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energy agency

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international centre for theoretical physics

ICTP 40th Anniversary

SMR.1555 - 21

Workshop on
Nuclear Reaction Data and Nuclear Reactors:
Physics, Design and Safety

16 February - 12 March 2004

Introduction to EMPIRE

Mike HERMAN
National Nuclear Data Center
Building 197D
Brookhaven National Laboratory
Upton, NY 11973
U.S.A.

Introduction to EMPIRE-II

-

a modular system for nuclear reaction calculations

(version: 2.18 Mondovi)
(version: 2.19beta12 Lodi)

M.Herman

Brookhaven National Laboratory

e-mail: mwherman@bnl.gov

EMPIRE developers

- R. Capote (Seville, Spain)
- M. Herman (BNL, US)
- P. Oblozinsky (BNL, US)
- M. Sin (Bucharest, Romania)
- A. Trkov (IAEA, Vienna)
- A. Ventura (ENEA, Bologna)
- V. Zerkin (IAEA, Vienna)

EMPIRE highlights

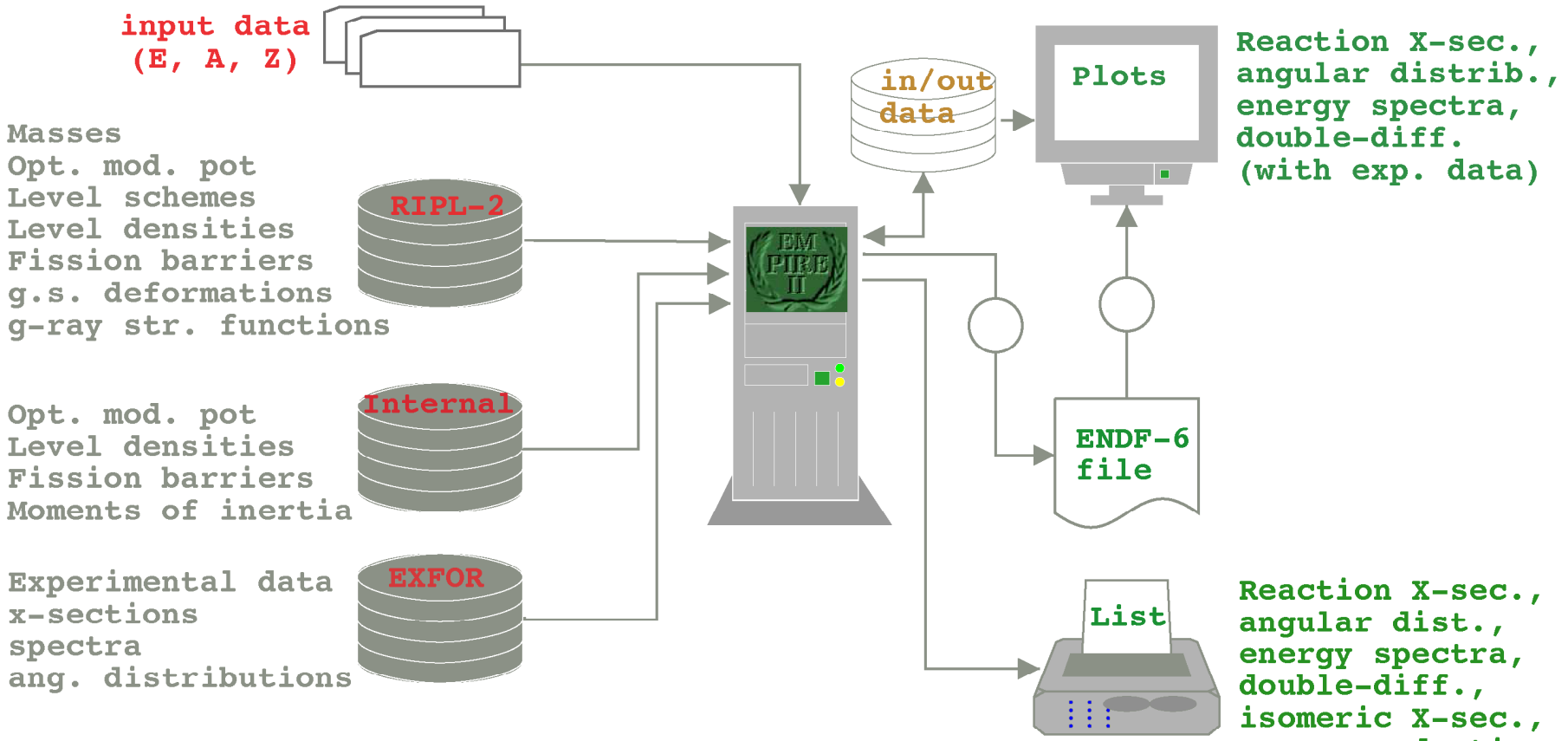
System of codes for modeling nuclear reactions:

- broad range of energies (up to ~200 MeV) and projectiles (any nucleon or HI)
- most important nuclear reaction models
- extensive input parameter library (RIPL-2)
- ENDF-6 formatting
- utility codes (ENDF-6 verification)

EMPIRE highlights (cont.)

- automatic retrieval of experimental data from EXFOR
- interactive plots of experimental and calculated results
  - excitation functions
  - angular distributions
  - inclusive emission spectra for n, p, α, and γ)
  - double differential spectra

EMPIRE layout



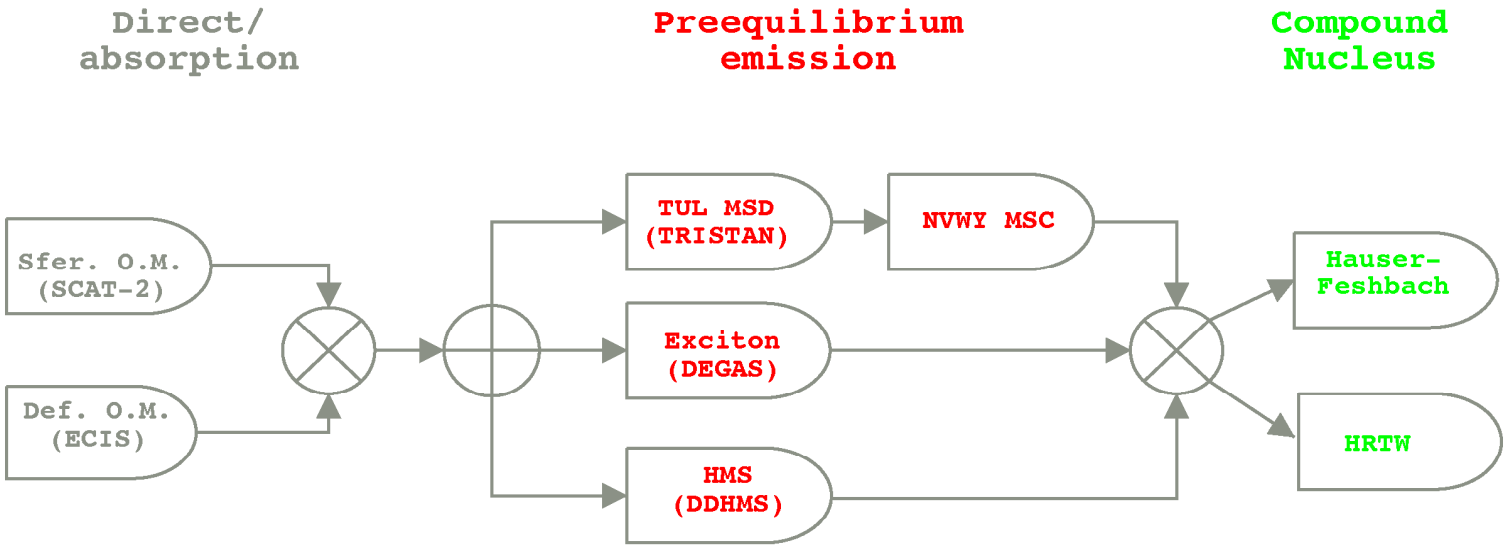
Reaction mechanisms

- optical model (SCAT2)
- coupled channels (ECIS)
- TUL Multi-step Direct (ORION + TRISTAN)
- NVWY Multi-step Compound with γ-emission
- second-chance preeq. emission
- exciton model (DEGAS)

Reaction mechanisms (cont.)

- Monte Carlo preequilibrium (DDHMS)
- HRTW for widths' fluctuations
- Hauser-Feshbach model with full γ-cascade and dynamical deformation effects
- State of the art fission (three-hump barrier)

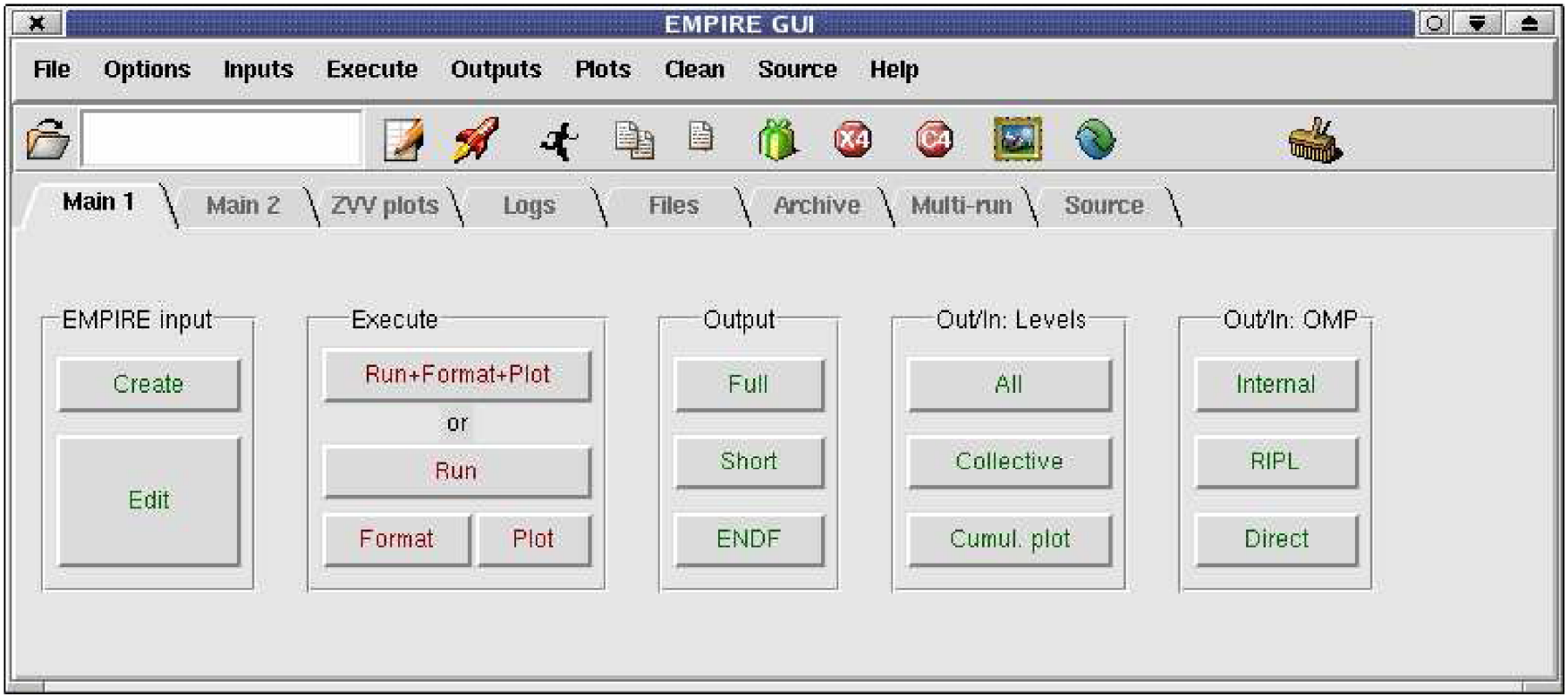
EMPIRE core


Direct/
absorption
Preequilibrium
emission
Compound
Nucleus
Sfer. O.M.
(SCAT-2)
Def. O.M.
(ECIS)
TUL MSD
(TRISTAN)
Exciton
(DEGAS)
HMS
(DDHMS)
NVWY MSC
Hauser-
Feshbach
HRTW

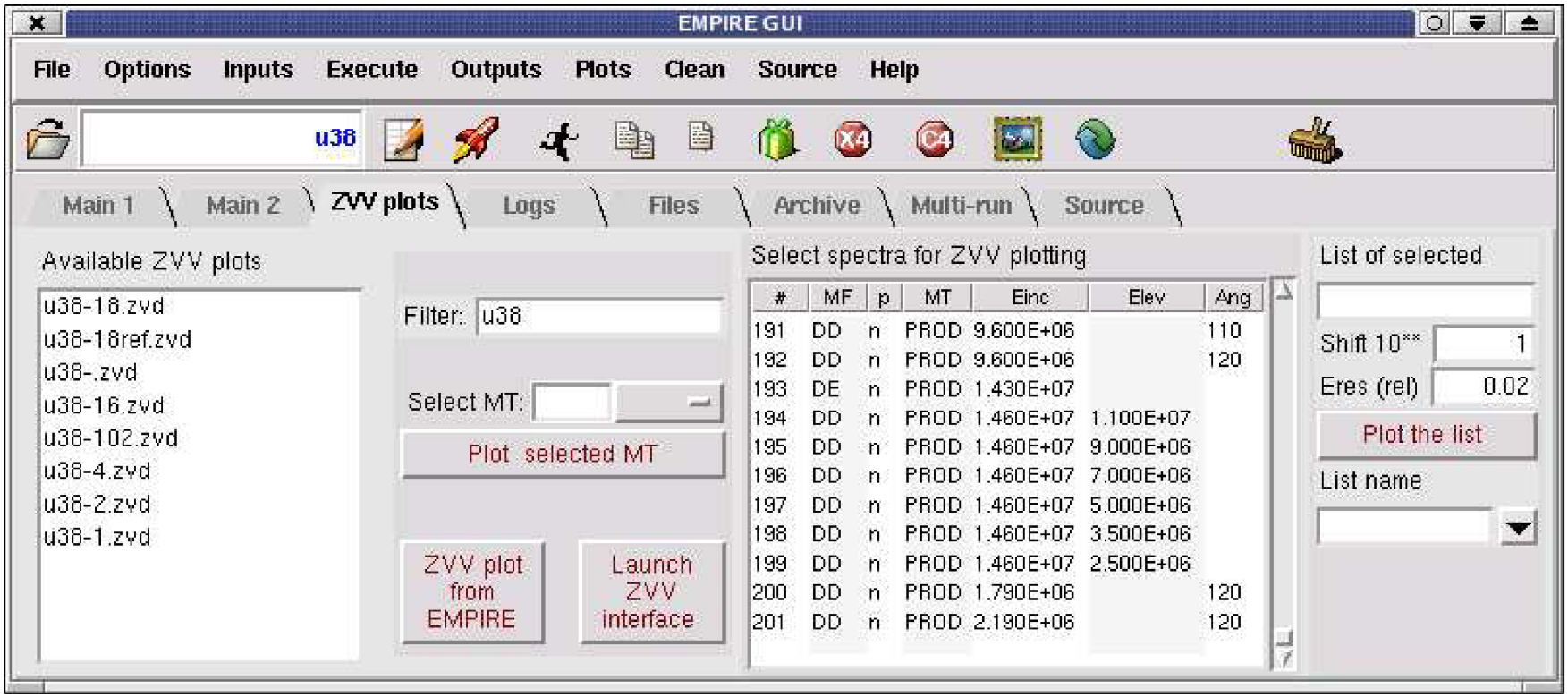
EMPIRE statistics

- EMPIRE core: >60 000 lines
- utility codes: >61 000 lines
- # of bash and Tcl/Tk scripts: 25
- size of the internal parameter library: 2 Mb
- size of the RIPL-2 library: 224 Mb
- size of the EXFOR library: 567 Mb

EMPIRE GUI (Main)



EMPIRE GUI (ZVV plots)



Operating systems

- languages: FORTRAN 77 (99%), C (mostly ZVView), bash, Tcl/Tk, awk
- operating systems:
  - **Linux** (developed on Red Hats up to version 9),
  - UNIX (any one should work but TLC might be needed)
  - Mac (reported to work)
  - MS Windows (EMPIRE core runs)
  - VMS (EMPIRE core used to run)

EMPIRE directory tree

- **source** - source of the EMPIRE code divided into modules and Makefile
- **RIPL-2** - input parameters from the RIPL-2 library
- **data** - library of input parameters (files: *ldp.dat, nix-moller-audi.dat, nparac.dat*, *mass-hms.dat*)
- **work** - input and output files, scripts

Directory structure (cont.)

- **EXFOR -** EXFOR library, index file (X4-INDEX.TXT) and retrieval tools
  - **subent -** 86 443 subentries

EMPIRE-2.19 (Lodi) will use EXFOR relational database (MySQL)

Directory structure (cont.)

- **util -** utility codes
  - **empend -** code converting EMPIRE results into the ENDF format
  - **endres** - merges resonances from the exsisting evaluation
  - **fixup** - used to reconstruct MT= 1, 4, 103, and 107
  - **recent** - reconstructs neutron cross sections form resonance parameters
  - **sigma1** - Doppler-broadens neutron induced cross sections

Directory structure (cont.)

- **util -** utility codes (cont.)
  - **x4toc4 -** code converting retrieved EXFOR data into the computational format
  - **c4sort** - sorts data in the computational format (file .c4)
  - **lsttab** - tabulates ENDF and EXFOR data in PLOTTAB format
  - **legend** - calculates linearly interpolable angular distributions from ENDF data
  - **sixtab** - converts ENDF file MF6 to Law 7 representation

Directory structure (cont.)

- **util -** utilty codes (cont.)
  - **plotc4 -** code plotting the comparison between calculated and experimental data
  - **c4zvd** - ZVView interactive plotting package
  - **zvvddx** - prepares data for double differential plots with ZVView

Directory structure (cont.)

- **util -** utilty codes (cont.)
  - **linear** - imposes linear interpolation in the ENDF formatted file
  - **endtab** - converts ENDF tabulated data to PLOTTAB format
  - **stanef** - converts ENDF file into a standard form

Directory structure (cont.)

- **util -** utilty codes (cont.)
  - **checkr** - checks ENDF format
  - **fizcon** - checks physics in the ENDF file
  - **psyche** - even more stringent physics test (energy balance)
  - **auxiliary -** icons , sound and pictures
- **doc** - documentation

Installation

Preferred OS: **Linux**

mount /mnt/cdrom
cd /mnt/cdrom
sh setup-emp

Installs EMPIRE-II on HD and compiles.
Space: ~55 Mb (~800 Mb with EXFOR and HF-BCS lev. dens.)

Installation (cont.)

For full functionality EMPIRE needs:

- FORTRAN 77(90) compiler
- C-compiler
- gnuplot
- ghostview (gv)
- gawk
- bash shell
- Tcl/Tk, itcl, Tix (latter not needed in version 2.19)

Parameter libraries

- **Masses**
  (*empire/data/nix-moller-audi.dat)*
  Nuclear masses for **9026** nuclides combining Moller and Nix (theo.) and Audi and Wapstra (95) recommendations.
- **RIPL-2 discrete levels**
  (*empire/RIPL-2/levels/*zxxx.dat)
  RIPL-2 library based on the ENSDF as of 1998, mass range A=1-266 and Z=0-109, **2546** nuclear level schemes, **113346** levels and **159323** γ-transitions.

Parameter libraries (cont.)

- **Level density parameters from the shell-model (*empire/data/nparac.dat*)**
  Level density parameters for **3962** nuclei between ^{12}C and ^{252}Sg derived from the spacings of the shell-model single-particle spectrum.

Parameter libraries (cont.)

- **RIPL-2 optical model parameters (empire/RIPL-2/optical/om-data/om-parameter-u.dat)**
  409 sets of omp for nuclei up to Lr (Z=103) for neutrons, protons, α-particles, d, t, and ^{3}He for energies up to 400 MeV.

Parameter libraries (cont.)

- **RIPL-2 HF-BCS level densities (*empire/RIPL-2/*densities/total/level-densities-hfbcs/zxxx.dat)**
  Tabulated level densities for 103 elements between Z=8 and Z=110, adjusted to discrete levels schemes and neutron resonance spacings.

Parameter libraries (cont.)

- **RIPL-2 experimental fission barriers (empire/RIPL-2/fission/fis-barrier-exp.dat)** Fission barrier parameters recommended for the trans-thorium nuclei by V.M.Maslov and for the pre-actinides by G.N.Smirenkin.
- **RIPL-2 theoretical fission barriers (empire/RIPL-2/fission/fis-barrier-etfsi.dat)** Fission barriers and saddle point deformations obtained within the Extended Thomas-Fermi plus Strutinsky Integral (ETFSI) method for 2301 nuclei with 78 <= Z <= 120.

Parameter libraries (cont.)

- **RIPL-2 theoretical level densities at inner/outer fission barrier (empire/RIPL-2/fission/fis-levden-hfbcs-inner(outer))**
  Nuclear level densities at the inner and outer fission saddle points for some 2300 nuclei with 78 <= Z <= 120 (included in the ETFSI compilation) based on the realistic microscopic single-particle level scheme determined within the HF-BCS mass model obtained with the MSk7 Skyrme force.

Parameter libraries (cont.)

- **abundances (empire/RIPL-2/masses/abundance.dat)**
  Reformatted version of the file from the Nuclear Wallet cards includes all stable isotopes.
- **RIPL-2 nuclear deformations (empire/RIPL-2/optical/om-data/om-deformations.dat)**
  Recommended deformation parameters (β_2 and β_3) for 1643 collective levels retrieved from the JENDL-3.2 evaluations, ENSDF and the literature.

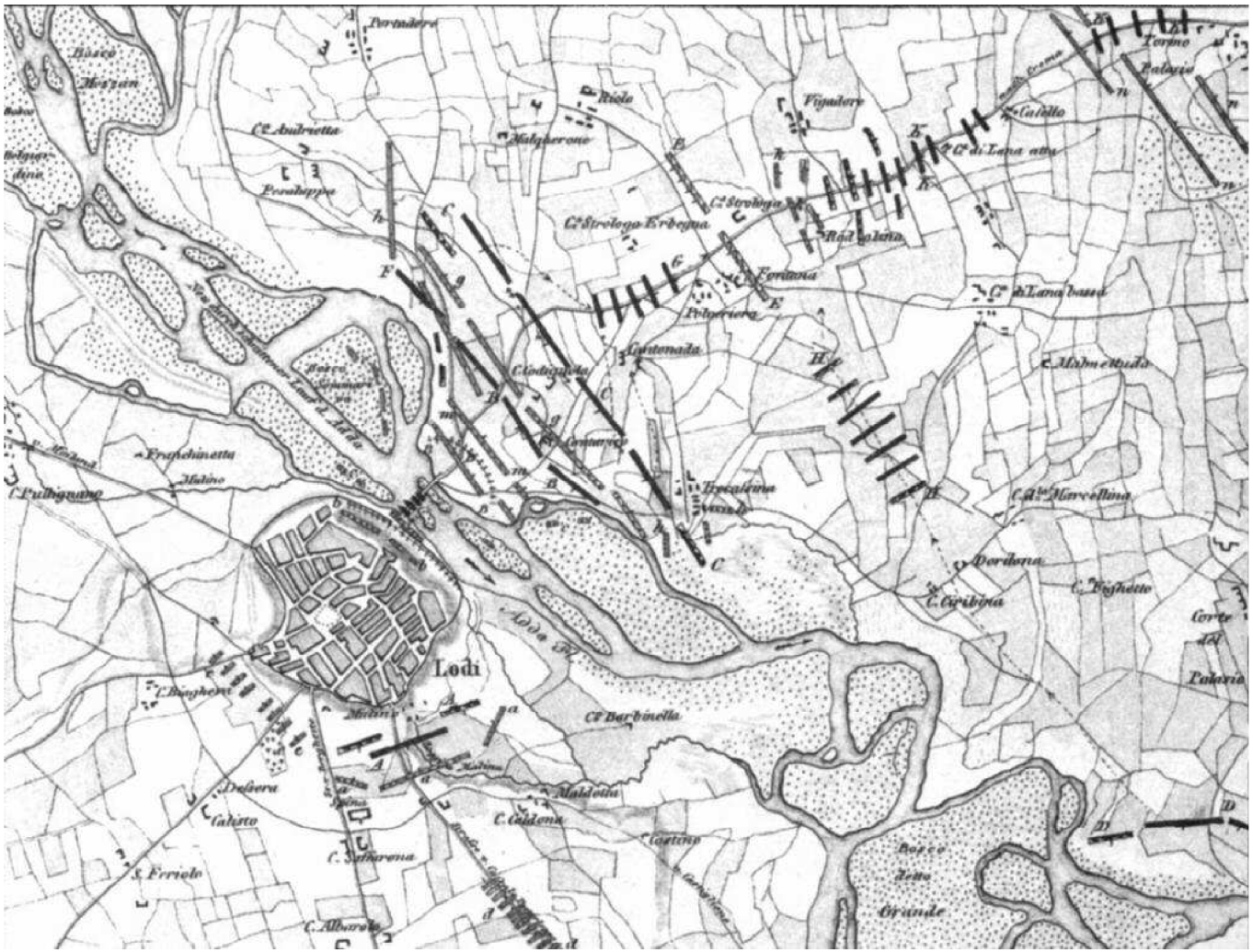
Historical note - Lodi

Lodi May 10, 1796

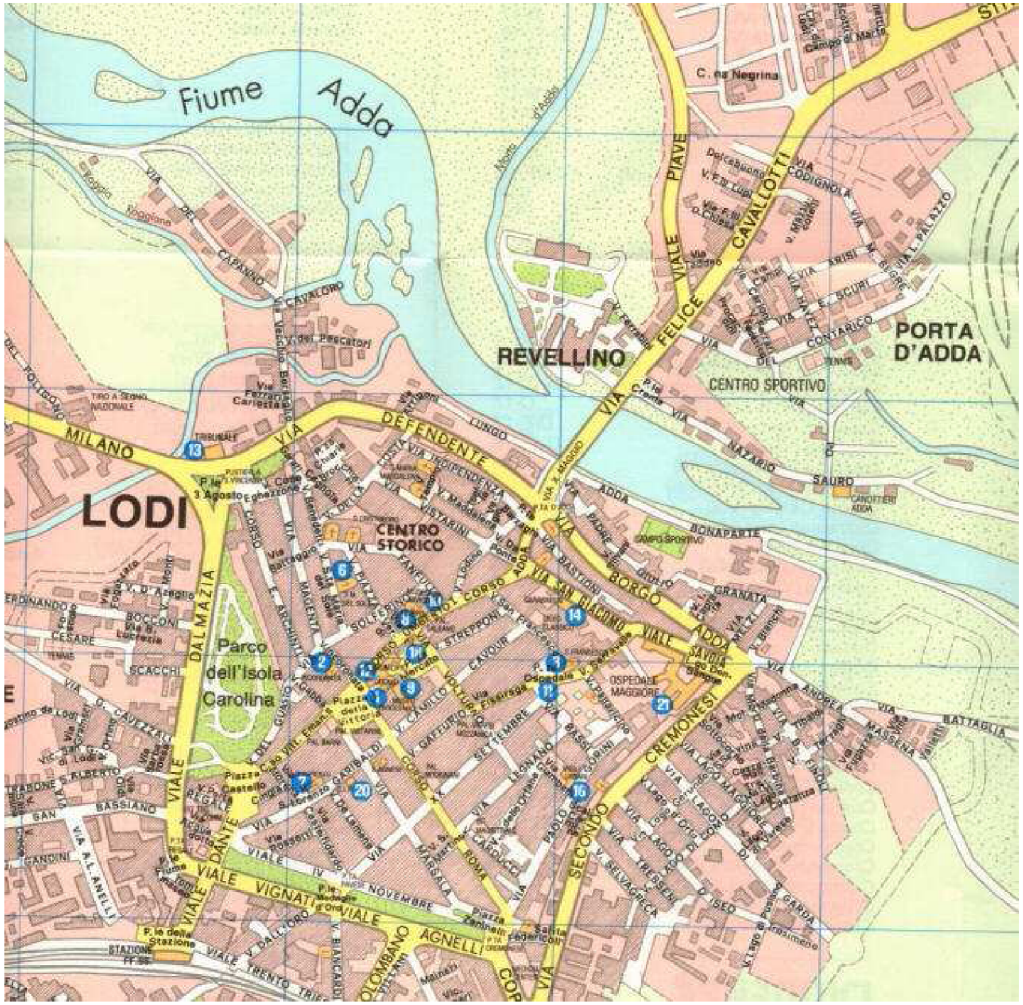
First italian campaign

1796

Historical map



Todays map of Lodi



Where the legend started

New bridge in Lodi

Mondovi April 21, 1796

Flow of calculations

1. read EMPIRE input file (*.inp*)
2. construct table of nuclei involved
3. read from the input parameter library (or input/output files if such exist)
   - discrete levels,
   - binding energies,
   - level density parameters,
   - shell corrections,
   - ground state deformations ,

Flow of calculations (cont.)

4. calculate
   - transmission coefficients
   - level densities
   - fission barriers
5. retrieve experimental data from the EXFOR library

Flow of calculations (cont.)

6. write input/output files
   - .exf
   - .omp
   - .lev
7. ECIS (CC elastic and inelastic scattering)
8. determine fusion cross section
9. select a compound nucleus for consideration

Flow of calculations (cont.)

10. MSD (for the first CN only)
11. MSC (for the first CN only)
12. DEGAS (for the first CN only)
13. HMS (for the first CN only)
14. HRTW (for the highest energy bin in the first CN only)
15. calculate particle and fission widths within Hauser-Feshbach

Flow of calculations (cont.)

16. normalize emission and fission widths with the Hauser-Feshbach denominator and fusion cross section
17. print results for the decay of the considered nucleus
18. select new nucleus and repeats steps 15 through 18 until all requested nuclei are treated
19. print inclusive spectra, reads new incident energy from the input file (.*inp*) and repeat steps 4 and 7 through 19

Executing EMPIRE

Three modes:

- manual
- script mode
- Graphic User Interface (GUI)

Script mode

- Scripts use UNIX bash-shell (!)

Script invoked with a root_name of the input file

```
run Mo100
```

File nameing convention

root_name[-distinction].extension

- **root_name** - any string chosen by the user (**no '.'**), eg., U238, fe56
- **extension** - set by EMPIRE (input must be 'inp', eg., U238.inp)
- **distinction** - set by EMPIRE to differentiate files with the same extensions eg., U238-18.zvd is a ZVView plot file displaying MT=18 (fission)

Scripts

runE	runs EMPIRE, retrieves EXFOR data and translates them into computational format
format	run EMPEND to transform .*out* output into ENDF format (produces .*endf* file)
plot	runs PLOTC4 to create comparison plots of experimental and calculated cross sections
run	does all above (runE + format + plot)

Scripts (cont.)

clean	removes files with extensions: *.lev, .endf, .lst, .out, .x42c4_errs, .x42c4_lst*, and *.exf*
zvd	create ZVView plot for the selected MT excitation function ('ZVV' button in GUI)
zvpl	create ZVView plot for the excitation function for any cross section printed in the main output ('Create ZVV' button in GUI)

Scripts (cont.)

zvcomb	merge several existing ZVView plots into one plot ('Merge ZVV' button in GUI)
mtacomp	create ZVView plot comparing experimental data with the results of up to three sets of calculations
acomp	the same as *mtacomp* but does the job for the whole list of MTs

Auxiliary scripts

store moves *all output* files for all projects (*.inp* files are copied rather than moved) to a subdirectory specified as a parameter to *store*

run-piece-wise runs up to 3 input files for the same case but in different, non-overlapping energy ranges. Used to apply different model parameters in separate energy ranges

cleanall removes all output files preserving inputs (no parameter)

GUI mode

Invoked by typing: **Xrun.tcl &**

- Creates input file
- Runs entire sequence of codes
- Creates and displays comparison plots
- Offers access to files and scripts with a mouse click
- Provides certain file-manager functionalities

ENDF formatting

select ENDF =1 or 2 in the input file (.*inp*)

- ENDF=1 (exclusive spectra)
  - EMPIRE rearranges exclusive emission spectra (d and dd)
  - dd spectra for recoils (for binary reactions exact, for two particle emission channels approximated, no recoils for 3 particle emission)

New algorithm for exclusive spectra implemented in version 2.19

ENDF formatting (cont.)

- ENDF=2 (inclusive spectra)
  - Inclusive light particle emission spectra (dx and ddx) in CM
  - Recoil spectra include correlations among subsequent emissions (LAB)
  - Arbitrary reaction can be handled (high incident energies)

ENDF formatting (cont.)

- EMPIRE output (.*out*) is processed and converted into ENDF format by running EMPEND code (not completed for ENDF=2)
- MF=1, 3, 4 and 6 are created
- MT=5 representation for ENDF=2
- ddx cross sections and angular distributions are expanded in Legendre polynomials
- Cross sections can be interpolated with a cubic spline

Input/Output files

.inp (main input)

- EMPIRE reads as much data as possible form the input parameter library (*empire/data*)
- User has to supply only those input parameters that the code **can not** know (incident energy, the projectile, the target and the number of neutron, proton, α, and light-ion emissions)

Input/Output files (cont.)

- Prioritized access to input data
  1. case specific files (*.lev, .fus, .omp*)
  2. input file (.*inp*)
  3. general input parameter library

Note, that *all (*except *.inp)* files are created by the code in the first run. User **only** has to create an .*inp* file
Editing *.lev, -omp.*,* and *.c4* files is a convenient method of adjusting some of the input data

Input/Output files (cont.)

Input file (*.inp)* consists of the mandatory and the optional part

Mandatory input

```
     14.8                  ;INCIDENT ENERGY (IN LAB)
56.  26.                   ;TARGET A , Z
1.    0.                  ;PROJECTILE A, Z
3                         ;NUMBER OF NEUTRONS TO BE EMITTED
1                          NUMBER OF PROTONS TO BE EMITTED
1                         ;NUMBER OF ALPHAS TO BE EMITTED
0.   0.   0.               ;NUMBER OF L.I. TO BE EMITTED
```

$$\sigma_{(n,3npa)} = \sigma_{(n,2npna)} + \sigma_{(n,np2na)} + \sigma_{(n,p3na)} + \cdots$$

Input/Output files (cont.)

.lst (long output)

- optional input
- 1-st incident energy
  - Compound Nucleus
  - 1-st residue
  - . . .
  - last residue
  - inclusive γ, n, p, α, and light ion spectra
- 2-nd incident energy

Input/Output files (cont.)

-ecis.in

- ECIS input produced by EMPIRE in each run (for checking)

-ecis.out

- ECIS output file (for the last energy)

-lev.col

- File with collective levels for ECIS produced by EMPIRE in the first run

Input/Output files (cont.)

.out (short output)

```
REACTION   6-C - 12 +  13-Al- 27 INCIDENT
ENERGY   50.1     MeV
COMPOUND NUCLEUS ENERGY   51.295 MeV
FUSION CROSS SECTION =   1285.1     mb
19-K - 39 production cross section 0.566424E-08 mb
   fission  cross section  0.0000     mb
g  emission cross section 0.15879     mb
n  emission cross section  250.52     mb
p  emission cross section  247.58     mb
He emission cross section  786.84     mb
```

With ENDF option this file is read by the EMPEND code

Input/Output files (cont.)

.fus

- User supplied fusion cross sections
- If present, will override any disposition in input
- A simple column of fusion cross sections for subsequent partial waves starting with *l* = 0
- Code will consider only those below actual value of NDLW
- Can be used for a single energy only

Input/Output files (cont.)

.lev

- Discrete levels for all nuclei involved in a calculation
- Produced by EMPIRE during the first run
- **.lev** often needs modifications:
  - cut-off some levels
  - missing branching ratios,
  - uncertain spins and/or parities
  - add levels

Input/Output files (cont.)

-omp.int

- Optical model parameters for various nucleus-ejectile combinations
- Produced, from built-in systematics, during the first run

```
 38-K   +  1-n         19038 +      1
Emin, Emax     0.0000    15.0000     1.0000     0.0000     1.2500
real
vol      54.1900    -0.3300     0.0000     0.0000     1.1980     0.6630
imag
vol       0.0000     0.0000     0.0000     0.0000     1.2950     0.5900
imag
surf      4.2800     0.4000     0.0000     0.0000     1.2950     0.5900
real
```

Input/Output files (cont.)

-omp.ripl

- Optical model parameters for various nucleus-ejectile combinations for which RIPL omp were specified in input
- Produced, from RIPL-2 omp library, during the first run.
- Reproduces RIPL-2 format.

Input/Output files (cont.)

-omp.dir

- Optical model parameters to be used in ECIS for CC or DWBA calculations
- Produced, from the RIPL-2 omp library or internal systematics during the first run
- Reproduces RIPL-2 or internal format

Input/Output files (cont.)

.endf

- EMPIRE results processed by EMPEND and RESEND into the ENDF format (final ENDF file)

-s.endf

- .**endf** file processed with utility codes (**to be used for plotting only**).

NOTE: depending on the setup of the ***run*** script there might be more files with **.endf** extension

Input/Output files (cont.)

.exf

- Relevant experimental data retrieved from the EXFOR library (in EXFOR format).

.c4

- EXFOR data translated into the computational format by the X4TOC4 code

Input/Output files (cont.)

.ps

- PostScript plots comparing calculations against experimental data produced by the PLOTC4 code. Plots are automatically produced for all matches between experimental and calculated data. If there is no match no plots are produced.
- Note that to be plotted EMPIRE results must be ENDF formatted

Input/Output files (cont.)

-cum.ps

- PostScript plot with cumulative plots of discrete levels compared against level densities
- Produced with the FITLEV$\neq 0$ input option (**highly recommended**)

Input/Output files (cont.)

-MT.zvd

- Input file for plotting MT reaction with ZVView (e.g., mn55-102.zvd)
- Created by invoking ZVView from the GUI
- Different **.zvd** files can be combined into a single plot directly from GUI

Input/Output files (cont.)

-log.name_of_code

- Log file produced by the code indicated by the extension (name_of_code)

.x42c4_lst

- Log: translation from EXFOR to computational format

Input/Output files (cont.)

.x42c4_errs

- List of EXFOR entries not translated by X4TOC4

.war

- List of warnings produced by EMPIRE extracted from the **.lst** file (checking this file is recommended)

Neutron capture

neutron capture on ^{100}Mo at 1.9 MeV

```
 1.9                    ;INCIDENT ENERGY (IN LAB)
100.   42.                ;TARGET  A , Z
1.      0.                ;PROJECTILE A, Z
0                        ;NUMBER OF NEUTRONS TO BE EMITTED
0                        ;NUMBER OF PROTONS  TO BE EMITTED
0                        ;NUMBER OF ALPHAS   TO BE EMITTED
0   0.   0.               ;NUMBER OF L.I. TO BE EMITTED
GO
-1.
```

Heavy Ion induced reaction

^{48}Ca + ^{248}Cm reaction $\Rightarrow$ Z=116.

```
240.0                    ;INCIDENT ENERGY (IN LAB)
248.  96.                ;TARGET  A , Z
48.   20.                ;PROJECTILE A, Z
6                        ;NUMBER OF NEUTRONS TO BE EMITTED
0                        ;NUMBER OF PROTONS TO BE EMITTED
0                        ;NUMBER OF ALPHAS TO BE EMITTED
0  0.  0.                 ;NUMBER OF LI TO BE EMITTED
IOUT        3.
NEX       100.
BETAV       8.6
SHRJ       20.
SHRD        3.
LTURBO      2.
GO
-1.
```

MSD+MSC+HF calculation

All reactions of the type
^{100}Mo(n, *x*n *y*p *z*α)
with *x*=0, 1, 2, *y*= 0, 1 and *z*=0, 1

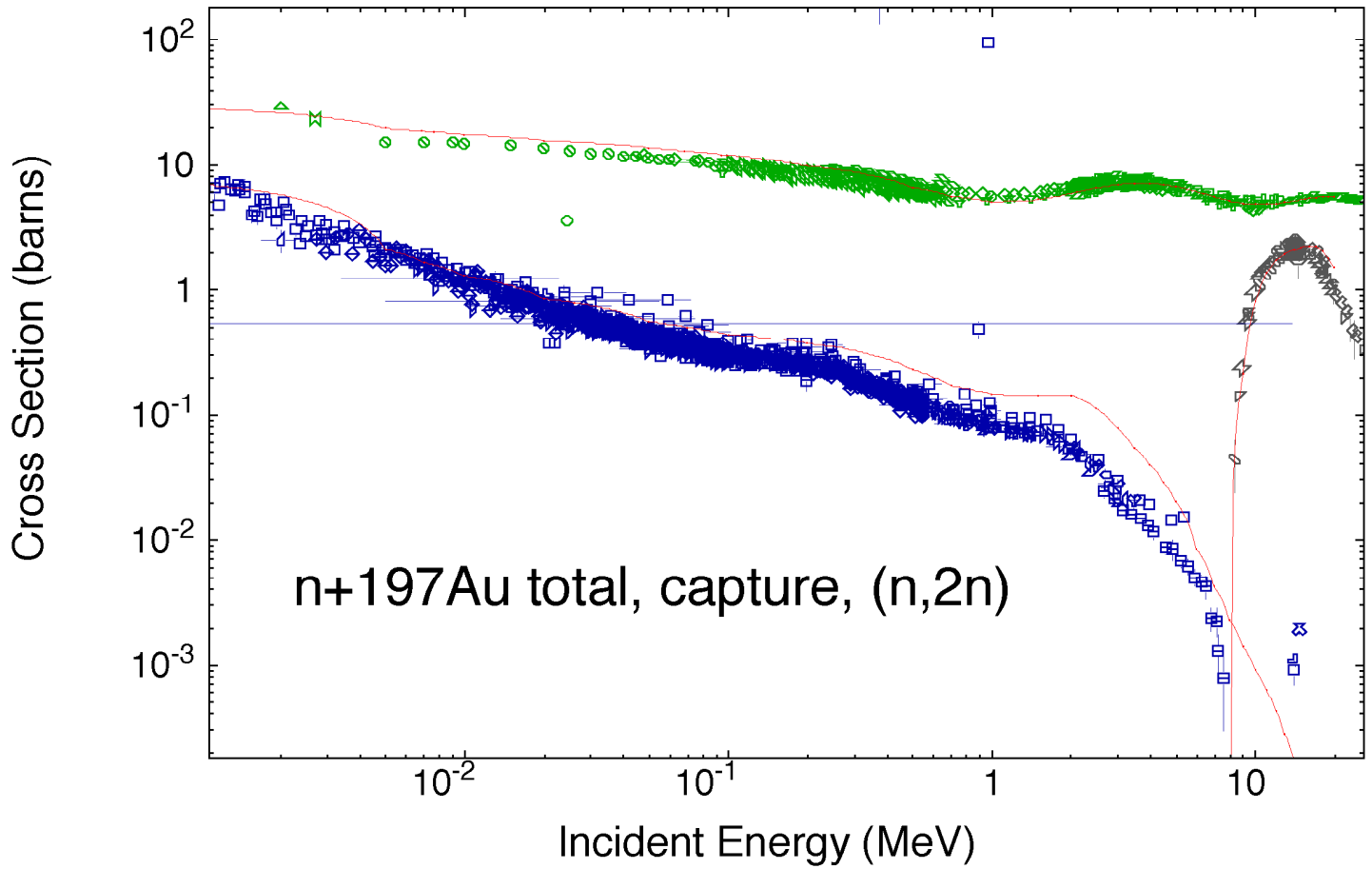
```
  0.1                    ;INCIDENT ENERGY (IN LAB)
100.  42.                ;TARGET A , Z
  1.   0.                ;PROJECTILE A, Z
2                        ;NUMBER OF NEUTRONS TO BE EMITTED
1                        ;NUMBER OF PROTONS TO BE EMITTED
1                        ;NUMBER OF ALPHAS TO BE EMITTED
0  0.  0.                 ;NUMBER OF L.I. TO BE EMITTED
IOUT        3.
LEVDEN      0.
NEX       100.
MSD         1.
MSC         1.
```

MSD+MSC+HF calculation (cont.)

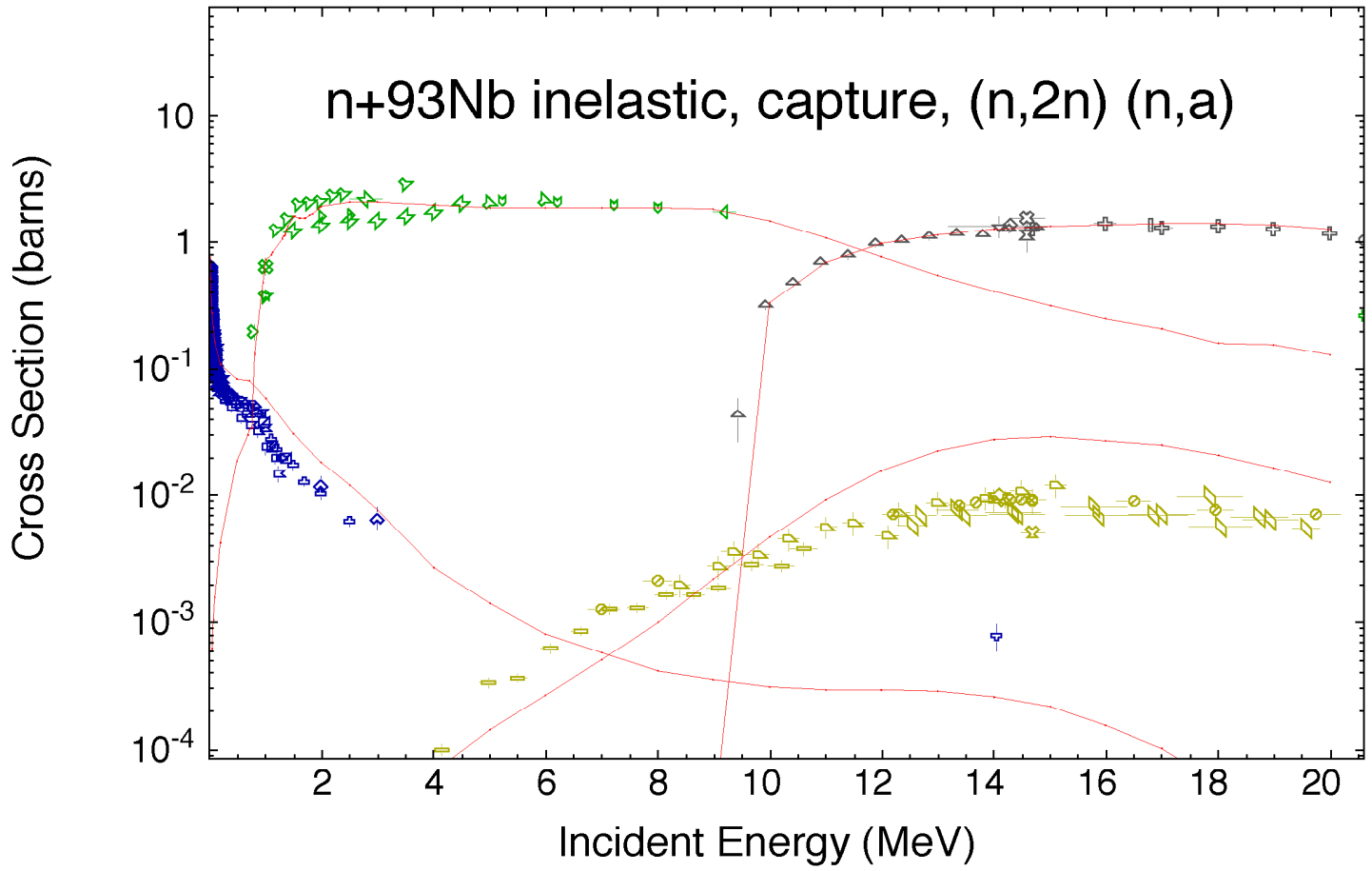
```
ENDF        1.
OMPOT       6.          1
GO
0.5
1.
2.
3.
...
17.
18.
20.

-1.
```

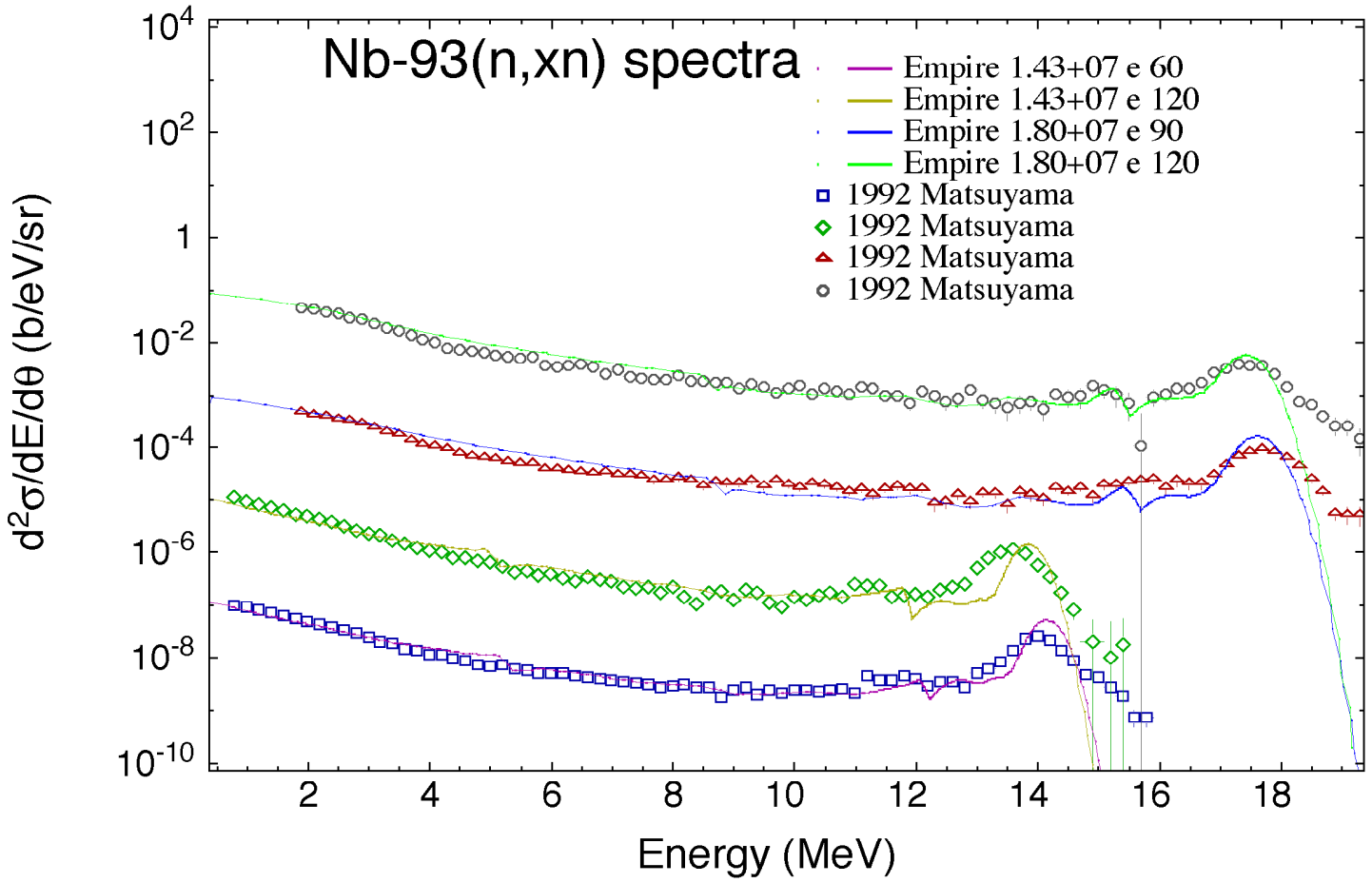
Default calculations



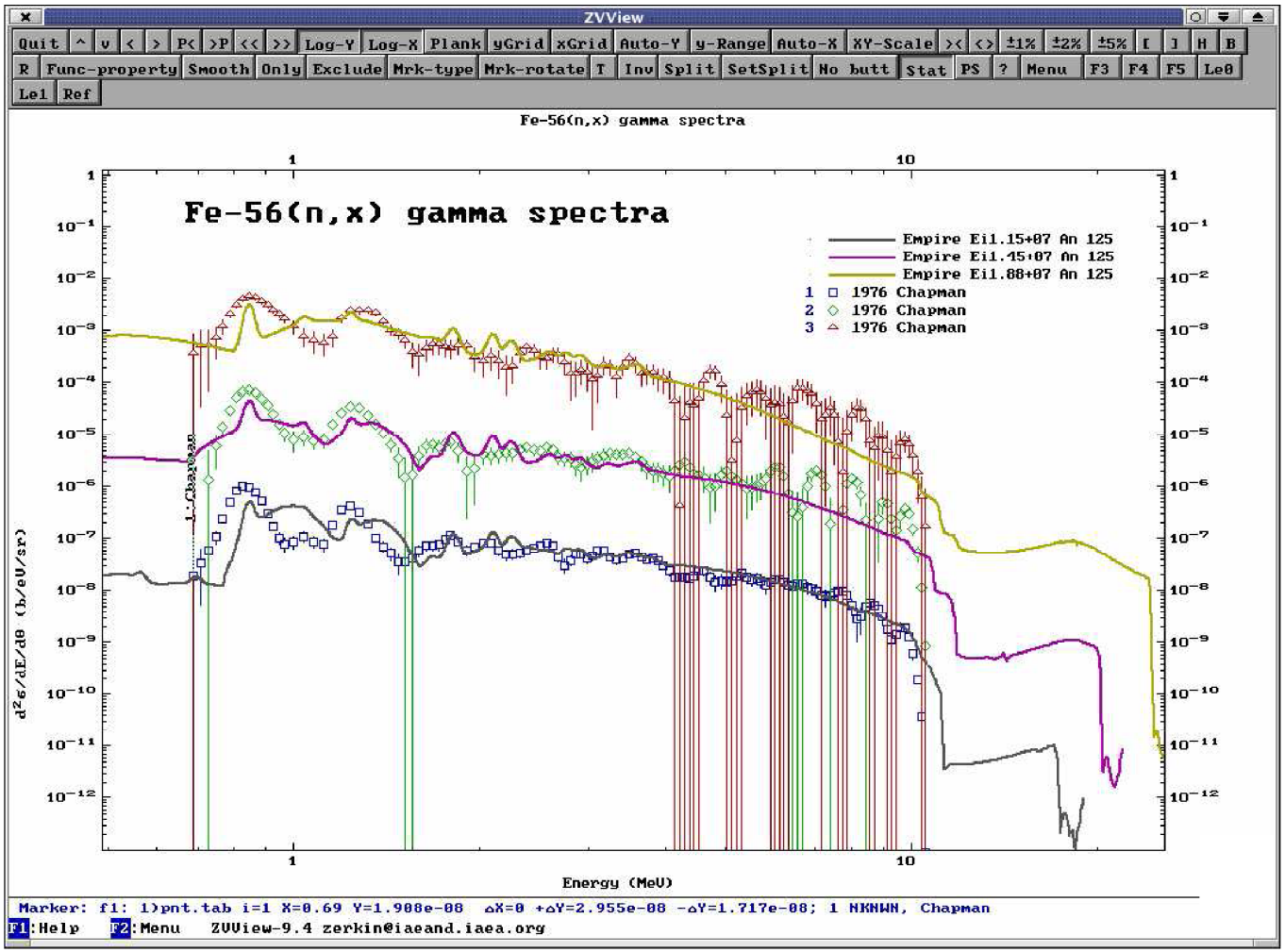
Default calculations



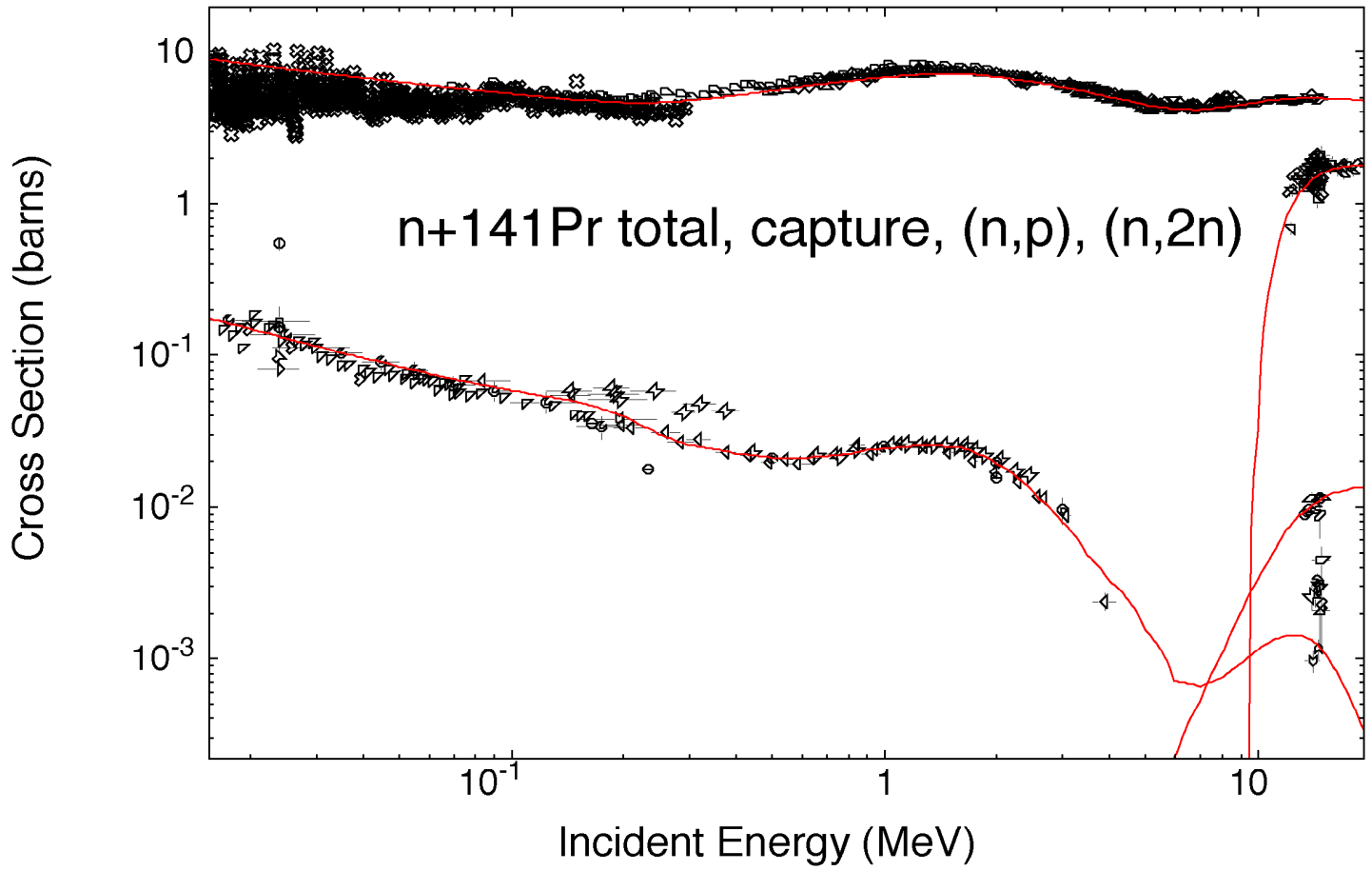
Default calculations



Default calculations



Adjusted calculations (evaluation)

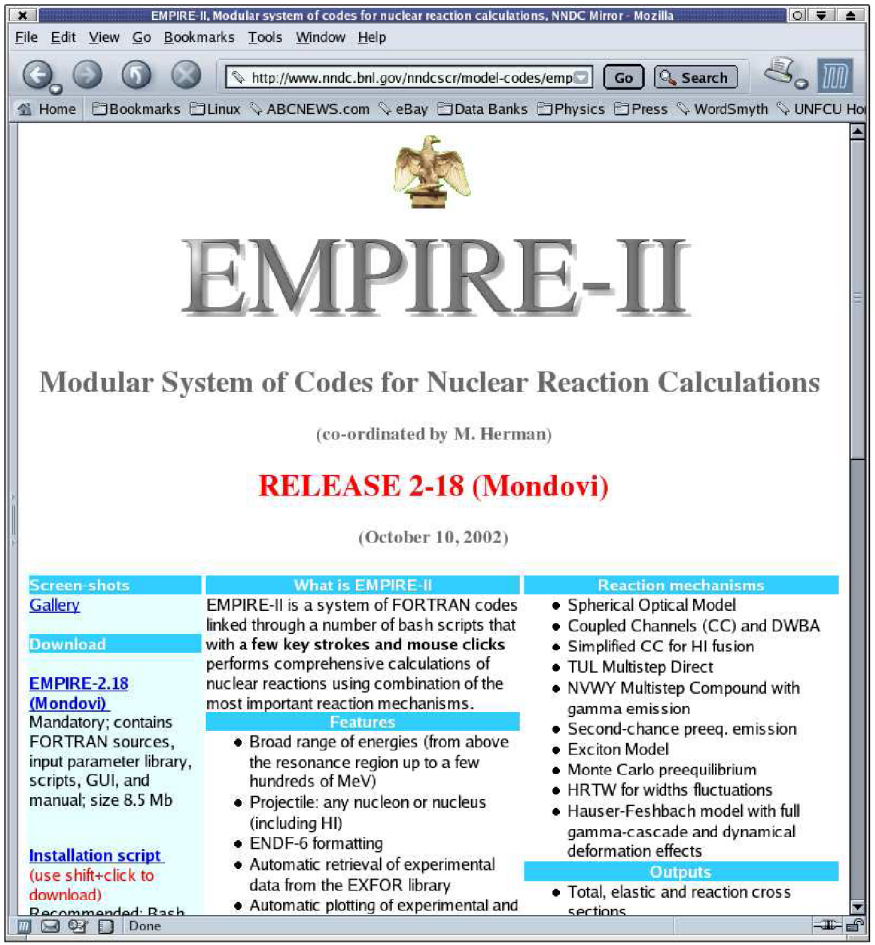


How to get EMPIRE

EMPIRE-2.18 (Mondovi) available at:

- http://www.nndc.bnl.gov/nndcscr/model-codes/empire-ii/
- http://www-nds.iaea.org/empire/
- CD-ROM can be requested from: http://www-nds.iaea.org/cd-catalog.html

EMPIRE Web page



Next release of EMPIRE

EMPIRE-2.19 (Lodi), expected release April/May 2004, will include:

- new fission channel
- reactions on excited targets
- preequilibrium emission of clusters
- merging of resonance region into the ENDF file
- improved exclusive spectra
- updated relational EXFOR database