

Expanding EMPIRE usability: portable package for Windows, Web interface, remote server calculations.

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Nuclear Data Section

IAEA workshop on Modelling and Evaluating Nuclear Reaction Data for Energy
and Non-energy Applications

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Topics:

1. Porting EMPIRE to Windows and Web. Concept.

2. Portable complete EMPIRE package for Windows

- 1) Tasks and requirements
- 2) Implementation. Common Tcl/Tk for Windows, Linux, Mac
- 3) Distribution:
 - a) “ready-to-run” system for Windows; DVD-ROM, USB, FTP
 - b) “express-system” for Linux

3. EMPIRE as Web application

- 1) General concept
- 2) Web interface to EMPIRE package
- 3) Current implementation: extension of ENDF Uploading system

4. EMPIRE with Web interface

- 1) Remote server calculations: problems and perspectives
- 2) Local calculations (on PC) using Web interface without Internet
- 3) Struggle for speed

1. Porting EMPIRE to Windows and Web

1. What do we have now?

- 1) System of Fortran and C codes called from interactive Tcl/Tk GUI via system of bash and python scripts using files-parameters.
- 2) Complete package works on Linux and Mac-OSX.
Part of the package works on Windows (without GUI).
- 3) The package requires installation including system components (Fortran and Active-Tcl/Tk).

2. What we can try to achieve?

- 1) Internet (Web) version of the package
- 2) Complete package for Windows (identical to Linux)
- 3) Portable version without installation of system components

Assess feasibility within a short time

3. How useful it can be? What would be the price?

- 1) Portable version for Windows can expand usability. (To discuss?)
- 2) Web version can be useful only if powerful server will be assigned
- 3) Price? Till now – 0. All was done for “academic interest”.

First version for Windows and Web are ready for testing by developers.

Process and status of the development

1. Original idea (2010)

- 1) To develop Web wrapping system for Empire package
- 2) To create PC system on Windows: Web interface + Empire package
- 3) To create “Empire in clouds”: Web-Empire on a remote Web server

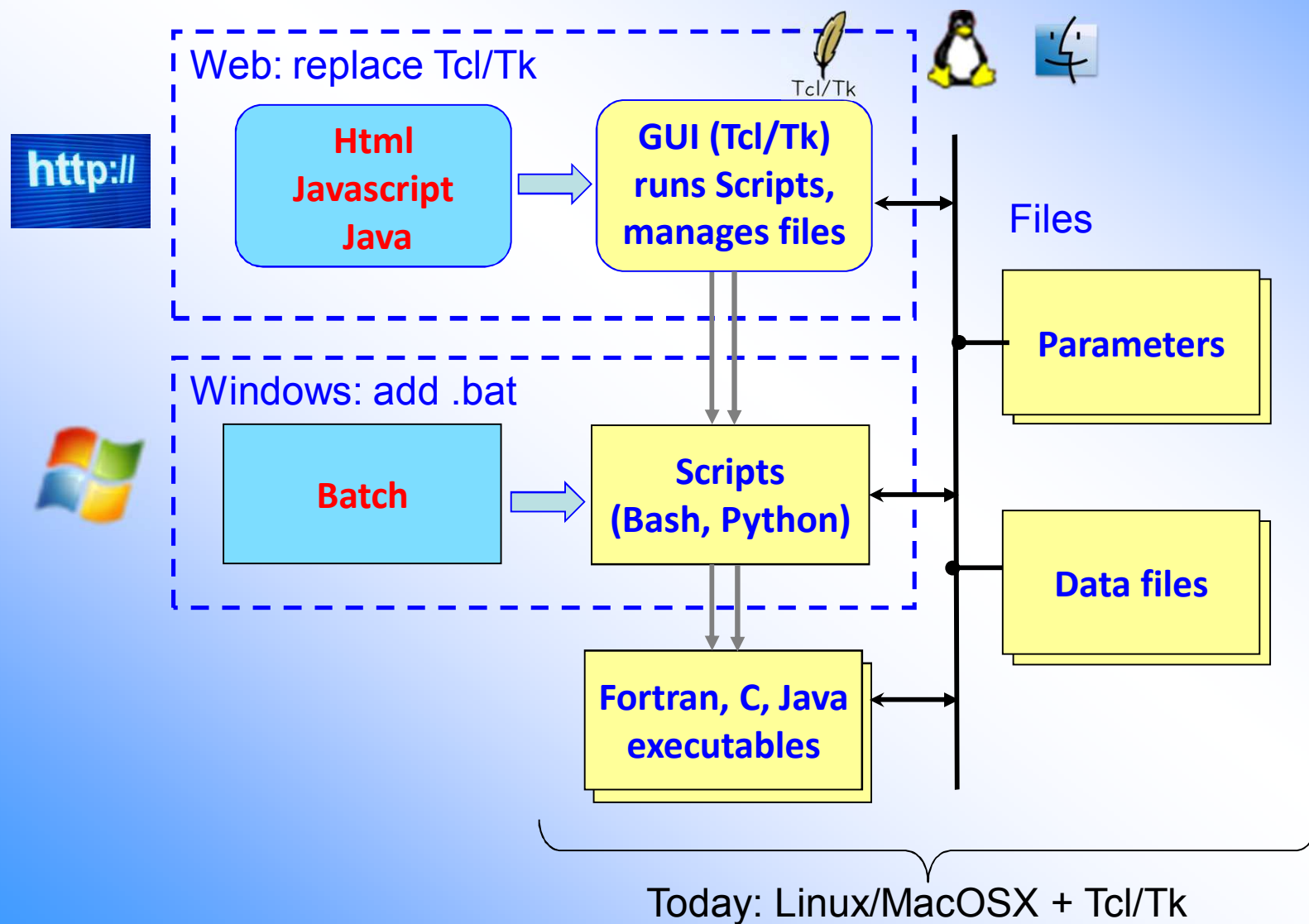
2. Steps of development (2013)

- 1) Web interface to run Empire core codes producing ENDF file (Sept.2013)
- 2) Porting core Empire codes to Windows (Oct.2013)
- 3) Individual Web Empire system on Windows (Oct.2013)
- 4) Understanding problems and practical needs
- 5) Struggle for speed (Oct. 2013)
- 6) Adaptation Empire Tcl/Tk for Windows (Oct.2013)
- 7) Portable version of Empire without installation for Windows (No. 2013)
- 8) Universal Tcl/Tk for Window/Linux/Mac
- 9) Express version of Empire for Linux (Nov.2013)

3. Status (as of end of 2013)

- 1) Original idea. “Empire in Clouds” - foggy perspectives.
- 2) Windows version: successful (may be included to official distribution)
- 3) Speed: may be important, should be re-done for 3.2 in systematic way

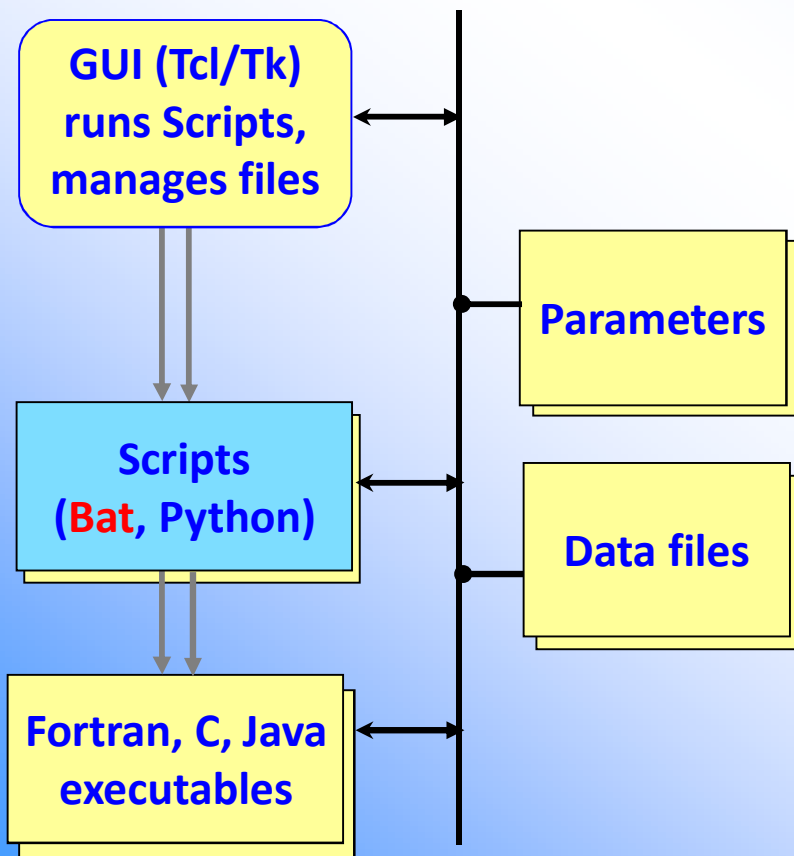
Porting EMPIRE to Windows and Web



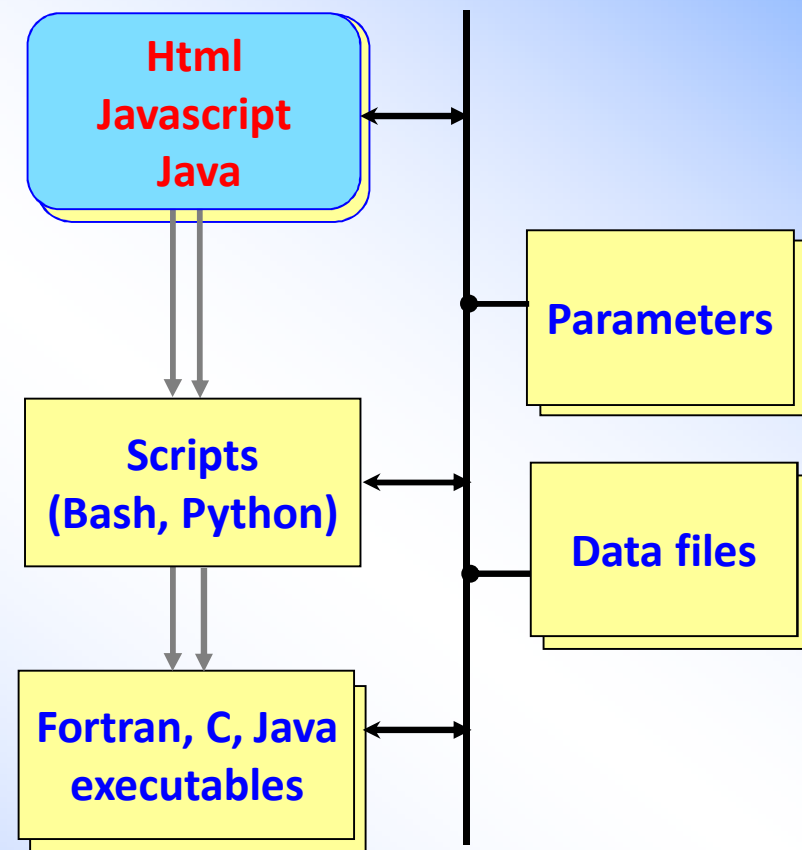
EMPIRE on Windows and Web



Windows + Tcl/Tk interface



Linux + Web interface



2. Full Empire package for Windows*

Tasks and requirements

- 1) To make main Tcl/Tk program Xrun.tcl executing MS-DOS commands running in popup terminal Window
- 2) Implement all basic GUI functions (including multiple selection) via MS-DOS scripts
- 3) Universal solution for call scripts either on Windows or Linux/Mac depending of platform (automatically detected)
- 4) The final system should not require any installation (only copying), i.e. to be fully portable

* *This project has appeared as “side-effect” during implementation of “Empire with Web interface”*

Porting Empire package to Windows

What was done

- 1) Modified main Tcl/Tk program Xrun.tcl executing both MS-DOS commands in popup terminal Window and xterm on Linux (including multiple selection)
- 2) 15 MS-DOS BAT-scripts implementing main functions
- 3) Portable version of EMPIRE for Windows is prepared for USB, DVD, FTP.

Portable version of EMPIRE for Windows

1. Empire with static executable 842Mb
2. Portable versions of:
 - 1) GNU Fortran (GCC) 8.4.0 199Mb
 - 2) Portable Python 2.7.5.1 591Mb
 - 3) Active Tcl/Tk 8.4.20 71Mb
 - 4) Postscript viewer 6Mb
 - 5) Text editor Notepad2 (LF, CR+LF) 1Mb
3. All directories are relative, .Xrunrc is in the working directory
4. No need for installation, no need for configuration.
All software is pre-configured and ready to run.
5. Start by [runme.bat](#) in working directory.
6. Size: ~2Gb. Works also from DVD-ROM (without copying to HD).

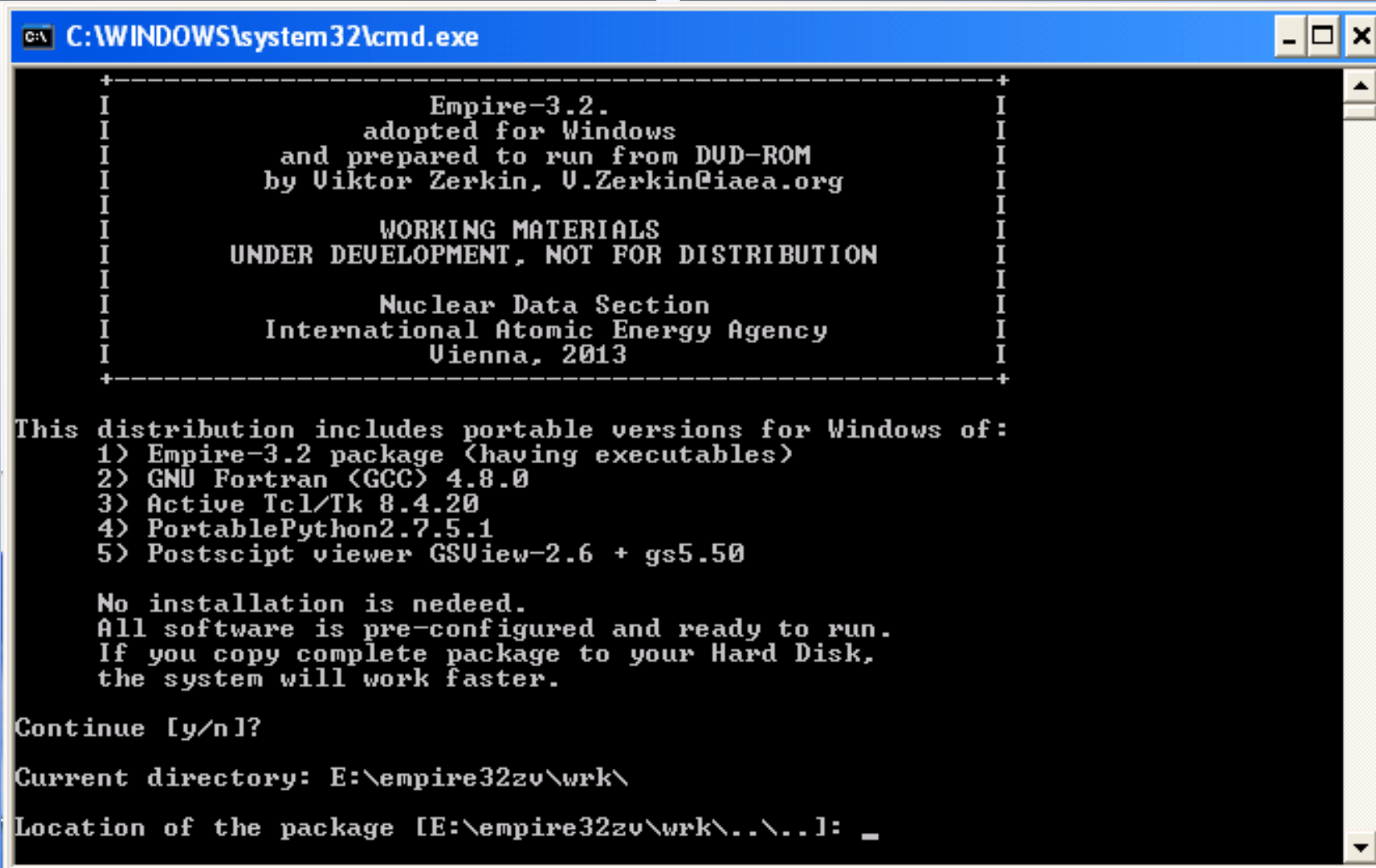
How to run portable Empire for Windows

How to install it?

- 1) No installation is needed!
- 2) Just copy **empire32zv** to your disk

How to run it?

- 1) Go to working dir **empire32zv\wrk**
- 2) Start file **runme.bat**



```
C:\WINDOWS\system32\cmd.exe
+-----+
|               Empire-3.2.               |
|               adopted for Windows        |
|               and prepared to run from  |
|               DUD-ROM                    |
|               by Viktor Zerkin, U.Zerkin@iaea.org |
|               |                           |
|               WORKING MATERIALS          |
|               UNDER DEVELOPMENT, NOT FOR DISTRIBUTION |
|               |                           |
|               Nuclear Data Section       |
|               International Atomic Energy Agency |
|               Vienna, 2013               |
+-----+

This distribution includes portable versions for Windows of:
1) Empire-3.2 package (having executables)
2) GNU Fortran (GCC) 4.8.0
3) Active Tcl/Tk 8.4.20
4) PortablePython2.7.5.1
5) Postscript viewer GSView-2.6 + gs5.50

No installation is needed.
All software is pre-configured and ready to run.
If you copy complete package to your Hard Disk,
the system will work faster.

Continue [y/n]?

Current directory: E:\empire32zv\wrk\
Location of the package [E:\empire32zv\wrk\..\..\]: _
```

Screenshot: Empire running on Windows

System Properties

System Restore Automatic Updates Remote
General Computer Name Hardware Advanced

System:
Microsoft Windows XP
Professional
Version 2002
Service Pack 3

Registered to:
IAEA
IAEA

About Empire-3.2

Welcome to Empire-3.2

Nuclear Reaction Model Code

Modular system of nuclear reaction codes for advanced modeling of nuclear reactions using various theoretical models. It consists of a number of FORTRAN codes, input parameter libraries, and experimental data library (EXFOR) - operated through the Graphic User Interface (GUI).

National Nuclear Data Center, BNL, USA
International Atomic Energy Agency, Vienna, Austria

<http://www.nndc.bnl.gov/empire/>

EMPIRE-3.2 (Malta), August 2013, Graphical User Interface (GUI). Test version adopted for Windows-XP, November 2013

File Options Inputs Execute Outputs Logs Plots Clean Source Help

Pd105w

Main 1 | Main 2 | ZVV plots | Files | Archive | Folders | Multi-run | Source

Execute

Create input

Edit input

MAT 1111

Run selected:

Select for running

- EMPIRE
- Formatting (EMPEND)
- Verification
- Preparing for plotting
- Adding resonances

Output

Full

Short

ENDF

Output/Input

Discrete levels

Collective levels

Cumul. plot

OM parameters

OMP for direct

Fission input

EXIT / SAVE SETTINGS

Developer: Pause after running scripts Show exec command Run exec immediately

Start time: 18:45.46 (18-11-2013)

EMPIRE - 3.2

MALTA

PLOT4	4 KB	LST
pnt.zvd	1 KB	ZVD
Present	14,339 KB	File
runme	3 KB	MS-I
SIGMA1	12 KB	LST

start Control... wrk McAfee... EMPIR... Pd105... About ... untitled... EN 19:54

Screenshot: Empire running on Windows

System Properties

System: Microsoft Windows XP Professional

About Empire-3.2

Welcome to Empire-3.2

Nuclear Reaction Model Code

Modular system of nuclear reaction codes for advanced modeling of nuclear reactions using various theoretical models. It consists of:

- Reaction codes, input parameter files, and nuclear data library (EXFOR) - ENDF/B-VI format.
- Public User Interface (GUI).

Developed at: Brookhaven National Laboratory, Upton, NY, USA
Institute for Nuclear Studies, University of Vienna, Vienna, Austria
Website: <http://www.bnl.gov/empire/>

```
C:\WINDOWS\system32\cmd.exe - E:\empire32zv\wrk\... \empire32zwin\script...  
===Define number of subentries  
lXrefs=0 lData=0 lDataMax=0  
===Allocate memory  
reactions: <003E2430> 300*0 =0  
data: <003E3FF8> 32*0 =0  
dataIndex: <003E3FE8> 4*0 =0  
xref: <003E2498> 172*0 =0  
===Fill in reactions list  
nReactions=0  
Processing: sorting of data===  
E:\empire32zv\wrk>E:\empire32zv\wrk  
vd31.exe LSTTAB.CUR cur.zvd  
Extract CUR file to ZUD file.  
U.Zerkin, IAEA, 2000-2006  
file:[LSTTAB.CUR]  
Comment: |Ei2.00E+6 An 201  
Comment: |Ei2.00E+6 An160|  
E:\empire32zv\wrk>echo #?zvview.exe  
E:\empire32zv\wrk>type pnt.zvd 1>>  
E:\empire32zv\wrk>type cur.zvd 1>>
```

ZVView

46-Pd-105(n,x) Ei2.00E+6 An160

Empire Ei2.00E+6 An160

$d^2\sigma/dE/d\Omega$ (b/eu/sr)

Energy (eV)

Marker: f2: Empire Ei2.00E+6 An160 i=11 X=169265 Y=9.88
F1:Help F2:Menu ZVView2-v1.023,2013/11/01 U.Zerkin@i

List of selected

20 21

Shift 10** 1

Eres (rel) 0.02

Maxwellian Temp. 1.382E+

Plot the list

List name

Compare to:

4 KB LST
1 KB ZVD
14,339 KB File
3 KB MS-I
12 KB LST

EMPIRE - 3.2

start Cont... wrk McAf... EMPI... Pd10... Abou... C:\W... ZVView EN 20:02

Express version for Linux

Includes: executables (static) and portable ActiveTcl-8.4.

Assumes: gfortran-4.6+, python-2.7+ are installed.

Files *.o and *.mod are removed; make can directly be done from Tcl/Tk GUI.

No installation. No configuration. Starts by [runme.sh](#). Size: ~230Mb (without EXFOR).

EMPIRE-3.2 (Malta), August 2013, Graphical User Interface (GUI). Test version adopted for Windows-XP, November 2013

File Options Inputs Execute Outputs Logs Plots Clean Source Help

Pd105w

Main 1 \ Main 2 \ ZVW plots \ Files \ Archive \ Folders \ Multi-run \ Source \

Available ZVW plots

- Pd105w-.zvd
- Pd105w-1.zvd
- Pd105w-4.zvd
- Pd105w-102.zvd
- Pd105w-Mu-bar.zvd
- Pd105w-preq-det.zvd
- Pd105w-preq.zvd
- Pd105w-z2n.zvd
- Pd105w-za.zvd
- Pd105w-zd.zvd
- Pd105w-zel.zvd
- Pd105w-zf-part.zvd
- Pd105w-ze.zvd

Filter: Pd105w

Select MT:

Plot selected MT

<= Delete selected

ZVW plot from EMPIRE

Launch ZVW interface

Select data for ZVW plotting (multiple allowed)

#	MF	MT	Ino	MT	Einc	Elev1/Eg	Elev2/Ang
15	10	103	n	p		1,0	
16	10	103	n	p		1,0	
17	XS	102	n	capt.			
18	XS	2	n	elast.			
19	XS	102	n	capt.			
20	DD	9000	n	Xn	2,000E+6		20,00
21	DD	9000	n	Xn	2,000E+6		160,00
22	DD	9000	n	Xn	1,000E+7		20,00
23	DD	9000	n	Xn	1,000E+7		160,00
24	DD	9000	n	Xn	1,400E+7		20,00
25	DD	9000	n	Xn	1,400E+7		160,00
26	DD	9000	n	Xn	2,000E+7		20,00
27	DD	9000	n	Xn	2,000E+7		160,00
28	DD	9000	n	Xn	6,000E+7		20,00

List of selected

20 21

Shift 10** 1

Eres (rel) 0,02

Maxwellian Temp. 1.

Plot the list

List name

Compare to:

Developer: Pause after running scripts Show exec command Run exec immediately






Execute: `xterm -e /home/zerkin/empire32linux/wrk/./empire/scripts/zvddx Pd105w & |` Run2

Useful?

New. Developer's options:

- 1) Show exec command
- 2) Run exec immediately
- 3) Pause after running scripts (Windows)

Who are users of Empire on Windows and express version for Linux?

- 1) Beginners? Yes. 
- 2) Potential users who are not yet sure? Yes. 
- 3) Old generation of physicists? Probably... 
- 4) Today's experienced users? No. 
- 5) Participants of Empire Workshop-2013 - 

3. Empire as Web application

Tasks and requirements

- 1) To make simple Web interface to Empire:
 - a) upload input file
 - b) run basic codes to produce ENDF file
 - c) display results (text, messages, plots)
- 2) To implement timeout, buttons to interrupt running codes, clean files, etc.
- 3) To organize file system for multi-users' work on Web server
- 4) To implement (if possible) all functions of Empire package
- 5) Do all above quickly
- 6) Assess and discuss results and perspectives

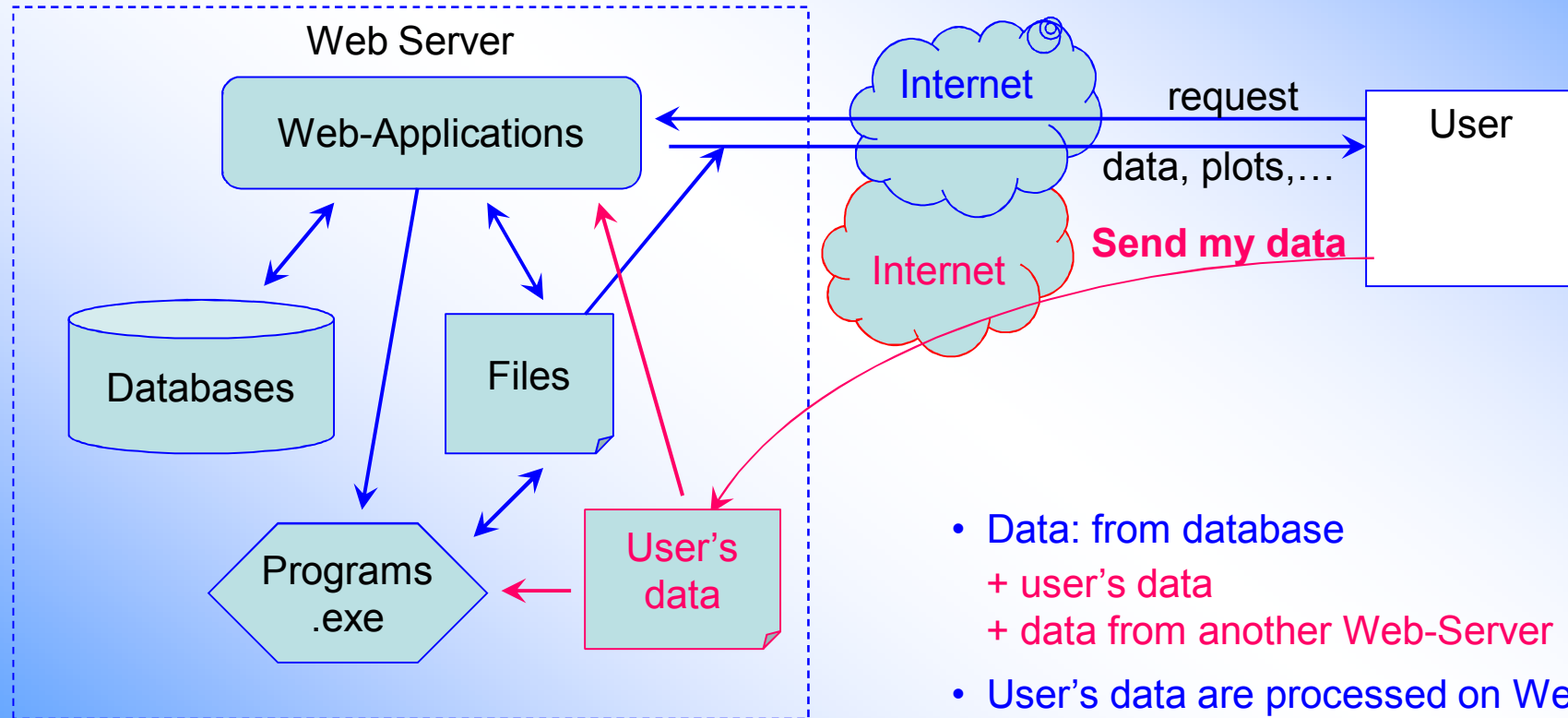
Today's solution:

To build-in Empire to NDS Web system via sending ENDF file to MyENDF Uploading system, to perform all operations using ENDF Utilities, run Prepro, send data to ENDF-EXFOR-ZVView Web 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

Web server applications and Web Empire

MyPlot	Plotting with Web-ZVView (2009)
MyEXFOR	Uploading System (2010)
MyENDF	Uploading System (2010-2011)
MyENSDF	Uploading System (2011)
EMPIRE-3.1	Web Interface to Empire /under development/ (2013)

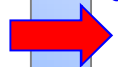
Web Empire functions (today):

- Running:
 - Empire-3.1
 - Formatting
 - Add resonances
- File management (view, sort, delete)
- Send ENDF file to MyENDF



MyENDF functions:

- Running on ENDF file:
 - Checking and verification
 - Re-formatting, endf2gnd
 - Prepro-2012, etc.
- File management (view, delete)
- Send ENDF file to ENDF-Retrieval



EXFOR Retrieval:

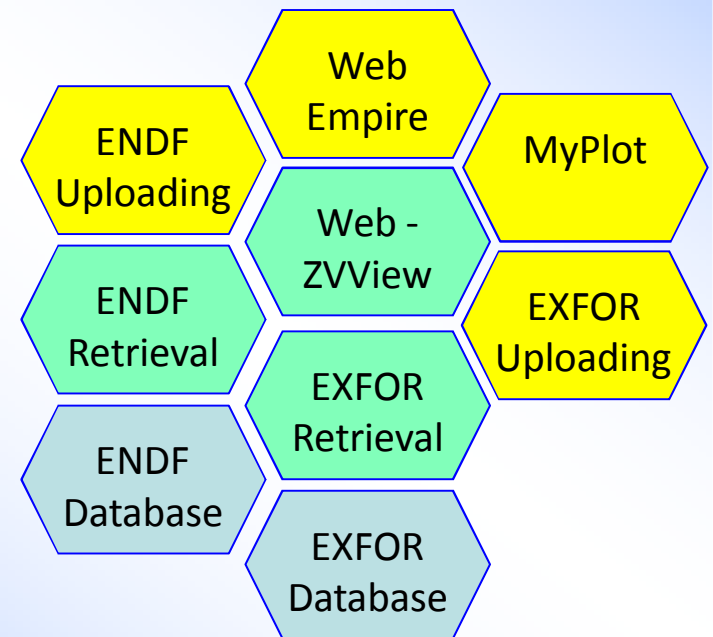
- Search in database
- Select and renormalize
- Display, plot



ENDF Retrieval:

- Search in database
- Display, plot
- Send request to EXFOR-Retrieval

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



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

```
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:

↓

Output:

↓

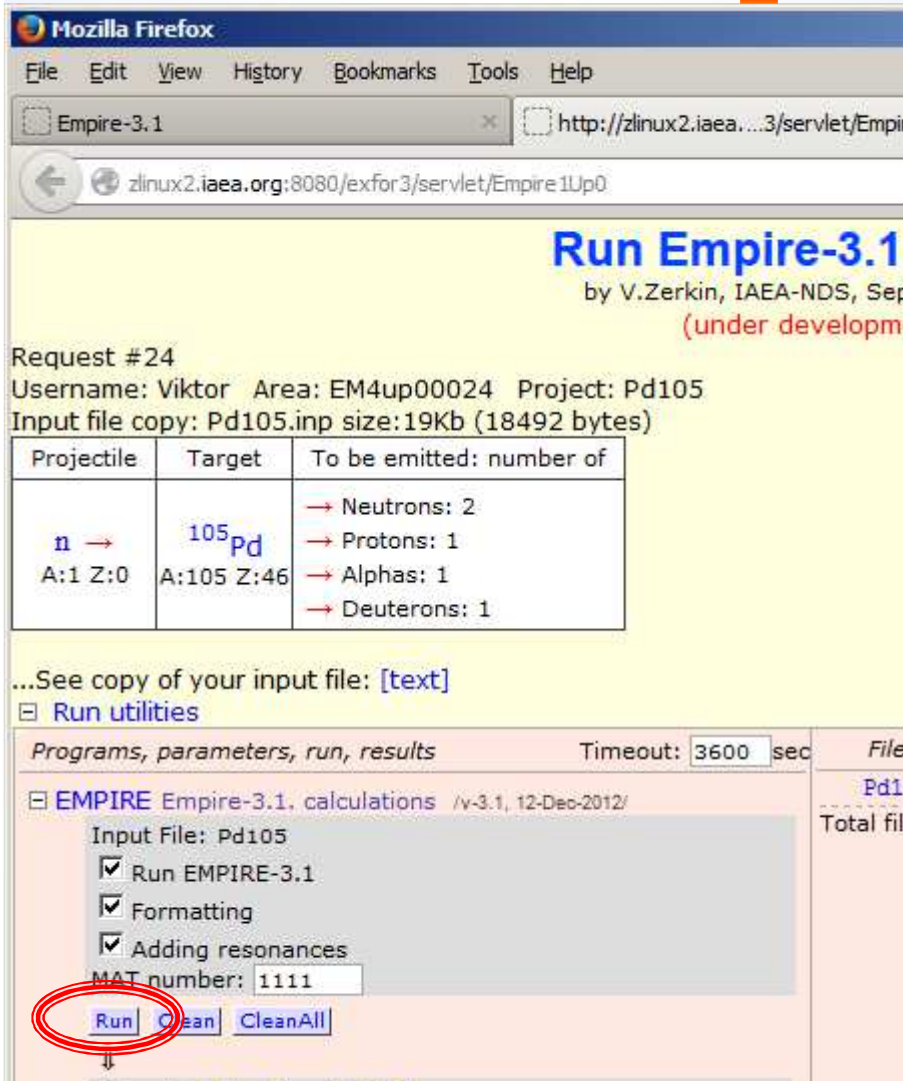
Next: ENDF to checking, pre-processing, plotting, comparing with ENDF libraries and EXFOR database, etc.

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

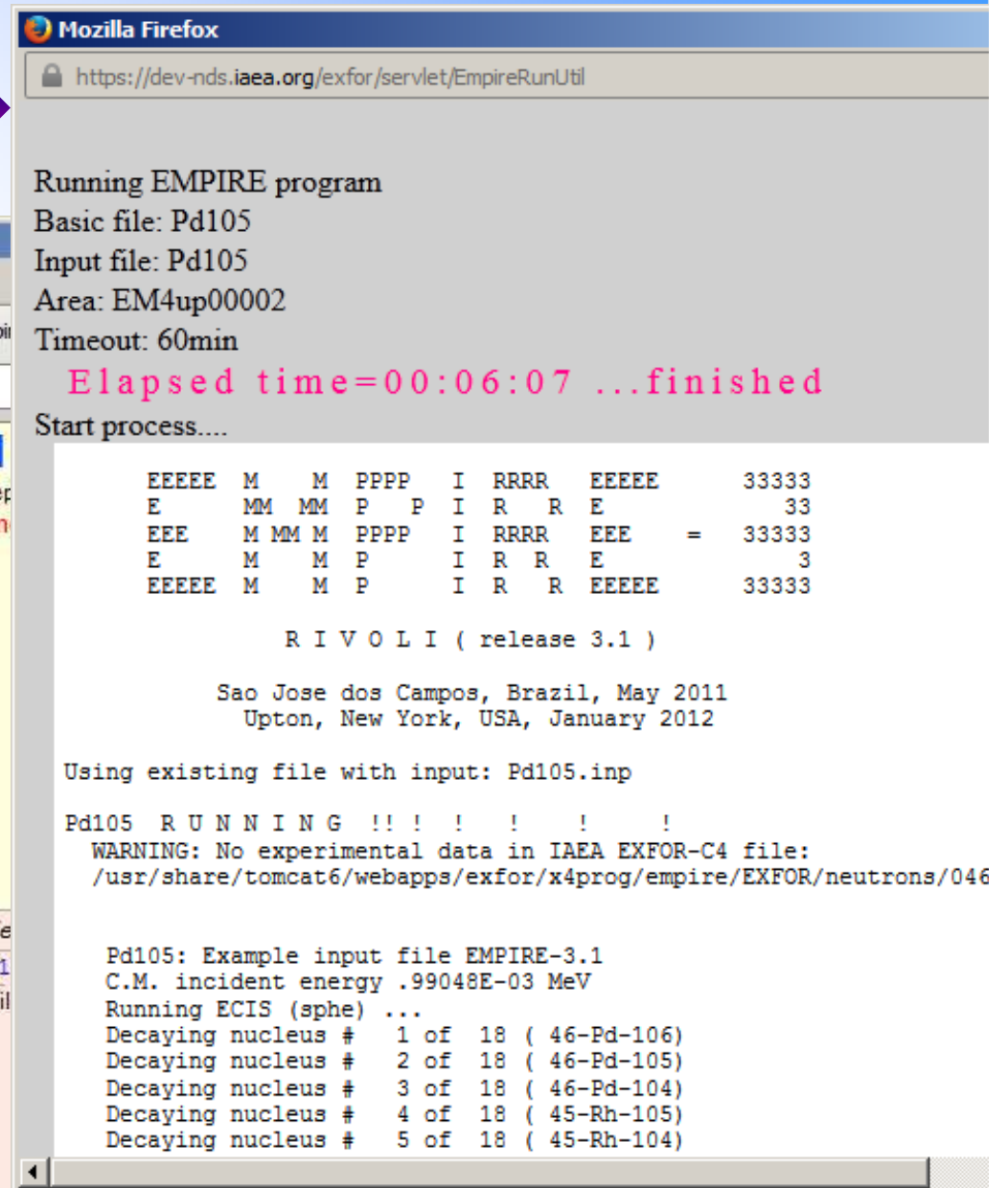
Input File: Pd105

Run EMPIRE-3.1

Formatting

Adding resonances

MAT number: 1111



```
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 EEEE 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 EEEE 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 →	¹⁰⁵ Pd	→ Neutrons: 2 → Protons: 1 → Alphas: 1 → Deuterons: 1
A:1 Z:0	A:105 Z:46	

...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]
↑ 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.addressonances.err	63	2013/12/03 01:09:58
× Pd105.addressonances.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 request details: "Request #1", "Username: Viktor", and "Uploading...". The main content area is titled "Programs, parameters, run, results" and contains a list of programs with their descriptions and versions. A "Run" button is visible. To the right, there is a "Your Files" section showing a list of files: "EE4up00001.endf-mfnt", "EE4up00001.endf", and "EE4up00001.txt". Below the file list, there is a "Manual search # 1" section with various search criteria. At the bottom, there is a "Data sections" section with a list of data sections and their descriptions. A "Go to retrieval systems" button is visible.

Request #1
Username: Viktor
Uploading...
ENDF file copy: EE4up00001.txt size:2Mb (1231281 bytes)
...Found Material(s): 1
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
...Materials: 1 Sections:390
...See: [your file] [working ENDF File]
Run utilities

Programs, parameters, run, results Timeout: 300 sec Your Files [refresh]

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 v-8.04, Jan-2011 Create directory, add tape label, convert numeric fields to binary format
- PSYCHE v-8.00, Aug-2008 More complicated physics checking code
- INTER v-8.07, Oct-2013 Calculate selected cross sections and integrals (run after PREPRO)
- endf2gnd v-4.00, May-2013 Convert ENDF file to GND (xml)

PREPRO 2012 Pre-processing ENDF files.
Produces data in pointwise format: linearized ENDF file with reconstructed resonances using Doppler broadening at a given temperature.

Input File: EE4up00001.endf
Reconstruct cross sections at the temperature 293.6 (Kelvin)
with accuracy 0.1 (per-cent)

Run

ENDF Materials in your file:
1) MAT=1111 IZA=46105 NSUB=10 LISO=0 Target=Pd-105
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;

Search similar data in ENDF and EXFOR databases...

Manual search # 1

ENDF EXFOR

Target Pd-105

Sub-Lib (projectile) N

MF (quantity) # 3

MT (reaction) # 1

X4-Reaction N,TOT

X4-Quantity CS

Data sections. Set up search / find data in ENDF and in EXFOR

NSUB=10 [N] Incident-Neutron Data

- 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
- Pd-105 MF=12 Photon production multiplicities and transition probabilities

209 N Pd-105 MF10 MT28 Pd-105(N,N+P),SIG/ACT ENDF: set go EXFOR: set go

210 N Pd-105 MF10 MT41 Pd-105(N,2N+P),SIG/ACT ENDF: set go EXFOR: set go

211 N Pd-105 MF10 MT103 Pd-105(N,P),SIG/ACT ENDF: set go EXFOR: set go

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*

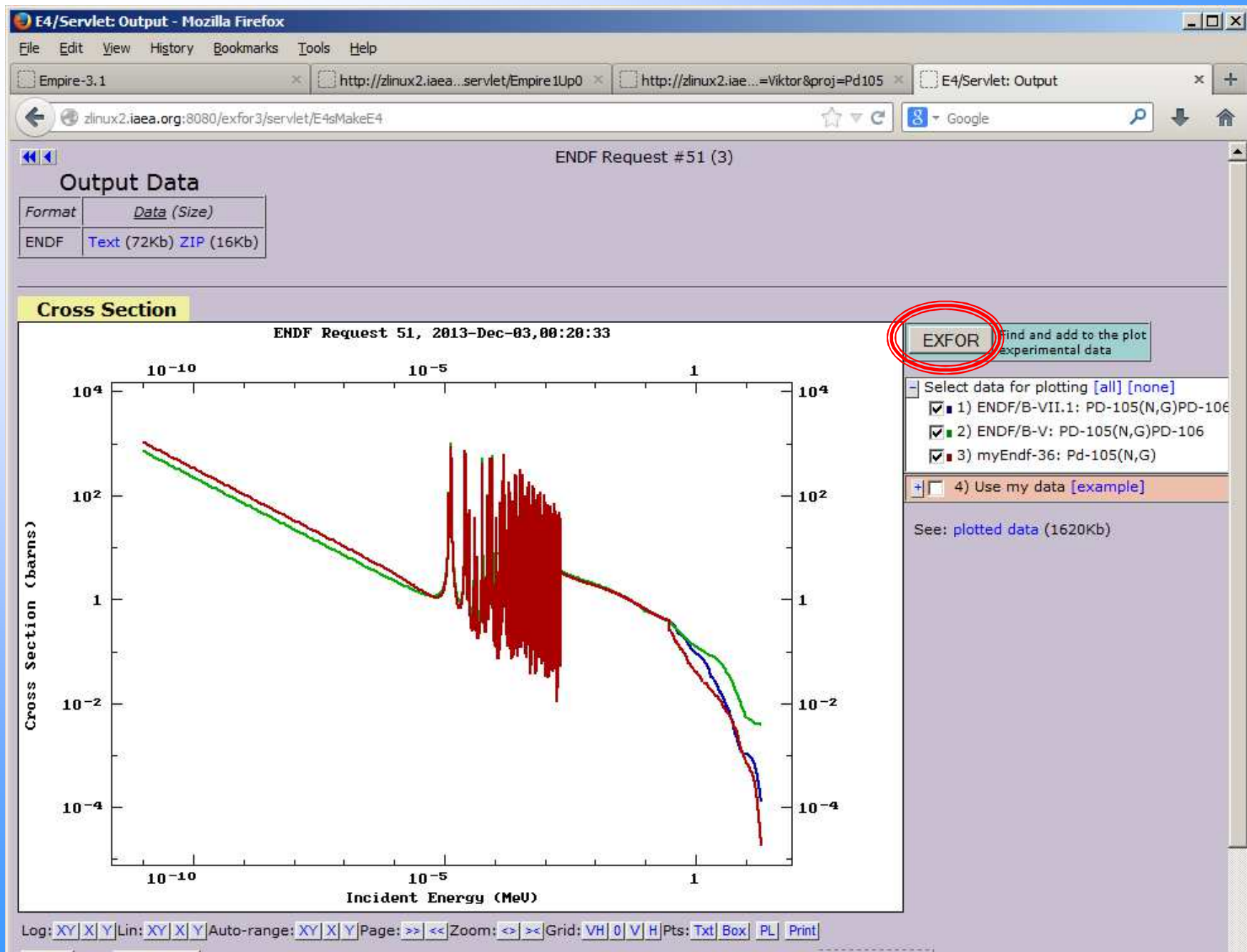
Sorted by: [Reactions] Reorder by: [Libraries] View: basic extended/get MAT/PEN, run Inter: resonance integrals, etc.

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. SCHMITTROTH

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

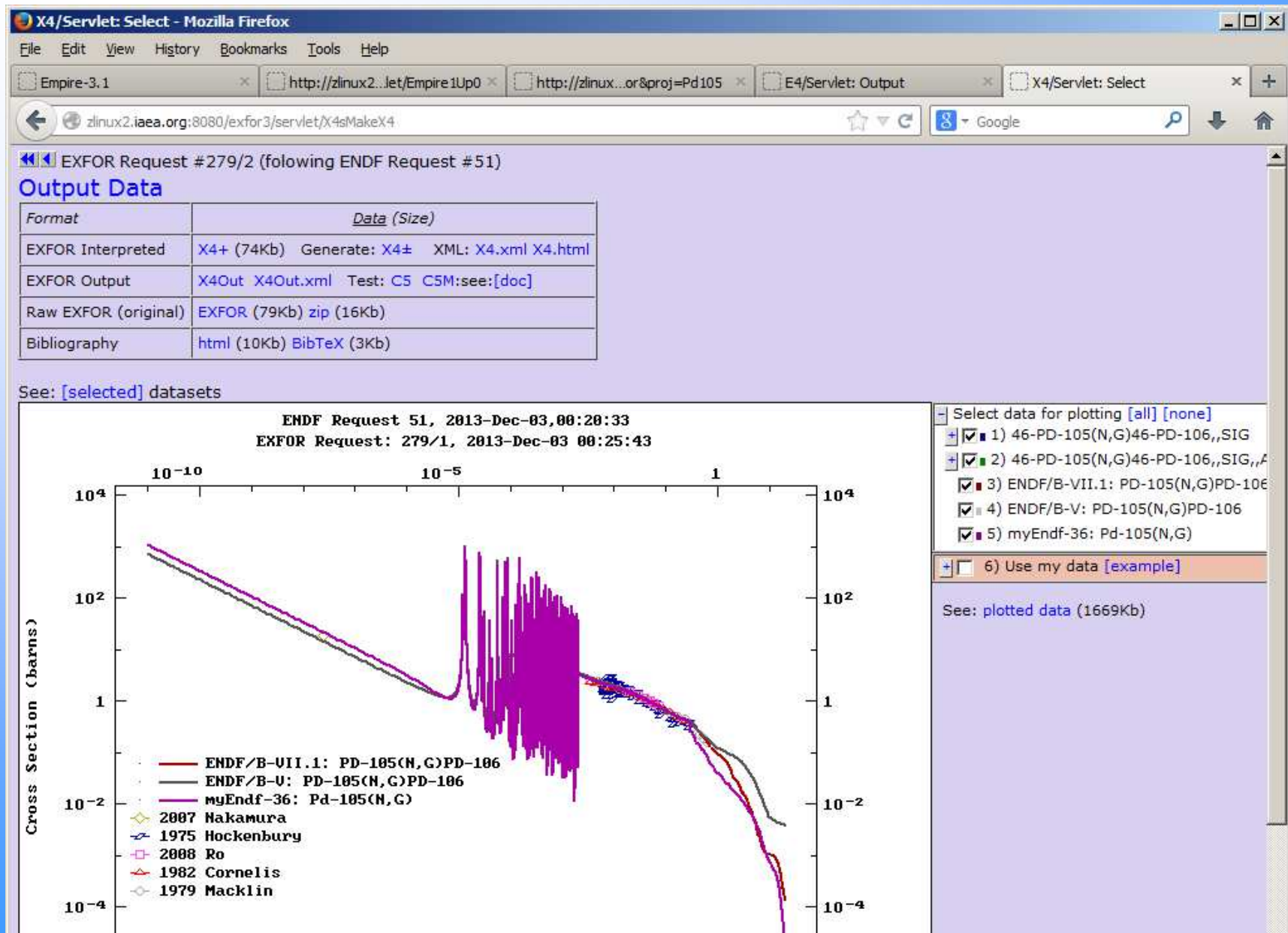
Output: X4+ EXFOR Bibliography TAB C4 PlotC4

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)	Info X4+ X4± T4 Cov	2007	S.Nakamura+	2.50e-2	1	[pdf]+ J,NST,44,103,2007	14133003	2007NA10
2)	Info X4+ X4± T4 Cov	1975	R.W.Hockenbury+	6.31e3 2.97e5	562	[pdf]+ C,75WASH,2,905,197503	10435004	
3)	Info X4+ X4± T4 Cov	2008	T.-I.Ro+	1.50e4 9.00e4	6	[pdf]+ J,NSTS,5,443,2008	23081002	
4)	Info X4+ X4± T4 Cov	1982	E.Cornelis+	3.00e3 3.00e5	16	[pdf]+ C,82ANTWER,,222,8209	21810002	1983CO2N
5)	Info X4+ X4± T4 Cov	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



4. Empire with Web interface

Having Empire-3.1 with Web interface it can be used:

- on remote Web server(s)
- on local systems (PC): Web without Internet

Remote server calculations: problems and perspectives

- 1) dedicated server(s)
- 2) providing IT security
- 3) long and regular calculations: accounts for users, self-cleaning
- 4) the system should be much faster (~ Web standards)

Empire with Web interface on Windows (PC)

- 1) nonsense if Windows version with Tcl/Tk exists

Conclusion

Empire with Web interface can have some practical sense only if the system will work much faster (typical cases should work 5-10 minutes)

Struggle for speed

Task: to make first run much faster

(second run was optimized to work much faster in version 2.19)

Steps:

- 1) diagnosis: how much time is spent by each part of the system
- 2) define for how much time is spent for types of operations
- 3) find out bottle-necks (if any)
- 4) accelerate program without changing the logic
- 5) analyse logic of the program and find possible acceleration
- 6) find faster computer(s)

Starting point:

- 1) Example from Empire-3.1 distribution Pt105.inp
- 2) 1-st run on old Linux web server (NNDC): 55 min
- 3) 1-st run on new powerful web server (NNDC): 9 min 45 sec

Goal: to achieve elapsed time ~5 min on PC and Web server

Struggle for speed: results

Platform	OS	Interface	Empire 3.1, original	Empire 3.1, modified	Ratio (modif./orig.)
PC's					
Old PC	Win-7	Script .bat	37min 2sec	14min 2sec	38%
New PC	Win-7	Script .bat	21min 41sec	<u>6min 44sec</u>	31%
New PC	Win-7	Web		7min 48sec	
New PC	Win-7	Tcl/Tk		7min 11sec	
zlinux2	Linux	Script .sh	45min 57sec	23min 51sec	52%
Laptop					
Fujitsu-2006	Win-XP	Tcl/Tk		20min 36sec	
Servers					
dev-nds	Linux	Web		<u>6min 3sec</u>	
www-nds	Linux	Web		12min 6sec	
dev-nndc	Linux	Web	9min 47sec		




Achieved:

- 1) Windows: program runs 3 times faster (HP Compaq Elite 8300 PC: **22min**→**7min**)
- 2) Linux: program runs 2 times faster best result on Linux server: **~6min**

Conclusion. Goal (5min) was not achieved.

Further acceleration need deep analysis of the program's logic (if possible at all)

Concluding remarks

- 1) Empire as cloud computing tool is not fast enough for practical usage, although fully working 
- 2) Struggle for speed can be considered as an “academic” exercise, but can be continued 
- 3) Portable Empire for Windows can “survive” and be prepared for distribution to end-users 

Thank you.