



*The Abdus Salam
International Centre for Theoretical Physics*



2055-25

Joint ICTP/IAEA School on Physics and Technology of Fast Reactor Systems

9 - 20 November 2009

Nuclear Data for Fast Reactor Systems - 2

Roberto Capote
*International Atomic Energy Agency
IAEA NAPC
Nuclear Data Section
Vienna*

Nuclear Data for Fast Reactor Systems: Nuclear reaction data evaluation



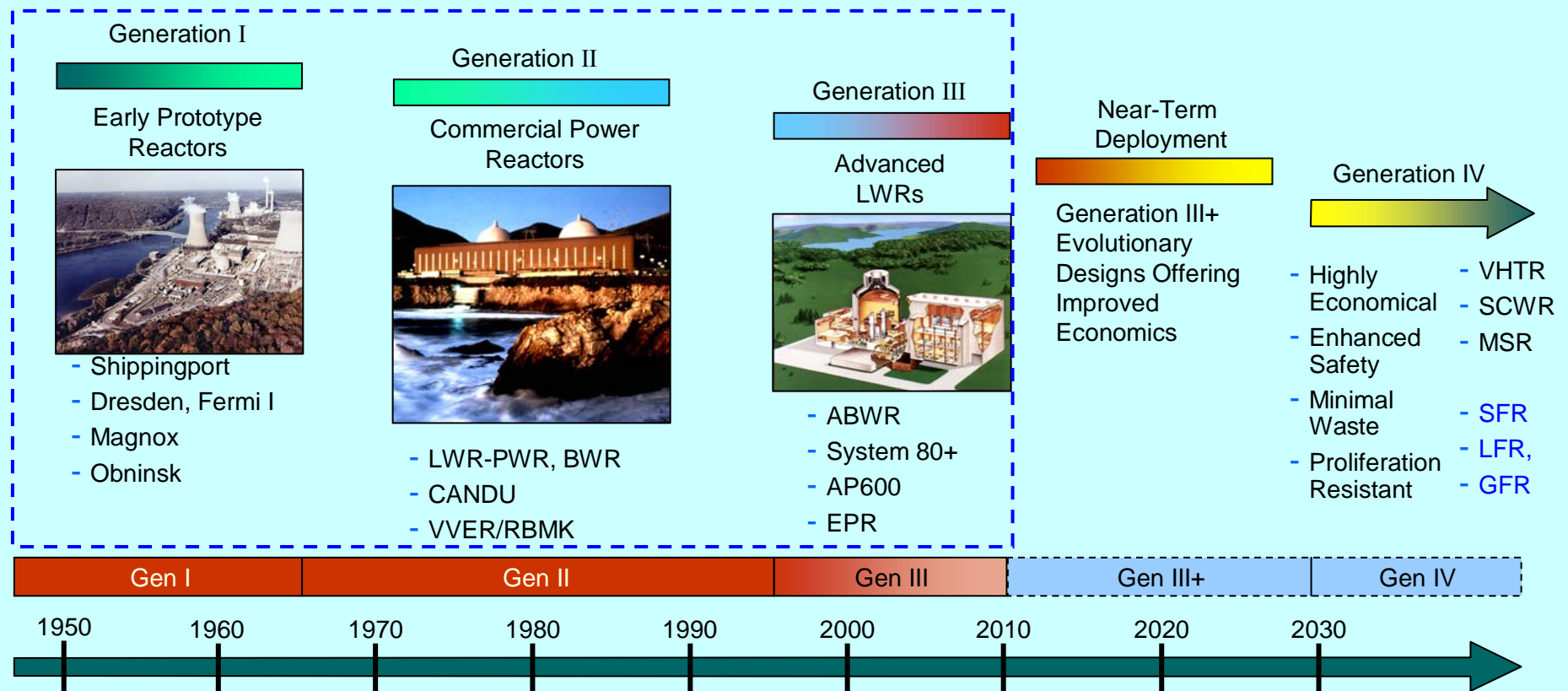
IAEA HQ
Vienna
Austria

Roberto Capote, IAEA NAPC - Nuclear Data Section

Andrej Trkov, Jožef Stefan Institute, Ljubljana, Slovenia

GENERATION IV

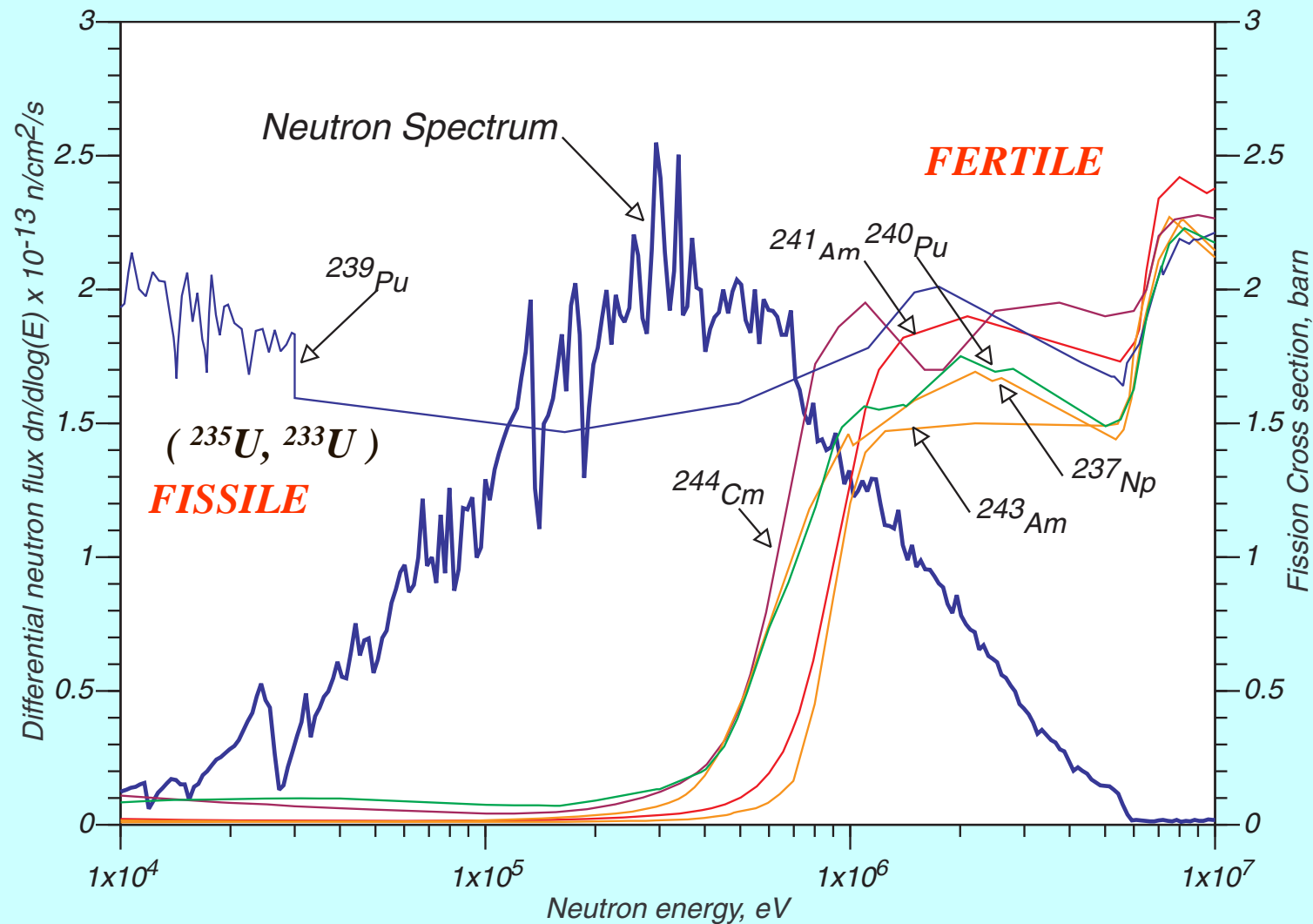
Nuclear energy systems deployable no later than 2030
in both developed and developing countries, for
generation of electricity and other energy products



Phillip Finck (ANL, USA), "The Future of Nuclear Energy and the Role of Nuclear Data", April 2005, Antwerp, Belgium



Why we need fast reactor systems?



What is Nuclear Data Evaluation?

Experimental nuclear physicist
Theoretician
Evaluator



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.*

see Giuseppe Palmiotti (INL, USA) lecture later this week

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** $^{238}\text{U}(\text{n},\text{inl})$ in the whole energy range up to 20 MeV and **on capture cross section** $^{238}\text{U}(\text{n},\gamma)$.

Cross sections, uncertainties and covariance data are strongly required



SCOPE

- ☐ Types of nuclear data
- ☐ Nuclear reaction data evaluation
- ☐ ENDF-6 format
- ☐ Data file verification and validation
- ☐ Processing for applications:
 - point-wise libraries for MC codes
 - group libraries for deterministic codes



OBJECTIVES

- ☐ Distinguish different ND types and understand the transformations
- ☐ Understand the basic principles of nuclear data evaluation
- ☐ Understand nuclear data verification and validation
- ☐ Get acquainted with methods of ND processing for applications



Nuclear reaction data types (I)

☐ Integral

From integral experiments

☐ Microscopic (or Differential)

☐ Differential in incident particle energy

☐ Differential in outgoing particle angle or energy

☐ Double differential in energy and angle

☐ Processed (result of data reduction)



Nuclear reaction data types (II)

□ Microscopic (or differential)

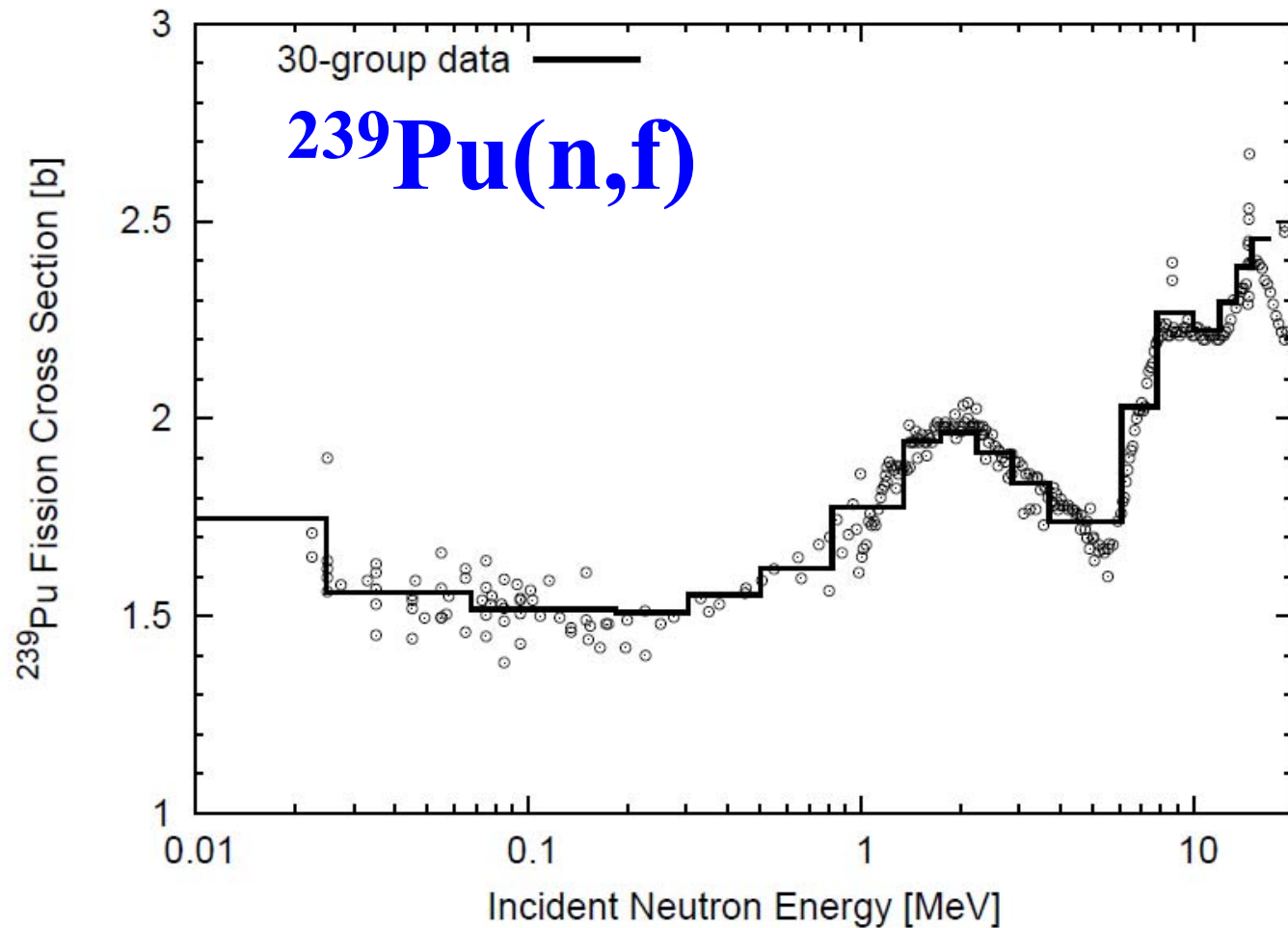
- Basic: Measured (**EXFOR**) or
Calculated (**models or model codes**)
- Evaluated (proper combination of **EXP + CALC**)

□ Processed

- Change of data representation
- Reformatting
- Group averaging (preparation of multigroup constants) \Rightarrow **Data Reduction**



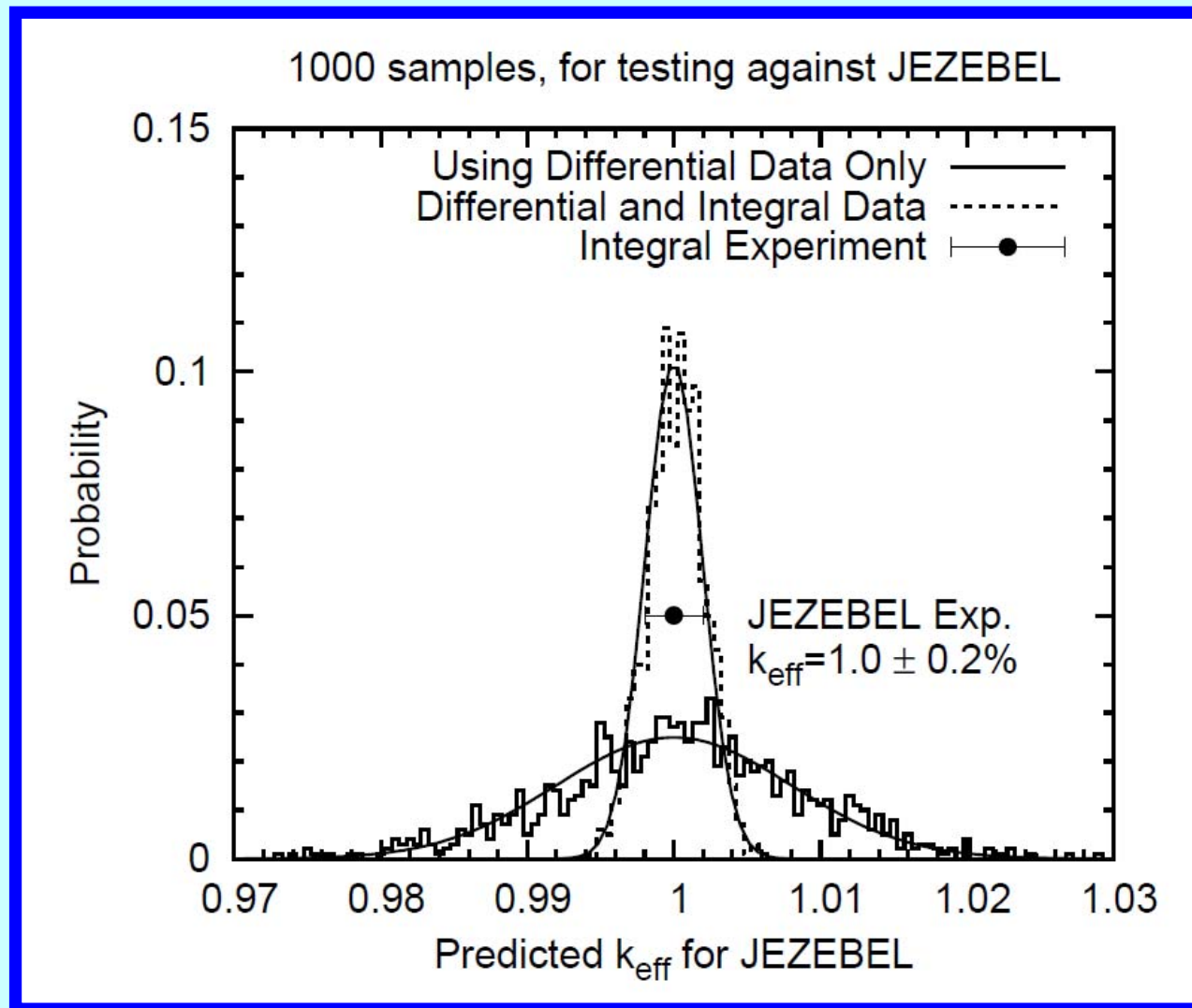
Differential and processed data



Kawano *et al.*
NSE 2006



Considering integral data on k_{eff}

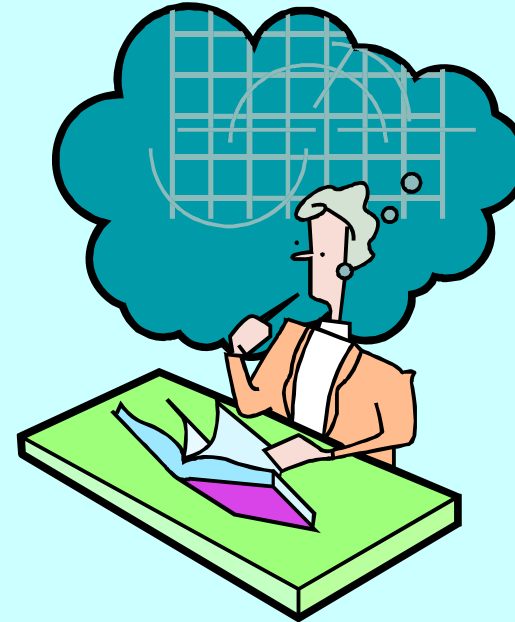


Kawano *et al.*
NSE 2006



What do engineers (you) need?

I need cross sections ...

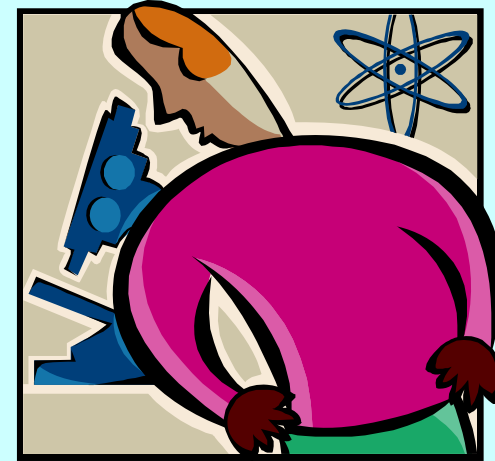


$$-\nabla D_{(1)} \nabla \phi_{(1)} + \Sigma_{a(1)} \phi_{(1)} = \frac{1}{k} \left[\sum_g \nu_{(g)} \Sigma_{f(g)} \phi_{(g)} \right] + \Sigma_{(2 \rightarrow 1)} \phi_{(2)}$$
$$-\nabla D_{(2)} \nabla \phi_{(2)} + \Sigma_{a(2)} \phi_{(2)} = \Sigma_{(1 \rightarrow 2)} \phi_{(1)}$$



What orthodox theoreticians provide?

Here you are ...
It is all described in
my article in the journal !



$$\sigma_a(U, J, \pi) = \frac{\pi}{k^2} \frac{(2J+1)}{(2I+1)(2i+1)} \sum_{S=|I-i|}^{I+i} \sum_{l=|J-S|}^{J+S} f(l, \pi) T_l^a(\varepsilon)$$

Or even worse ...
Please use my calculations ...

1.00000E-03	2.43758E+01	1.26322E+01	1.17435E+01
5.00000E-03	1.75172E+01	5.98889E+00	1.15283E+01
1.00000E-02	1.58838E+01	4.55133E+00	1.13325E+01
2.00000E-02	1.46751E+01	3.66517E+00	1.10099E+01
4.00000E-02	1.36734E+01	3.19591E+00	1.04775E+01
7.00000E-02	1.28627E+01	3.03899E+00	9.81379E+00

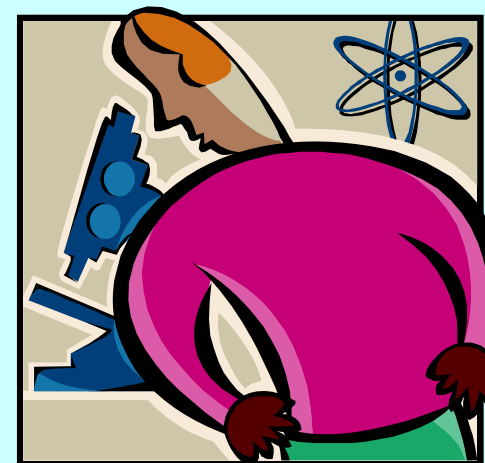


Dialogue?

**What do I do with that?
My codes cannot read journals!
What data you got there?**



**Do what you want!
It's not my job...**



Nice guy/girl comes along...

**We now have a code
that turns theory
into numbers ...
Retrieve data from the web**



**We can compare measured
and calculated data ...**

... plot pictures ...



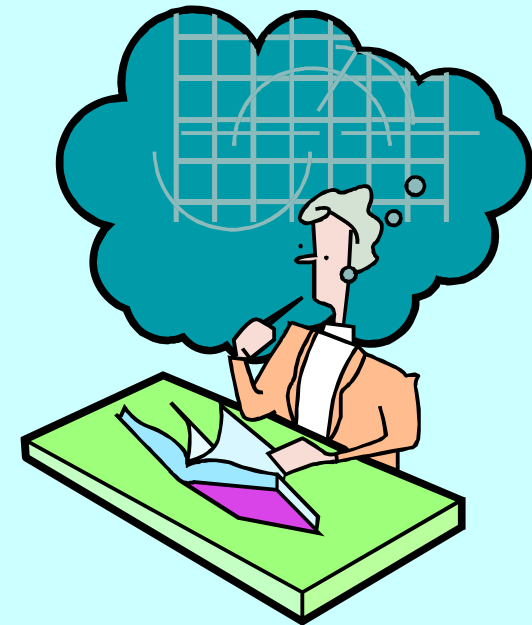
Are we there yet?

Nice numbers ...

Lots of numbers !

Too many numbers !!!

Besides: which one is right ?

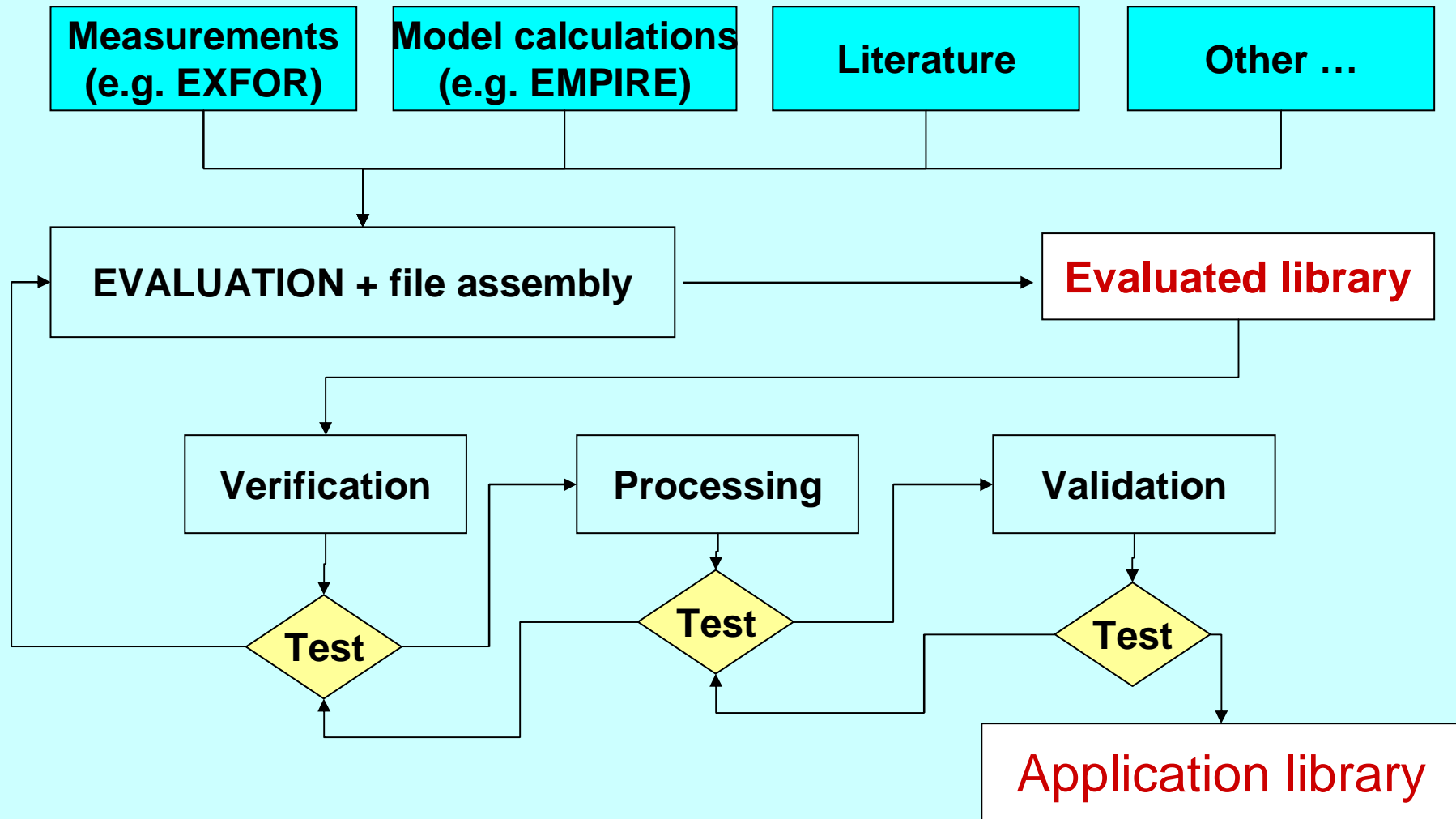


What needs to be done?

- ❑ ND evaluation → computer-readable format
- ❑ ND reduction (**processing**)
 - Averaging by energy (deterministic transport)
=> group-averaged cross sections
 - Reformatting point-wise (Monte Carlo transport)
 - Homogenisation and condensation =>
macroscopic cross sections that engineers need
- ❑ Whole-core reactor calculation with thermo-hydraulic feedbacks ...



What needs to be done?



Nuclear reaction data evaluation

- ☐ Evaluation and formatting
- ☐ Complete file assembly
- ☐ Data file verification
- ☐ Processing for applications
- ☐ Validation = Benchmarking

feedback loop to evaluation

Loop-2

- ☐ Final validation

**Now we know at least what numbers
are (probably) right !**

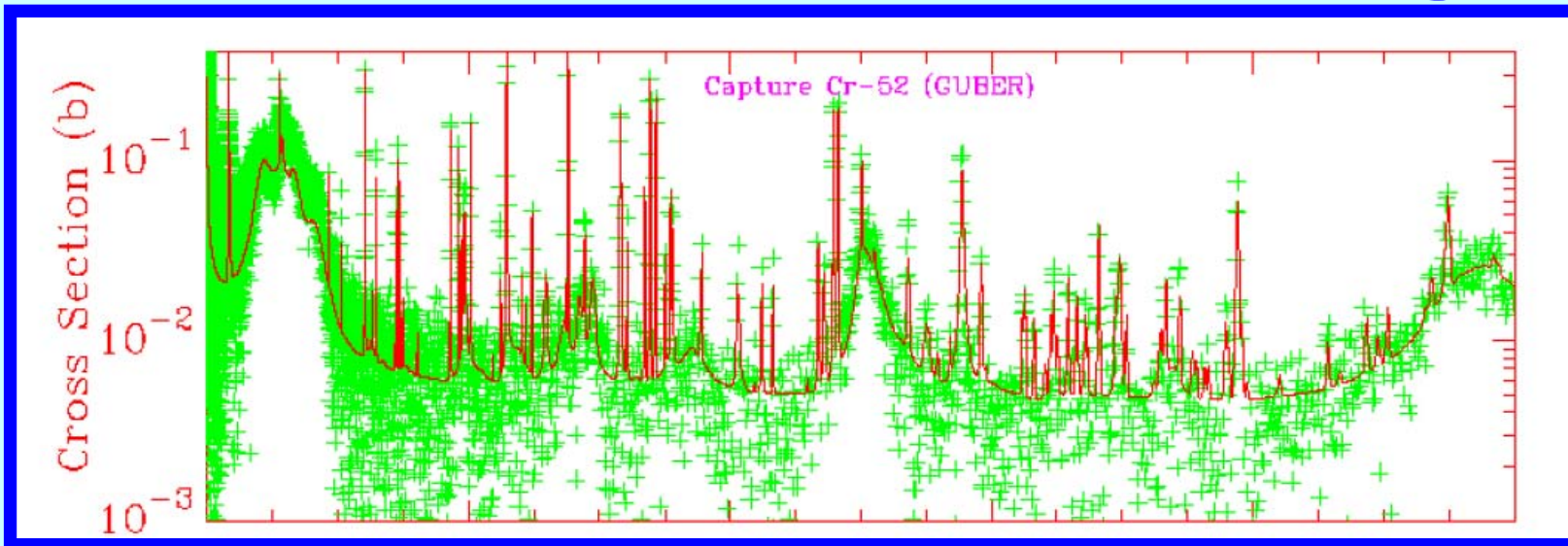


Nuclear reaction data evaluation

- ❑ Resonance energy range ($\Gamma \ll D$)
- ❑ Fast neutron range ($\Gamma \gg D$ stat models)
keV for actinide, MeV for Ni, Fe, Cr,...
- ❑ Unresolved resonance range (in between)
(self-shielding)



Evaluation – resonance range

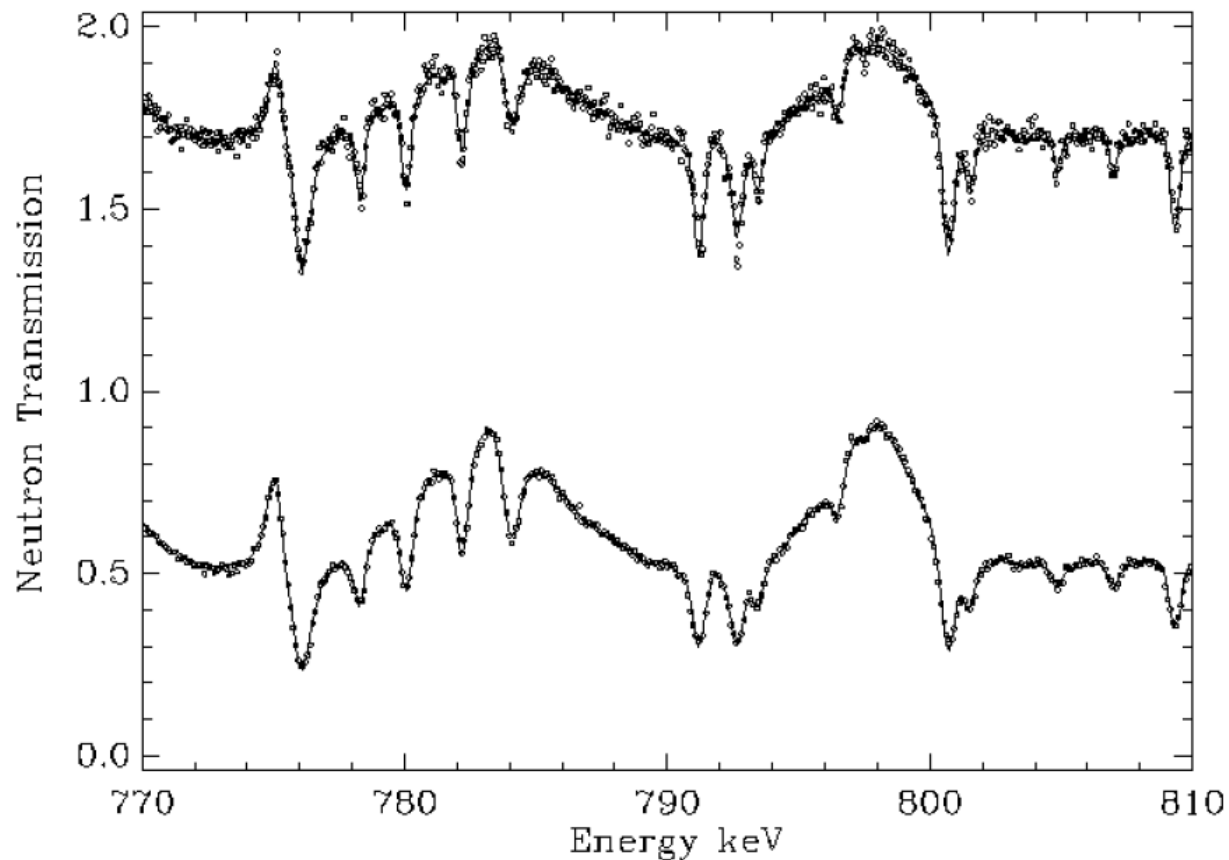


- ☐ Theoretical predictions not possible yet
- ☐ Resonance parameters must be obtained from fitting experimental data
- ☐ Modern resonance fitting codes produce “best fit” parameters as well as their covariances (e.g. **SAMMY**, **REFIT**, **CONRAD**, etc.)

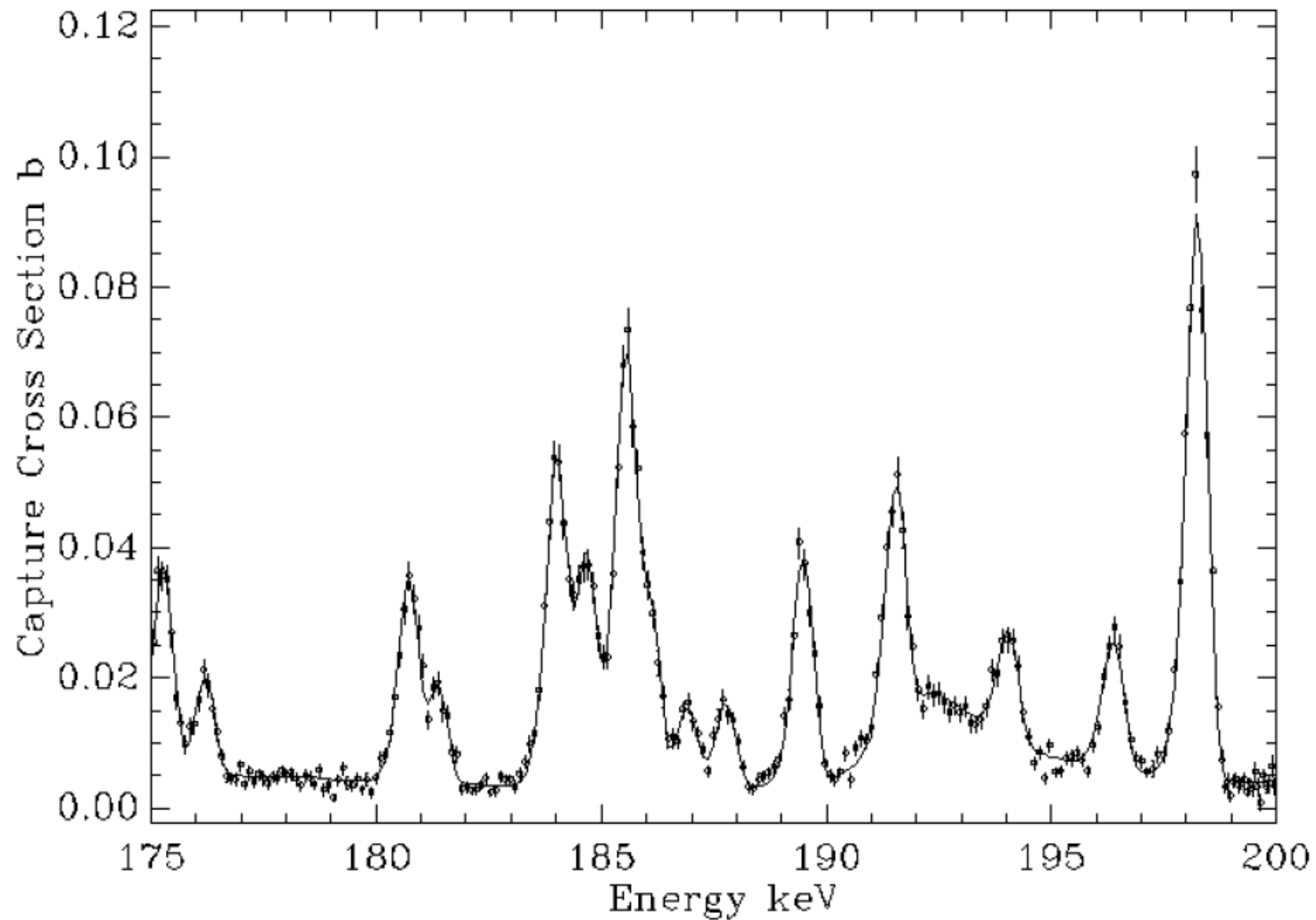


Evaluation – resonance range - example

^{58}Ni Neutron Transmission in the energy range 770 keV to 810 keV from Brusegan et al. (upper part), and Perey et al. (lower part). The smooth curve represents the transmission calculated by SAMMY. Brusegan data were multiplied by 2 for clarity of the figure



^{58}Ni effective capture cross section in the energy range 175 keV to 200 keV from Guber et al. The smooth curve represents the effective cross section calculated by SAMMY from the resonance parameters



Evaluation – resonance range - results

⁵⁸Ni Evaluation

- 487 resonances from thermal to 812 keV
- 61 s-wave; 204 p-wave; 222 d-wave
- Average spacing for s-wave: $D_0 = 12.65 \pm 0.70$ keV
- Neutron Strength Function from fit to PT distribution:
 - $S_0 = 3.38 \pm 0.61 \times 10^{-4}$
 - $S_1 = 0.48 \pm 0.08 \times 10^{-4}$
 - $S_2 = 2.27 \pm 0.30 \times 10^{-4}$
- Thermal Capture : 4.27 ± 0.15 b compared to the ENDF/B-VII 4.62 b
- Capture Integral: 2.095 ± 0.07 b compared to the ENDF 2.20 b



Evaluation – fast energy range

- ☐ Use state-of-the-art **nuclear model code** (e.g. **EMPIRE**)
 - ☐ Choose **adequate model** options
 - ☐ Determine **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-1**
- ☐ From **model parameter uncertainties** and **model uncertainties** generate **covariance matrix prior**



NEW EMPIRE VERSION 3.0

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



**Nuclear Data
Sheets**

Nuclear Data Sheets 110 (2009) ?? (accepted)

www.elsevier.com/locate/nds

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

R. Capote,¹ M. Herman,^{1,2} P. Obložinský,^{1,2} P.G. Young,³ S. Goriely,⁴ T. Belgia,⁵ A.V. Ignatyuk,⁶ A.J. Koning,⁷
S. Hilaire,⁸ V.A. Plujko,⁹ M. Avrigeanu,¹⁰ O. Bersillon,⁸ M.B. Chadwick,³ T. Fukahori,¹¹ Zhigang Ge,¹²
Yinlu Han,¹² S. Kailas,¹³ J. Kopecky,¹⁴ V.M. Maslov,¹⁵ G. Reffo,¹⁶ M. Sin,¹⁷ E.Sh. Soukhovitskii,¹⁵ and P. Talou³



Evaluation - fast energy range

Mn-55: Neutron cross sections

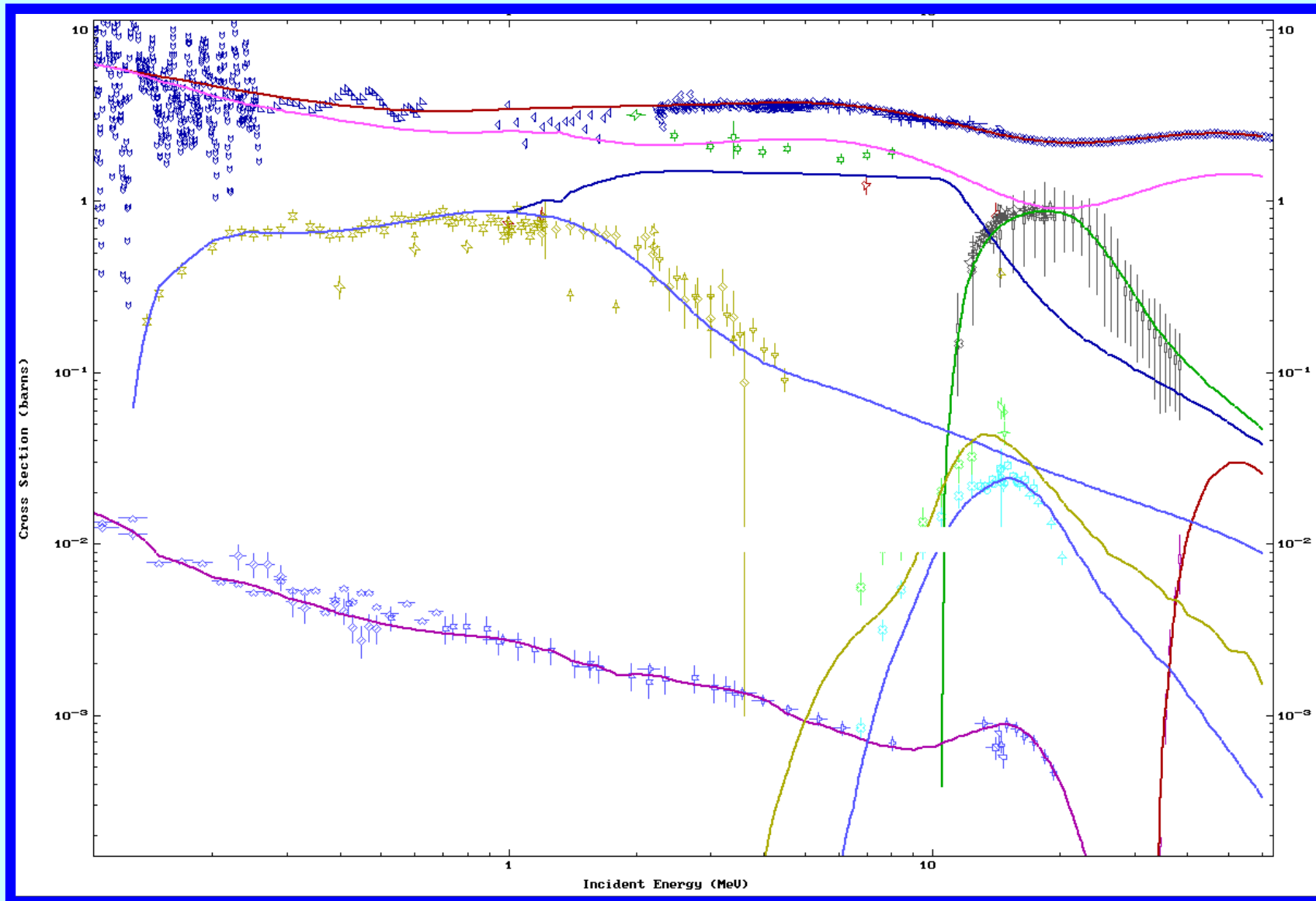
Structural material

Th-232: Neutron cross sections

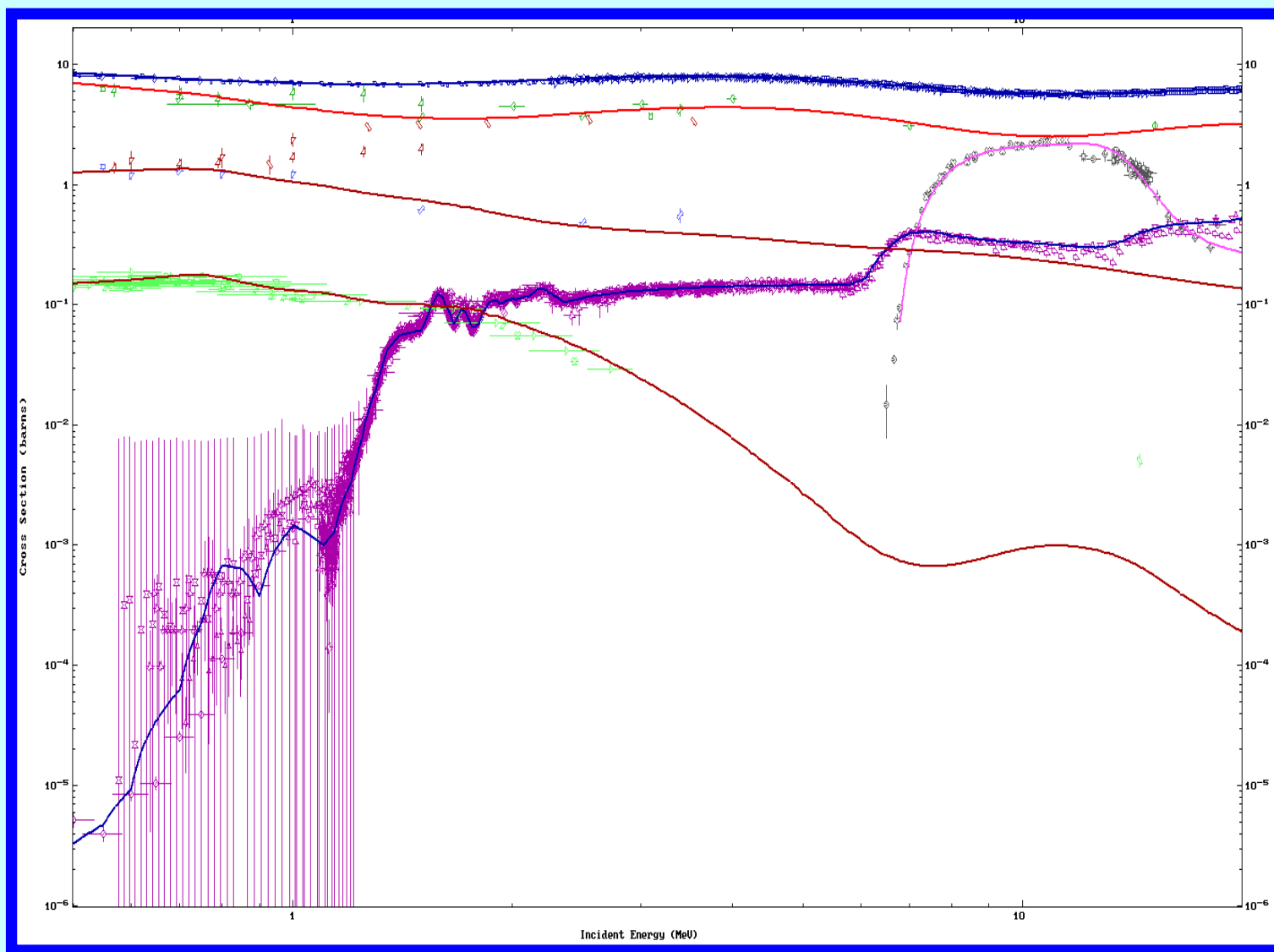
Fertile nucleus



$n + {}^{55}\text{Mn}$



$n + {}^{232}\text{Th}$



Evaluation - fast energy range

Mn-55: Neutron cross sections

Structural material

Th-232: Neutron cross sections

Fertile nucleus

What about uncertainties & covariances?



Covariances – fast energy range

- ❑ Prior by random sampling of model parameters and model uncertainties within their uncertainties
- ❑ Introduce measured data (microscopic cross sections and other quantities) to constrain the uncertainties (e.g. **GANDR**)
- ❑ Covariances must be consistent with the evaluated cross section data !

IAEA Visualization of covariance data

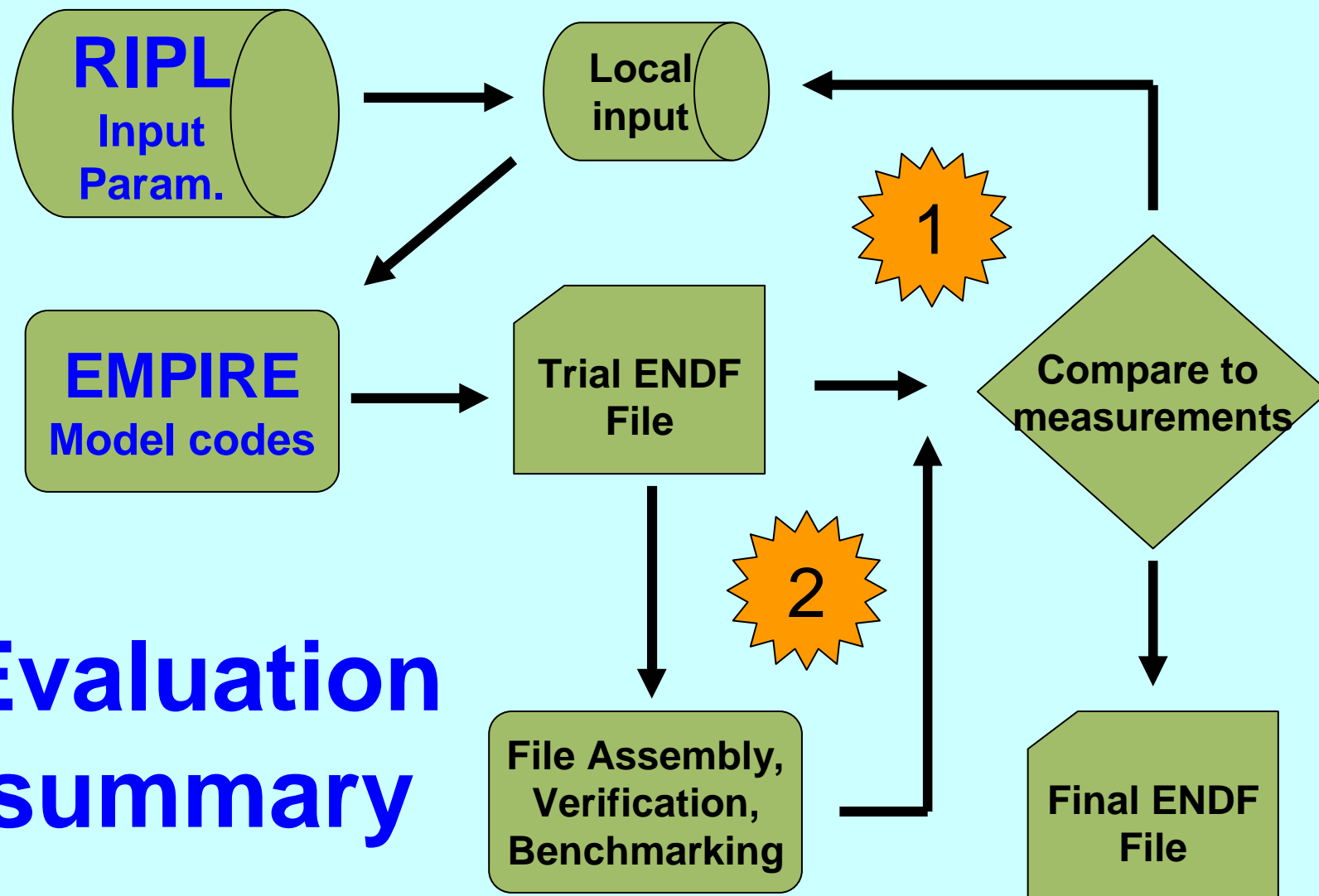


Evaluated data file assembly

- Data for the resonance and fast range must be assembled consistently
- Patching into the file covariance data from another evaluation is *dangerous !*



Evaluation summary



ENDF-6 format

- ❑ **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 !**



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 !



ENDF-6 format (Cont.)

What's in the name?

- Evaluated Nuclear Data File (ENDF)
- “/B” full library from U.S.A. (as opposed to partial evaluations denoted “/A”)
- Roman numerals denote library version (ENDF/B-VI)
- Several releases (updates) may exist (Rel.8)
- Format designation without “/B” and with arabic numerals for version designation.

ENDF/B-VII.0 (Rel. 0)– Library from U.S.A.

ENDF-6 Format (maintained by BNL, U.S.A.)



Nuclear Data verification



ENDF-6 evaluated file verification

□ ENDF Utility codes

- **STANEF**: utility to standardise number representation, dictionary, etc.
- **CHECKR**: check formal correctness of format
- **FIZCON**: check physical consistency of the data
- **PSYCHE**: more advanced checking of the file contents



Evaluated file verification (Cont.)

- **Pre-Pro** ENDF Pre-Processing codes
 - Linearisation, resonance reconstruction, Doppler broadening, etc.
 - First test of data processability.
- **ENDVER** graphical display package
 - Heavy usage of Pre-Pro codes
 - Comparison with experimental data from EXFOR
 - Reconstruction of elemental data from isotopic
 - Reactions defined by summation
 - Differential and double-differential data



Nuclear Data processing



Nuclear data processing

- ❑ Reformatting and basic operations
 - Linearization
 - Resonance reconstruction
 - Doppler broadening, etc.
- ❑ Data reduction
 - Averaging over energy
 - Averaging over space
- ❑ Assembly of application libraries



Nuclear data reduction: Group averaging over energy

Reaction Rates $\sigma_g \varphi_g = \int_g \sigma(E) \cdot \varphi(E) dE$

Average Cross Sections

$$\varphi_g = \int_g \varphi(E) dE$$

$$\sigma_g = \frac{\int_g \sigma(E) \varphi(E) dE}{\int_g \varphi(E) dE}$$

Scattering Matrices

$$\sigma_{(l)g \rightarrow h} = \frac{\int_{-1}^1 d\mu \int_g dE \cdot \varphi(E) \int_h dE' \cdot \sigma(E \rightarrow E', \mu) \cdot P_l(\mu)}{\int_g \varphi(E) \cdot dE}$$



Nuclear data reduction: Group averaging over space

Reaction Rates

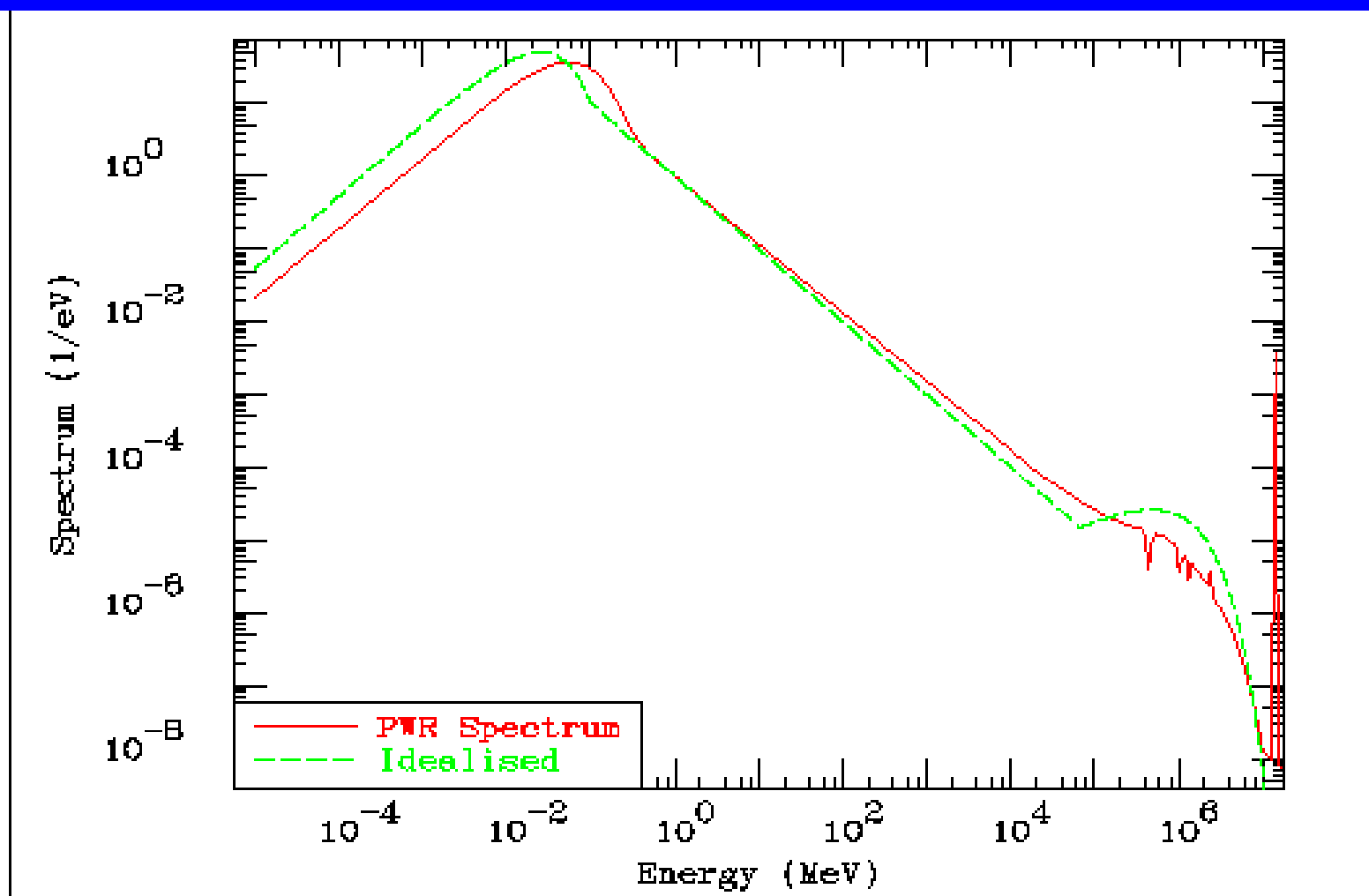
$$\langle \Sigma_g \rangle \langle \phi_g \rangle = \int_V \Sigma(\vec{r}) \phi(\vec{r}) dV$$

Average flux and cross sections

$$\langle \phi_g \rangle = \int_V \phi(\vec{r}) dV \quad \langle \Sigma_g \rangle = \frac{\int_V N \sigma(\vec{r}) \phi(\vec{r}) dV}{\int_V \phi(\vec{r}) dV}$$



Weighting spectra:



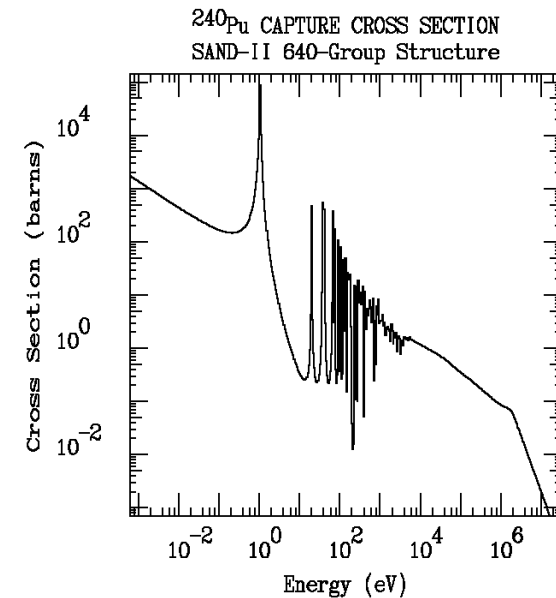
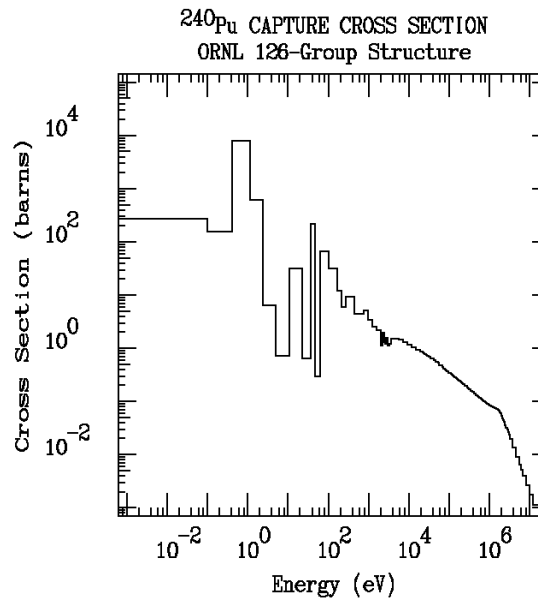
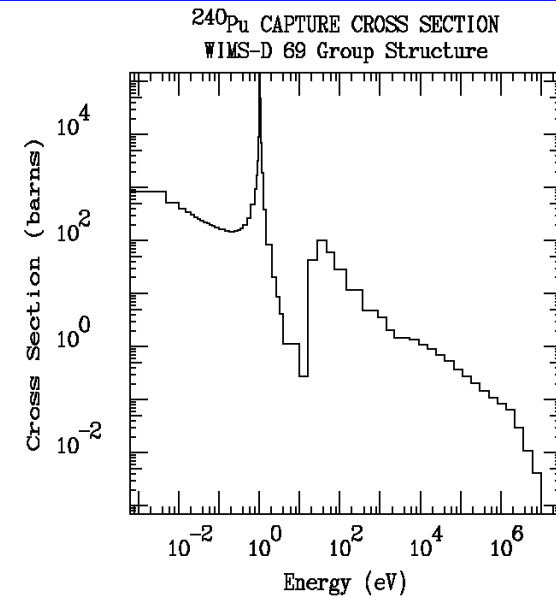
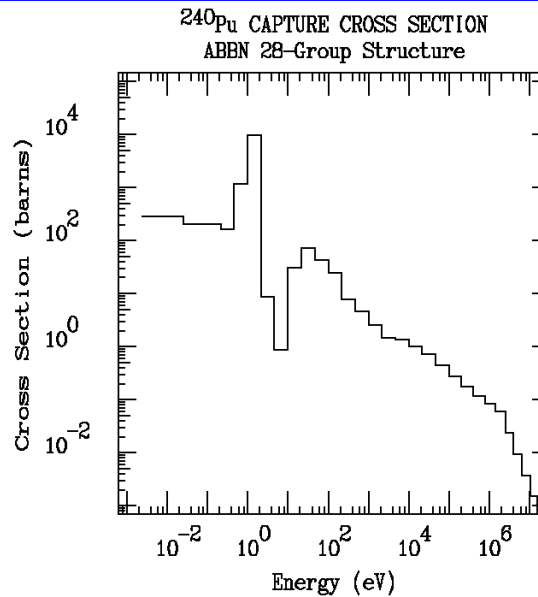
Group averaged data - Definitions

- ❑ Fine group data ($>$ about 600 groups)
- ❑ Multigroup (20 – 600 groups)
 - Application-dependent (fast reactors, thermal reactors, fusion applications, accelerator shielding, etc.)
- ❑ Few-group (1-20 groups)
 - Local material properties (macroscopic cross sections, homogenised coarse-mesh spatial grid)



ABBN 28-g
WIMS-D 69-g

ORNL 128-g
SAND-II 640-g



Data Processing codes

- ❑ **Pre-Pro**: ENDF Pre-Processing codes perform basic operations on nuclear data
- ❑ **NJOY** is a comprehensive system for generating application libraries, developed at Los Alamos National Laboratory
- ❑ **AMPX** is a comparable system developed at Oak Ridge National Laboratory
- ❑ **GALILEO** is a comparable system developed at CEA



Nuclear Data validation

= Benchmarks



Nuclear data validation

- ❑ Before use, verification of application libraries is needed (processing errors)
- ❑ Validation of evaluated data files is implicit in the validation of application libraries
- ❑ Validation of application libraries is done by modelling integral benchmarks and comparing calculated and measured integral parameters
- ❑ Validity of such libraries is limited to problems, which resemble the benchmark test cases.



Nuclear data validation (cont.)

- Verification: CHECKR, FIZCON, PSYCHE, EMPEND...
- Processing: NJOY (for deterministic and/or Monte Carlo codes) → test application library
- Validation: benchmark databases ICSBEP, SINBAD ... → Compare C/E



CONCLUSIONS

- Evaluation steps described
- Verification steps defined
- Validation:
 - Processing
 - Benchmark calculations
 - Feedback to evaluation
 - **Validity**: cases similar to benchmarks

RIPL + evaluation code (EMPIRE, TALYS, ...)



Application deadline: January 31 2010

① http://cdsagenda5.ictp.trieste.it/full_display.php?smr=0&ida=a09144

Joint ICTP-IAEA Workshop on

Nuclear Reaction Data for Advanced Reactor Technologies

3 May – 14 May 2010

Venue: LB (Euler Lecture Hall)

Trieste, Italy

Directors: R Capote, A Stanculescu, V. Pronyaev



Evaluation Loop 1

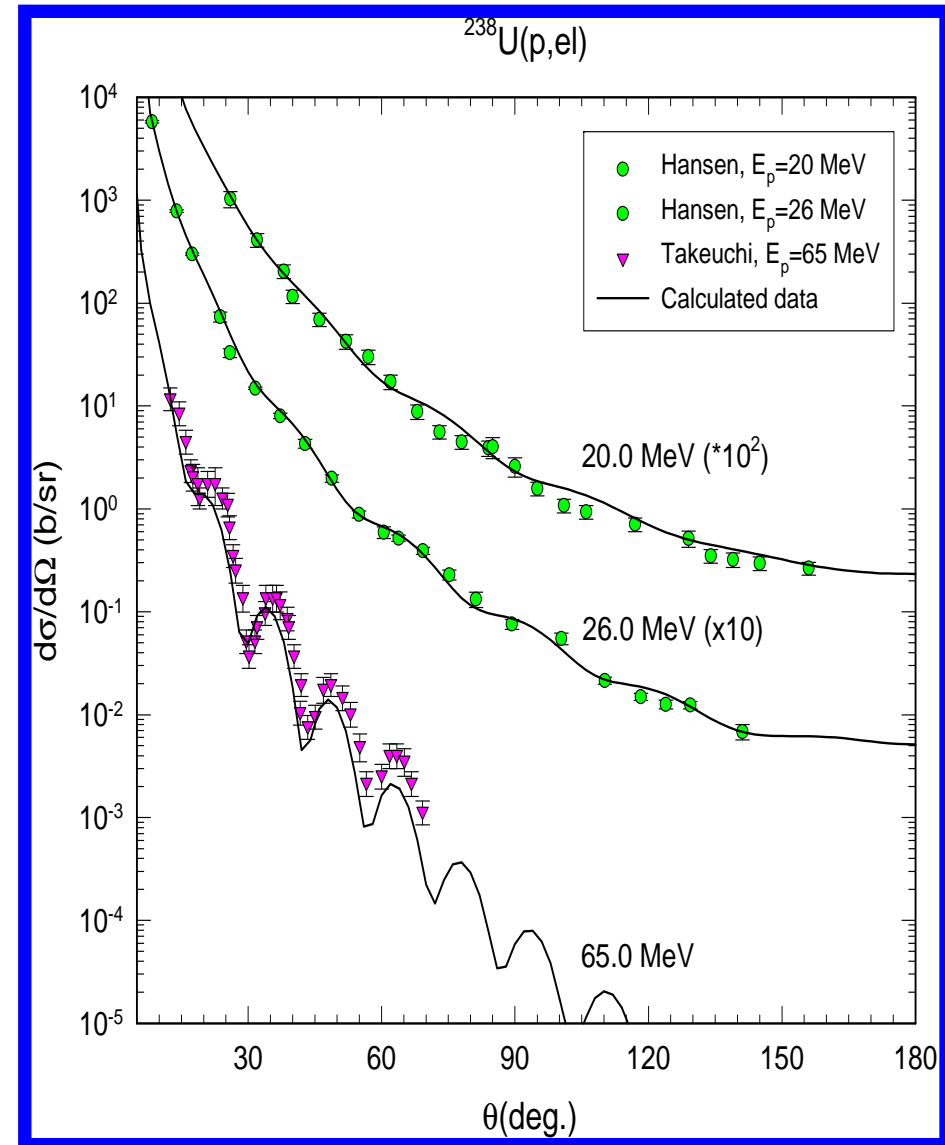
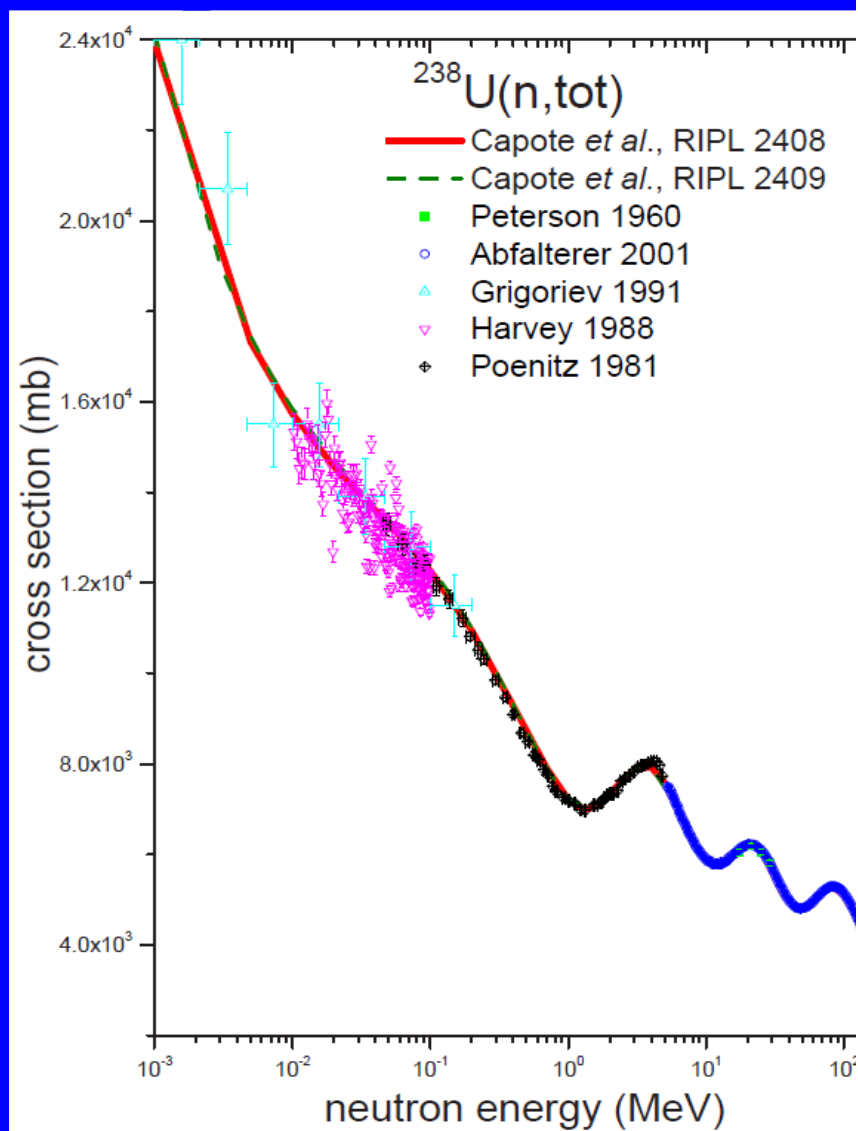


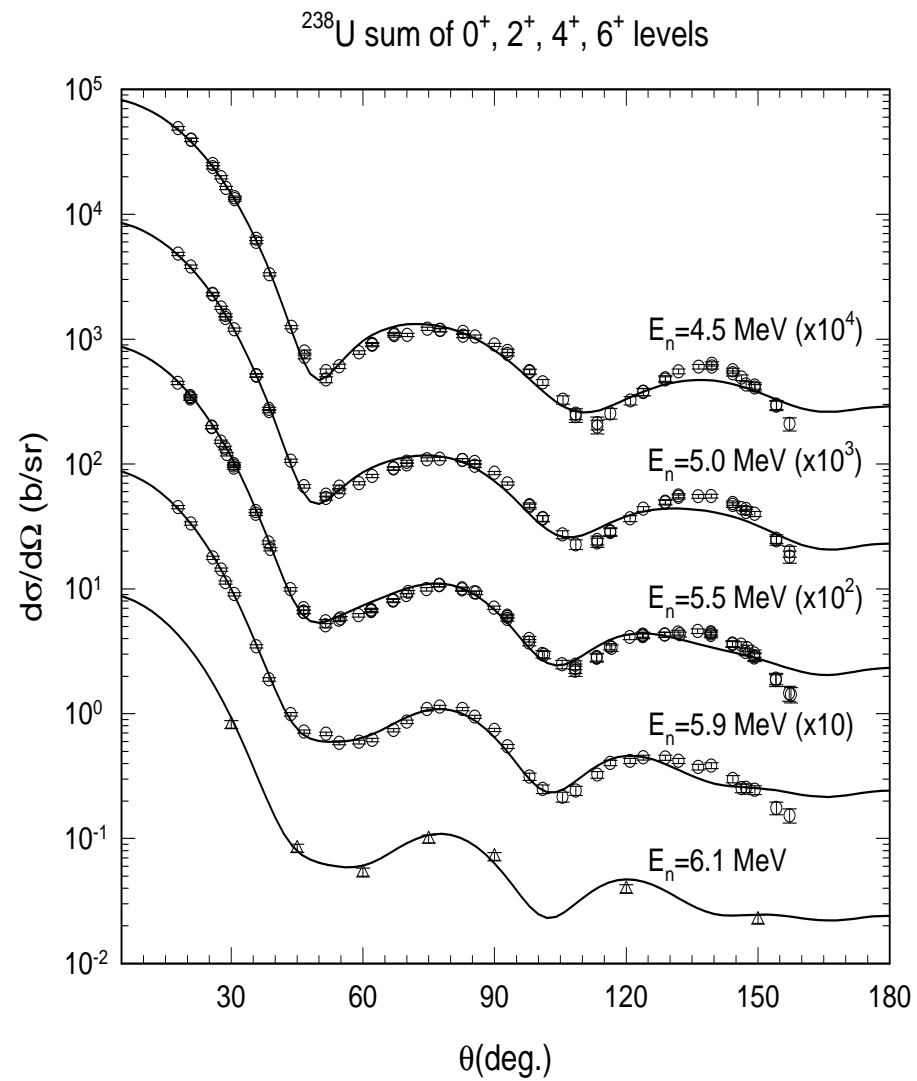
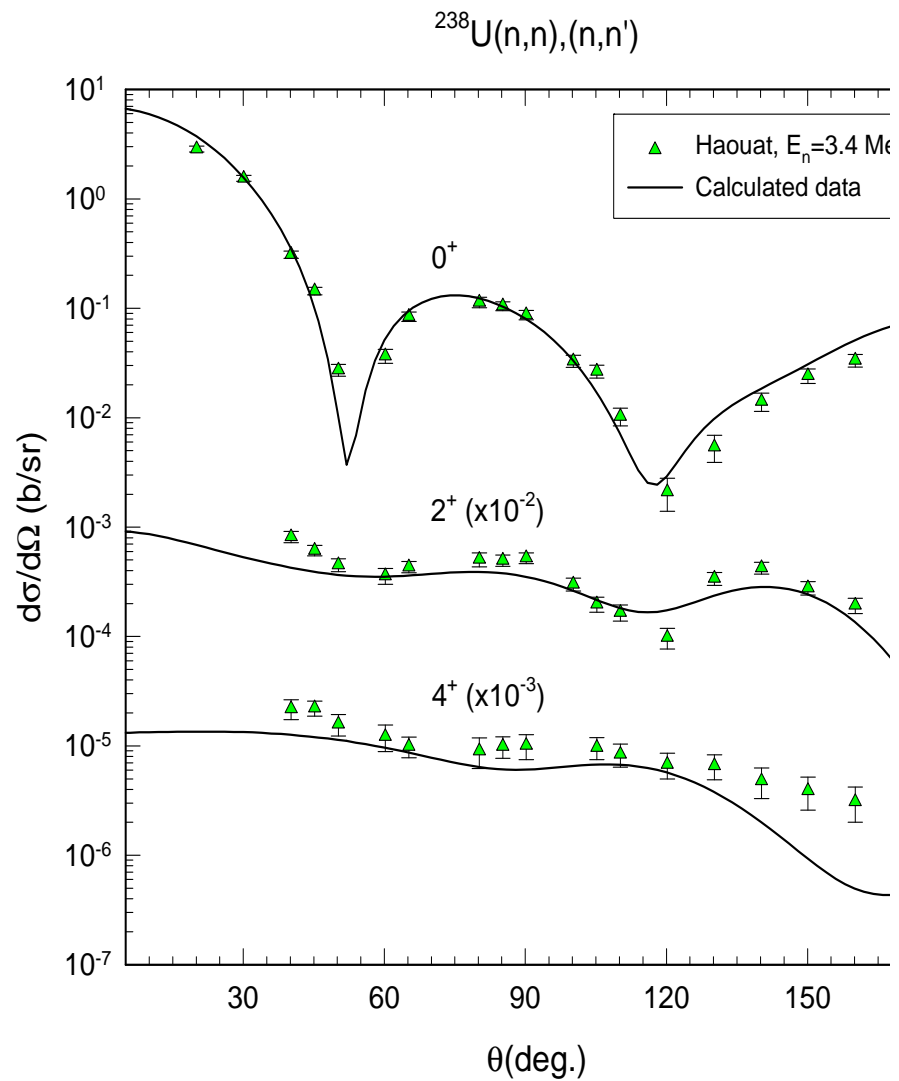
SUMMARY: Modelling advances

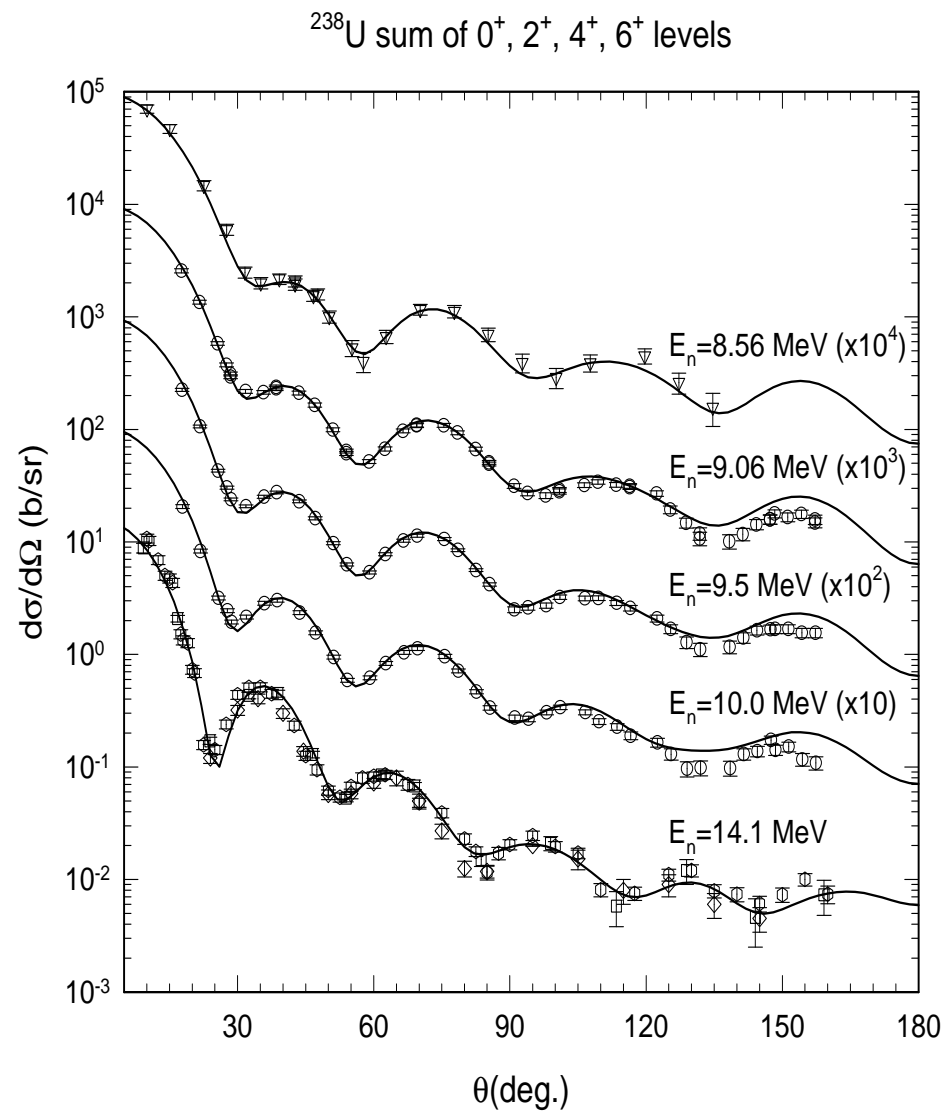
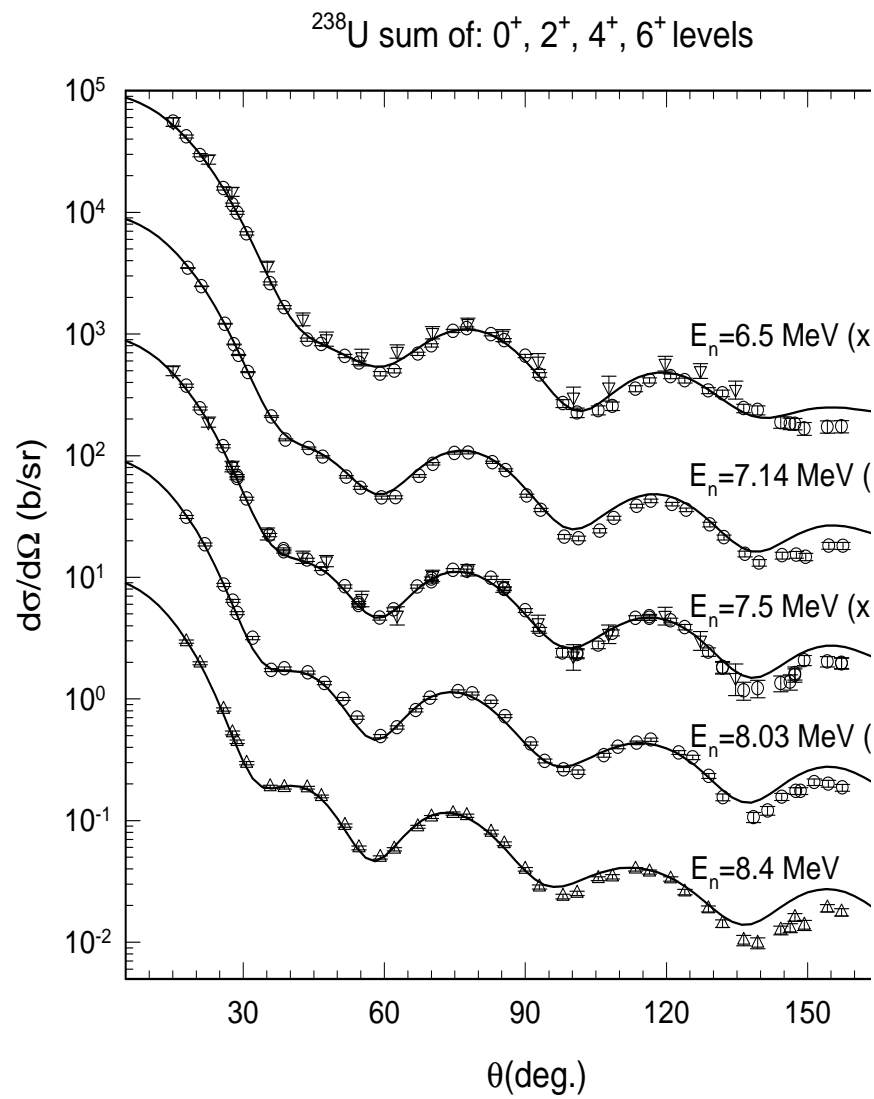
- ❑ *Dispersive and Lane consistent coupled-channel OMP:
neutron inelastic scattering to discrete levels;*
- ❑ *improved neutron emission spectra
(**MSD+MSC**) to calculate **neutron inelastic scattering** to the continuum;*
- ❑ *EGSM level density parameterization (**EGSM**):
all statistical cross sections*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

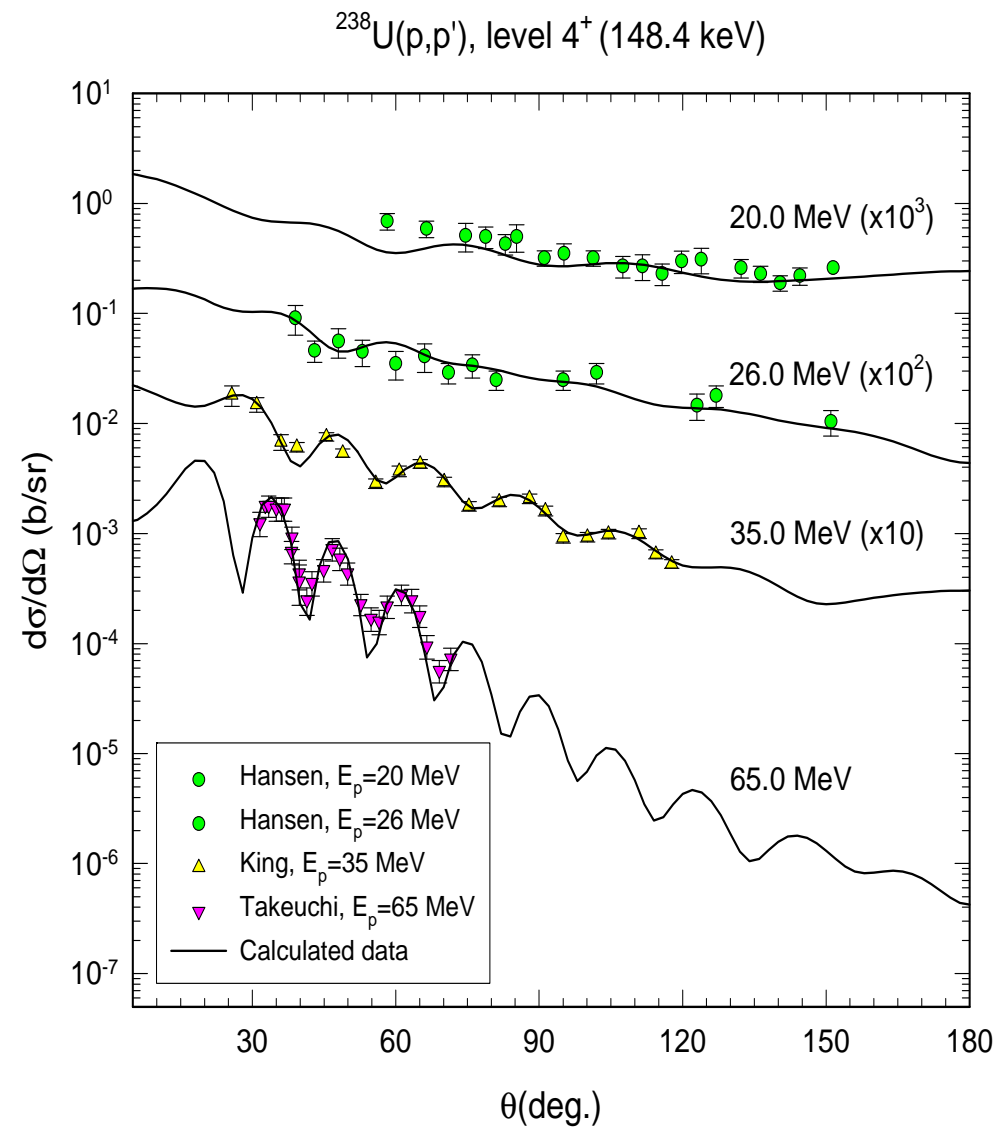
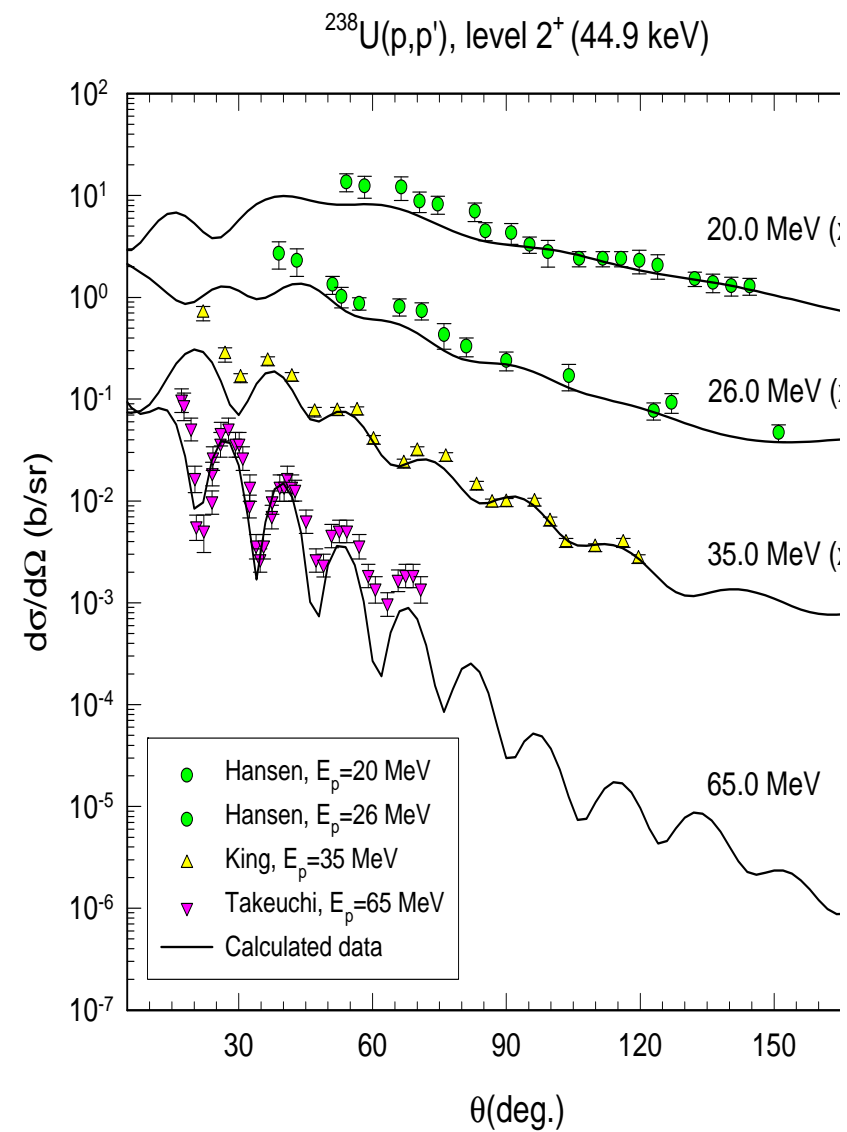


Dispersive and La

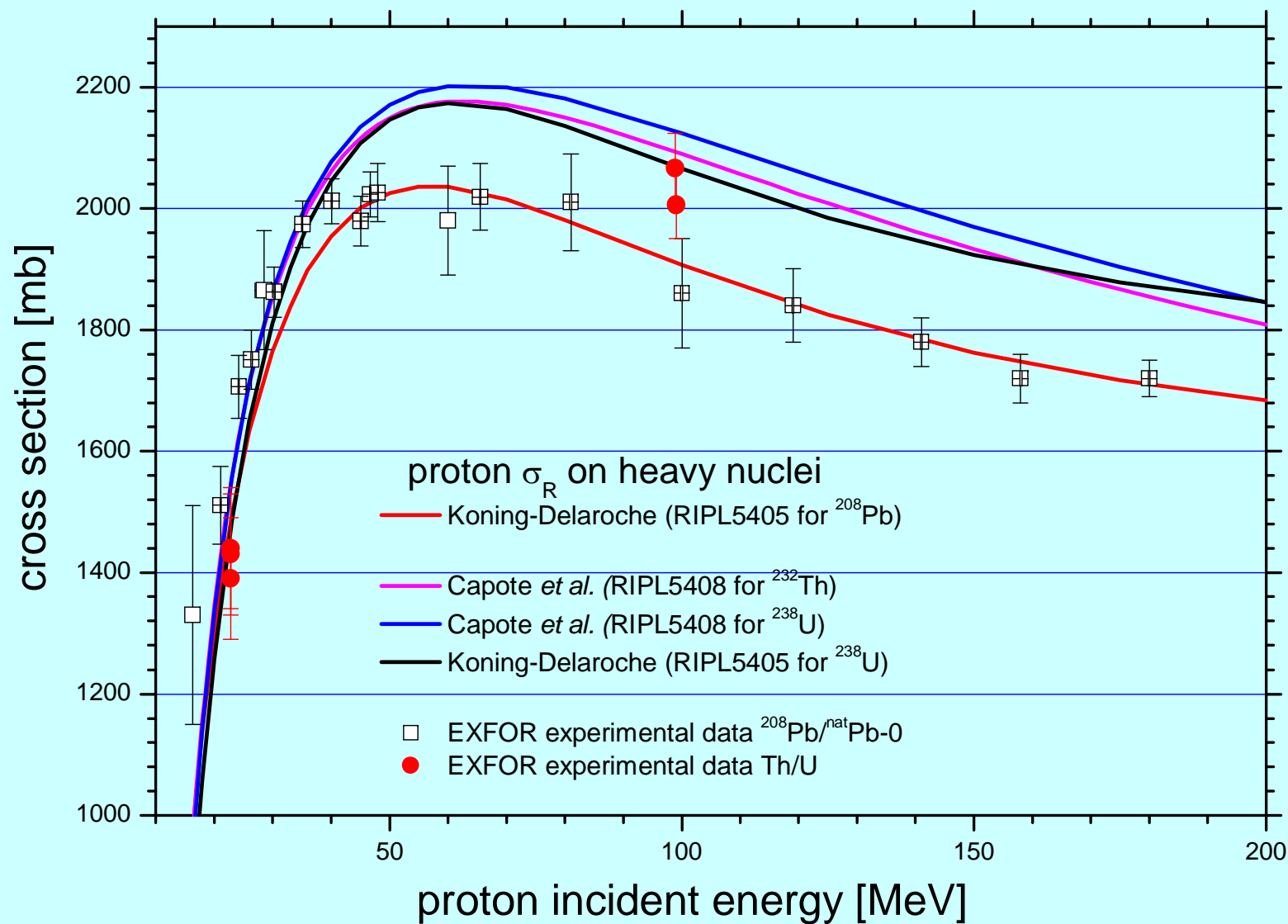




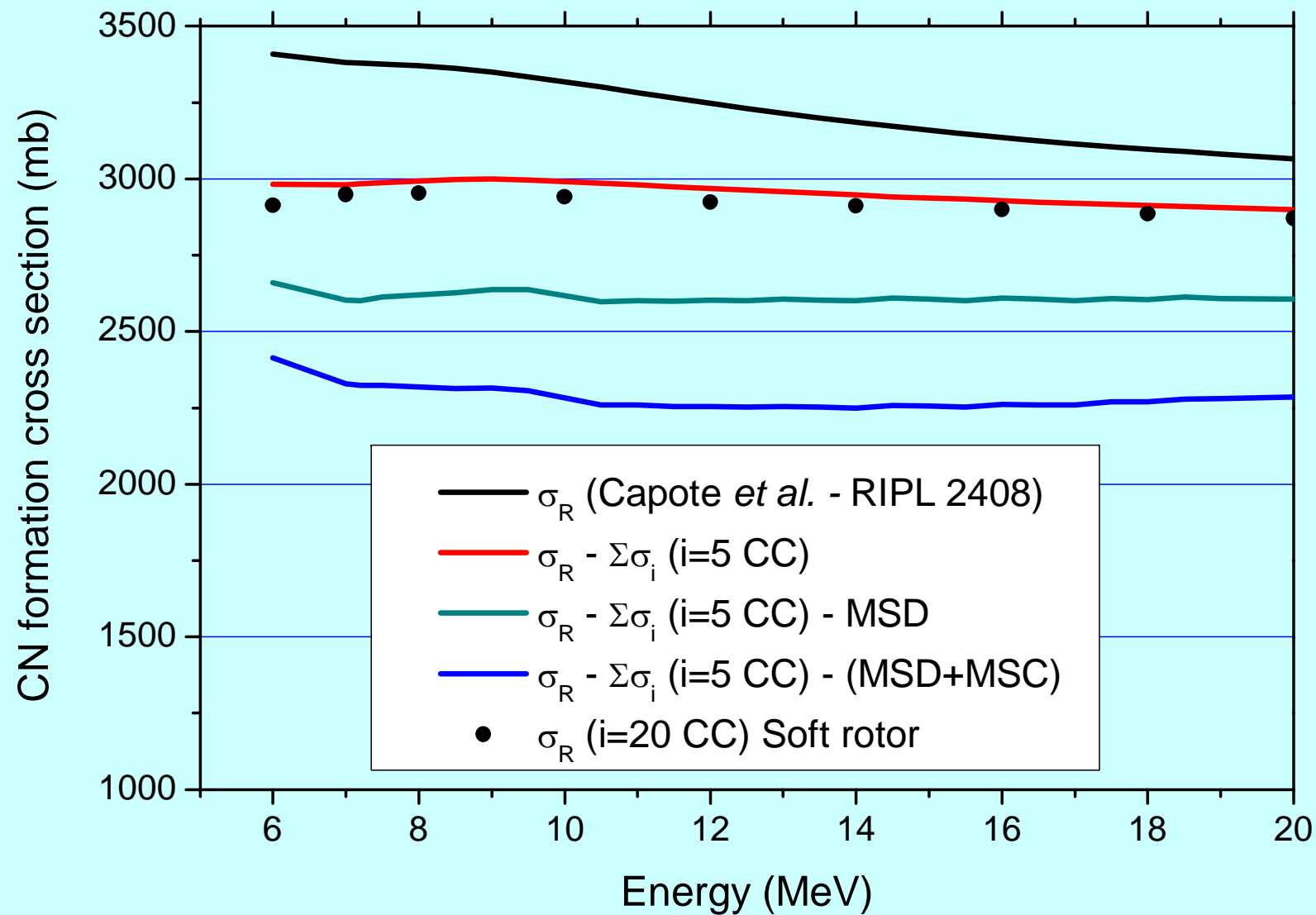




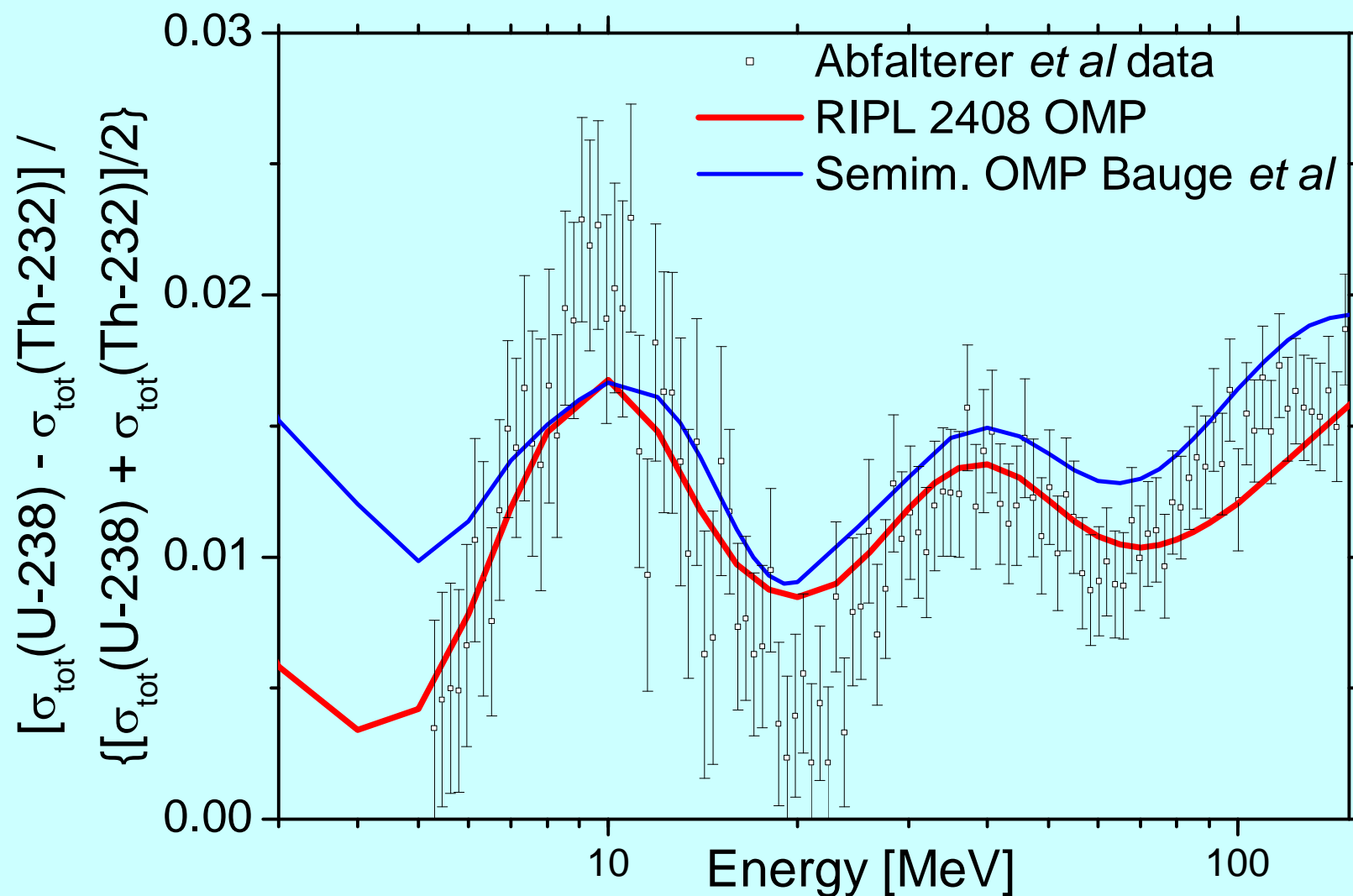
Dispersive and Lane consistent OMP (5)



Impact of MDS+MSC on CN formation



Dispersive and Lane consistent OMP (1)



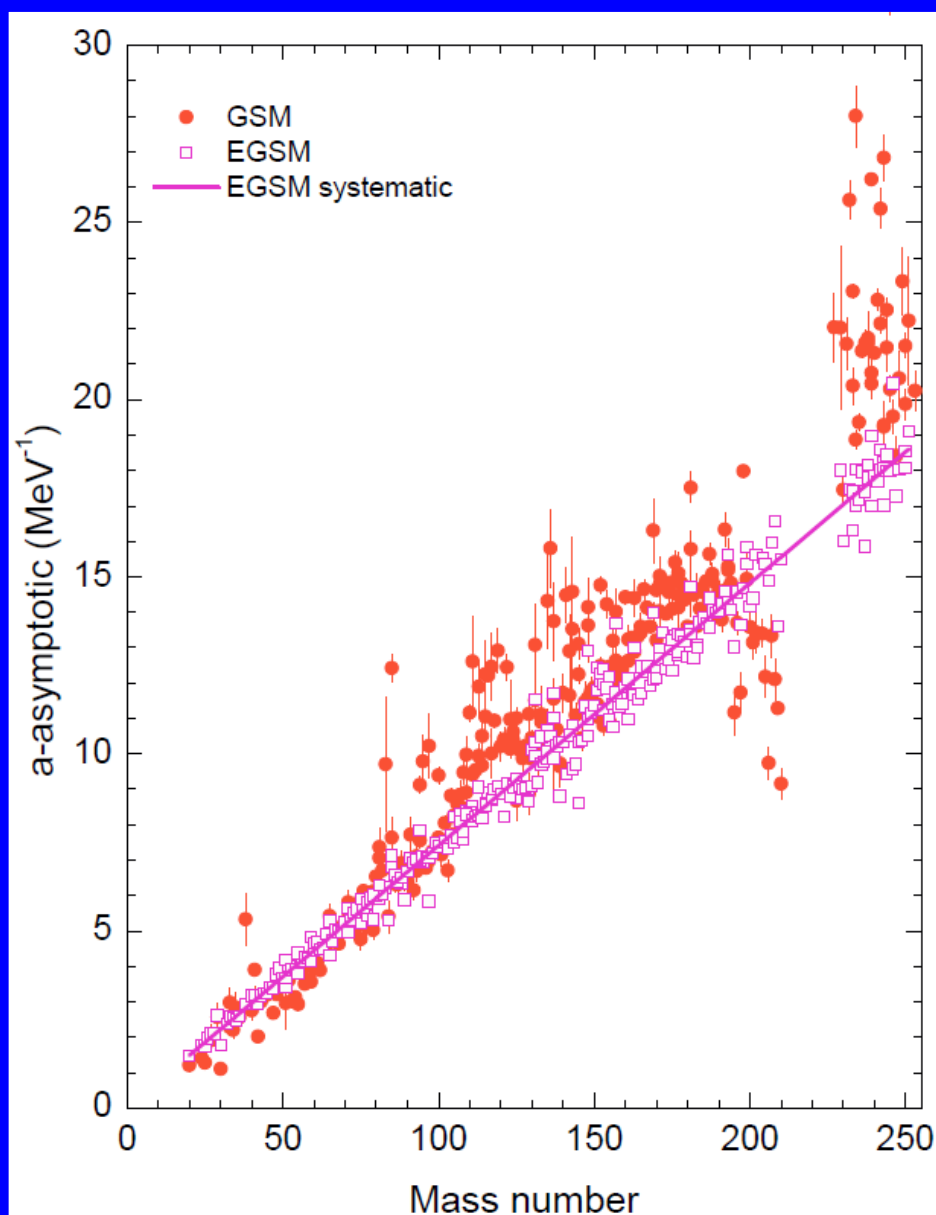
EGSM level density



Improved level density - EGSM

Notable features of the EGSM parametrization 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 favour of the collective enhancements and shell corrections adopted in the EGSM.

RIPL paper Nucl.Data Sheets 2009

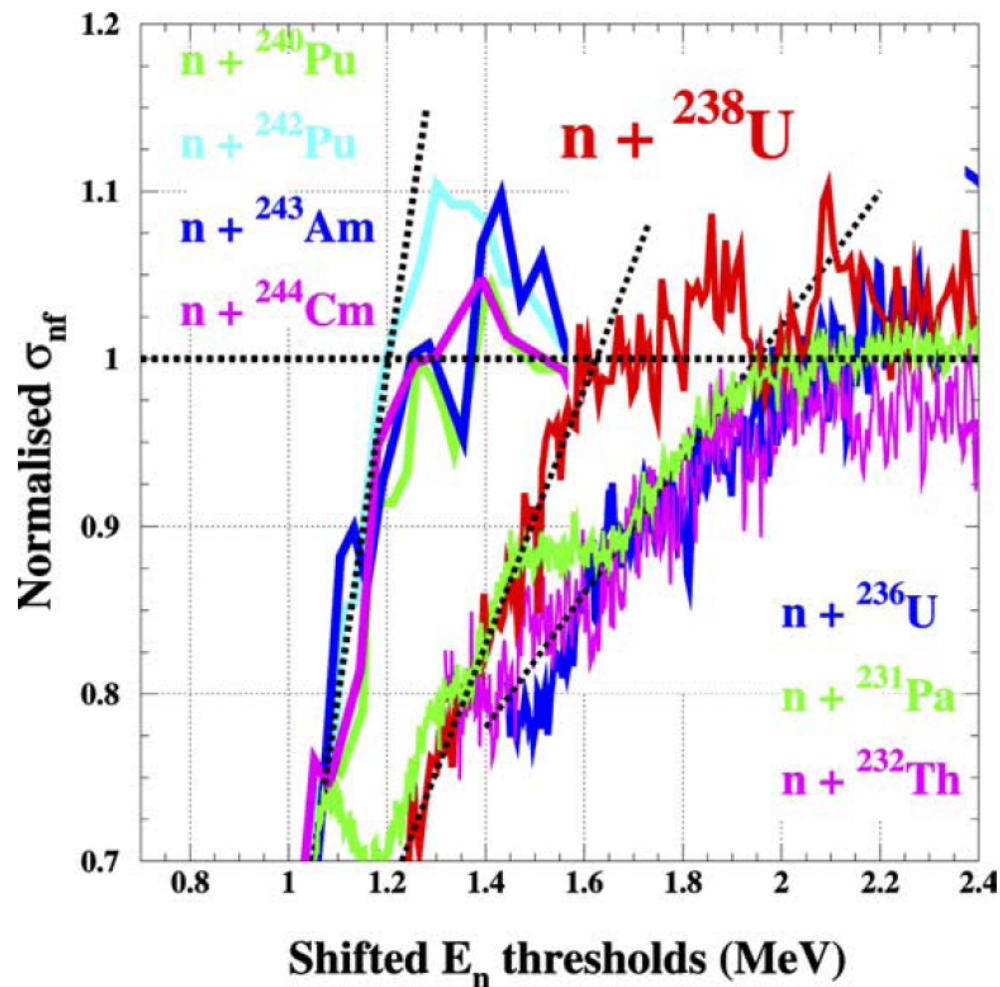


Fission modelling



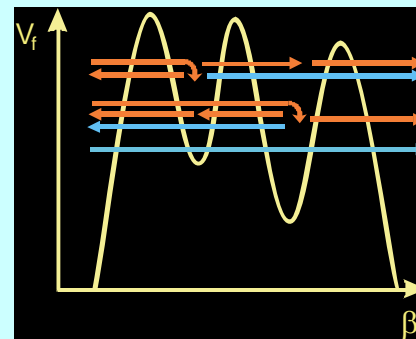
Triple vs Double humped barrier ?

M.J. López Jiménez et al. / Annals of Nuclear Energy 32 (2005) 195–213



Improved fission modelling

Fission mechanisms



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

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

M. Sin

Nuclear Physics Department, Bucharest University, Bucharest-Magurele, Romania

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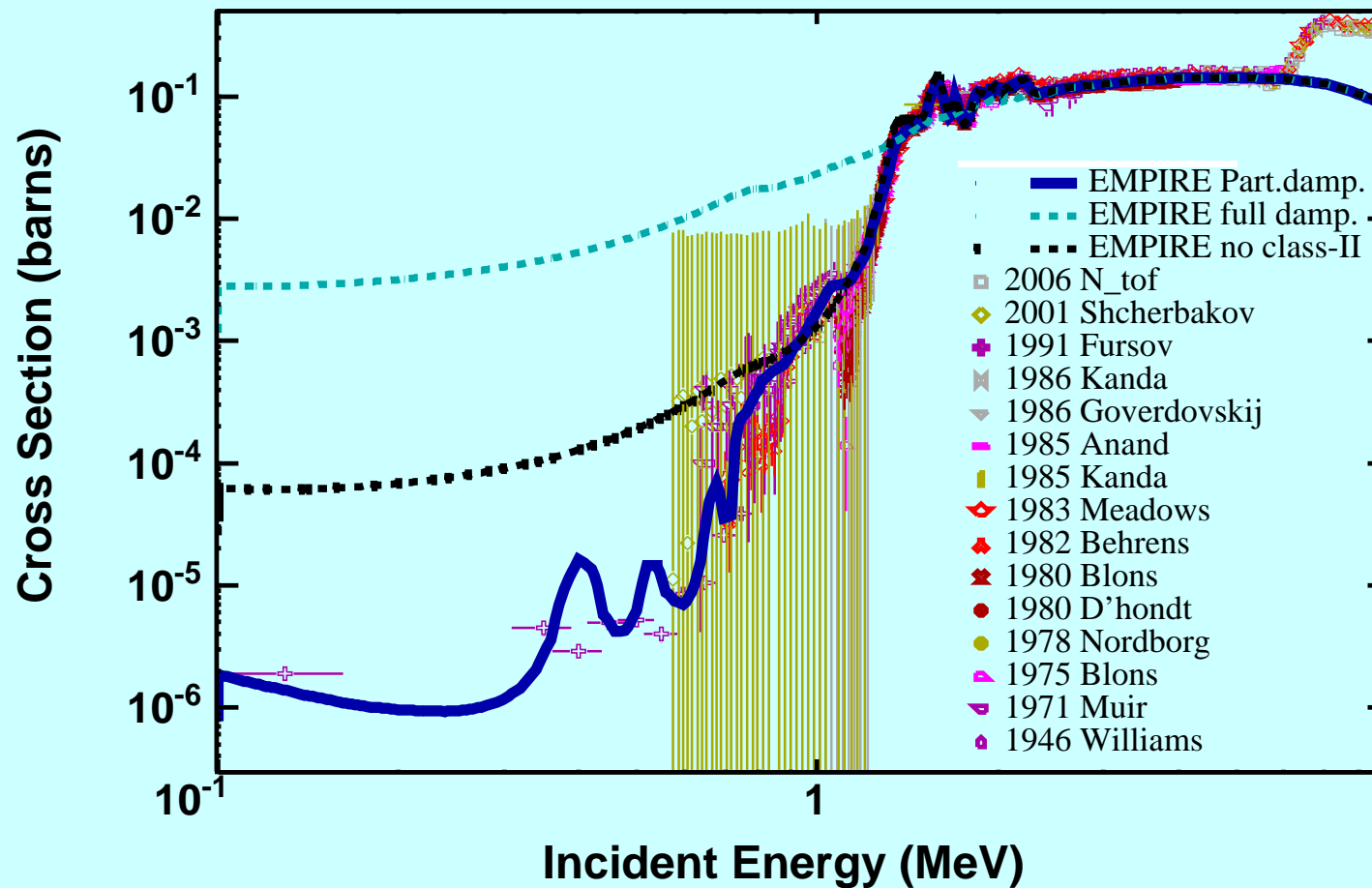
A fission formalism which describes transmission and absorption through multiple humped barriers using a recursive method is proposed. Developed within the optical model for fission, it accounts for the fission mechanisms associated to the different degrees of damping of the vibrational states accommodated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



Improved fission modelling

Barriers + Wells (includes absorption)

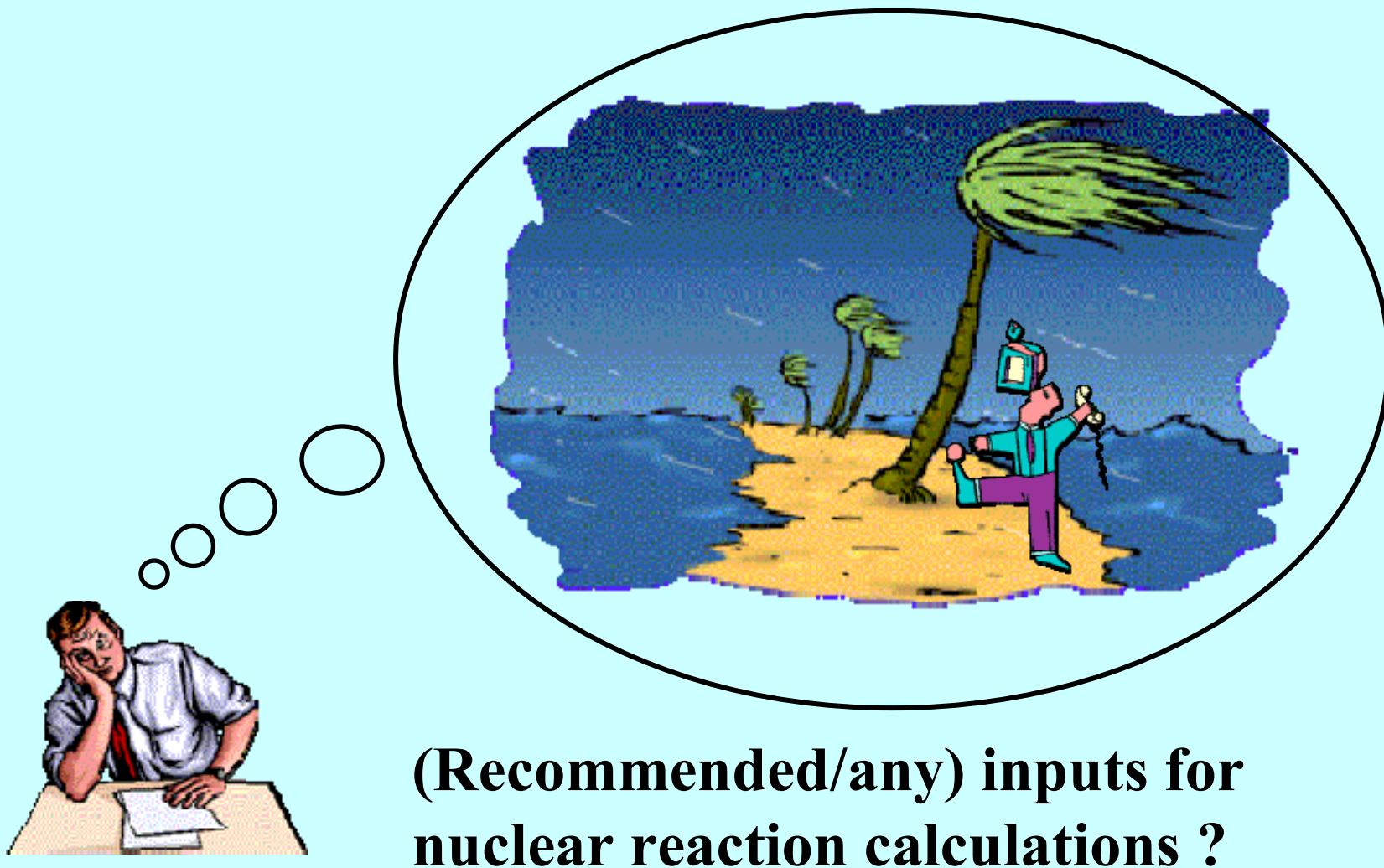
Full damping vs Partial damping.



RIPL



A long time ago before RIPL ...



**(Recommended/any) inputs for
nuclear reaction calculations ?**

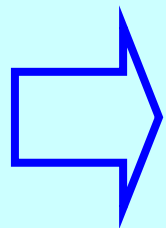


RIPL Background

- Nuclear reaction theory: sufficiently advanced to meet most of the requirements for a number of applications
- Major sources of uncertainty are the **input parameters** needed to perform theoretical calculations

RIPL Objective

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



Improved description of nuclear reactions, easier calculations allowing for a much better understanding

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IAEA Nuclear Data Section has addressed these needs through a series of Coordinated Research Projects dedicated to the production of a **Reference Input Parameter Library (RIPL)**

1993 – 2008

The longest running IAEA/NDS project

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RIPL-II and RIPL-III participants

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RIPL-III participants

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Reference Input Parameter Library

Electronic Starter File (known as Reference Input Parameter Library-1) was developed and made available to users throughout the world in 1997 (**compilation**)

- 1994-1997: RIPL-1 starter file (<http://www-nds.iaea.org/ripl/>)

Second CRP was initiated on “*Nuclear Model Parameter Testing for Nuclear Data Evaluation (Reference Input Parameter Library: Phase II)*”, and completed in 2003. Revision, extension and validation of the original RIPL-1 Starter File to produce a consistent RIPL-2 library of **recommended** input parameters.

- 1998-2003: RIPL-2 database (<http://www-nds.iaea.org/RIPL-2/>)

Main goal: Energy applications, $E < 20\text{MeV}$

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RIPL-3 additional requirements

- Reactions at high energies for ADS (up to 150 MeV), production of medical radioisotopes (up to 100 MeV) and radiotherapy (up to 250 MeV)
- Reactions on nuclei far from stability for ADS and astrophysics
- Charged-particle reactions for all non-energy applications
- Number of simple routines for the calculation of basic input data from the parameters contained in the library will be provided to reduce a risk of misusing the parameters

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Reference Input Parameter Library

Third (and final) CRP: “Parameters for Calculation of Nuclear Reactions of Relevance to Non-Energy Nuclear Application (Reference Input Parameter Library: Phase III)” started in 2003. The project is close to completion. The update of the RIPL-2 database will be released in September 2008.

2003-2008: RIPL-3 database (<http://www-nds.iaea.org/RIPL-3/>)

No	Directory	Contents
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1	MASSES	Atomic Masses and Deformations
2	LEVELS	Discrete Level Schemes
3	RESONANCES	Average Neutron Resonance Parameters
4	OPTICAL	Optical Model Parameters
5	DENSITIES	Level Densities (Total, Partial)
6	GAMMA	Gamma-Ray Strength Functions
7	FISSION	Fission Barriers and Level Densities

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RIPL: Nuclear Data Sheets 110 (2009)



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**Nuclear Data
Sheets**

Nuclear Data Sheets 110 (2009) ?? (accepted)

www.elsevier.com/locate/nds

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

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