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

Viktor Zerkin
International Atomic Energy Agency
Nuclear Data Section

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

Topics:
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)
   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

Web: replace Tcl/Tk

GUI (Tcl/Tk) runs Scripts, manages files

Files

Parameters

Data files

Web: replace Tcl/Tk

Html Javascript Java

Windows: add .bat

Batch

Scripts (Bash, Python)

Fortran, C, Java executables

Today: Linux/MacOSX + Tcl/Tk
EMPIRE on Windows and Web

Windows + Tcl/Tk interface

GUI (Tcl/Tk) runs Scripts, manages files

Scripts (Bat, Python)

Fortran, C, Java executables

Parameters

Data files

Linux + Web interface

Html Javascript Java

Scripts (Bash, Python)

Parameters

Data files

Fortran, C, Java executables
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`
Screenshot: Empire running on Windows

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

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

Start time: 18:43.48 (18-11-2013)
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.
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 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

MyEXFOR functions:
- Running on ENDF file:
  - Search in database
  - Select and renormalize
  - Display, plot

EXFOR Retrieval:
- Search in database
- 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

Copy – paste your Empire input file
Run Empire-3.1 on Web
by V.Zerkin, IAEA-NDG, September 2013
(under development)

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

<table>
<thead>
<tr>
<th>Projectile</th>
<th>Target</th>
<th>To be emitted: number of</th>
</tr>
</thead>
<tbody>
<tr>
<td>105Pd</td>
<td></td>
<td>→ Neutrons: 2</td>
</tr>
<tr>
<td>A:105 Z:46</td>
<td></td>
<td>→ Protons: 1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>→ Alphas: 1</td>
</tr>
<tr>
<td>n →</td>
<td>1:0</td>
<td>→ Deutrons: 1</td>
</tr>
</tbody>
</table>
A:1: Z:0

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

Programs, parameters, run, results

EMPIRE Empire-3.1. calculations /v3.1,12-Dec2012/

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.
Running Empire in “Web-terminal” window

Mozilla Firefox

https://dev-nds.iaea.org/exfor/servlet/EmpireRunUtil

Running EMPIRE program
Basic file: Pd105
Input file: Pd105
Area: EM4up00002
Timeout: 60min

Elapsed time=00:06:07 ...finished

Start process...

<table>
<thead>
<tr>
<th>EEEE</th>
<th>M</th>
<th>M</th>
<th>PPPP</th>
<th>I</th>
<th>RRRR</th>
<th>EEEE</th>
<th>33333</th>
</tr>
</thead>
<tbody>
<tr>
<td>R</td>
<td>MM</td>
<td>MM</td>
<td>P</td>
<td>P</td>
<td>I</td>
<td>R</td>
<td>R</td>
</tr>
<tr>
<td>EEE</td>
<td>M</td>
<td>MM</td>
<td>M</td>
<td>P PPP</td>
<td>I</td>
<td>RRRR</td>
<td>EEE</td>
</tr>
<tr>
<td>R</td>
<td>M</td>
<td>M</td>
<td>P</td>
<td>I</td>
<td>R</td>
<td>R</td>
<td>E</td>
</tr>
<tr>
<td>EEEE</td>
<td>M</td>
<td>M</td>
<td>P</td>
<td>I</td>
<td>R</td>
<td>R</td>
<td>EEEE</td>
</tr>
</tbody>
</table>

RIVOLI (release 3.1)
Sao Jose dos Campos, Brazil, May 2011
Upton, New York, USA, January 2012

Using existing file with input: Pd105.inp

Pd105 RUNNING !!! ! ! ! !
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

Run Empire-3.1 on Web
by V. Zerkin, IAEA-NDS, September 2013
(under development)

Results of calculation

Upload data to further processing

Input and output Empire files
Result of Empire calculation (ENDF file) sent into the ENDF Uploading system

ENDF-uploading system
by V. Zerkin, IAEA-NDS, November 2010 - November 2013

Request #1
Username: Viktor
Uploading...
ENDF file copy: EEup00001.txt, size: 2Mb (1231281 bytes)
...Found Material(s): 1
  1) MAT=1111, IZA=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, 6, 10, 12, 14
     ...Materials: 1 Sections: 990
     ...See: [your file] [working ENDF File]
  Run utilities

<table>
<thead>
<tr>
<th>Parameters, programs, run, results</th>
<th>Timeout: 300 sec.</th>
<th>Bac</th>
</tr>
</thead>
<tbody>
<tr>
<td>Check: 3, Run 3 standard checking codes: CHECKR, FIZCON, STANEF</td>
<td>CHECKR</td>
<td></td>
</tr>
<tr>
<td>FIZCON</td>
<td>v.0.7, Jan-2011 Procedures &amp; Simple Physics Checking Code</td>
<td></td>
</tr>
<tr>
<td>STANEF</td>
<td>v.0.4, Jan-2011 Create directory, add tape label, convert numeric fields to binary format</td>
<td></td>
</tr>
<tr>
<td>PSYCHE</td>
<td>v.4.0, Aug-2008: More complicated physics checking code.</td>
<td></td>
</tr>
<tr>
<td>INTER</td>
<td>v.0.7, Oct-2010: Calculate selected cross sections and integrals (run after PREPRO).</td>
<td></td>
</tr>
<tr>
<td>endf2gnd</td>
<td>v.4.0, May-2013 Convert ENDF file to GND (xml)</td>
<td></td>
</tr>
<tr>
<td>PREPRO</td>
<td>2012 Pre-processing ENDF files. Produces data in pointwise format: finalised ENDF file with reconstructed resonances using Doppler broadening at a given temperature</td>
<td></td>
</tr>
</tbody>
</table>

ENDF Materials in your file:
1) MAT=1111 IZA=46105 NSUB=10, LISO=0, Target=Pd-105
    Found in: ENDF/B-VII.1; ENDF/B-IV.0; PTEND-2.2; CENDL-3.1; JENDL-3.3/300; ENDF/B-VL-8-300; ROSFOND-2010; JEFF-3.1/A; EAF-2010; MENDEL-2; TENDL-2012; ...

Go to retrieval systems

Libraries in database having the same NSUB & Material

ENDF File structure

Go to retrieval systems
After running Prepro:search in ENDF database
Compare ENDF file from Empire with ENDF libraries
Search similar data in EXFOR database

**Data Selection (for ENDF Request #51)**

- **Retrieve**
- **Output:**
  - X4
  - EXFOR
  - Bibliography
  - TAB
  - C4
  - PlotC4
- **Plot:**
  - Quick-plot (cross-sections only)
  - Advanced plot [how-to]
  - converting ratios to cross sections using [IAEA-standards,2006]

<table>
<thead>
<tr>
<th>n</th>
<th>Display</th>
<th>Year</th>
<th>Author-1</th>
<th>Energy range, eV</th>
<th>Points</th>
<th>Reference</th>
<th>Subentry#</th>
<th>NSR-Key</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>46-DO-108(K,0)→6-DO-106, SIG, AV C4: MF3 MT102</td>
<td>1975 R.W. Mocrenbury+</td>
<td>6.31e3</td>
<td>2.97e5</td>
<td>562</td>
<td>[pdf] C,75WASH,2,905,197503</td>
<td>10435004</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>46-DO-108(K,0)→6-DO-106, SIG, AV C4: MF3 MT102</td>
<td>1982 E. Cornelisse+</td>
<td>3.00e3</td>
<td>3.00e5</td>
<td>16</td>
<td>[pdf] C,82ANTWER,222,8209</td>
<td>21811002</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>46-DO-105(K,0)→6-DO-106, SIG C4: MF3 MT102</td>
<td>1979 R.L. Macklin+</td>
<td>3.00e3</td>
<td>7.00e5</td>
<td>18</td>
<td>[pdf] J,NST,71,182,7908</td>
<td>10868008</td>
<td></td>
</tr>
</tbody>
</table>

[IAEA-standards,2006]
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

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

**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.