE-3.1

Formatting

Adding resonances

MAT number: 1111

[Run](#) [Clean](#) [CleanAll](#)

↓

Output: [Full](#) [Short](#) [ENDF](#)

↓

Next: [Send](#) ENDF to checking, pre-processing, plotting, comparing with ENDF libraries and EXFOR database, etc.

Pd105.inp 18,492 2013/12/03 00:41:06

Total files: 1, length: 18492 bytes

Check your input

Running Empire in “Web-terminal” window

Request #24
Username: Viktor Area: EM4up00024 Project: Pd105
Input file copy: Pd105.inp size:19Kb (18492 bytes)

Projectile	Target	To be emitted: number of
n → A:1 Z:0	¹⁰⁵ Pd A:105 Z:46	→ Neutrons: 2 → Protons: 1 → Alphas: 1 → Deuterons: 1

...See copy of your input file: [\[text\]](#)

Run utilities

Programs, parameters, run, results Timeout: 3600 sec File

EMPIRE Empire-3.1, calculations /v-3.1, 12-Dec-2012/ Pd1

Input File: Pd105
 Run EMPIRE-3.1
 Formatting
 Adding resonances
MAT number: 1111

Run Clean CleanAll

```
Running EMPIRE program
Basic file: Pd105
Input file: Pd105
Area: EM4up00002
Timeout: 60min
Elapsed time=00:06:07 ...finished
Start process....

EEEE M M PPPP I RRRR EEEEE 33333
E MM MM P P I R R E 33
EEE M MM M PPPP I RRRR EEE = 33333
E M M P I R R E 3
EEEE M M P I R R EEEEE 33333

R I V O L I ( release 3.1 )

Sao Jose dos Campos, Brazil, May 2011
Upton, New York, USA, January 2012

Using existing file with input: Pd105.inp

Pd105 R U N N I N G ! ! ! ! ! ! ! !
WARNING: No experimental data in IAEA EXFOR-C4 file:
/usr/share/tomcat6/webapps/exfor/x4prog/empire/EXFOR/neutrons/046

Pd105: Example input file EMPIRE-3.1
C.M. incident energy .99048E-03 MeV
Running ECIS (sphe) ...
Decaying nucleus # 1 of 18 ( 46-Pd-106)
Decaying nucleus # 2 of 18 ( 46-Pd-105)
Decaying nucleus # 3 of 18 ( 46-Pd-104)
Decaying nucleus # 4 of 18 ( 45-Rh-105)
Decaying nucleus # 5 of 18 ( 45-Rh-104)
```


After calculations have been finished

Running EMPIRE prog
Basic file: Pd105
Input file: Pd105
Area: EM4up00002
Timeout: 60min
Elapsed time
Start process....

```
EEEEEE M M  
E MM MM  
EEE M MM M  
E M M  
EEEEEE M M  
  
R I  
Sao Jose  
Upton,  
  
Using existing file  
Pd105 R U N N I N  
WARNING: No exper  
/usr/share/tomcat  
  
Pd105: Example i  
C.M. incident en  
Running ECIS (sp  
Decaying nucleus  
Decaying nucleus  
Decaying nucleus  
Decaying nucleus
```

Request #24
Username: Viktor Area: EM4up00024 Project: Pd105
Input file copy: Pd105.inp size:19Kb (18492 bytes)

Projectile	Target	To be emitted: number of
n → A:1 Z:0	¹⁰⁵ Pd A:105 Z:46	→ Neutrons: 2 → Protons: 1 → Alphas: 1 → Deuterons: 1

...See copy of your input file: [text]
Run utilities

Programs, parameters, run, results Timeout: 3600 sec

EMPIRE Empire-3.1. calculations /v-3.1, 12-Dec-2012/
Input File: Pd105
 Run EMPIRE-3.1
 Formatting
 Adding resonances
MAT number: 1111
Run Clean CleanAll

Output: Full Short ENDF

Next: Send ENDF to checking, pre-processing, plotting, comparing with ENDF libraries and EXFOR database, etc.

Files Refresh sorting by [name] [extension] [length] [time]

Files	Refresh	sorting by	[name]	[extension]	[length]	[time]
↑ Pd105-e.endf	1,139,589	2013/12/03	01:08:25			
↑ Pd105-endres.endf	1,199,448	2013/12/03	01:09:57			
↑ Pd105-f.endf	1,143,639	2013/12/03	01:09:55			
Pd105-fiss.xsc	0	2013/12/03	00:44:09			
Pd105-log.empend	360,278	2013/12/03	01:08:25			
Pd105-log.endres	2,403	2013/12/03	01:09:57			
Pd105-log.fixup	18,448	2013/12/03	01:09:55			
↑ Pd105-z2n.zvd	1,430	2013/12/03	01:08:12			
↑ Pd105-za.zvd	1,430	2013/12/03	01:08:12			
↑ Pd105-ze1.zvd	1,430	2013/12/03	01:08:12			
↑ Pd105-zg.zvd	1,430	2013/12/03	01:08:12			
↑ Pd105-zn.zvd	1,430	2013/12/03	01:08:12			
↑ Pd105-znon.zvd	1,430	2013/12/03	01:08:12			
↑ Pd105-zp.zvd	1,430	2013/12/03	01:08:12			
↑ Pd105-ztot.zvd	1,430	2013/12/03	01:08:12			
× Pd105.addresonances.err	63	2013/12/03	01:09:58			
× Pd105.addresonances.tt	20,204	2013/12/03	01:09:58			
× Pd105.empire.err	194	2013/12/03	01:08:12			
× Pd105.empire.tt	36,309	2013/12/03	01:08:12			
↑ Pd105.endf	1.231.281	2013/12/03	01:09:58			

Input and output Empire files

Results of calculation

Upload data to further processing

Result of Empire calculation (ENDF file) sent into the ENDF Uploading system

The screenshot shows the ENDF-uploading system interface. At the top, it displays the title "ENDF-uploading system" and the author "by V.Zerkin, IAEA-NDS, November 2010 - November 2013". Below this, it shows the details of a request: "Request #1", "Username: Viktor", and "Uploading...". The main content area shows the upload progress: "ENDF file copy: EE4up00001.txt size:2Mb (1231281 bytes)", "...Found Material(s): 1", and a list of materials: "1) MAT=1111 ZA=46105 Target=Pd-105 AWR=104.004 NSUB=10 LISO=0 EMAX=2.0E7 ZSYNAM= 46-Pd-105 ALAB=EMPIRE EDAT ---MF:1,2,3,4,6,8,10,12,14". Below this, there are links for "[your file]" and "[working ENDF File]".

The interface is divided into two main sections. The left section, titled "Programs, parameters, run, results", contains a list of utilities: "CHECKR", "FIZCON", "STANEF", "PSYCHE", "INTER", "endf2gnd", and "PREPRO". The "PREPRO" utility is selected, and its parameters are shown: "Input File: EE4up00001.endf", "Reconstruct cross sections at the temperature 293.6 (Kelvin)", and "with accuracy 0.1 (per-cent)". A "Run" button is visible below these parameters.

The right section, titled "Your Files [refresh]", shows a list of uploaded files: "EE4up00001.endf-mfnt", "EE4up00001.endf", and "EE4up00001.txt". Below this list, it states "Total files: 3, length: 2470755 (byte)".

Below the utility list, there is a section titled "ENDF Materials in your file:" which lists the materials found in the file: "1) MAT=1111 IZA=46105 NSUB=10 LISO=0 Target=Pd-105". Below this, it lists the databases found: "Found in: ENDF/B-VII.1; JEFF-3.1.2; JENDL-4.0; BROND-2.2; CENDL-3.1; JENDL-3.3/300; ENDF/B-VI.8-300; ROSFOND-2010; JEFF-3.1/A; EAF-2010; MENDL-2; TENDL-2012;".

At the bottom of the interface, there is a search section titled "Search similar data in ENDF and EXFOR databases...". It contains a table of search results for "NSUB=10 [N] Incident-Neutron Data". The table lists various materials and their corresponding data types, such as "Pd-105 MF=2 Resonance parameters", "Pd-105 MF=3 Cross sections", "Pd-105 MF=4 Angular distributions of secondary particles", "Pd-105 MF=6 Product energy-angle distributions", "Pd-105 MF=8 Radioactive decay data", "Pd-105 MF=10 Cross sections for production of radioactive elements", and "Pd-105 MF=12 Photon production multiplicities and transition probabilities".

There are three yellow callout boxes with red borders and black text. The first callout box, located near the "Run" button, contains the text "Run Prepro-2012". The second callout box, located near the "Your Files" section, contains the text "Libraries in database having the same NSUB & Material". The third callout box, located near the search results table, contains the text "Go to retrieval systems".

Run Prepro-2012

Libraries in database having the same NSUB & Material

ENDF File structure

Go to retrieval systems

After running Prepro:search in ENDF database

Request #51
ENDF Data Selection +myEndf#36

Retrieve **Plot** Selected Unselected All Reset

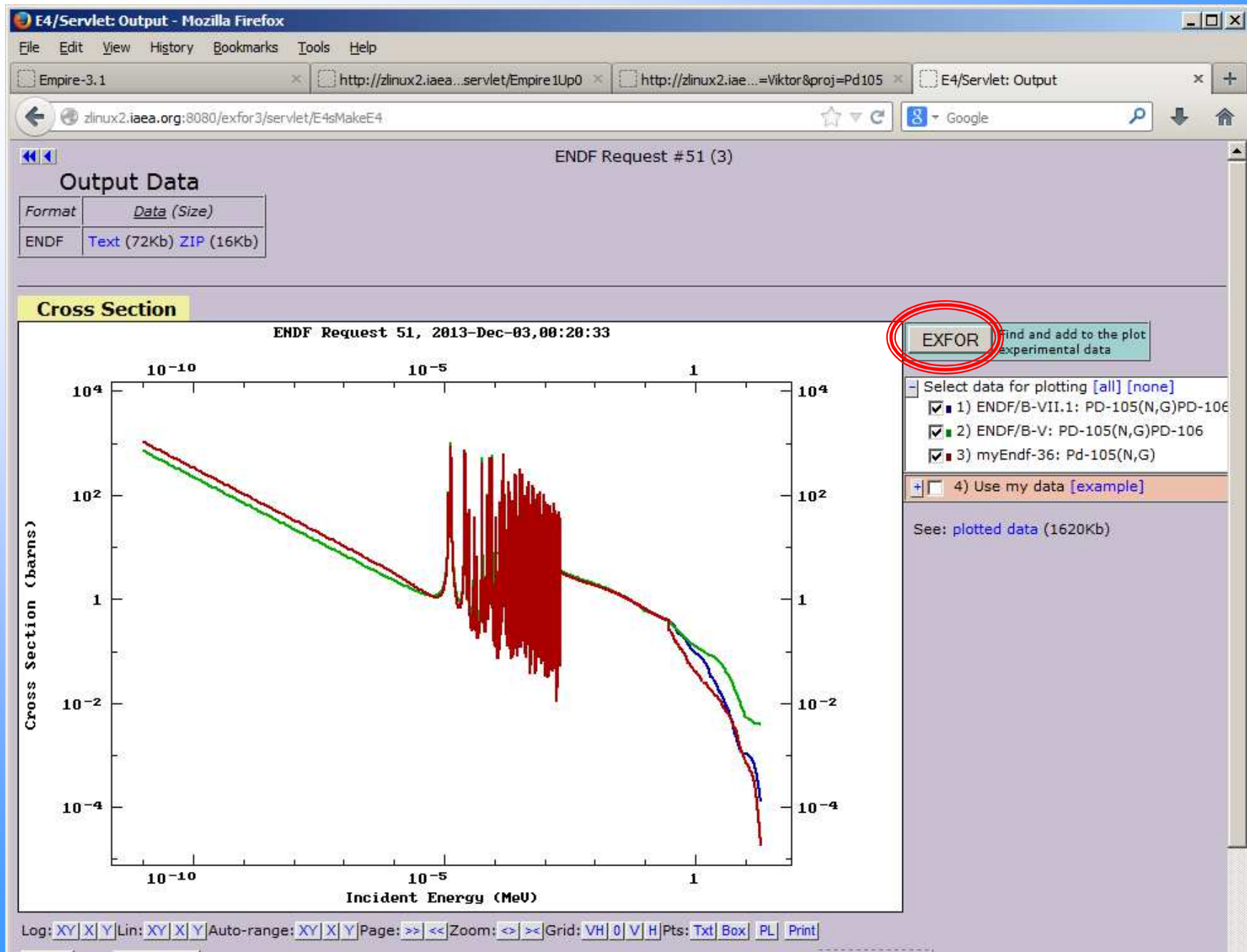
Plotting options: Quick plot (cross-sections only: σ)
Universal plot ($\sigma \pm \Delta\sigma$, $d\sigma/d\Omega$, $d\sigma/dE$, $d^2\sigma/dE/d\Omega$) *beta version*

Sorted by: [Reactions] Reorder by: [Libraries] View: basic extended/get MAT/PEN, run Inter: resonance integrals, etc.

1) PD-105 (N,G), SIG MI=102 MF=3 NSUB=10
MF3: [SIG] Cross sections MT102: [N,G] Radiative capture.

1	<input checked="" type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	myEndf-36	E=20MeV Lab=EMPIRE	
2	<input checked="" type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	ENDF/B-VII.1	E=20MeV Lab=BNL, KAERI Date=20111222	Kim, Herman, Oh, Mughabghab+
3	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	ENDF/B-VII.0	E=20MeV Lab=BNL, KAERI Date=DIST-DEC06	Kim, Herman, Oh, Mughabghab+
4	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	JEFF-3.1.2	E=20MeV Lab=BNL, KAERI Date=DIST-APR-11	Kim, Herman, Oh, Mughabghab+
5	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	JEFF-3.1	E=20MeV Lab=NEA Date=090105	H. GRUPPELAAR. E. MENAPACE
6	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	JENDL-4.0	E=20MeV Lab=JAEA Date=20100119	N. Iwamoto, K. Shibata
7	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	JENDL-3.3	E=20MeV Lab=JNDC Date=20020222	JNDC FP NUCLEAR DATA W.G.
8	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	JENDL-3.3	E=20MeV Lab=JNDC Date=20020222 T=300	JNDC FP NUCLEAR DATA W.G.
9	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	ENDF/B-VI	E=30MeV Lab=BNL, KAERI+ Date=20011108	S. Y. Oh, S. F. Mughabghab, P. Young
10	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	ENDF/B-VI	E=30MeV Lab=BNL, KAERI+ Date=20010926 T=300	S. Y. Oh, S. F. Mughabghab, P. Young
11	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	BROND-2.2	Lab=CJD Date=840712	IGNATYUK A. V., KRAVCHENKO I. V.
12	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	ROSFOND-2010	E=20MeV Lab=IPPE Date=DIST-DEC06	NIKOLAEV. M. N.
13	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	ROSFOND-2008	E=20MeV Lab=IPPE Date=DIST-DEC06	NIKOLAEV. M. N.
14	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	CENDL-3.1	E=20MeV Lab=NJU, NWU Date=DIST-DEC09	J. W. ZHAO, W. N. SU, Z. J. ZHANG, X. Q. SUN
15	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	JEFF-3.1/A	E=20MeV Lab=UKAEA Date=DIST-JUL03 T=293	Forrest, Kopecky, Sublet, Koning
16	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	JEFF-3.0	E=20MeV Lab=NEA Date=DIST-APR02	H. GRUPPELAAR. E. MENAPACE
17	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	JEF-2.2	Lab=NEA Date=920101	H. GRUPPELAAR. E. MENAPACE
18	<input type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	EAF-2010	E=60MeV Lab=CCFE, NRG Date=DIST-SEP11 T=293	
19	<input checked="" type="checkbox"/>	ENDF-6	Interpreted	σ	Plot	ENDF/B-V	Lab=HEDL, RCN Date=0	R. E. SCHENTER AND F. SCHMITTROT

Compare ENDF file from Empire with ENDF libraries



Search similar data in EXFOR database

X4/Servlet: Select - Mozilla Firefox

File Edit View History Bookmarks Tools Help

Empire-3.1 http://zlinux2...et/Empire1Up0 http://zlinux...or&proj=Pd105 E4/Servlet: Output X4/Servlet: Select

zlinux2.iaea.org:8080/exfor3/servlet/X4sSearch5

Request #279
Access-Level=2
Results: Reactions: 2 Datasets: 5

Data Selection (for ENDF Request #51)

Retrieve Selected Unselected All Reset

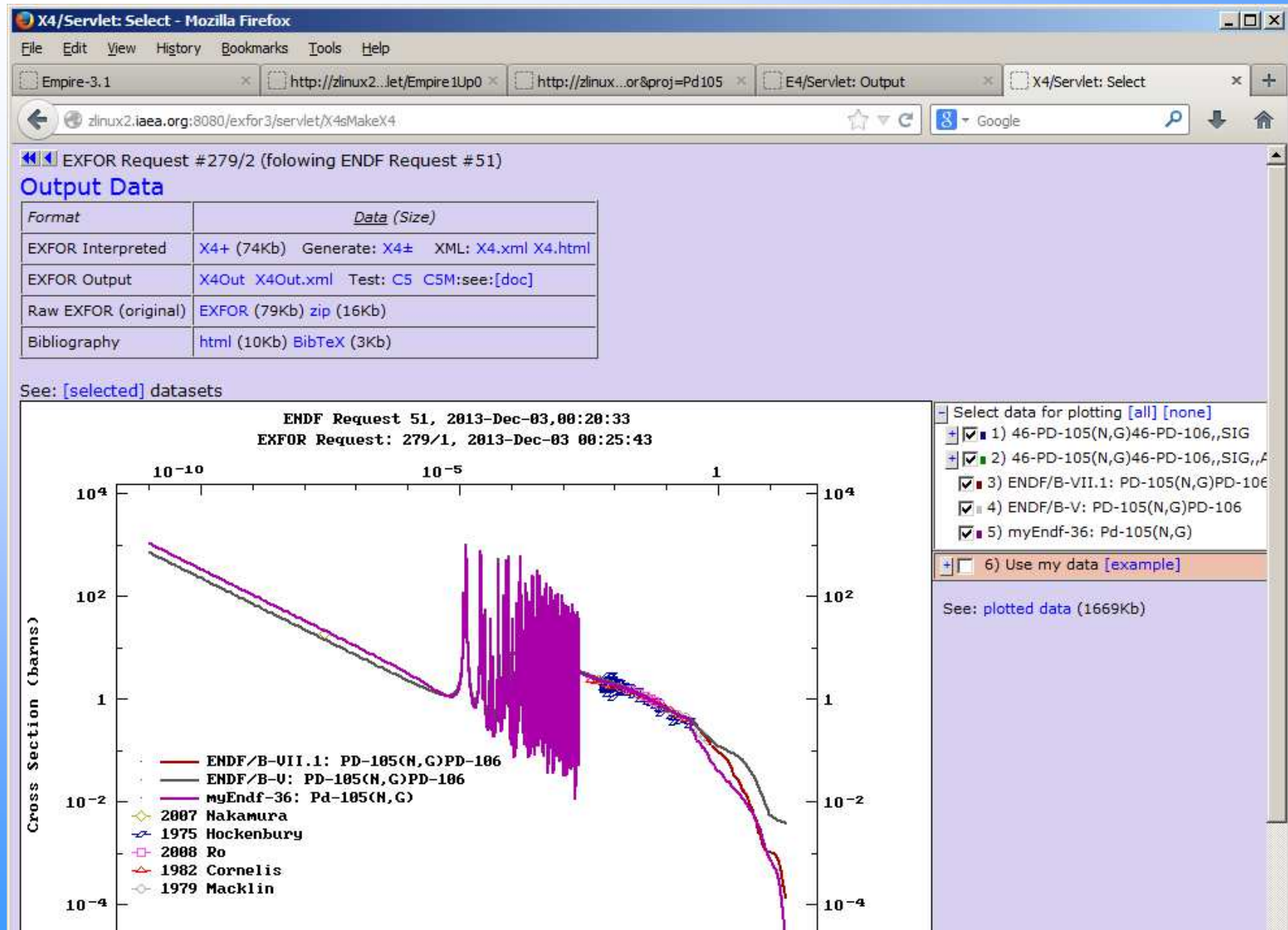
Output: X4+ EXFOR Bibliography TAB C4 PlotC4

Plot: Quick-plot (cross-sections only) Advanced plot [how-to] using C5 and converting ratios to cross sections using [IAEA-standards,2006]

Apply(1A) Data re-normalization (for advanced users, results in: C4, TAB and Plots)

n	Display	Year	Author-1	Energy range, eV	Points	Reference	Subentry#	NSR-Key
1	46-PD-105 (N,G) 46-PD-106,,SIG	2007	S.Nakamura+	2.50e-2	1	[pdf]+ J,NST,44,103,2007	14133003	2007NA10
2	46-PD-105 (N,G) 46-PD-106,,SIG,,AV	1975	R.W.Hockenbury+	6.31e3 2.97e5	562	[pdf]+ C,75WASH,2,905,197503	10435004	
3	46-PD-105 (N,G) 46-PD-106,,SIG,,AV	2008	T.-I.Ro+	1.50e4 9.00e4	6	[pdf]+ J,NSTS,5,443,2008	23081002	
4	46-PD-105 (N,G) 46-PD-106,,SIG,,AV	1982	E.Cornelis+	3.00e3 3.00e5	16	[pdf]+ C,82ANTWER,,222,8209	21810002	1983CO2N
5	46-PD-105 (N,G) 46-PD-106,,SIG,,AV	1979	R.L.Macklin+	3.00e3 7.00e5	18	[pdf]+ J,NSE,71,182,7908	10868008	1979MA34

Compare data from Empire calculation with ENDF and EXFOR databases



Calling ENDF-GND software (LLNL) on-line

Request #446
Username: Viktor
Uploading...
Remote file: <https://localhost/exfor/x4guide/gnd>
ENDF file copy: EE4up00446.txt size:629Kb (64...)
...Found Material(s): 1
1) MAT=525 ZA=5010 Target=B-10 AWR=9.926
--MF:1,2,3,4,6,12,13,14,33
...Materials:1 Sections:108
...See: [your file] [working ENDF File]
Run utilities

Programs, parameters, run, results
Timeout: 300 sec

- Check-3 Run 3 standard checking codes: CHECKR, FIZCON, STANEF
- CHECKR v-8.11, Jan-2011 Format Checking Code
- FIZCON v-8.07, Jan-2011 Procedures & Simple Physics Checking Code
- STANEF add tape binary for
- PSYCH physics of
- INTER cross section
- PREPRO
- endf2gnd to GND (x)
- Input
- Run
- PREPRO

Running xsltproc 18:43:28.....
..... This was last program. 1
-----File: EE4up00446.endf
Running FUDGE package:
2014-05-02 18:43:25
2014-05-02 18:43:25 rePrint.py
2014-05-02 18:43:28 xsltproc
2014-05-02 18:43:28 finished OK

A Generalized Nuclear Data File

XML files (such as GND) can be easily transferred and automatically generated using an XML stylesheet.

About this file:

- Incident channel: $n + B10$
- Format: *gnd version 1.2*
- Temperature: *0 K*
- Available styles for this reactionSuite:
 - Style: *evaluated*; Library: *ENDF*

Documentation:
[endfDoc: click to expand](#)

Particles used in this evaluation:
[click to expand](#)

Resonance region:
[Scattering radius \(1e-5 eV - 1e4 eV\)](#)

List of reactions:

Inclusive (summed) channels:

- total
- nonelastic
- (z,n)
- (z,p)
- (z,alpha)

Exclusive (regular) channels:

- $n + B10$
- $n + B10_e1$
- $n + B10_e2$
- $n + B10_e3$
- $n + B10_e4$
- $n + (B10_e5 \rightarrow He4 + Li6)$
- $n + (B10_e6 \rightarrow He4 + Li6)$
- $n + B10_e7$
- $n + (B10_e8 \rightarrow He4 + Li6)$
 - Native cross section is in linear format
 - Pointwise lin-lin cross section: [Show data](#) [Plot](#)
 - Product n:
 - angular distribution
 - Product B10_e8:
 - none distribution
- $n + (B10_e9 \rightarrow He4 + Li6)$
- $n + (B10_e10 \rightarrow He4 + Li6)$
- $n + (B10_e11 \rightarrow He4 + Li6)$
- $n + (B10_e12 \rightarrow H2 + He4$ [multiplicity: ...])
- $n + (B10_e13 \rightarrow He4 + Li6)$
- $n + (B10_e14 \rightarrow H2 + He4$ [multiplicity: ...])
- $n + (B10_e15 \rightarrow H1 + Be9)$
- $n + (B10_e16 \rightarrow He4 + Li6)$
- $n + (B10_e17 \rightarrow He4 + Li6)$
- $n + (B10_e18 \rightarrow H2 + He4$ [multiplicity: ...])
- $n + (B10_e19 \rightarrow He4 + Li6)$
- $n + (B10_e20 \rightarrow H2 + He4$ [multiplicity: ...])

The plot shows the cross section in barns (b) as a function of incident energy in eV. The y-axis ranges from 0 to 0.0081 b, and the x-axis ranges from 0 to 2.10e+7 eV. The data points, represented by green circles connected by a red line, show a sharp resonance peak at approximately 10^7 eV, reaching a maximum cross section of about 0.0081 b. The cross section decreases significantly as the incident energy increases beyond the resonance region.

Concluding remarks

- 1) Empire code is working on Web-cloud
(but not yet fast enough for practical usage)
- 2) ENDF Uploading system provides Web interface to ENDF utility codes, Prepro-2012, allows to use ENDF and EXFOR retrieval tools together with users' data on-line
- 3) ENDF Uploading system provides Web interface to converter ENDF to GND (LLNL) including Html interpretation and plotting on-line

Thank you.