The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

2141-31

Joint ICTP-IAEA Workshop on Nuclear Reaction Data for Advanced Reactor Technologies

3 - 14 May 2010

Introduction to Nuclear Model Code EMPIRE

CAPOTE R.

IAEA
Vienna
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EMPIRE code as a tool for nuclear reaction data evaluations

IAEA HQ
Vienna
Austria

Roberto Capote

International Atomic Energy Agency, NAPC - Nuclear Data Section

OUTLOOK

- Principles of nuclear data evaluation
- EMPIRE overview
- EMPIRE as a ND evaluation tool
- Selected evaluations and modelling results

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Motivation for new ND evaluations

OECD/NEA WPEC Subgroup 26 Final Report:
"Uncertainty and Target Accuracy Assessment for Innovative Systems Using Recent Covariance Data Evaluations",
M Salvatores (coordinator), R. Jacquemin (monitor),
Technical report NEA No. ***6410****, OECD 2008.*

The request for improved cross sections and emission spectra and their accuracies for neutron induced reactions on ^{238}U is an important issue that emerges in several of cases studied. High accuracy requirements were placed on inelastic cross-sections ^{238}U(n,inl) in the whole energy range up to 20 MeV and on capture cross section ^{238}U (n,γ).

Cross sections uncertainties and covariance data are strongly required

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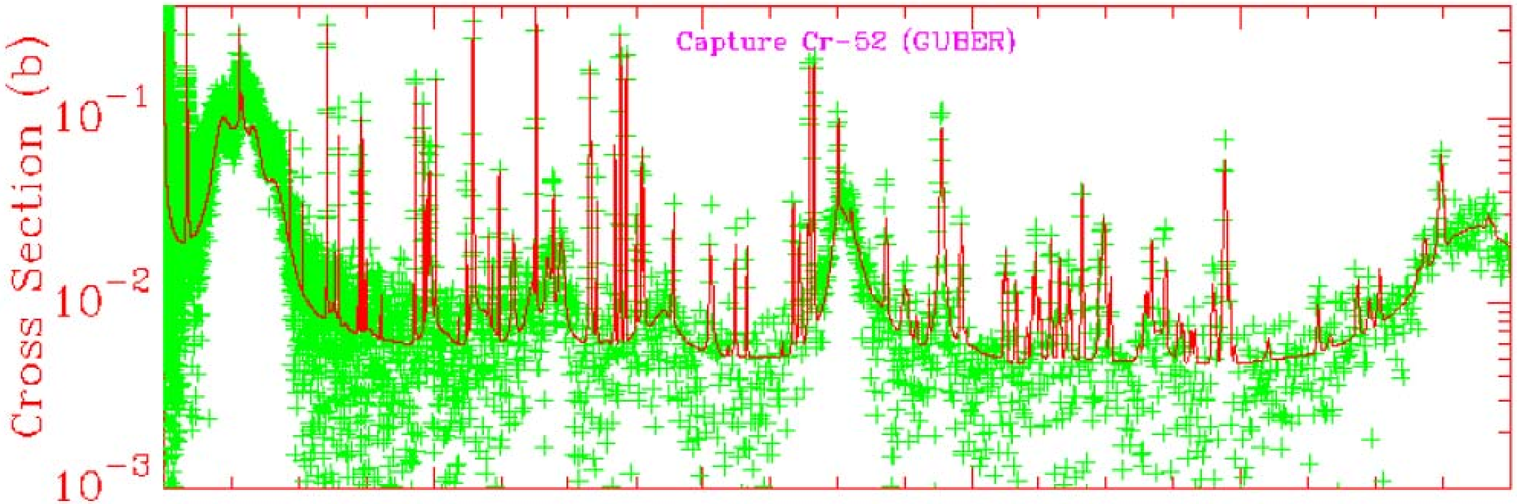
ND evaluation: energy ranges



- Resonance energy range (Γ << D)
- Unresolved resonance range (in between)
  (self-shielding)
- Fast neutron range (Γ >> D stat models)
  keV for actinides, MeV for Ni, Fe, Cr,…

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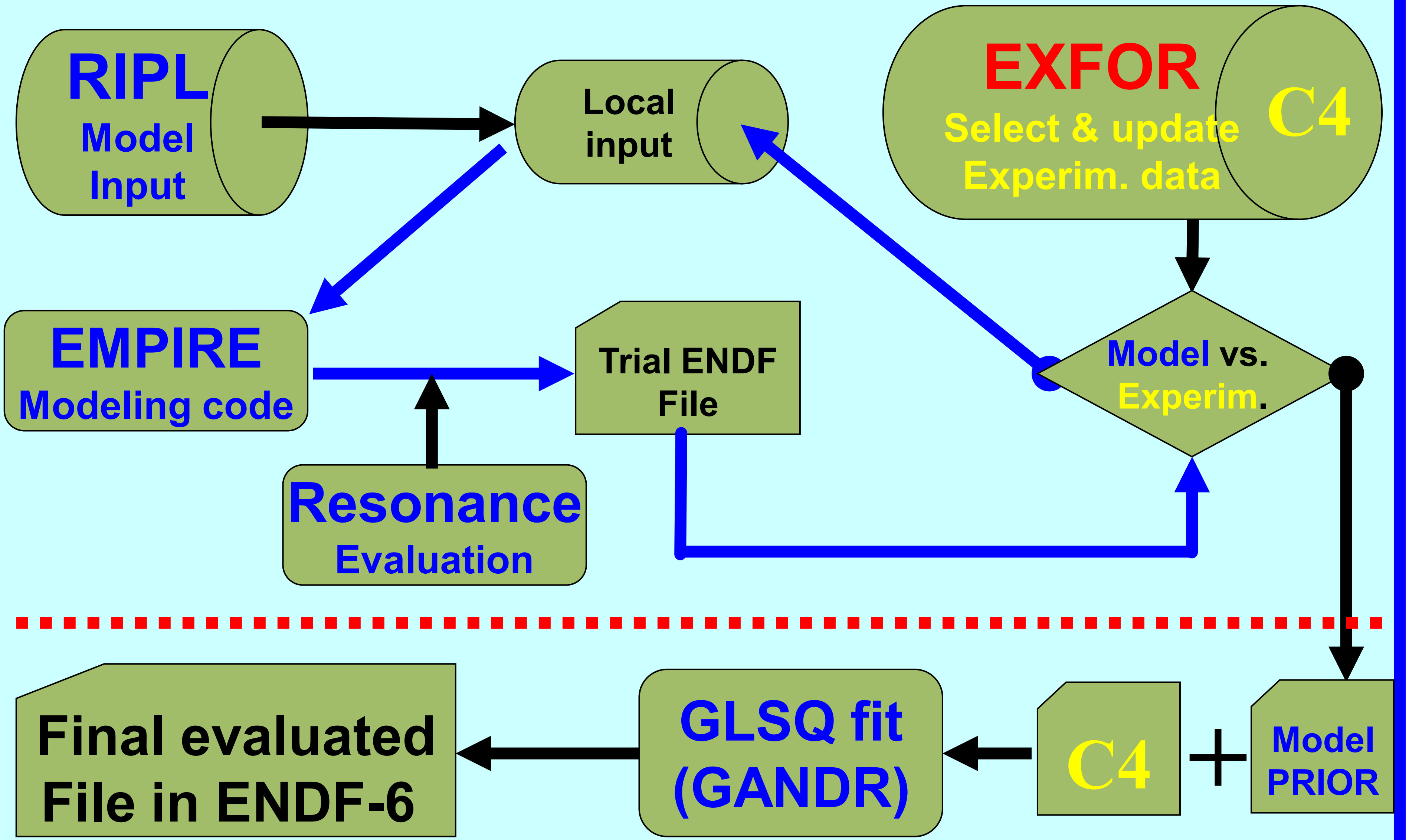
Nuclear Data Evaluation process



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What is Nuclear Data Evaluation?

A properly weighted combination (usually by GLSQ fit) of selected experimental data and nuclear reaction modelling results.

Alternatives:

- ❑ GLSQ model can be replaced by Unified Monte Carlo

  (see my Thursday lecture)

- ❑ MC sampling can be extended (TMC), no covariance formatting

  (see Koning's lecture in the morning)

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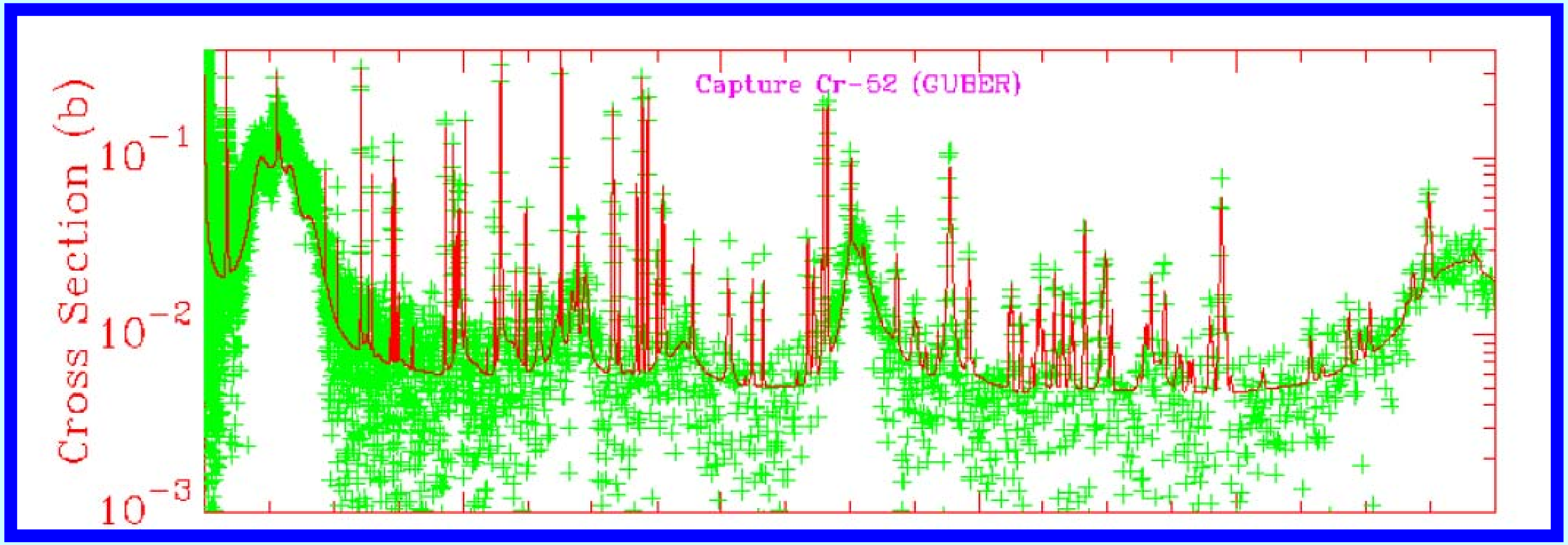
ND evaluation – resonance range



- Theoretical predictions not possible yet
- Resonance parameters must be obtained from fitting experimental data
- Modern resonance fitting codes produce “best fit” parameters as well as their covariances (e.g. SAMMY, REFIT, CONRAD, etc.)

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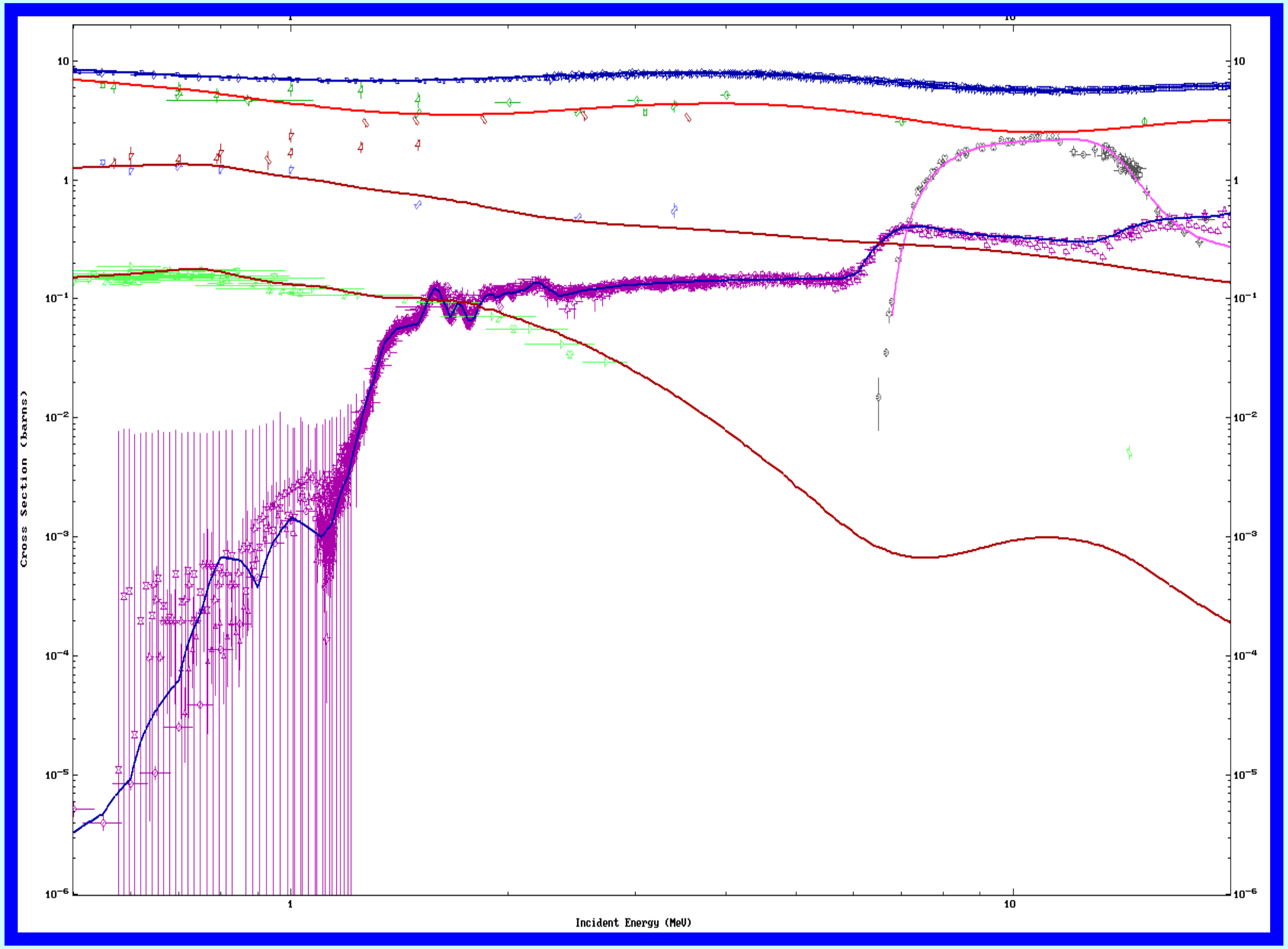
Evaluation – fast energy range



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Evaluation – fast energy range

- Use modern nuclear model code (e.g. EMPIRE or TALYS)
- Choose adequate reaction models
- Define recommended input parameters (RIPL)
- Calculate cross sections and other quantities
- Compare calculated values to selected measured data (after correcting for new stds, discarding discrepant, etc)
- Fine-tune the input model parameters

Loop

- From model parameter uncertainties and model uncertainties generate covariance matrix prior

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EMPIRE overview

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https://ndclx4.bnl.gov/gf/project/empire/

Extension of the nuclear reaction model code
EMPIRE
to actinides' nuclear data evaluation

@NNDC: http://www.nndc.bnl.gov/empire219/   @IAEA: http://www-nds.iaea.org/empire/

ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

Nuclear Data Sheets 108 (2007) 2655–2715

Nuclear Data Sheets

www.elsevier.com/locate/nds

EMPIRE: Nuclear Reaction Model Code System for Data Evaluation

M. Herman[1,*], R. Capote[2], B.V. Carlson[3], P. Obložinský[1], M. Sin[4], A. Trkov[5], H. Wienke[6], and V. Zerkin[2]

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[3] Departamento de Física, Instituto Tecnológico de Aeronáutica, 12228-900, SP, Sao José dos Campos, Brazil
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[5] Jozef Stefan Institute, Reactor Physics Division R-1, Jamova 39, 1000 Ljubljana, Slovenia and
[6] Belgonucleaire, Dessel, B2480, Belgium

EMPIRE developers

- M. Herman (BNL, NNDC) – coordinator
- R. Capote (IAEA, Vienna)
- B.V. Carlson (ITA, Dao Jose dos Campos)
- P. Oblozinsky (BNL, NNDC)
- M. Sin (Univ. Bucharest)
- A. Trkov (JSI, Lubljana)
- H. Wienke (Belgonucleaire)
- V. Zerkin (IAEA, Vienna)

Contributors:

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EMPIRE highlights

System of codes for modelling nuclear reactions:

- broad range of energies (up to ~150 MeV) and projectiles
- most important nuclear reaction mechanisms
- choice of models and parameterizations
- extensive input parameter library (RIPL)
- automatic retrieval of experimental data from EXFOR
- highly automated fit of optical model parameters
- determination of covariances (Monte Carlo, Kalman filter)
- easy input (extensive use of defaults, built-in internal logic)

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EMPIRE highlights (continued)

- ❑ easy operation via Graphic User Interface (GUI)
- ❑ interactive plots of experimental and calculated results
    - ◦ excitation functions
    - ◦ angular distributions
    - ◦ inclusive emission spectra for n, p, …
    - ◦ double differential spectra

  Plots use ZVView (see V. Zerkin lecture)

- ❑ ENDF-6 formatting (EMPEND, see A. Trkov lecture)
- ❑ utility codes (ENDF-6 verification)

Full path from experiment to validated ENDF-6 file

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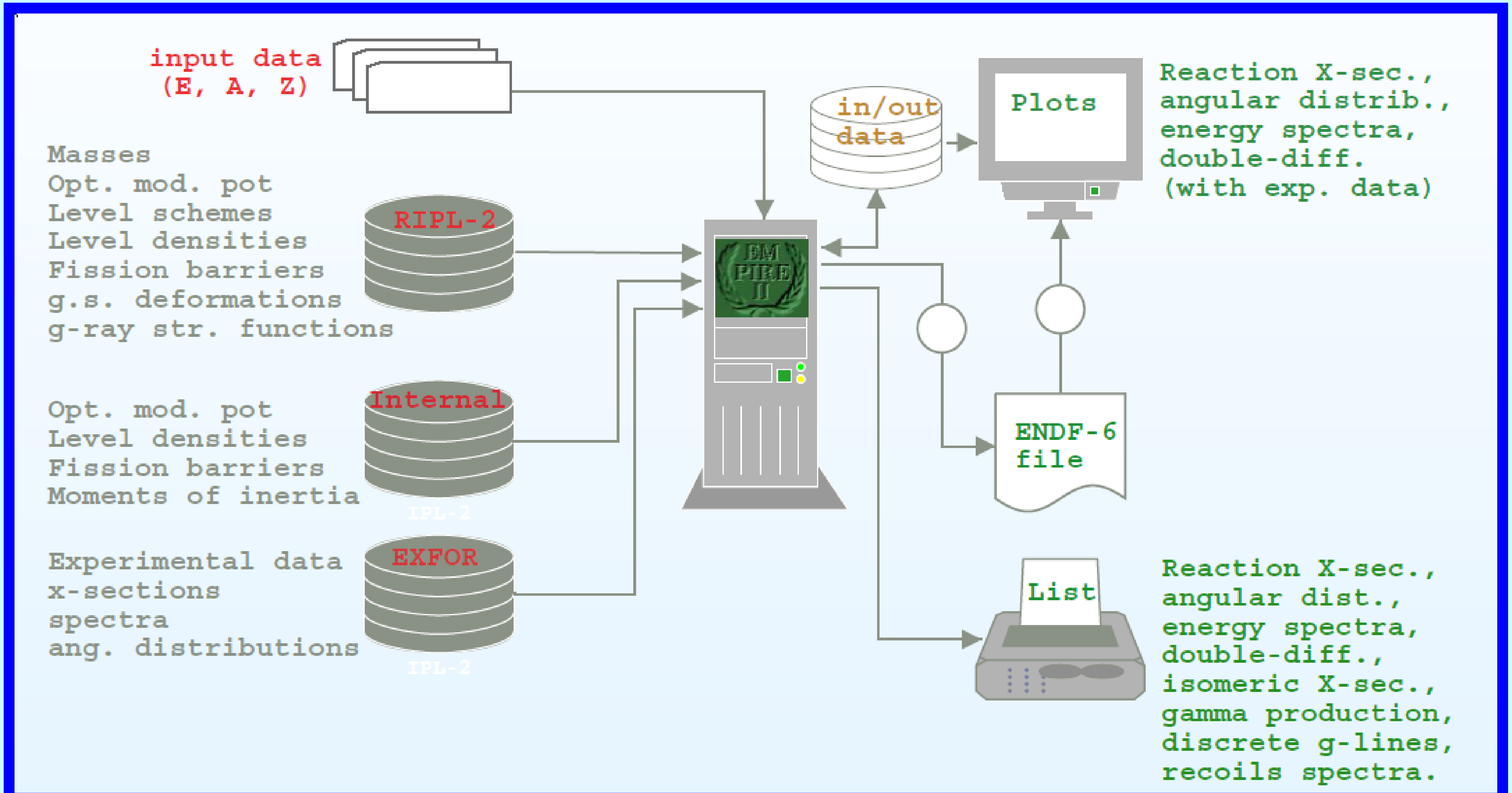
EMPIRE layout



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Intermezzo storico opus 1

Table 1: Major releases of the EMPIRE code.

Version	Year	Location	Comments
EMPIRE	1980	Warsaw	CN+HYBRID
EMPIRE MSC	1983	Warsaw	FKK(MSC)
EMPIRE HI	1988	Messina	heavy-ion version
EMPIRE HMS	1991	Bologna	NVWY(MSC)+TUL(MSD)
EMPIRE-2.13	2001	Vienna	totally rewritten
EMPIRE-2.17 (Montenotte)	2002	Vienna	ECIS, HRTW, EXFOR, HMS, DEGAS, RIPL-2, plotting
EMPIRE-2.18 (Mondovi)	2002	Vienna	
EMPIRE-2.19 (Lodi)	2005	Brookhaven	advanced fission, photo-nuclear reactions, PE clusters (PCROSS), OMP fitting, merging resonances, mixed inclusive/exclusive spectra, checking codes, NJOY support, used for ENDF/B-VII.0
EMPIRE-3.0 (Arcola)	2008	Brookhaven	deformed TUL(MSD) Monte-Carlo sampling of input parameters improved fission formatting of isomers

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EMPIRE: reaction models

- ❑ spherical optical model (ECIS-2006),
- ❑ DWBA, coupled channels (ECIS-2006),

- ❑ TUL Multistep Direct (ORION + TRISTAN),
- ❑ NVWY Multistep Compound with -emission,
- ❑ exciton model (PCROSS, DEGAS),
- ❑ Monte Carlo preequilibrium (DDHMS),

- ❑ HRTW for widths' fluctuations,
- ❑ Hauser-Feshbach model with full -cascade and dynamical
- ❑ deformation effects ,
- ❑ State of the art fission (multi-hump barriers, microscopic barriers, optical model for fission, multimodal fission)

(see M Sin lecture)

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EMPIRE statistics

- EMPIRE core: more than 79 000 lines (ECIS: 23860)
- utility codes: more than 109 000 lines
- number of bash and Tcl/Tk scripts: 40
- number of python scripts: 16 and growing!
- size of the internal parameter library: 31.6 Mb
- size of the RIPL-3 library: 91 (+129) Mb (micro LDs)

- Interactive plotting through ZVView
- Results converted into the ENDF-6 format (EMPEND)
- Verification using PREPRO system

Total size: ~ 350 Mb

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EMPIRE platforms

Languages:

- ❑FORTRAN 77 (99%),
- ❑C (mostly ZVView),
- ❑Bash (scripts),
- ❑Tcl/Tk (GUI),
- ❑Python (scripts), (awk)

Operating systems:

- ❑Linux (Red Hat, Fedora, Ubuntu, ...),
- ❑UNIX (any one should work but TLC might be needed)
- ❑Mac (X11 needed for ZVView and xterm)
- ❑MS Windows (EMPIRE core runs, close to be fully operational)

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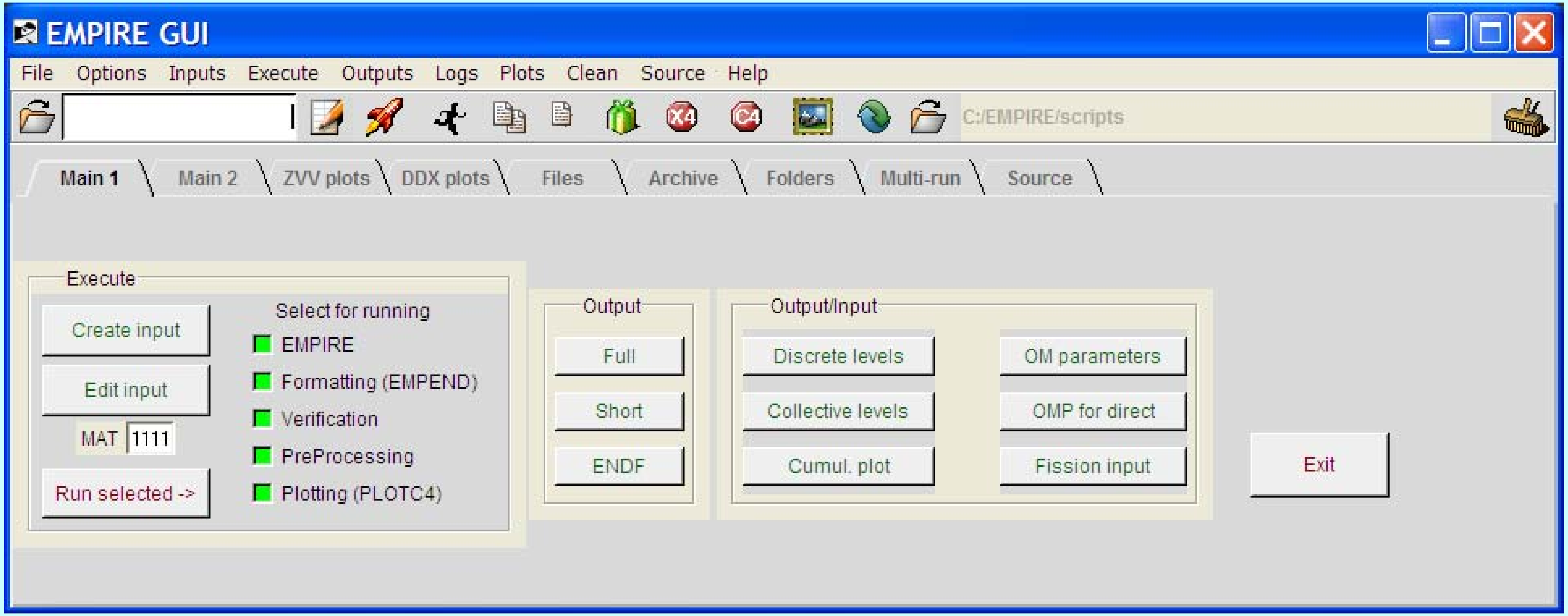
GUI interface (Main 1)



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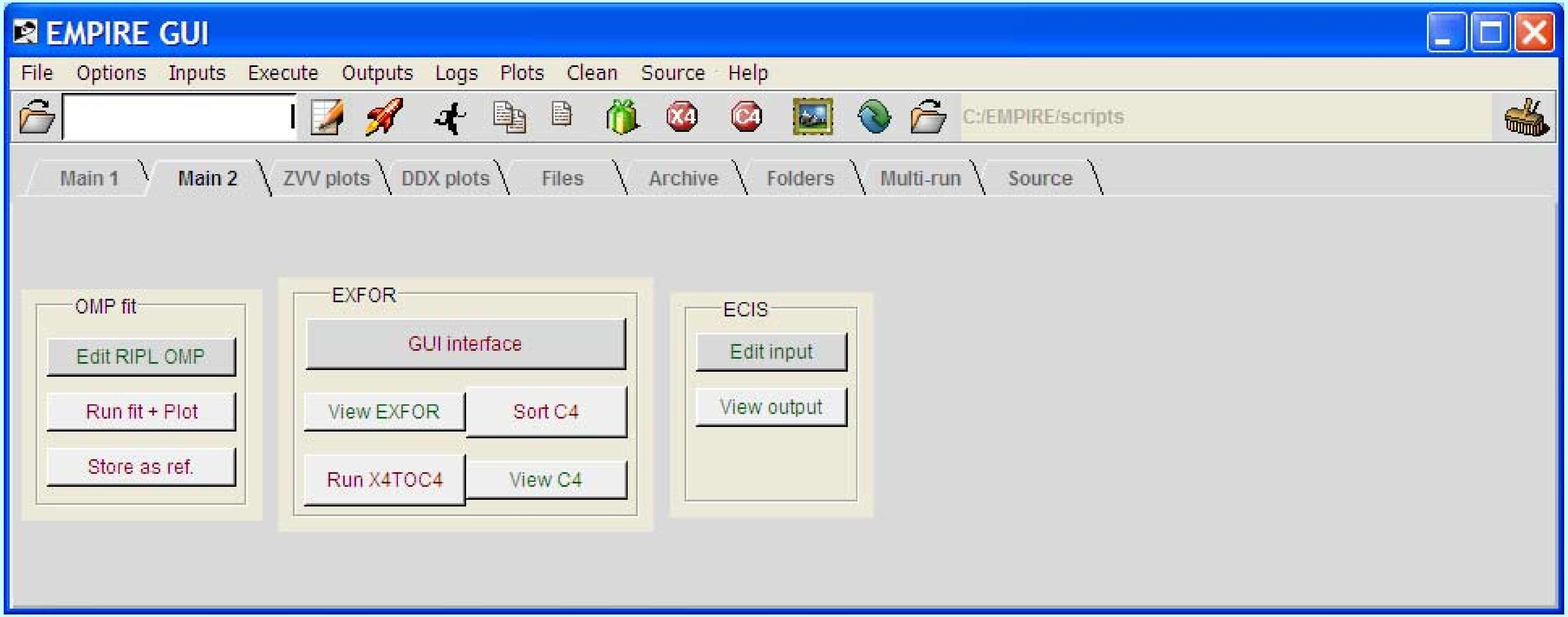
GUI interface (Main 2)



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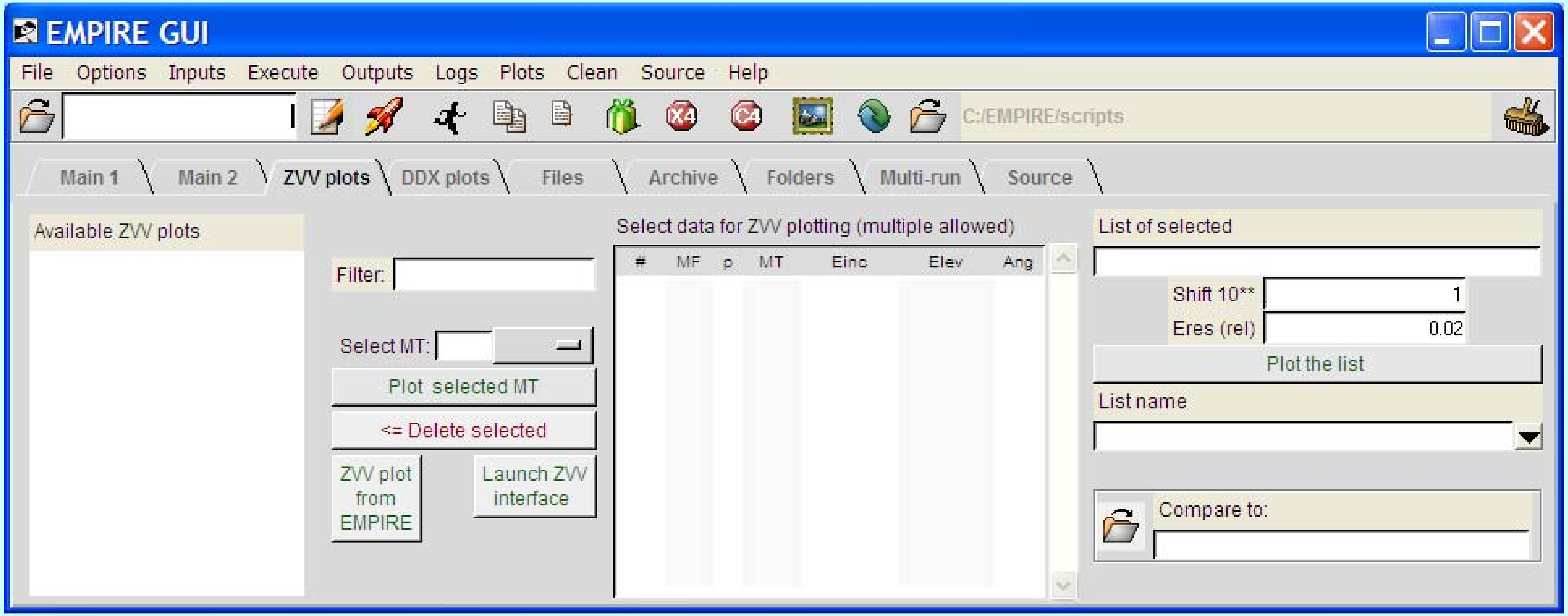
GUI interface (zvv plots)



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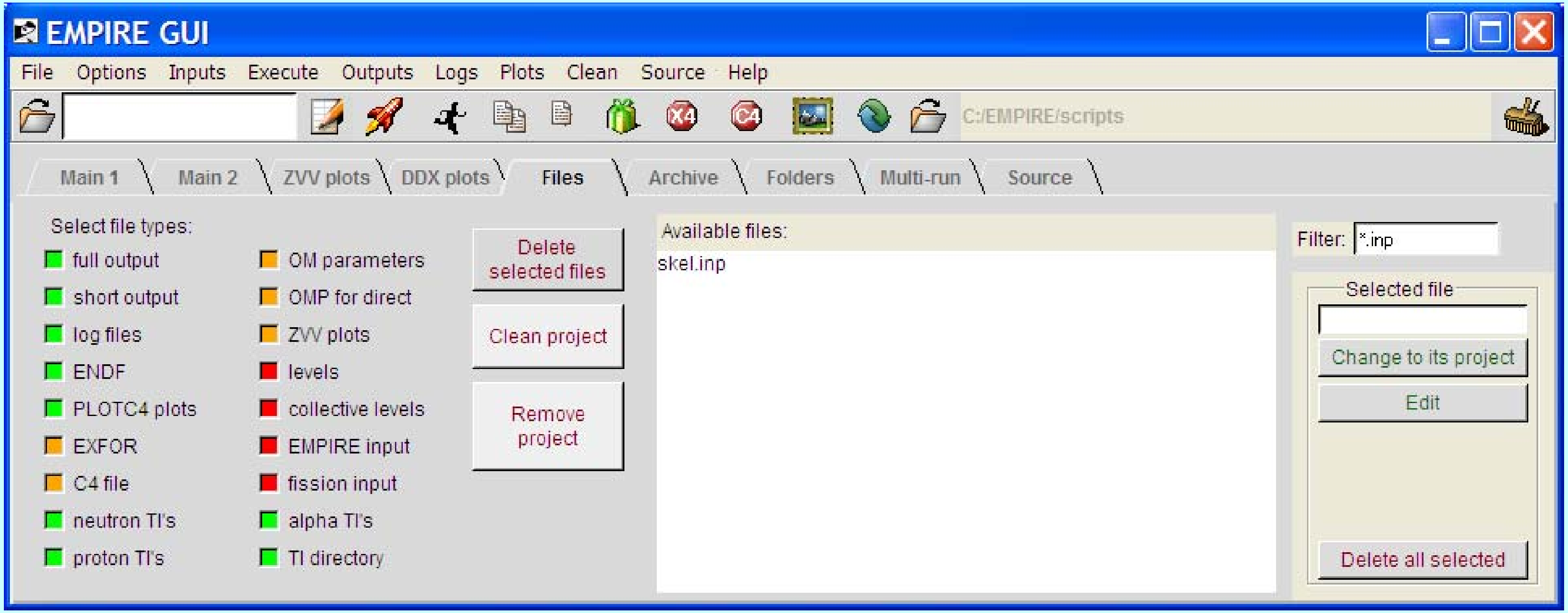
GUI interface (Files)



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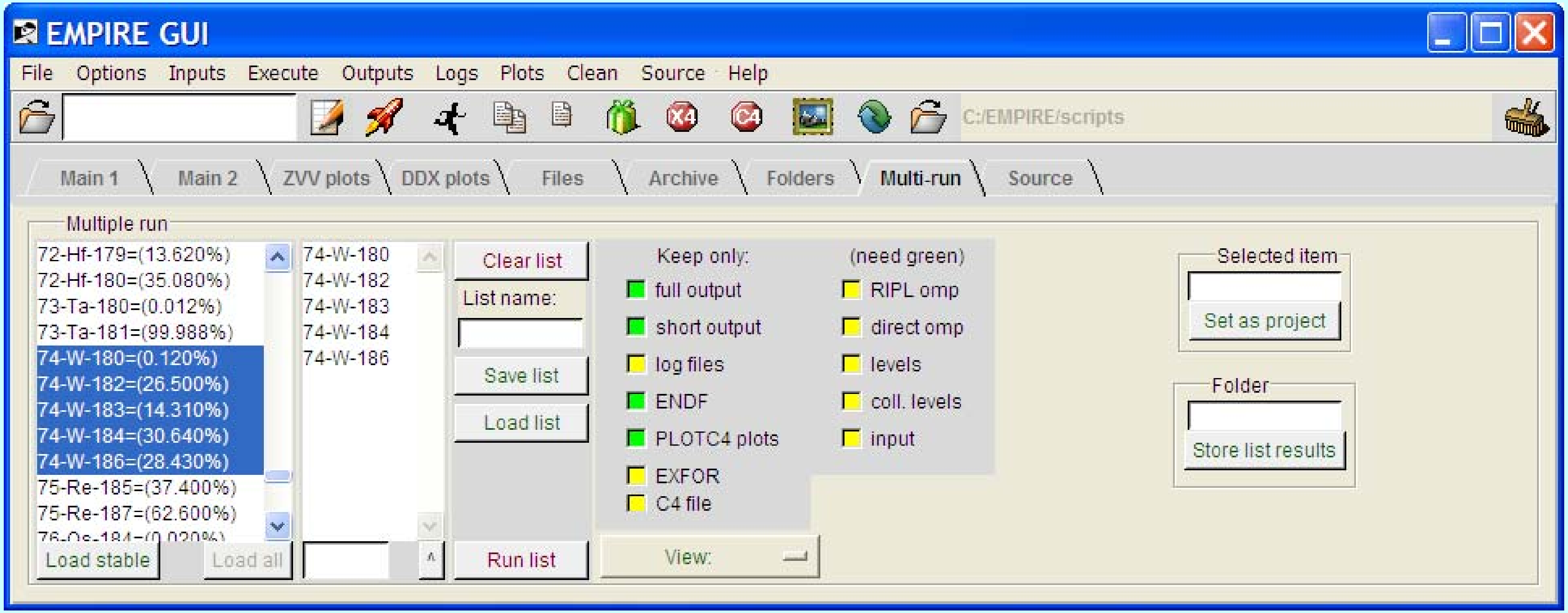
GUI interface (Multi-run)



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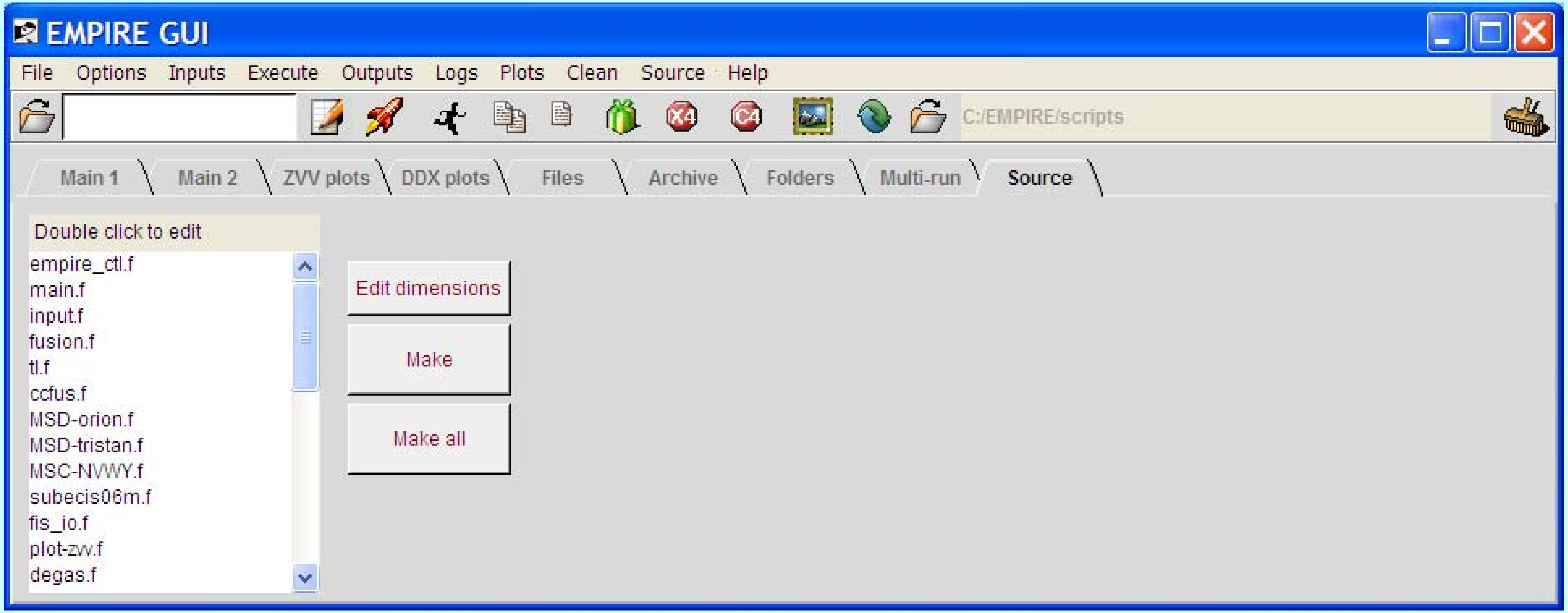
GUI interface (Source)



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Evaluation using EMPIRE

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EMPIRE produces ENDF-6 data

- Reasonable compromise between what:
  - Experimentalists can measure
  - Theoreticians can model
  - Engineers can use
- Well documented (ENDF-102.pdf – June 2009)

  Precise definitions, >300 pages manual
- Adopted by all major national projects

  USA, EU, Japan, Russia, China …
- **Supported by processing codes !**

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ENDF-6 formatted file

```
 2.505500+4 5.446610+1          0          0          1          01111 2151     1
 2.505500+4 1.000000+0          0          0          1          01111 2151     2
 0.0        0.0                 0          0          1          91111 2151     3
 9.000000+0 2.000000+0          0          0          0          01111 2151     4
 1.000000-5 6.368000-1 9.000000+4 6.225000-1 1.000000+5 6.049000-11111 2151     5
 1.100000+5 5.937000-1 1.250000+5 5.766000-1 1.350000+5 5.612000-11111 2151     6
 1.500000+5 5.406000-1 2.000000+5 5.140000-1 2.500000+5 4.810000-11111 2151     7
 1.000000-5 8.000000+4          1          1          1          91111 2151     8
 2.500000+0 0.0                 0          0          1          01111 2151     9
 5.446610+1 0.0                 0          0         24          41111 2151    10
-3.449970+3 2.000000+0 1.078210+0 3.282100-1 7.500000-1 0.0        1111 2151    11
-1.149970+3 2.000000+0 1.078210+0 3.282100-1 7.500000-1 0.0        1111 2151    12
 1.150030+3 2.000000+0 1.078210+0 3.282100-1 7.500000-1 0.0        1111 2151    13
 3.450030+3 2.000000+0 1.078210+0 3.282100-1 7.500000-1 0.0        1111 2151    14
                                                                   1111 2  099999
                                                                   1111 0  0     0
 2.505500+4 5.446610+1          0          0          0          01111 3  1     1
 0.0        0.0                 0          0          1        3791111 3  1     2
        379          2                                             1111 3  1     3
 1.000000-5 4.093599+1 1.084651-5 3.932864+1 1.175671-5 3.779880+11111 3  1     4
 1.273421-5 3.634307+1 1.378259-5 3.495820+1 1.494930-5 3.359273+11111 3  1     5
 1.620380-5 3.229340+1 1.755104-5 3.105730+1 1.899598-5 2.988168+11111 3  1     6
```

Processing codes clearly needed !

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EMPIRE: Modelling advances

- ❑ Full access to RIPL OM database: dispersive and Lane consistent coupled-channel OMPs

  neutron inelastic scattering to discrete levels;
- ❑ improved neutron emission spectra (MSD+MSC) to calculate **neutron inelastic scattering** to the continuum;
- ❑ EGSM level density parameterization (EGSM): all statistical cross sections
- ❑ improved fission formalism and parameters;

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DISPERSIVE OPTICAL MODEL POTENTIAL

Energy dependence (I)

Functional form of the real and imaginary potentials:

$$V_{HF}(E) = V_0 \cdot exp(-\alpha_{HF}(E - E_F))$$

$$W_V(E) = A_V \frac{(E - E_F)^4}{(E - E_F)^4 + (B_V)^4}$$

$$W_S(E) = A_S \frac{(E - E_F)^4}{(E - E_F)^4 + (B_V)^4} \cdot exp(-C_S|E - E_F|)$$

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DISPERSIVE OPTICAL MODEL POTENTIAL

$$\Delta V(E) = \frac{\mathcal{P}}{\pi} \int_{-\infty}^{\infty} \frac{W(E')}{E' - E} dE'$$

$$V_V(E) = V_{HF}(E) + \Delta V_V(E) + \Delta V_<(E) + \alpha_V \Delta V_>(E)$$

$$V_S(E) = \Delta V_S(E) + \alpha_S \Delta V_>(E)$$

$W(E)$ must be defined in the interval $-\infty < E < \infty$

Analytical/numerical solutions for ΔV(E) published

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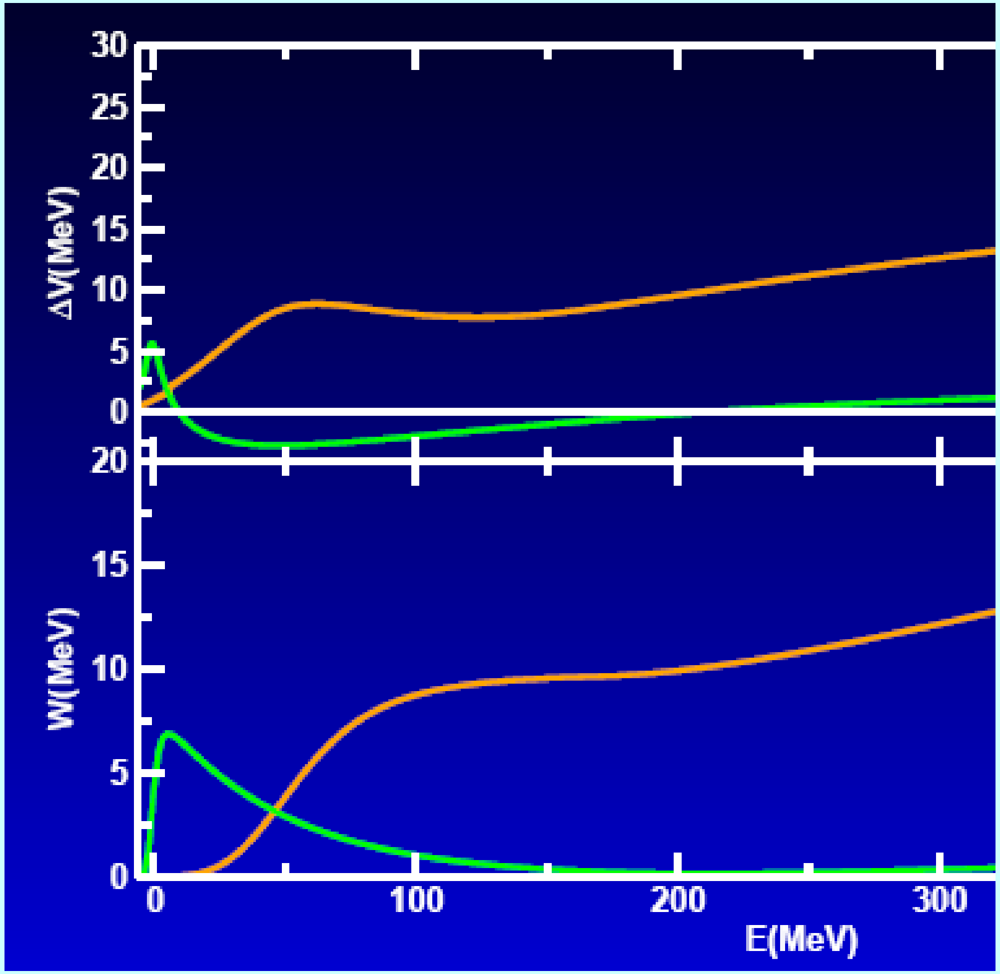
DISPERSIVE OPTICAL MODEL POTENTIAL

Dispersive

Imag OMP



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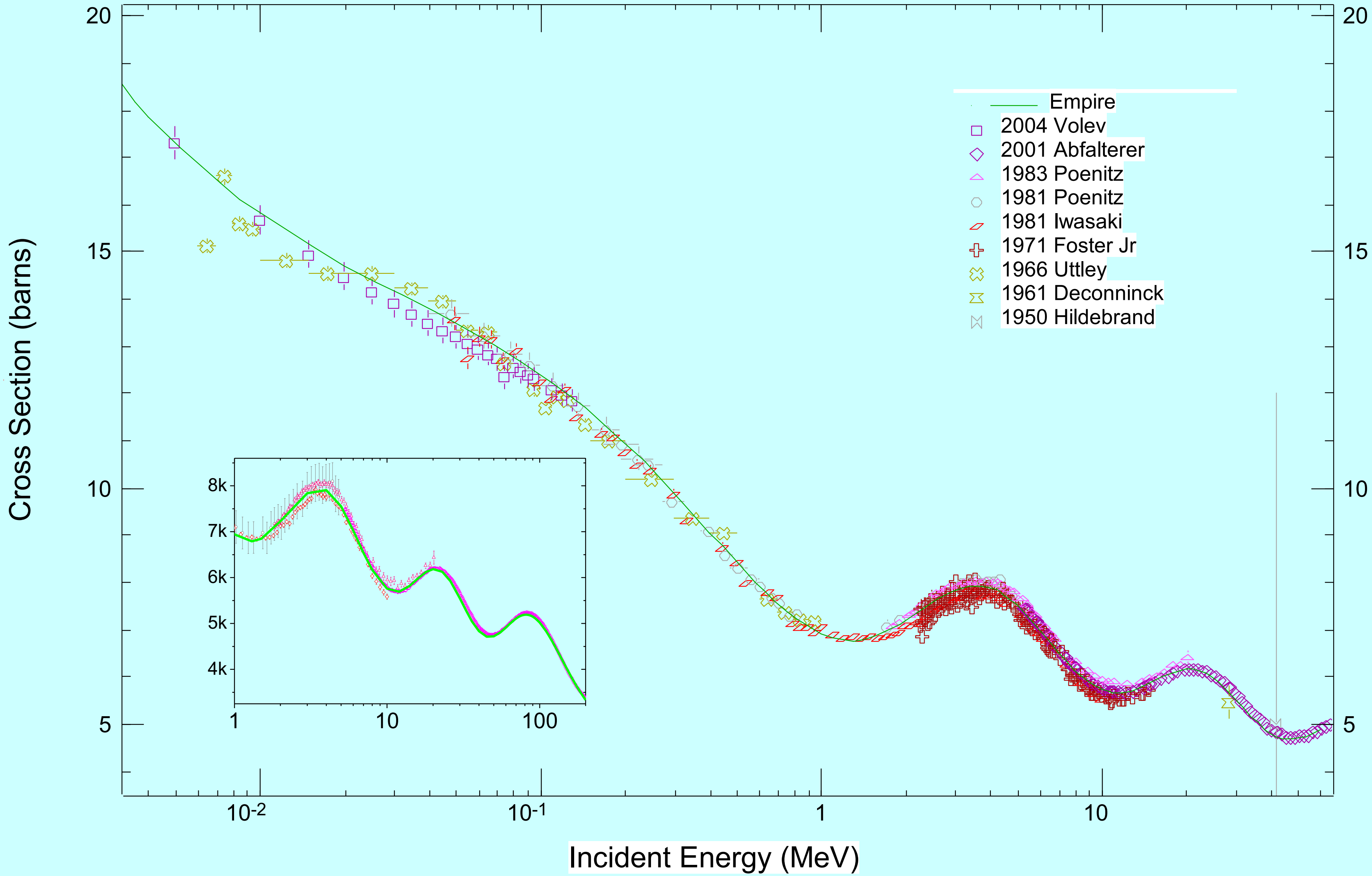
Total cross section (DCCOMP)



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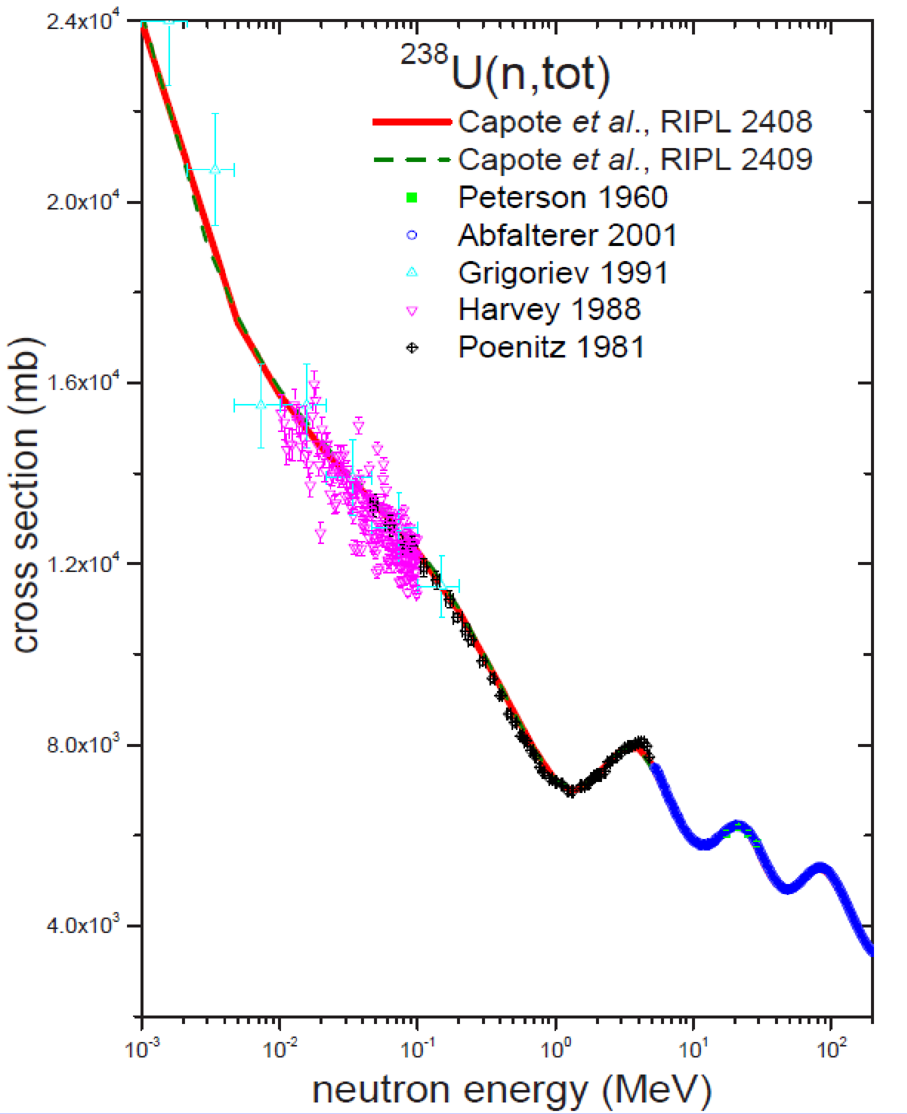
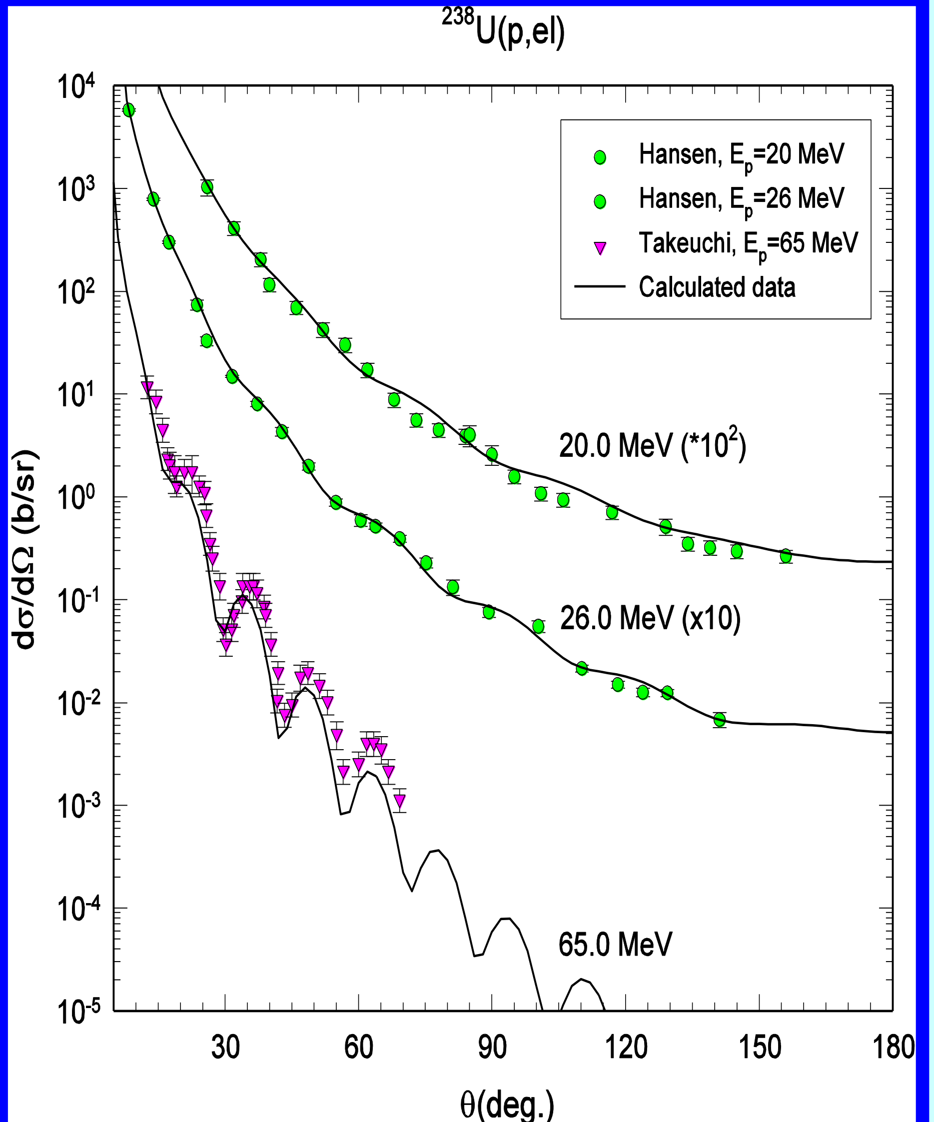
Dispersive and Lane consistent OMP (1)





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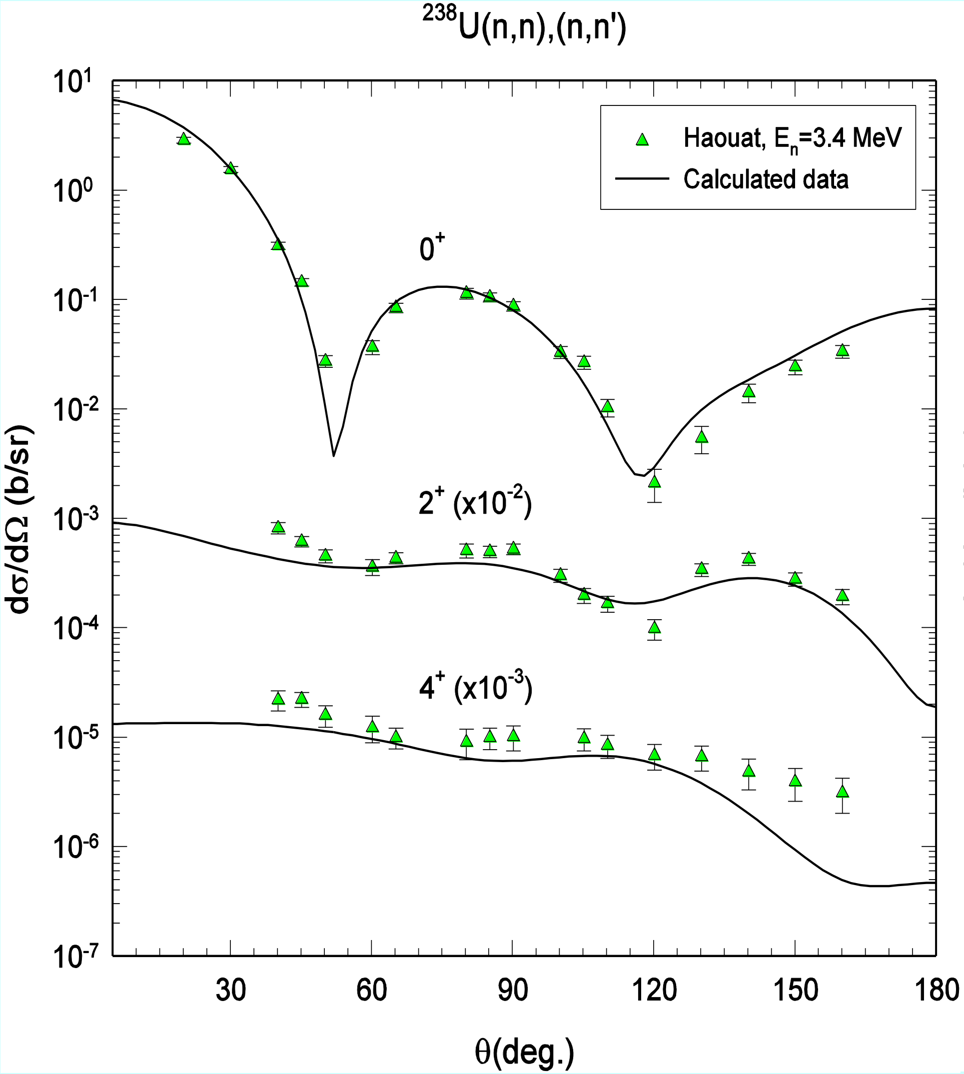
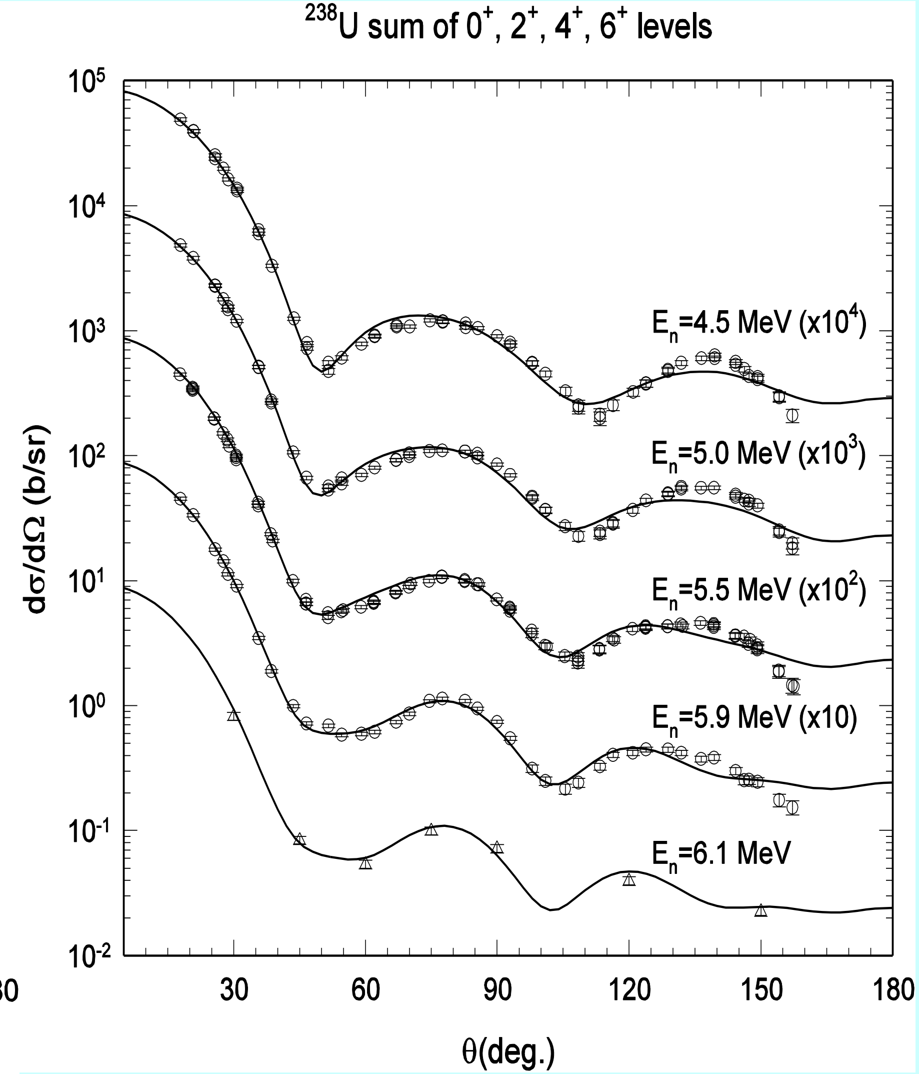
Dispersive and Lane consistent OMP (2)





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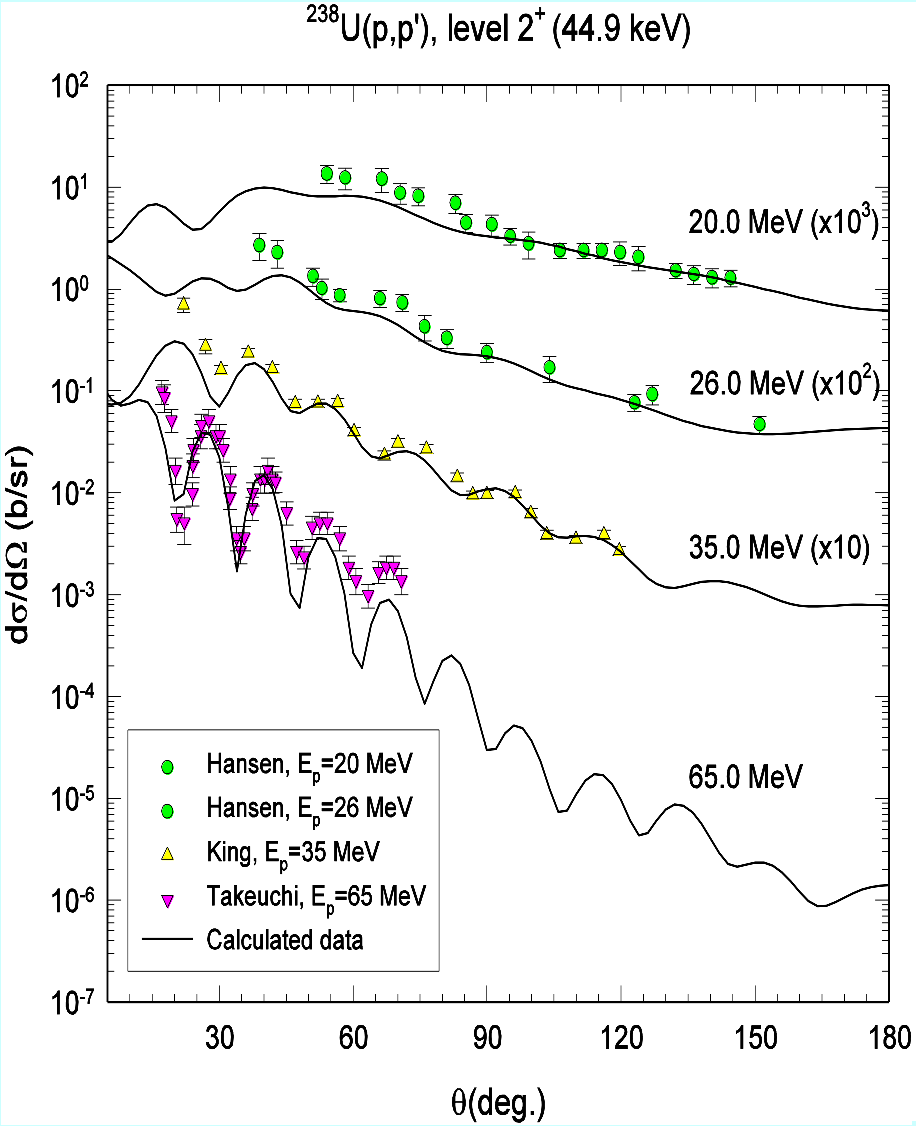
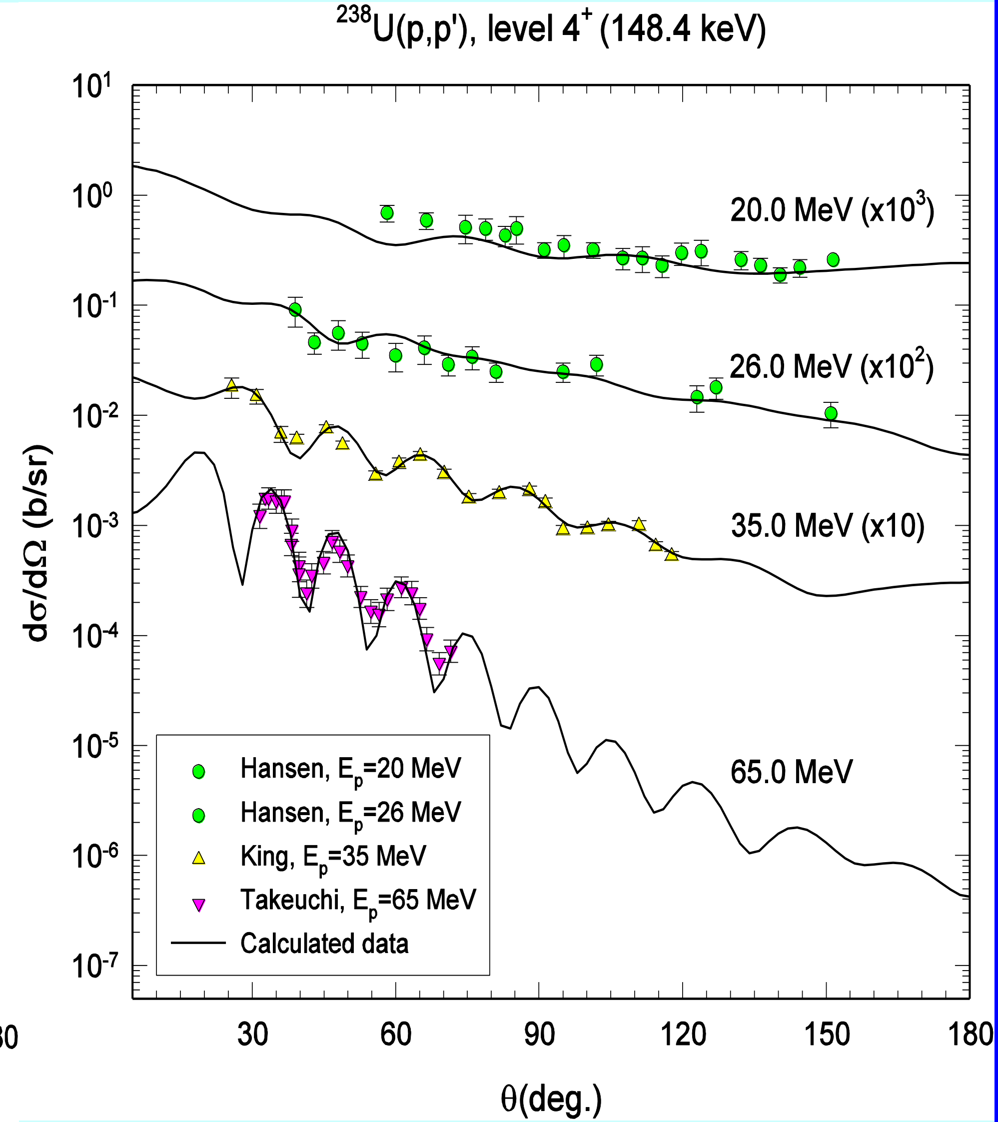
Dispersive and Lane consistent OMP (3)





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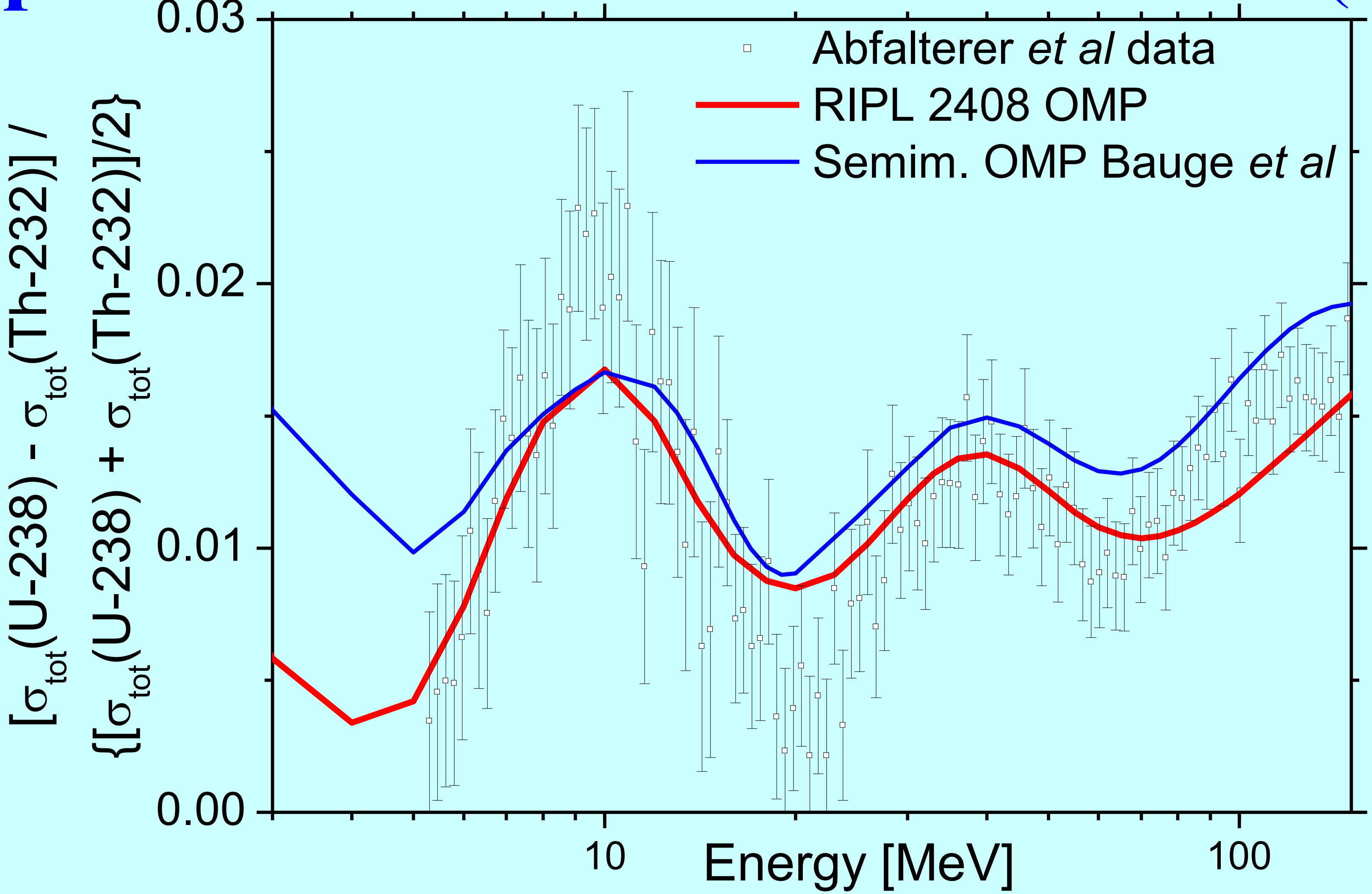
Dispersive and Lane consistent OMP (4)



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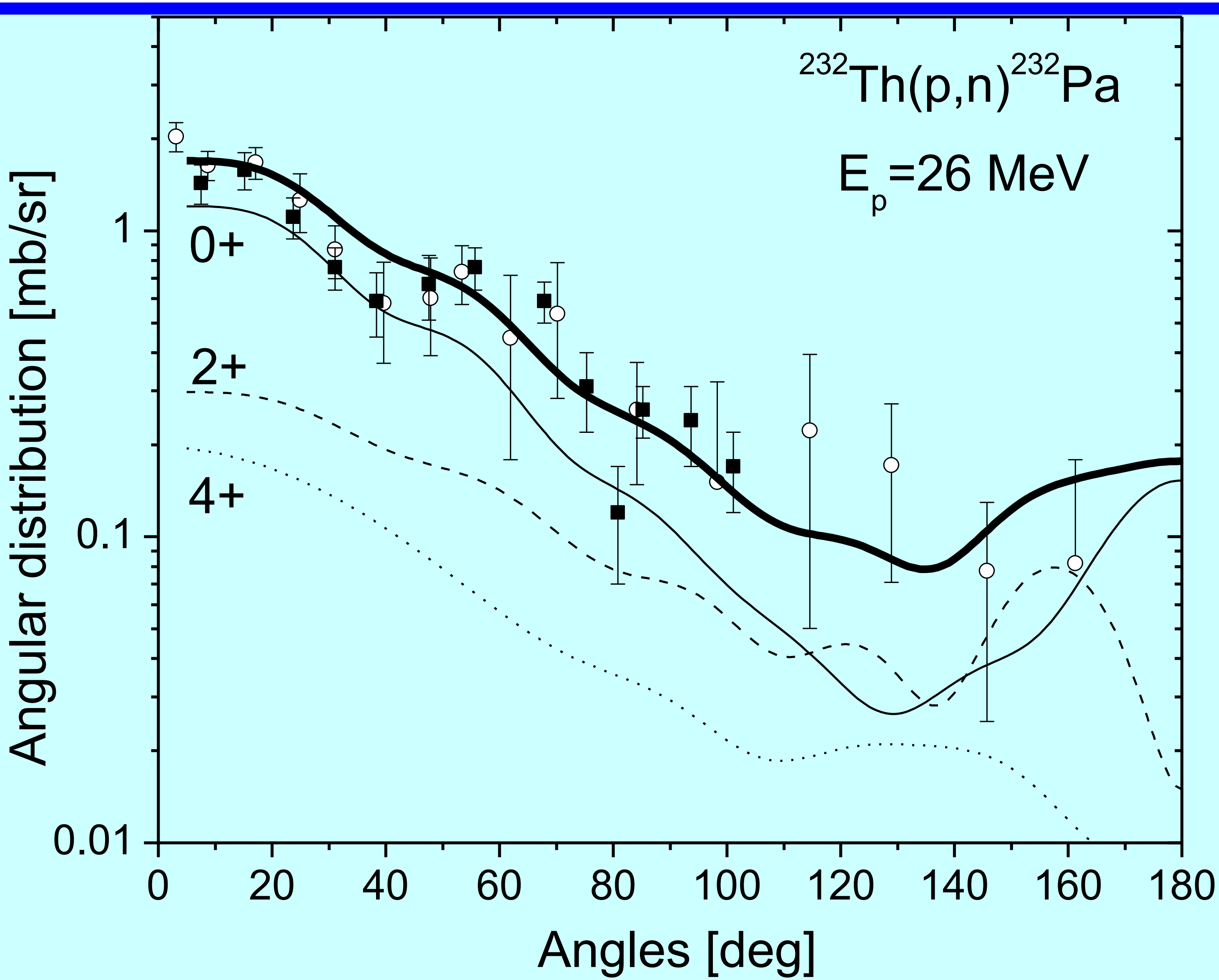

• Dispersive and Lane consistent OMP (5)

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AVERAGE RESONANCE PARAM.

For dispersive OMP, the real potential is almost flat toward the low energies, by a combination of the increasing contribution of the smooth "Hartree-Fock" potential with the decreasing dispersive contribution (which goes to zero at Fermi energy).

Average resonance parameters for DCCOMP (Th232+n)

Present work (evaluated at 2 keV)			Evaluated values		
$S_0, (eV)^{-1/2} 10^{-4}$	$S_1, (eV)^{-1/2} 10^{-4}$	R', fm	$S_0, (eV)^{-1/2} 10^{-4}$	$S_1, (eV)^{-1/2} 10^{-4}$	R', fm
0.853	1.80	9.58	0.935 (0.05) [35]	1.81 (0.03) [35]	9.53 (0.05) [35]
			0.87 (0.07) [64]		

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Th-232 and Pa-231 EVALUATION

- Optical model (total, inelastic to low-lying collective levels, angular distributions, elastic and non-elastic XS calculations)
- Capture (Hauser-Feshbach + HRTW)
- Neutron emission spectra (1-15 MeV)

  (DWBA + exciton model + Hauser-Feshbach)
- Total Inelastic, (n,2n) and (n,3n)
- Fission and prompt fission neutrons

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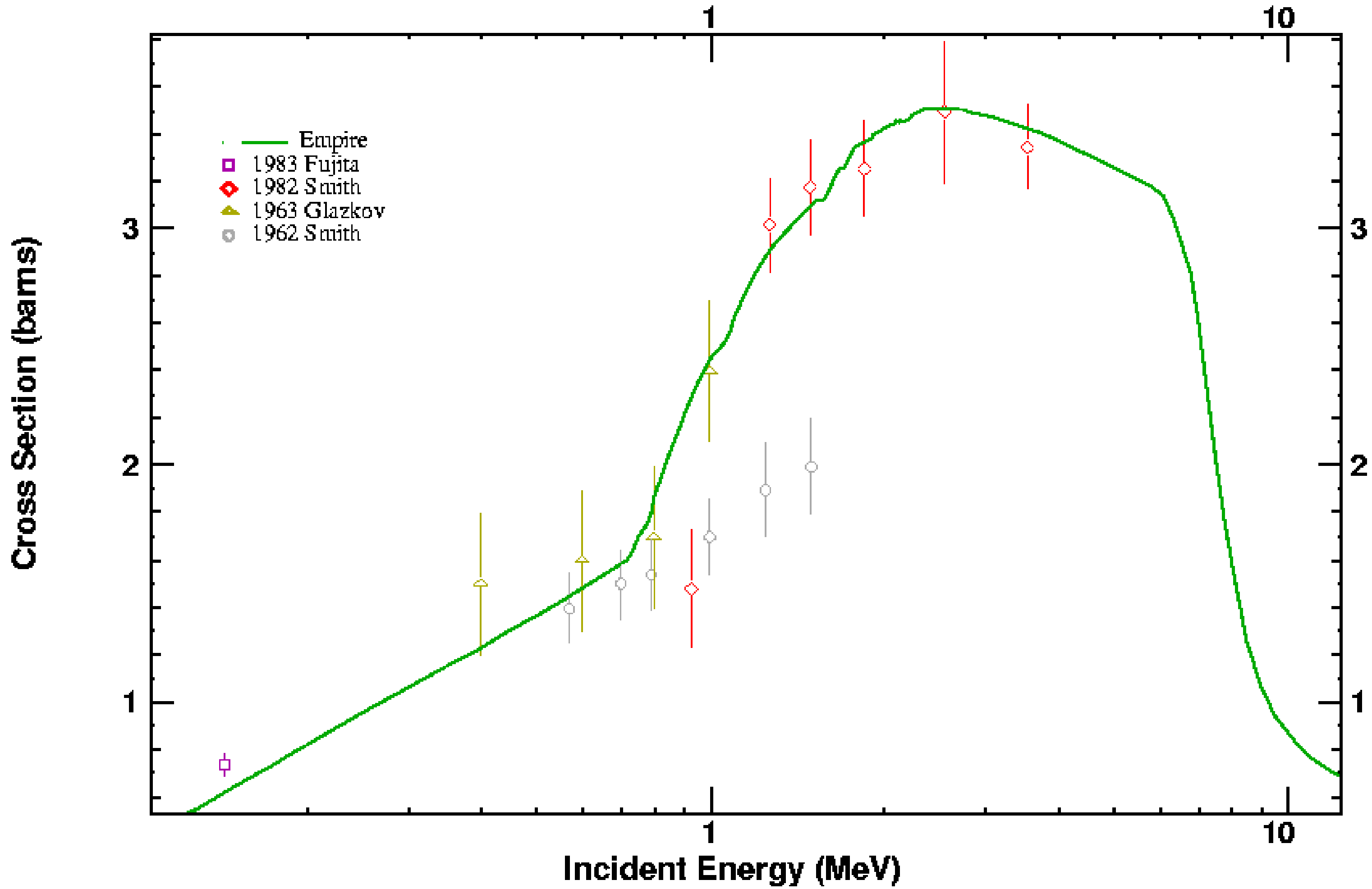
(n,INL)



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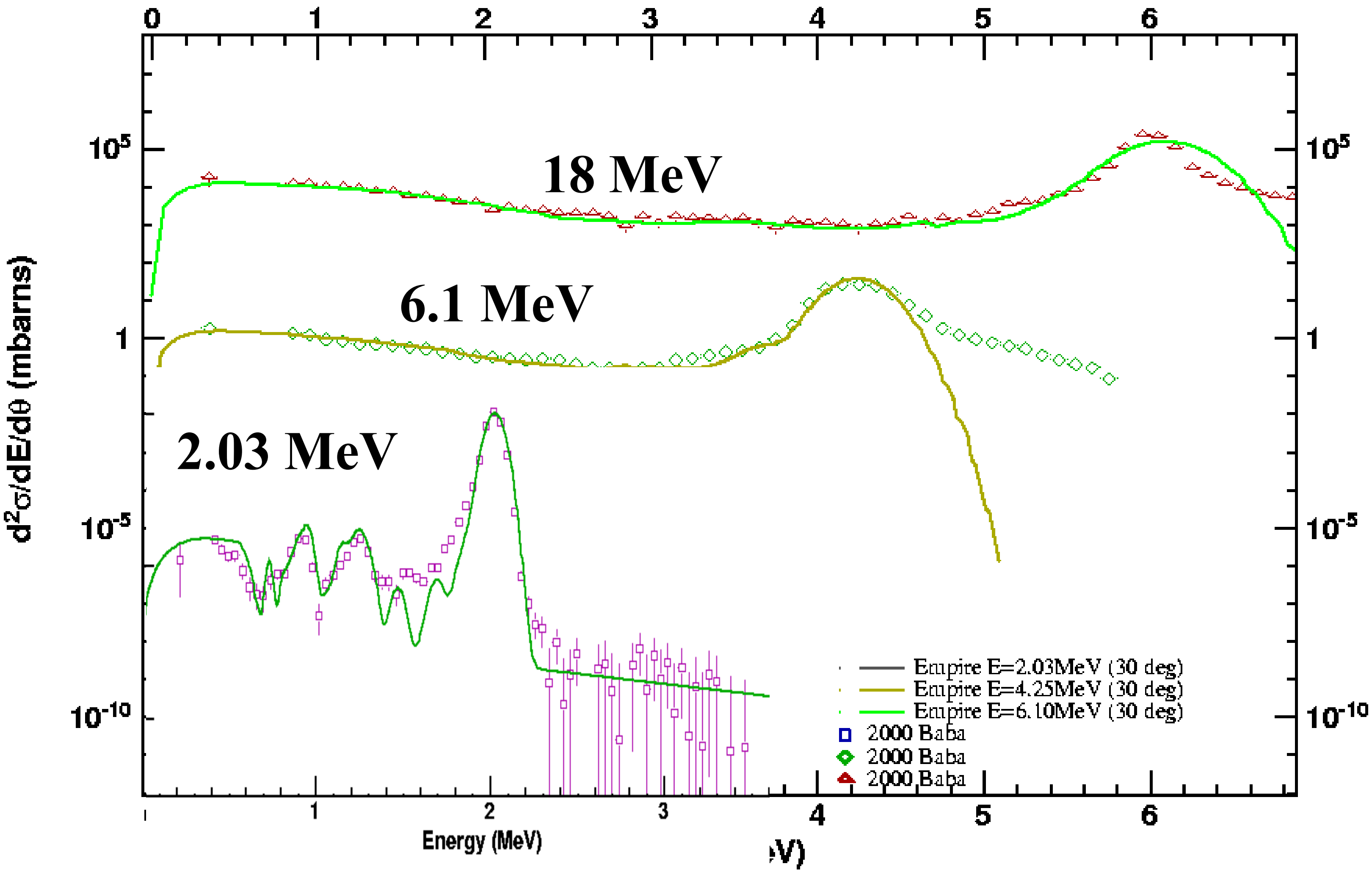
DDXS at 2.03, 6.1 and 18 MeV



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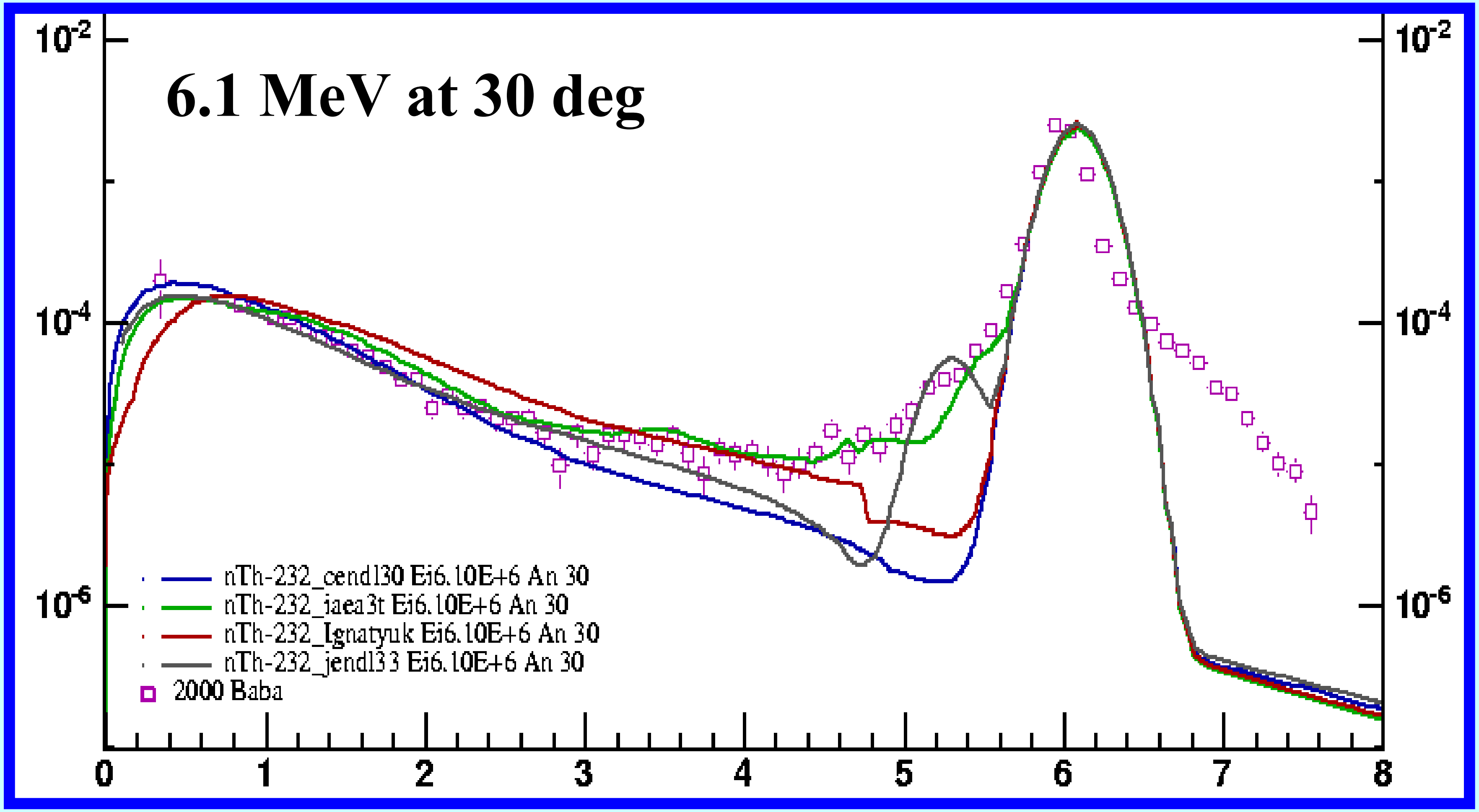
Recent evaluations (DDXS)



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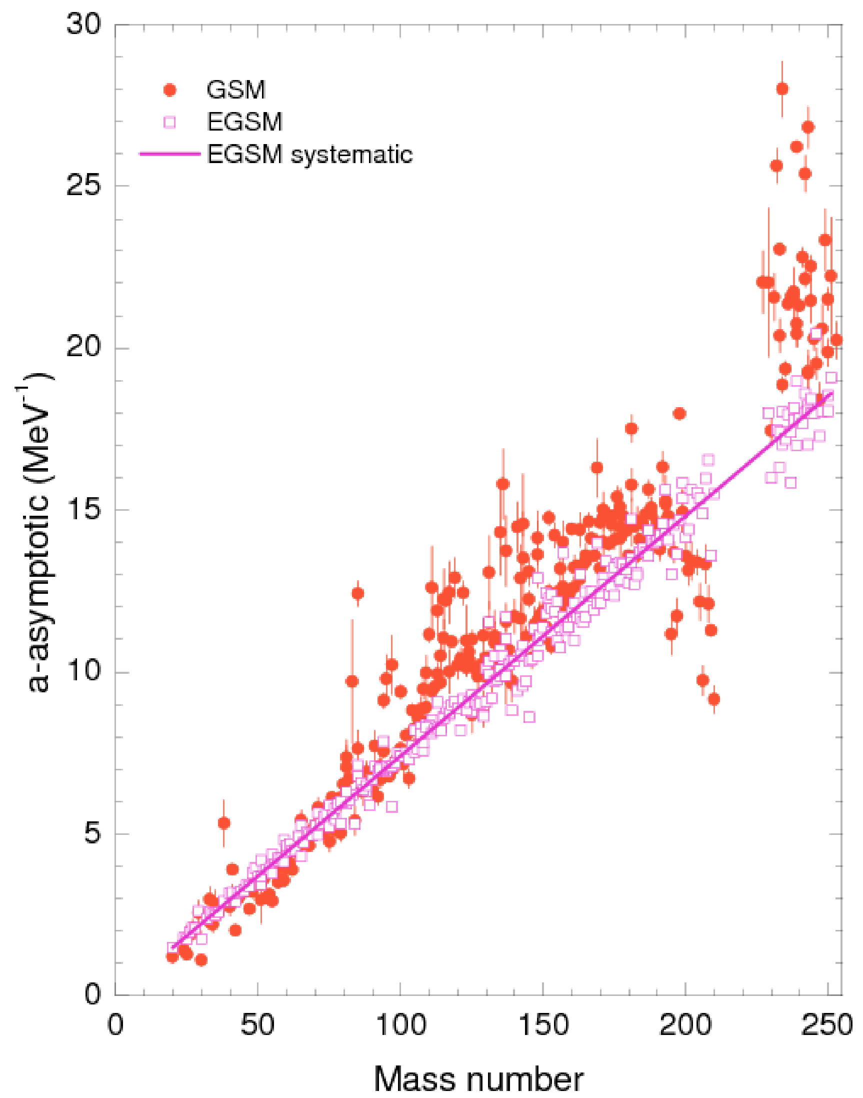
EGSM level density model



$$\alpha = 0.0741,$$
$$\beta = 0.0003,$$
$$\gamma_0 = 0.5725.$$

f_{rms}=1.70

Notable features of the EGSM parameterization are the vanishing role of the nuclear surface term (β parameter is negligible compared to α in Eq. (52)), and the linear dependence of "experimental" asymptotic $\tilde{a}$ values on mass number A ($\tilde{a} \approx 0.0741A = A/13.5$). The derived asymptotic value of the level density parameter is very close to the theoretical value of the Fermi gas model of Eq. (44); the complete absence of the shell effects in the mass dependence of $\tilde{a}$ is a strong argument in favor of the collective enhancements and shell corrections adopted in the EGSM.

γ-RAY STRENGTH FUNCTION

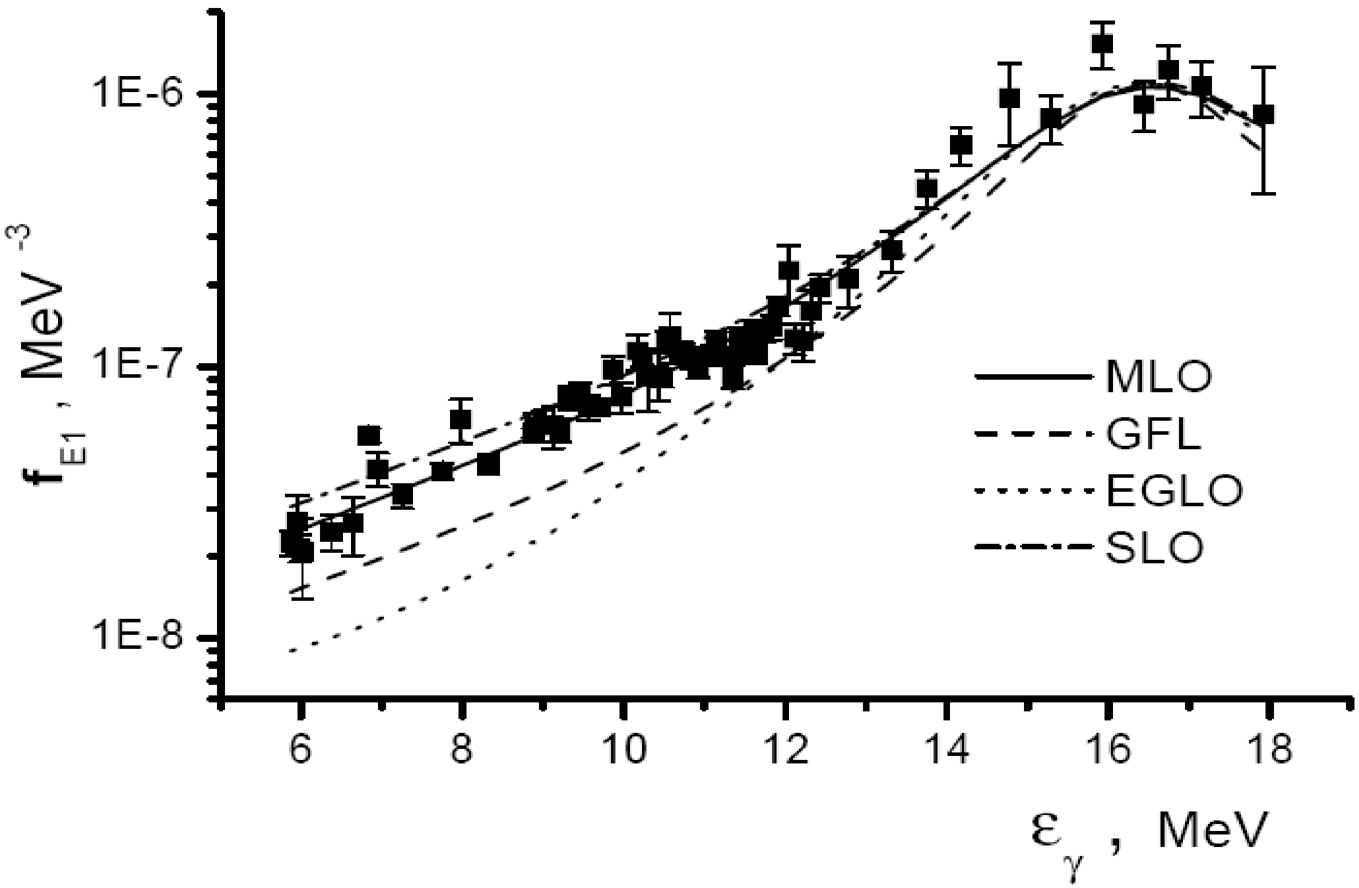


Figure 7.2: $E1$ gamma-decay strength function plotted against energy ϵ_{γ} for ^{90}Zr.

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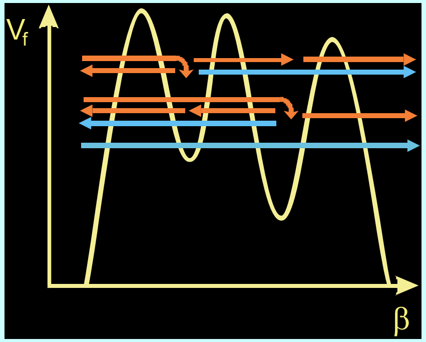
Improved fission modelling

Fission mechanisms



PHYSICAL REVIEW C **77**, 054601 (2008)

Transmission through multi-humped fission barriers with absorption: A recursive approach

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(Received 18 February 2008; published 7 May 2008)

A fission formalism which describes transmission and absorption through multiple humped barriers using a recursive method is proposed. Developed within the optical model for fission, it accounts for the fission mechanisms associated to the different degrees of damping of the vibrational states accommodated by the minima of the fission path. It can provide accurate description of experimental fission cross sections, including

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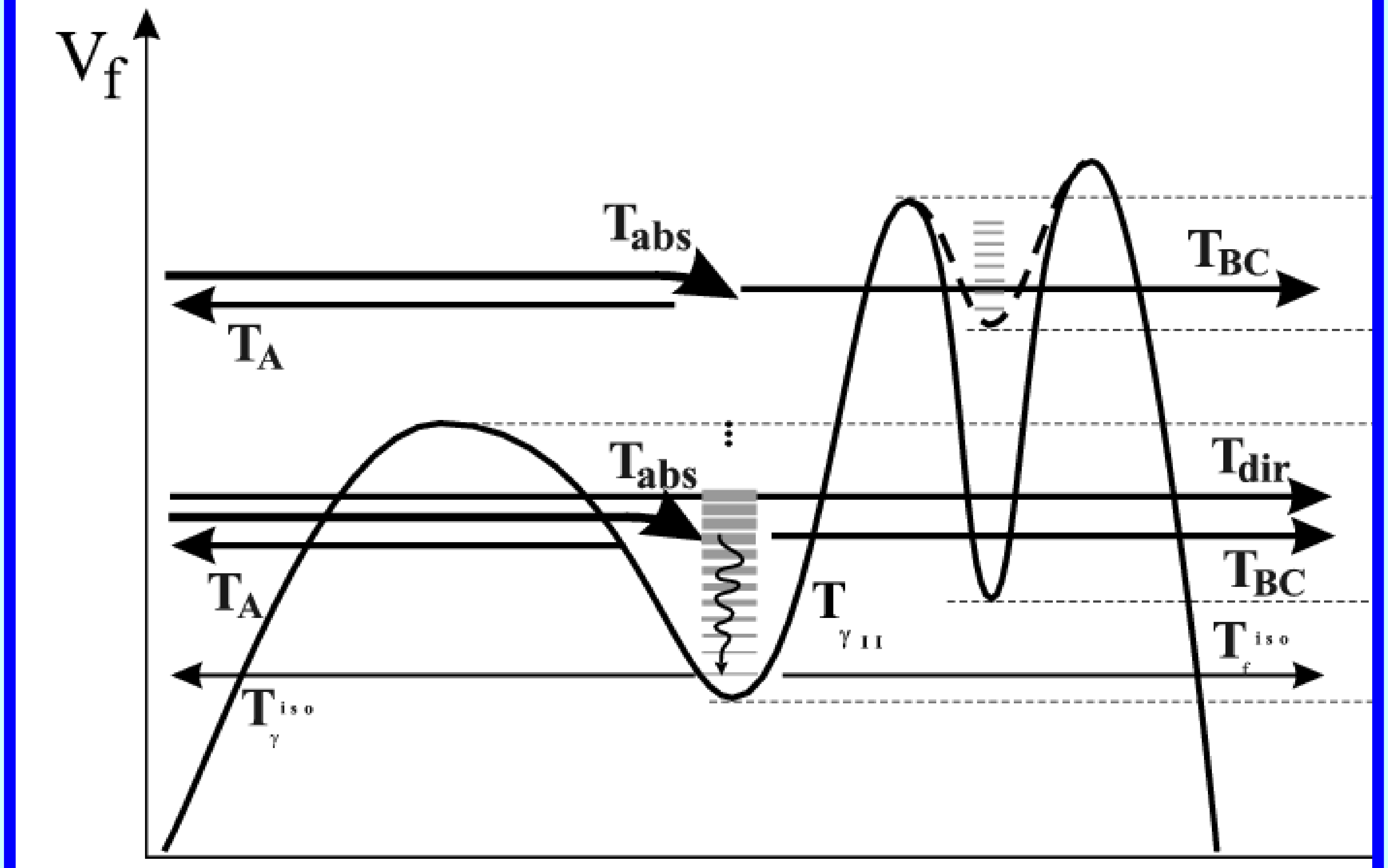
Improved fission modelling



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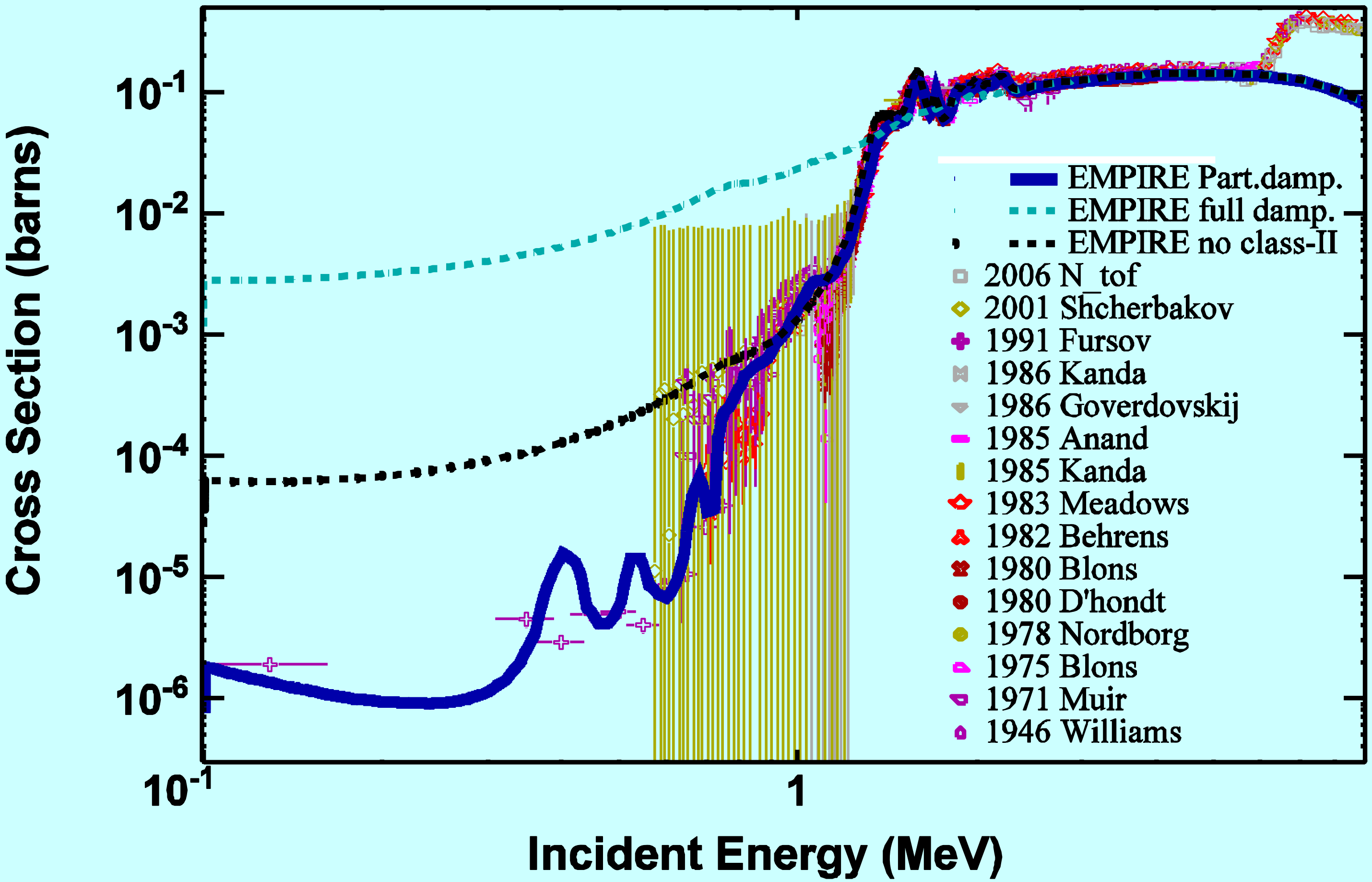
Improved fission modelling

Barriers + Wells (includes absorption)

Full damping vs Partial damping.



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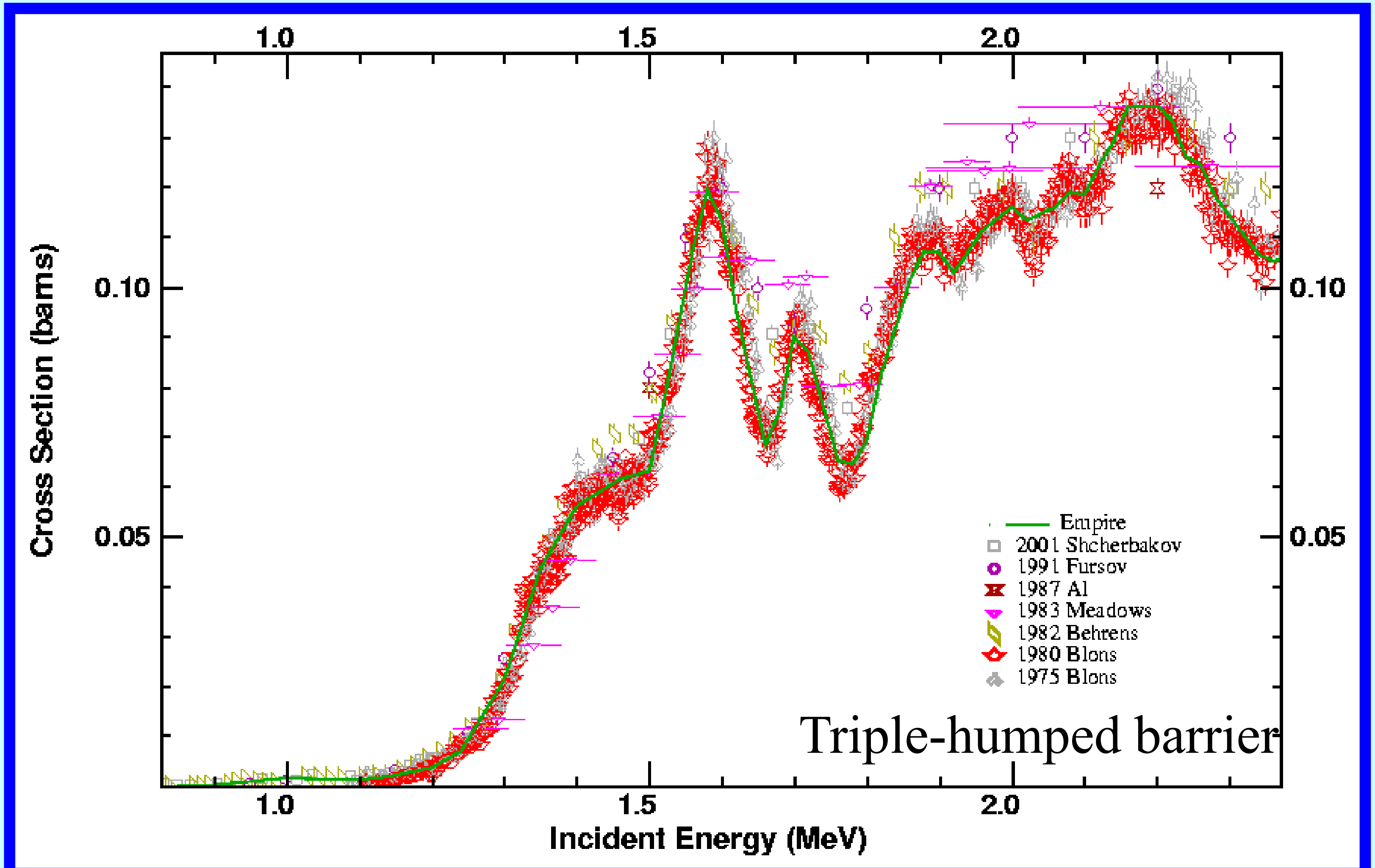
Near-barrier fission structure – ^{232}Th



ICTP workshop 2141, ND
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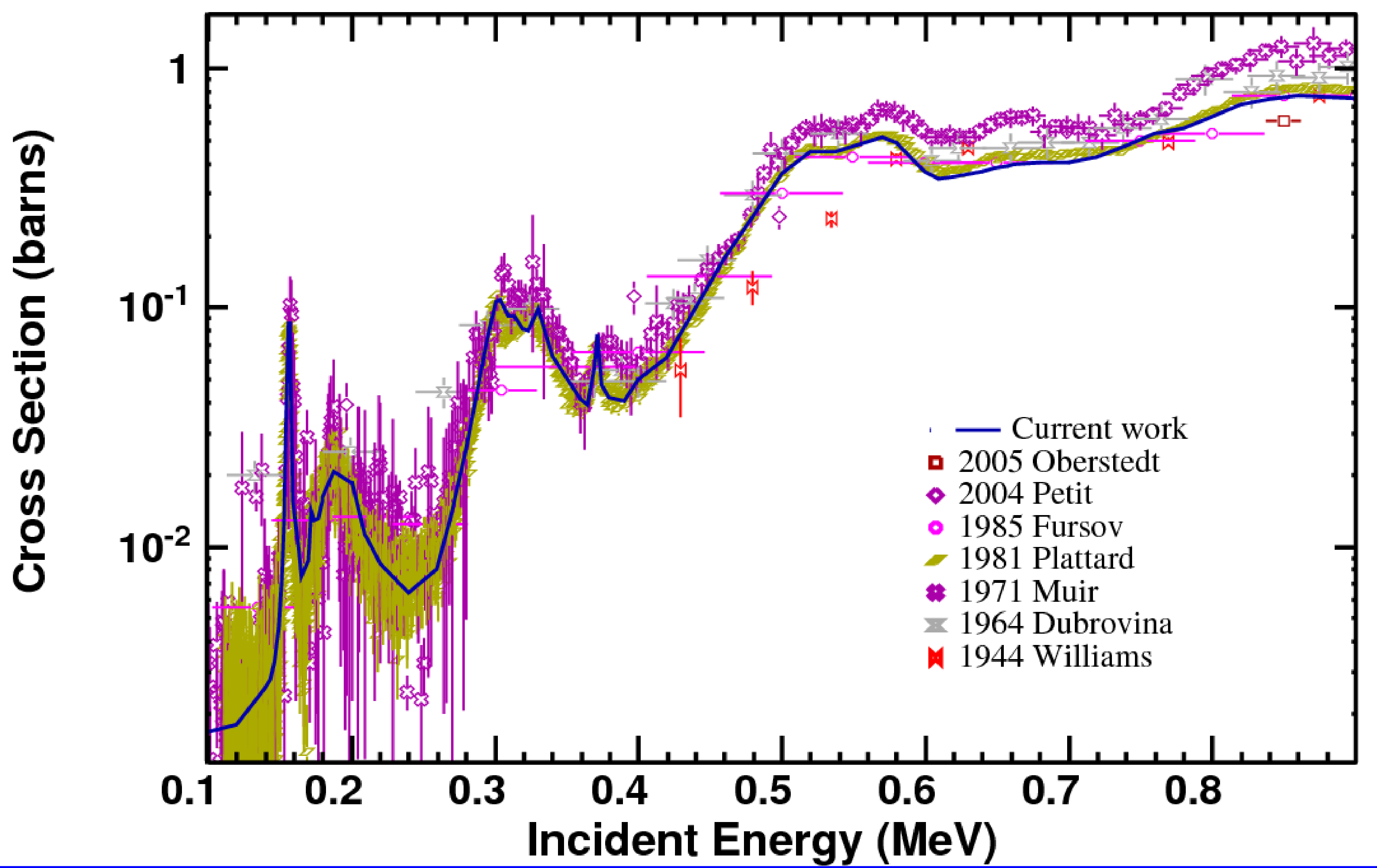
Near-barrier fission structure - ^{231}Pa



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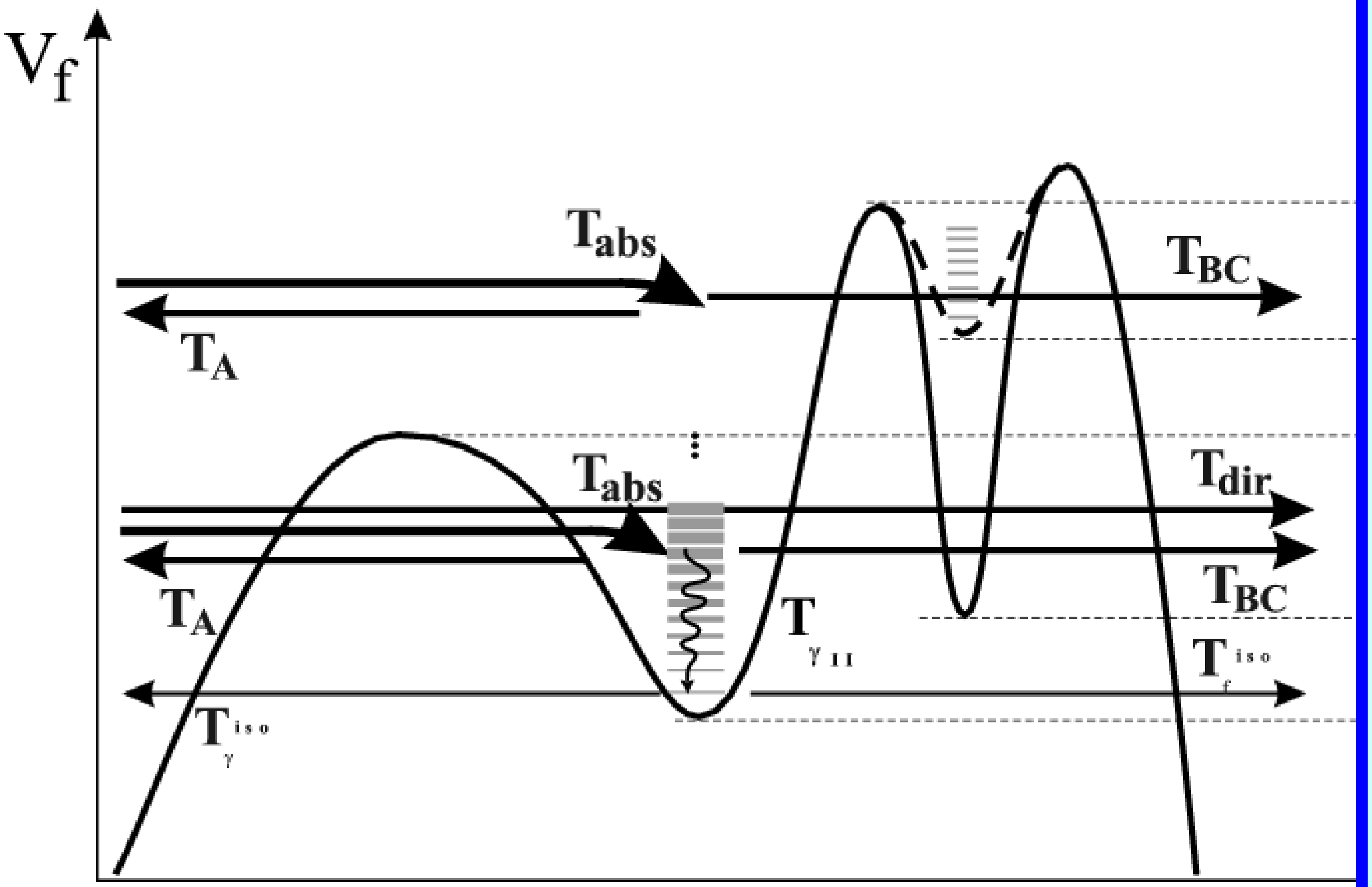
Improved fission modelling



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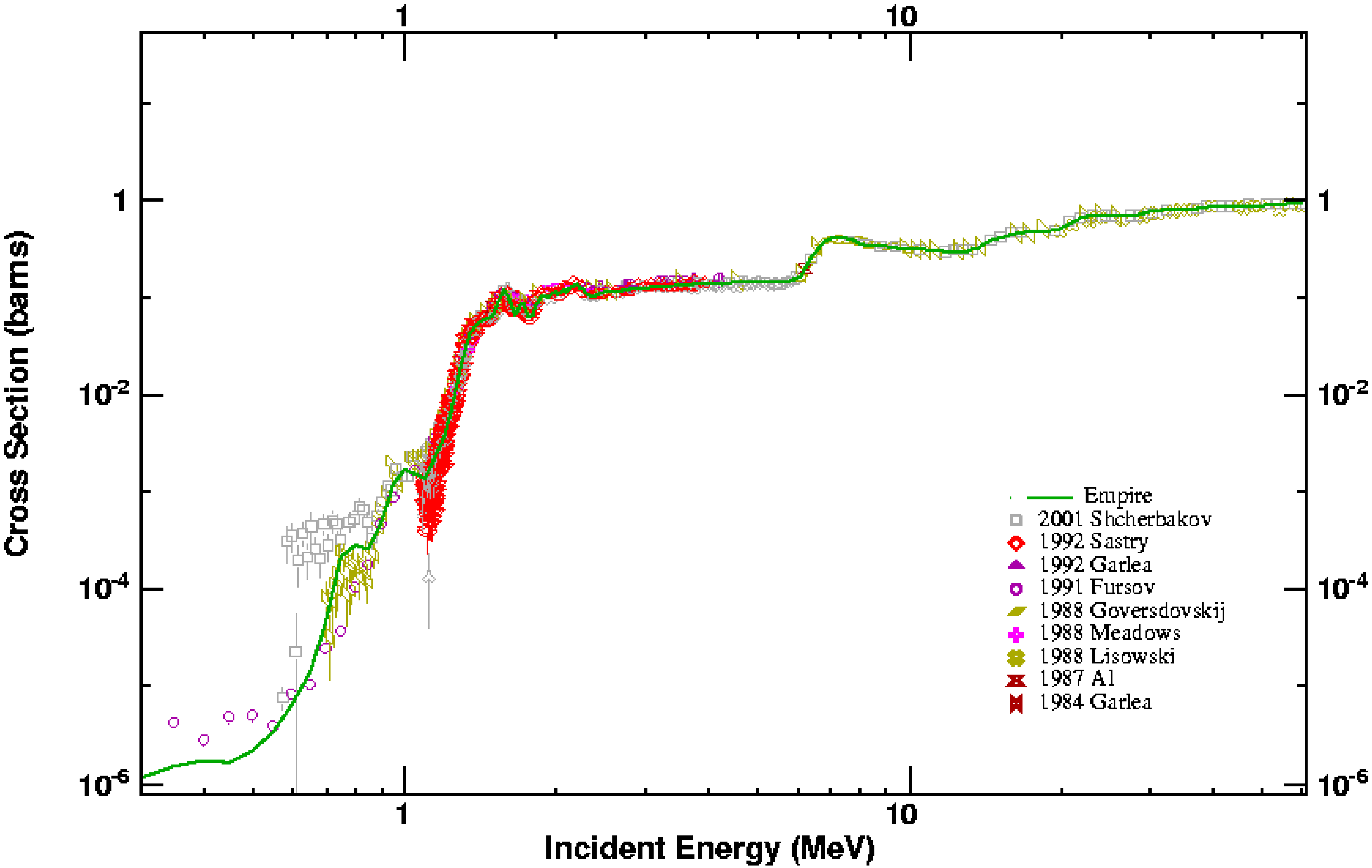
Fission cross section



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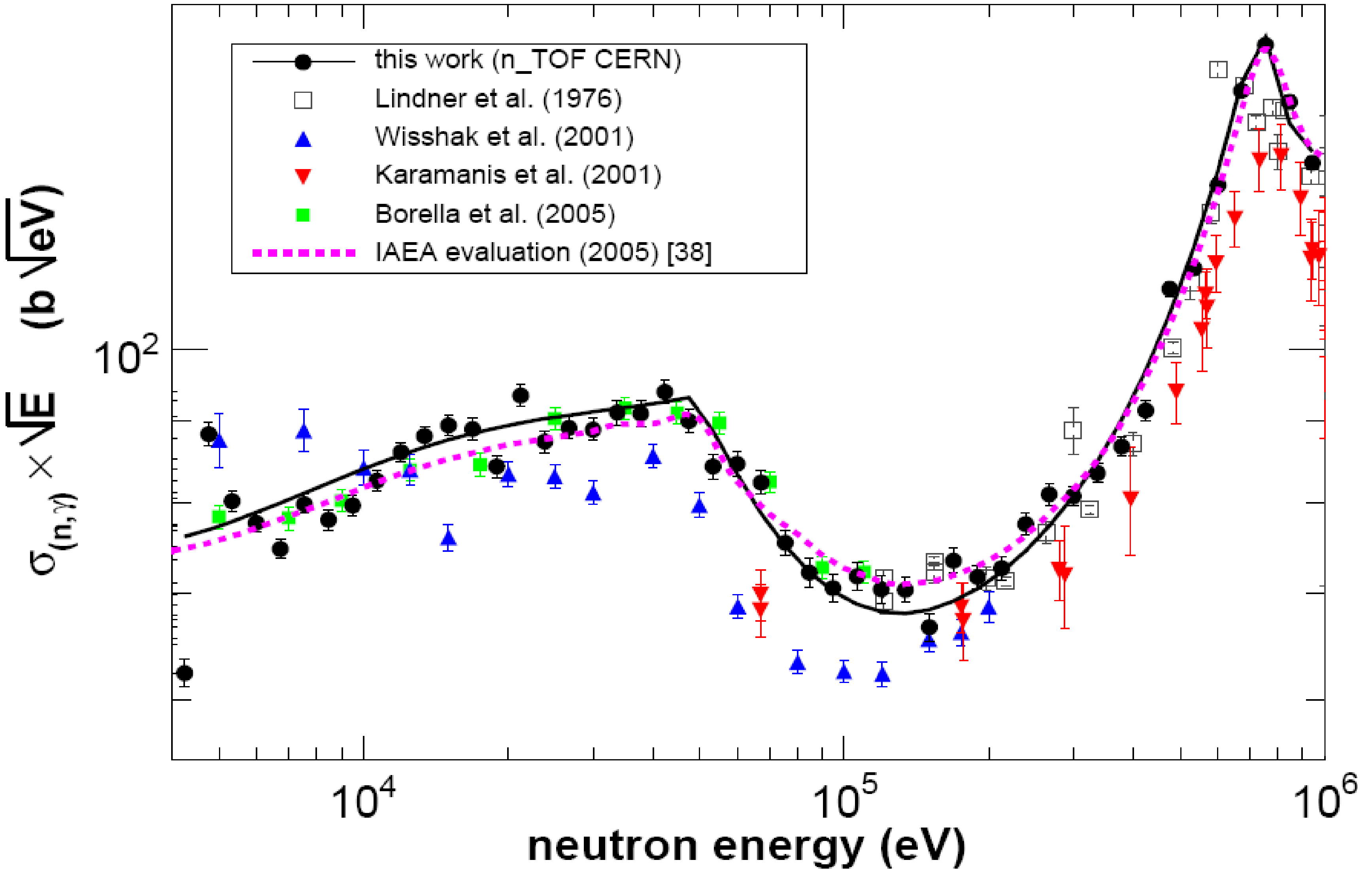
Neutron Capture



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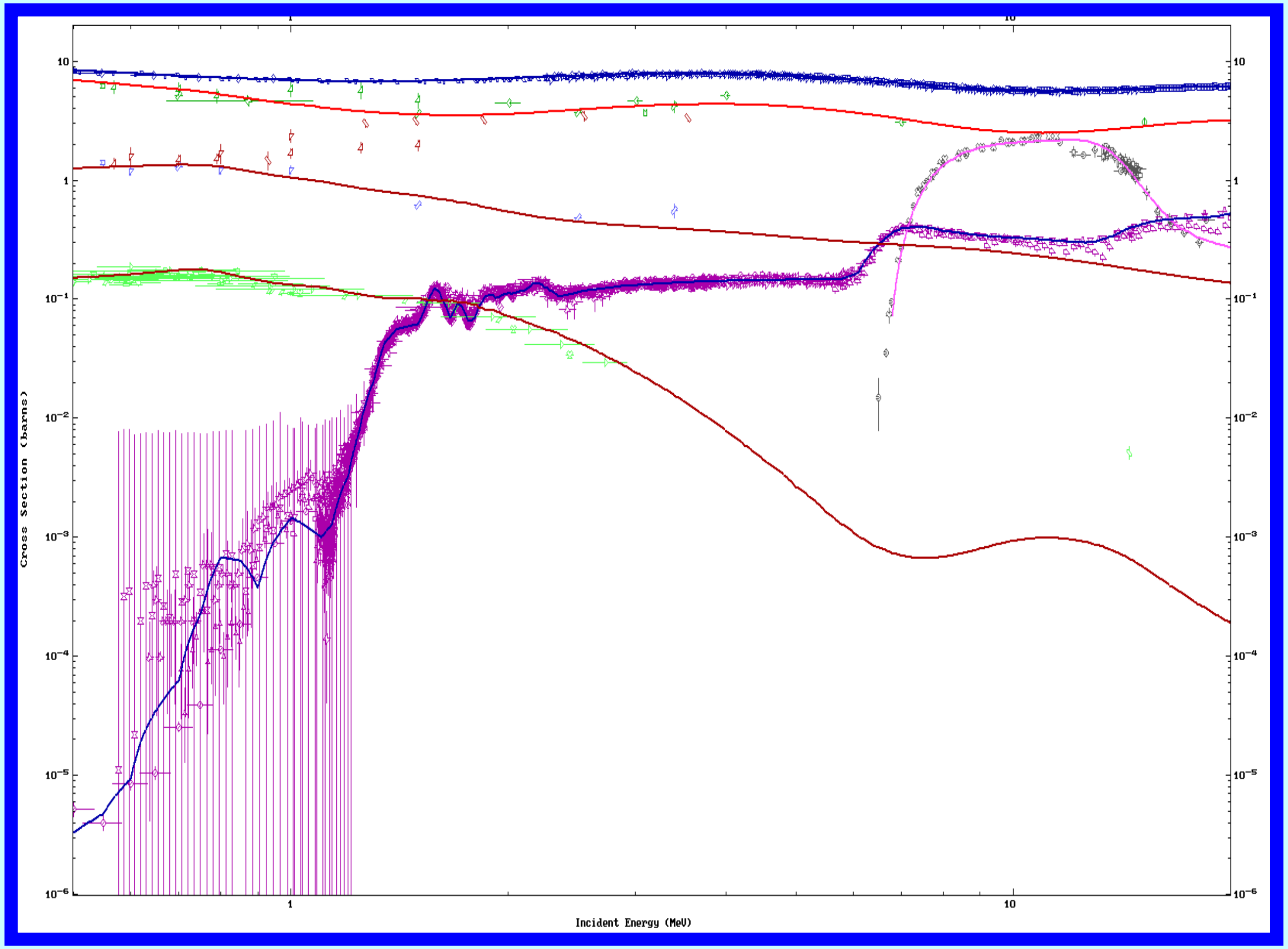
Evaluation: fast energy range n + ^{232}Th



What about uncertainties & covariances?

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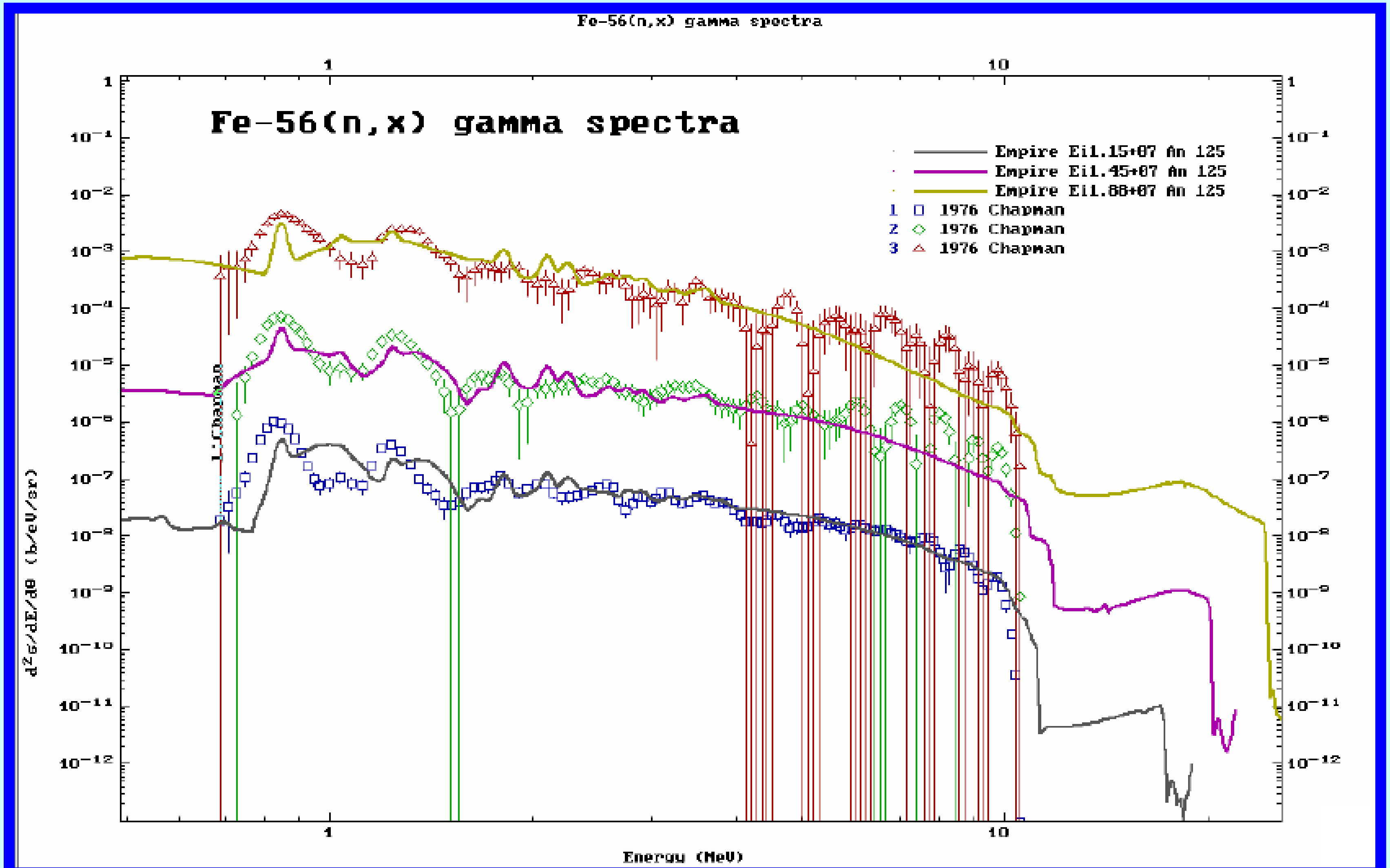
Some additional results



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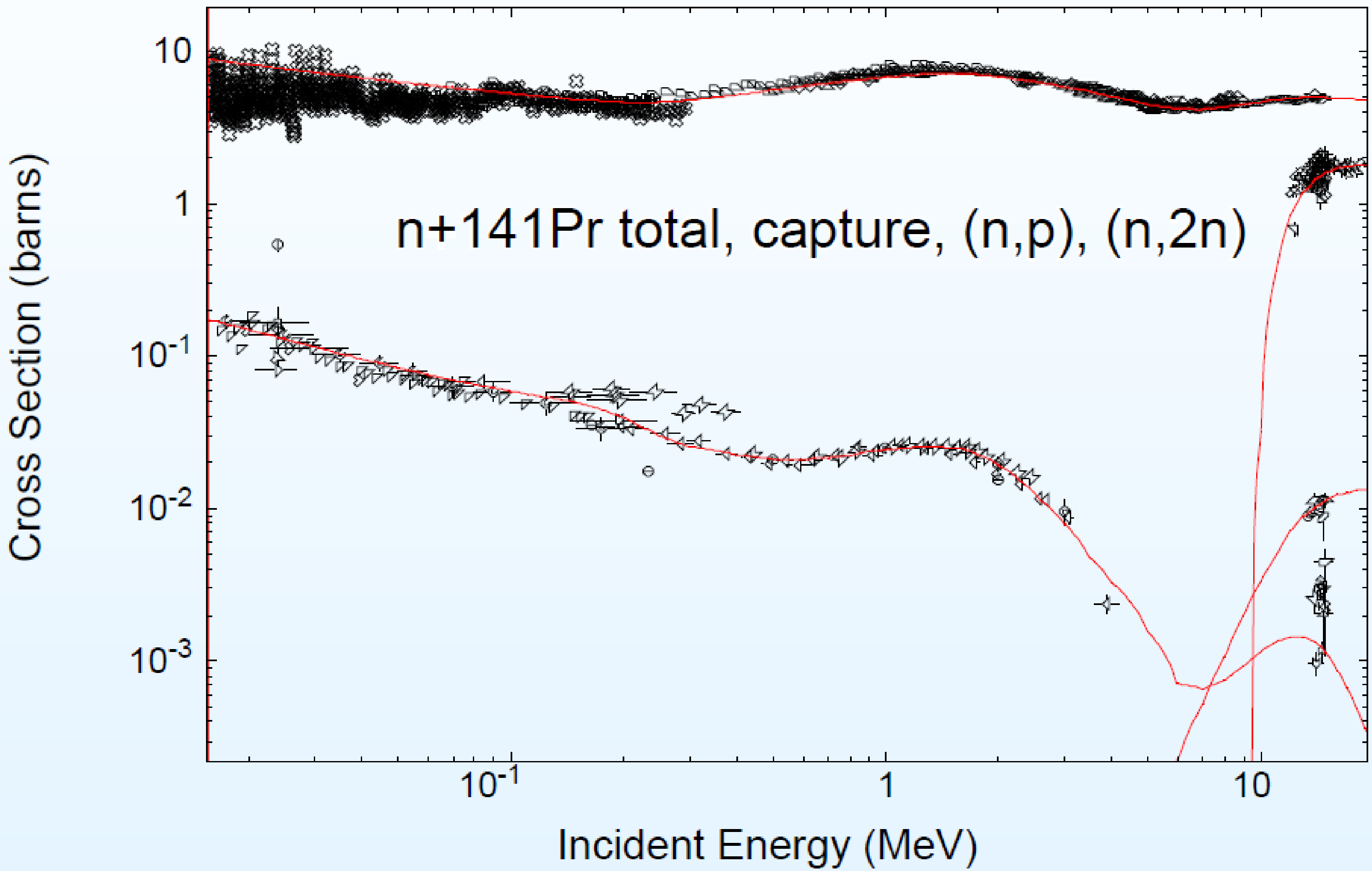
Some additional results



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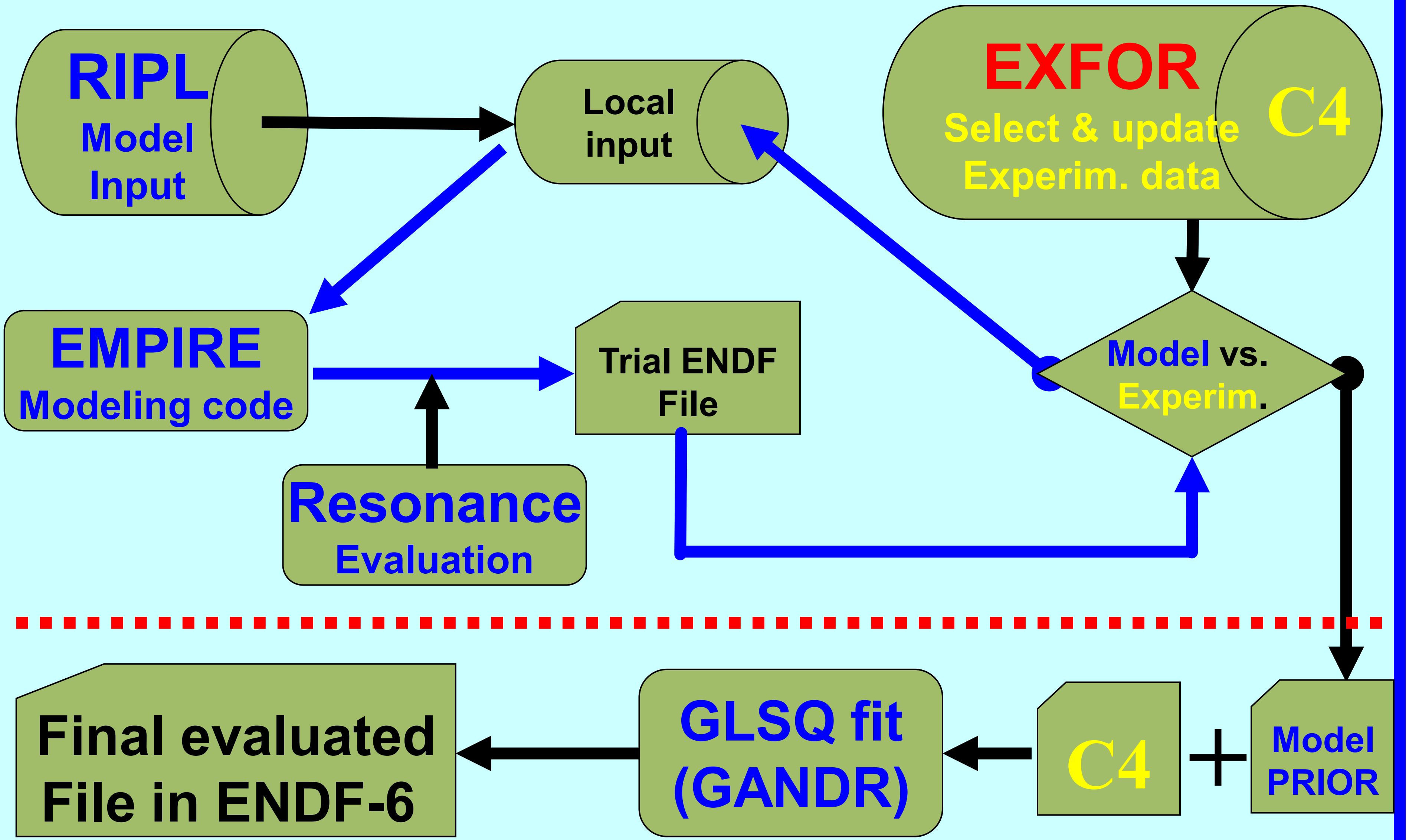
Nuclear Data Evaluation process



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https://ndclx4.bnl.gov/gf/project/empire/

Extension of the nuclear reaction model code

EMPIRE

to actinides' nuclear data evaluation

@NNDC: http://www.nndc.bnl.gov/empire219/ @IAEA: http://www-nds.iaea.org/empire/

Available online at www.sciencedirect.com

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Nuclear Data Sheets 108 (2007) 2655–2715

Nuclear Data Sheets

www.elsevier.com/locate/nds

EMPIRE: Nuclear Reaction Model Code System for Data Evaluation

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RIPL Objective (1993)

Improve the methodology of nuclear data evaluation by increasing predictive power, accuracy and reliability of theoretical calculations by nuclear reaction model codes

1994 – 2009

The longest running IAEA/NDS project

Nuclear Data Sheets **110** (2009) 3107–3214

RIPL – Reference Input Parameter Library for Calculation of Nuclear Reactions and Nuclear Data Evaluations

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