NUCLEAR DATA EVALUATION METHODOLOGY INCLUDING ESTIMATES OF COVARIANCE

Roberto Capote

International Atomic Energy Agency, NAPC - Nuclear Data Section

OUTLINE

- Overview of Nuclear Data Evaluation Methods
- Selection of experimental data and EXFOR
- Experimental uncertainties and correlations
- Modelling uncertainties
  - Model defects
  - Model parameters
- Evaluation based on GLSQ
- (UMC formulation)
- (UMC+TMC)

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

What is Nuclear (Reaction) Data Evaluation?

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

Bayesian approaches:

- ❑ “Non-model” GLSQ fit: standards
- ❑ Model prior + GLSQ fit

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Nuclear Data Evaluation

Evaluated cross sections and covariance matrices

Experimental Input

Inter and -intra experiment correlations

Experimental cross sections

Prior Knowledge

Model Defects

Parameter Uncertainties

Model cross sections

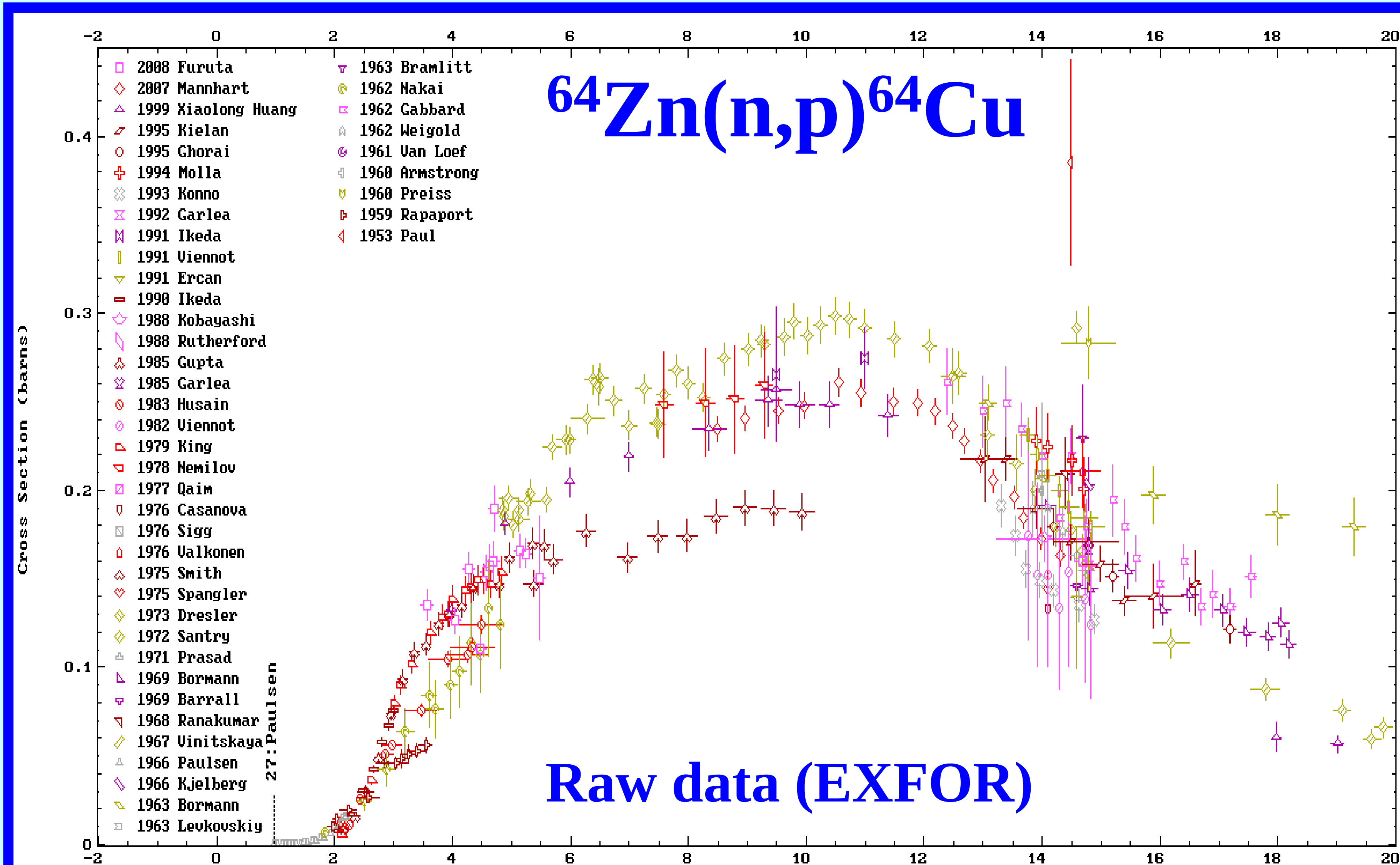
From D. Neudecker, S. Gundacker, H. Leeb *et al.*, ND2010, Jeju Isl., Korea

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Experimental uncertainties

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

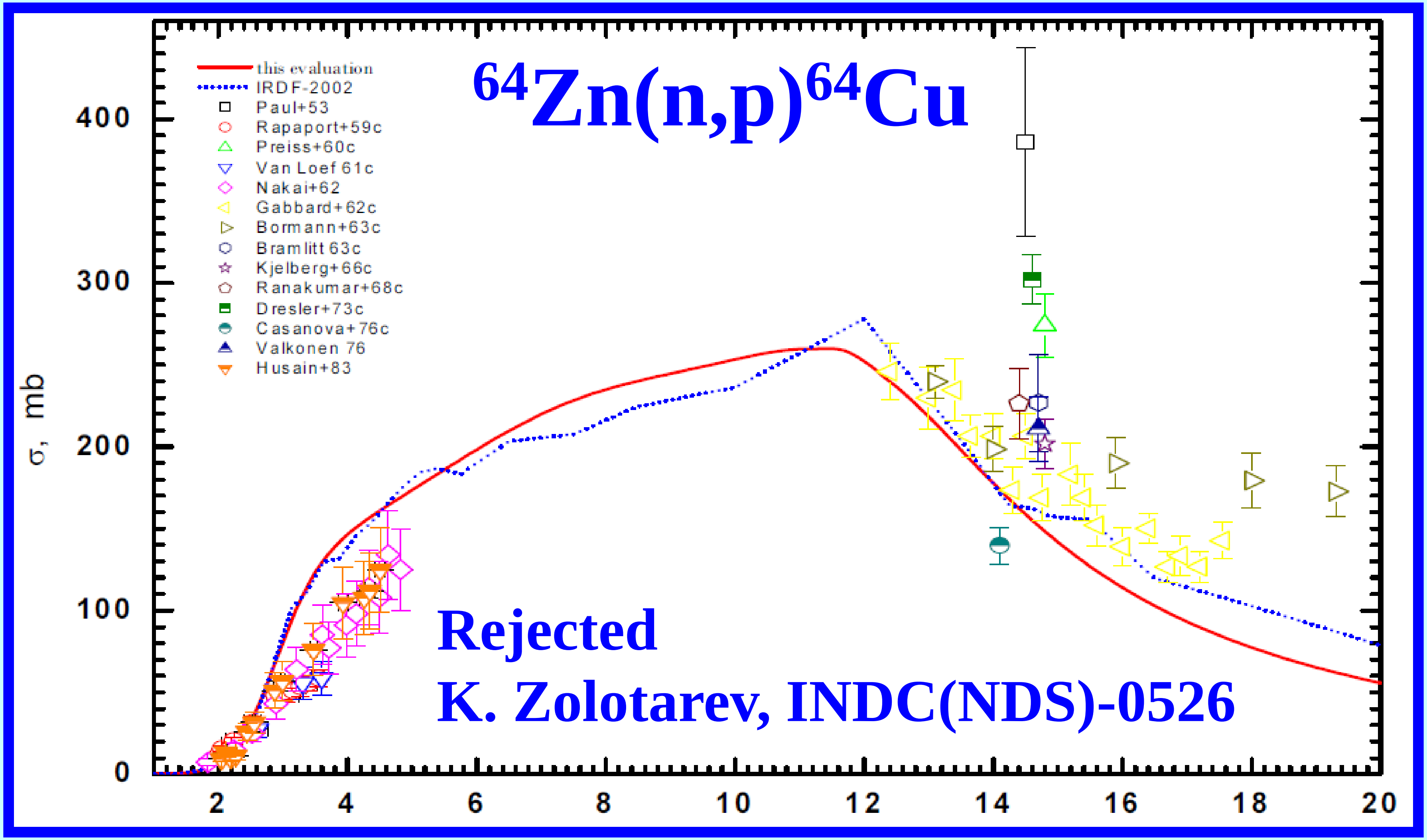
Selection of experimental data (1)



1st RCM, IAEA CRP on Nuclear Data for charged-particle monitor reactions …", 3-7 December 2012, Vienna, Austria

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

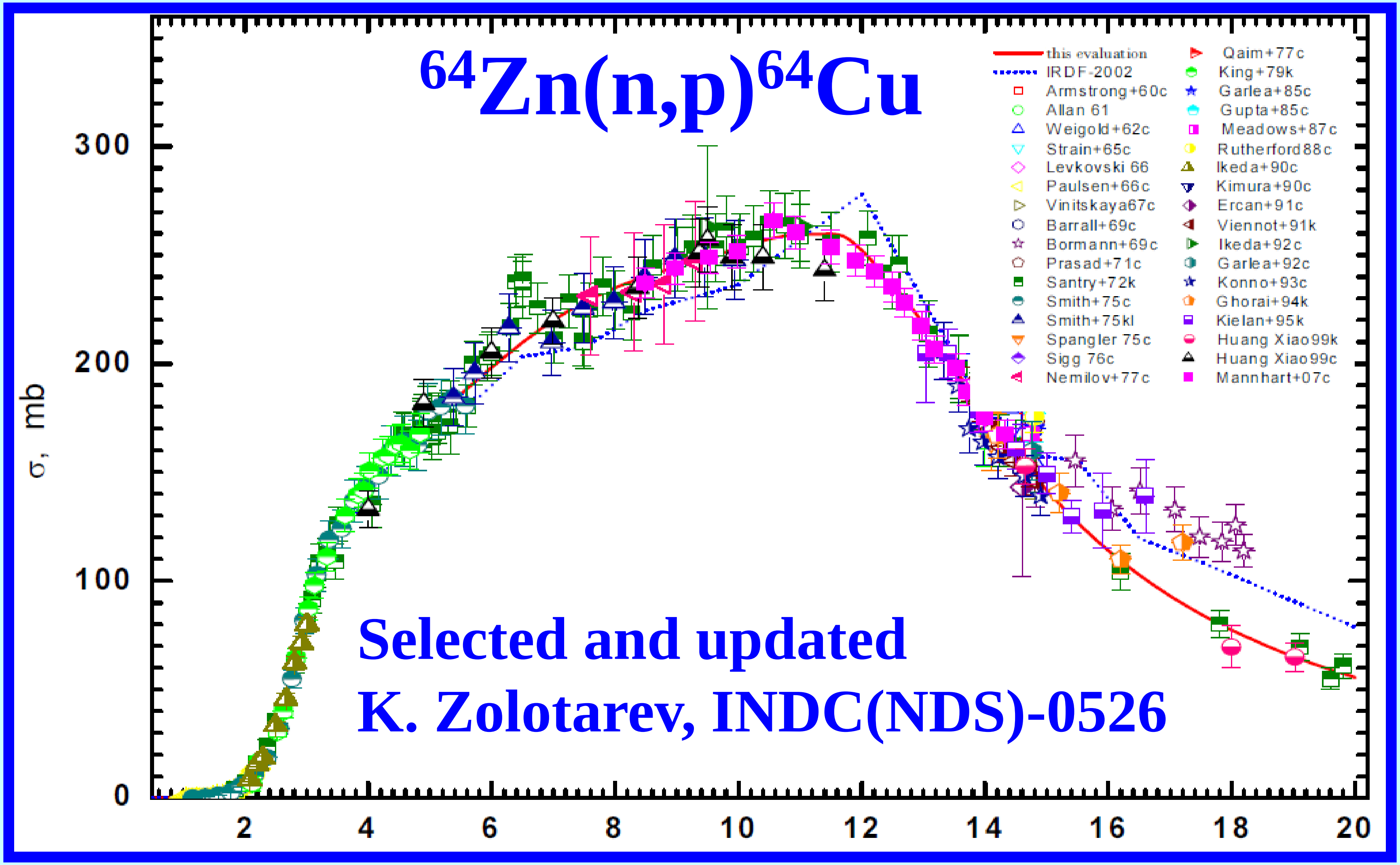
Selection of experimental data (2)



http://www-nds.iaea.org/reports-new/indc-reports/indc-nds/indc-nds-0526.pdf

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Selection of experimental data (3)



http://www-nds.iaea.org/reports-new/indc-reports/indc-nds/indc-nds-0526.pdf

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Experimental correlations

"Evaluation of measurement data - Guide to the expression of uncertainty in measurement"

Joint Committee for Guides in Metrology,

JCGM 100:2008, www.bipm.org (2008)

- Intra experiments correlations:
  Short and long term correlations within a single experiment can and should be estimated
  (statistical and systematic uncertainty)
- Inter-experiments correlations
  (very often neglected, default zero !!!)

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Experimental uncertainties

JRC
EUROPEAN COMMISSION

Activation reporting

ICTP-IAEA 10 and 11 May 2010

Energy (MeV)	σ_{Am} (mb)	Unc. (%)	Correlation matrix (x100)								
8.34(15)	96.8	6.5	100								
9.15(15)	162.9	5.7	35	100							
13.33(15)	241.8	4.6	37	42	100						
16.10(15)	152.4	4.6	38	43	53	100					
17.16 (3)	116.1	4.4	40	45	57	58	100				
17.90(10)	105.7	4.4	41	45	57	59	84	100			
19.36(15)	89.5	8.2	21	24	30	31	39	39	100		
19.95 (7)	102.1	5.8	30	34	44	45	58	59	51	100	
20.61 (4)	77.9	8.8	20	22	29	30	40	42	39	65	100

A. Plompen, ND workshop, ICTP, Trieste 2010

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Model uncertainties

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Model parameter uncertainties

D.L. Smith, "Covariance Matrices for Nuclear Cross-Sections Derived from Nuclear Model Calculations". Report **ANL/NDM-159**, Argonne National Laboratory, 2005

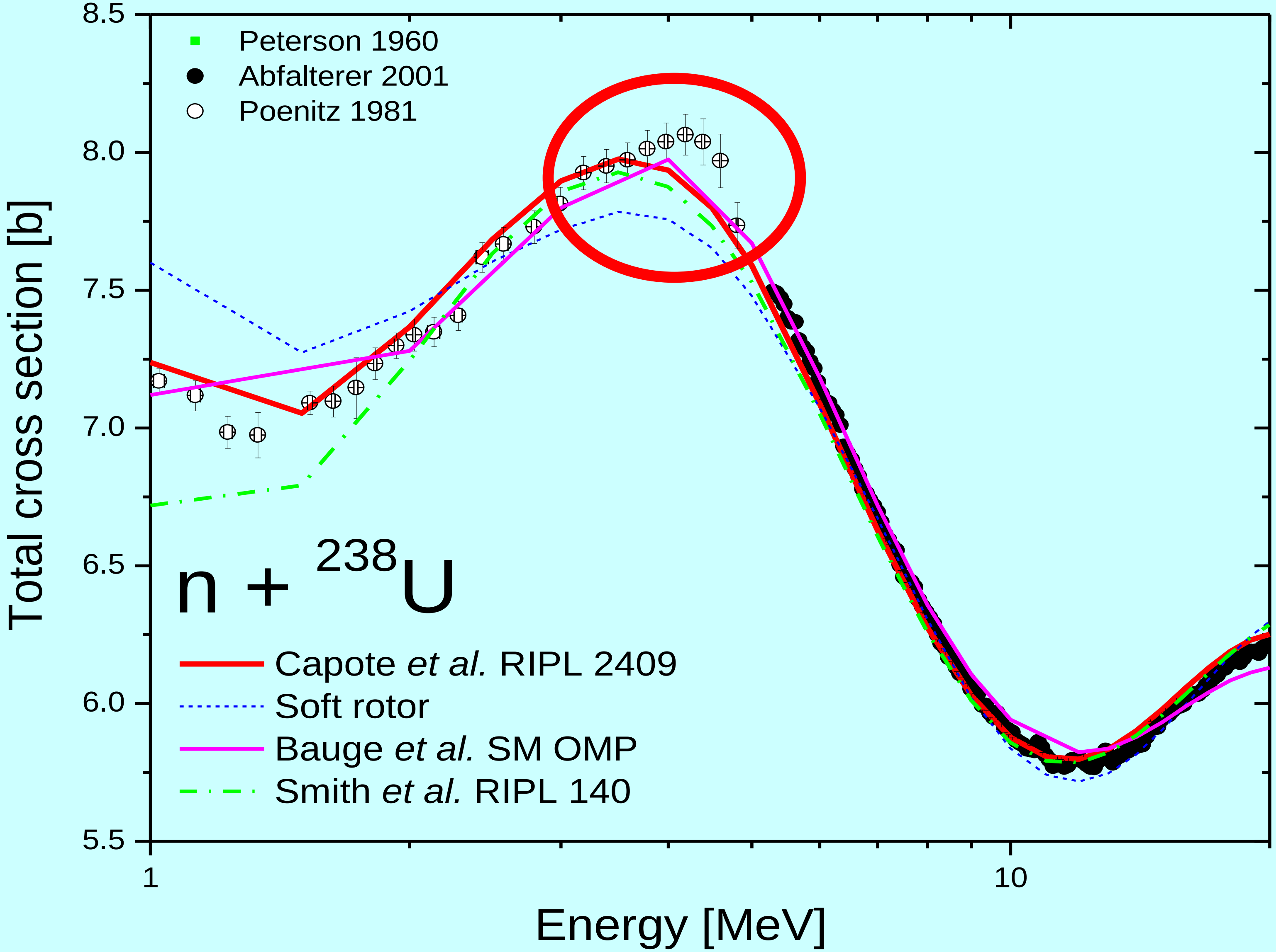
$$\overline{\sigma}_i = \frac{1}{K}\sum_{k=1}^{K}\sigma_{ik} \qquad V_{ij} = \overline{\sigma_i \sigma_j} - \overline{\sigma}_i \times \overline{\sigma}_j$$

i,*j* - energy indexes

Monte Carlo calculation of covariance first tested by A. Koning

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Model defects



EMPIRE code & RIPL database

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 110 (2009) 3107–3214

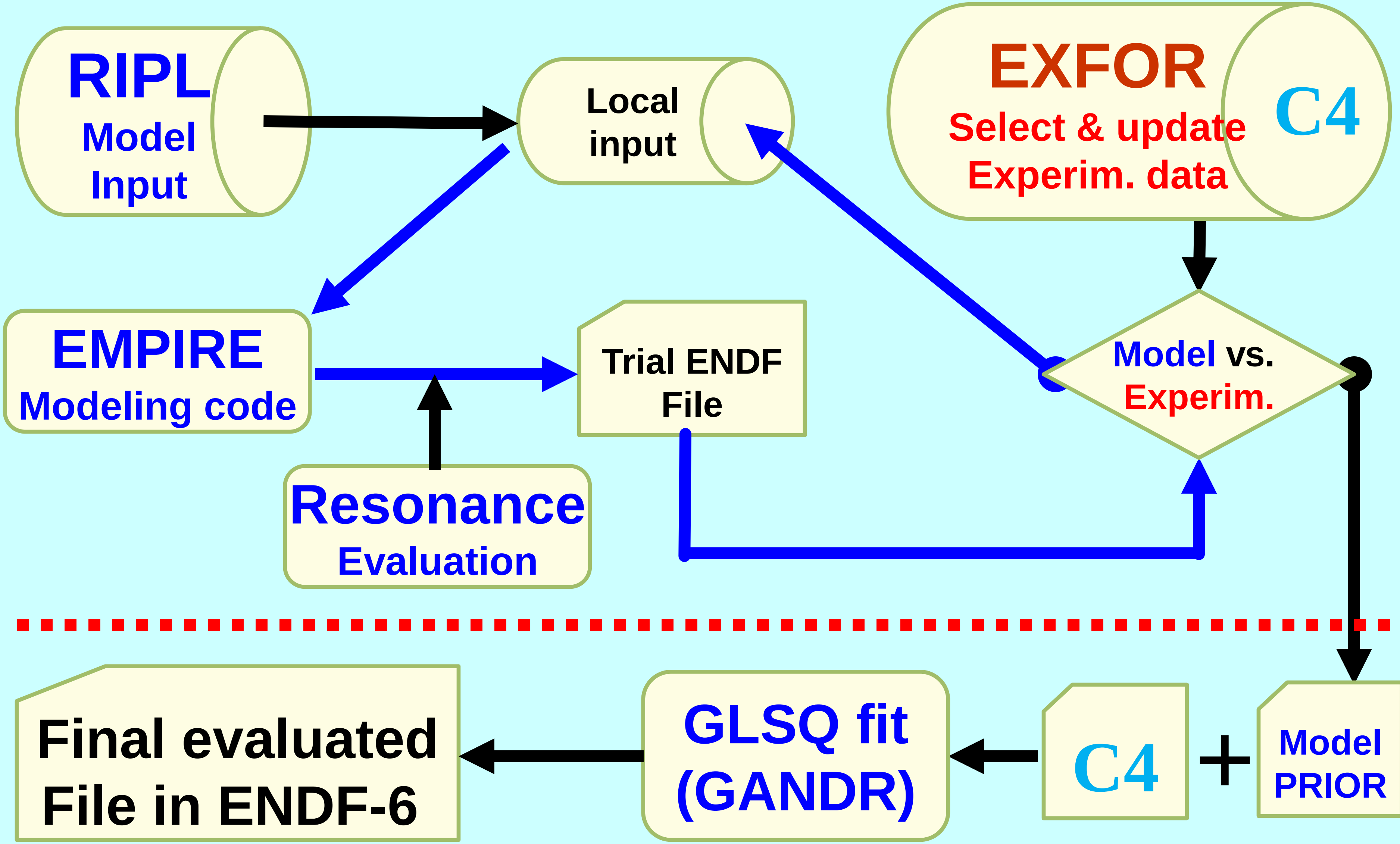
Nuclear Data Sheets

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. Belgya,[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. Talou[3]

Nuclear Data Evaluation process



Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Evaluation – fast energy range

- Use 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

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Evaluation methods

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Model prior +GLSQ fit

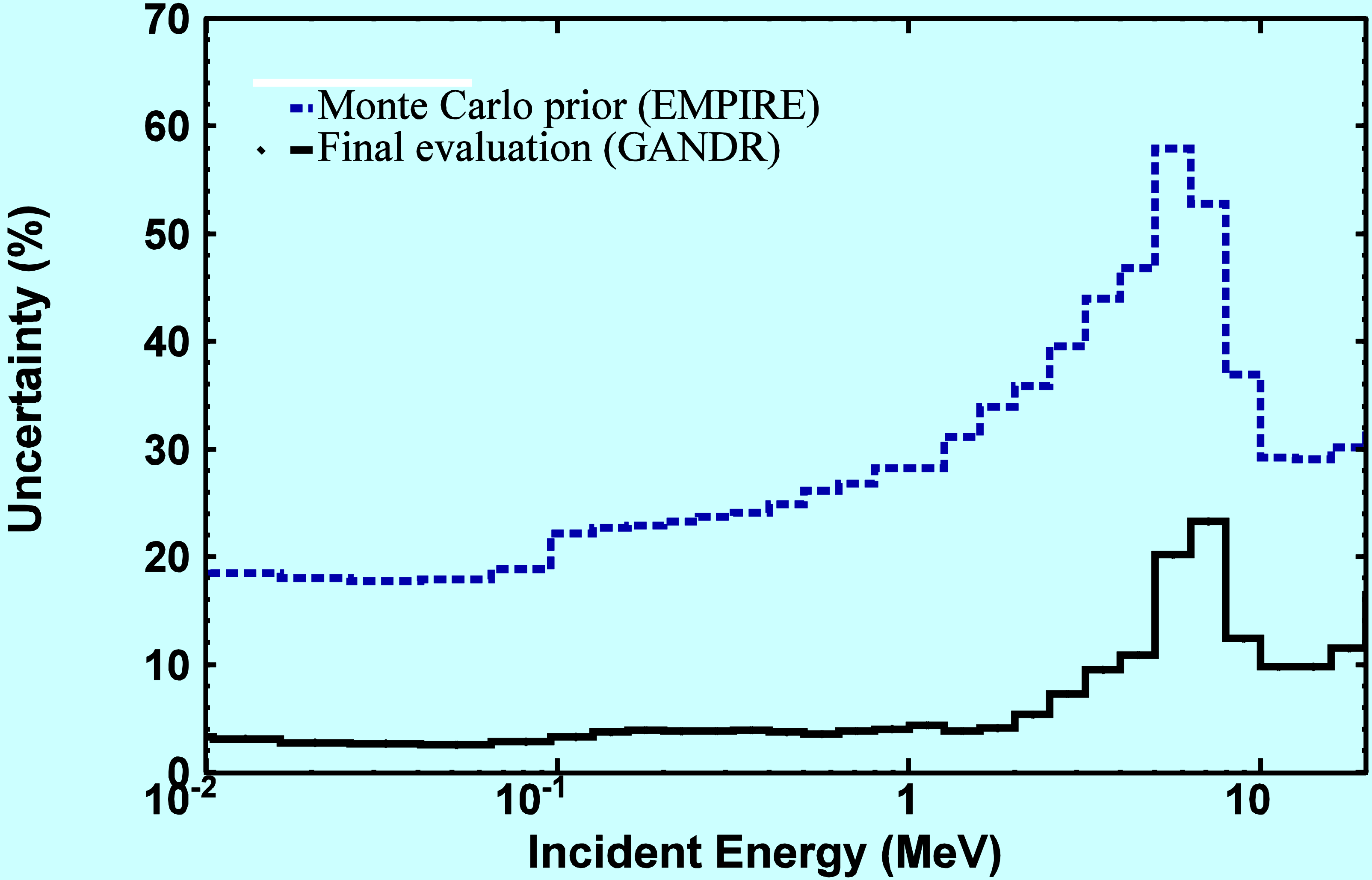
Monte Carlo prior (model) + *GANDR* (*GLSQ*)

A. Trkov and R. Capote, "Cross-Section Covariance Data", Th-232 evaluation for ENDF/B-VII.0 (MAT=9040 MF=1 MT=451); Pa-231 and Pa-233 evaluations for ENDF/B-VII.0 (MAT=9133 and 9137 MF=1 MT=451), National Nuclear Data Center, BNL (http://www.nndc.bnl.gov), 15 December 2006.

D.W. Muir, ***GANDR*** *project (IAEA)*, Online at www-nds.iaea.org/gandr/.

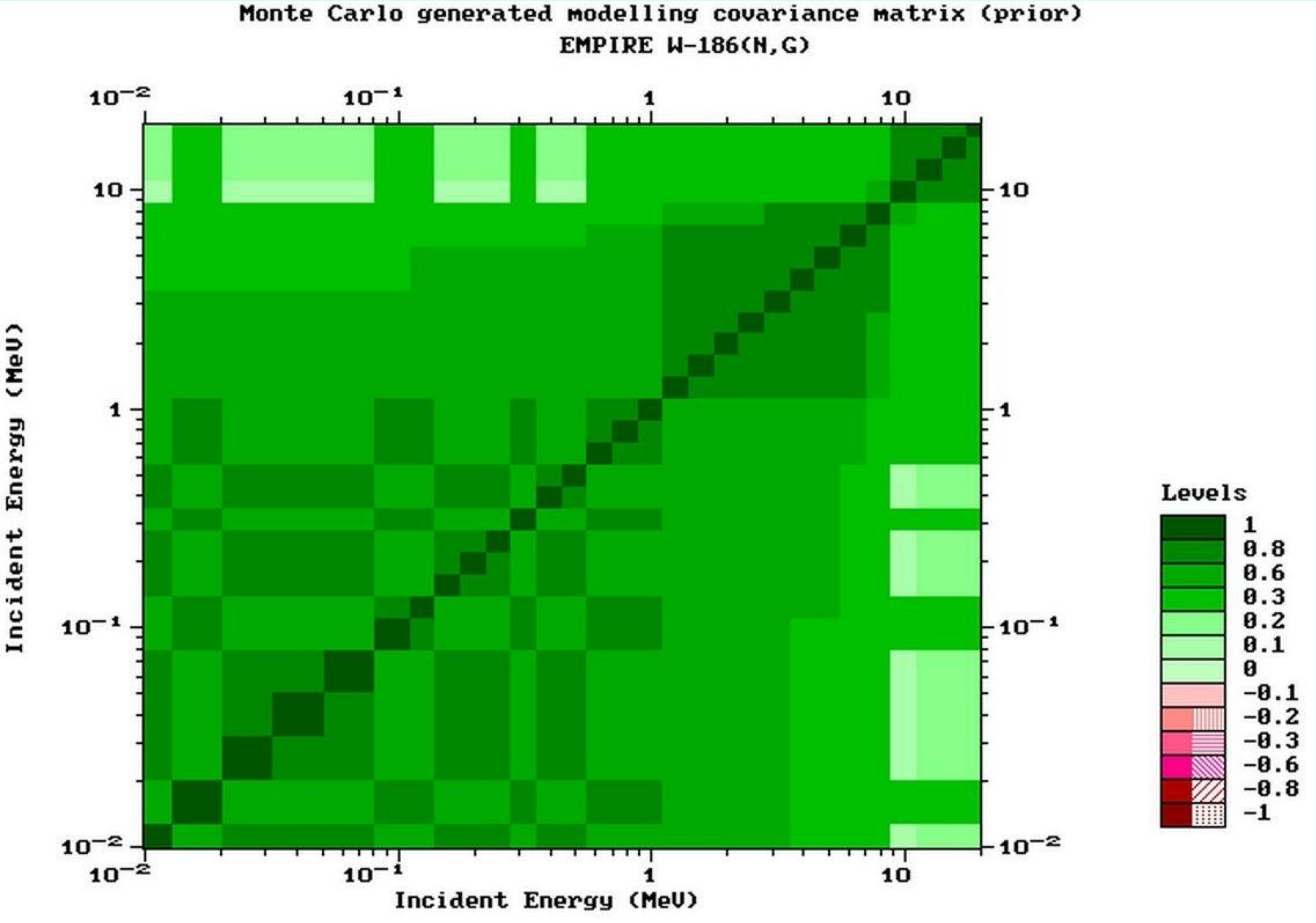
Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Uncertainties – model *vs* evaluated



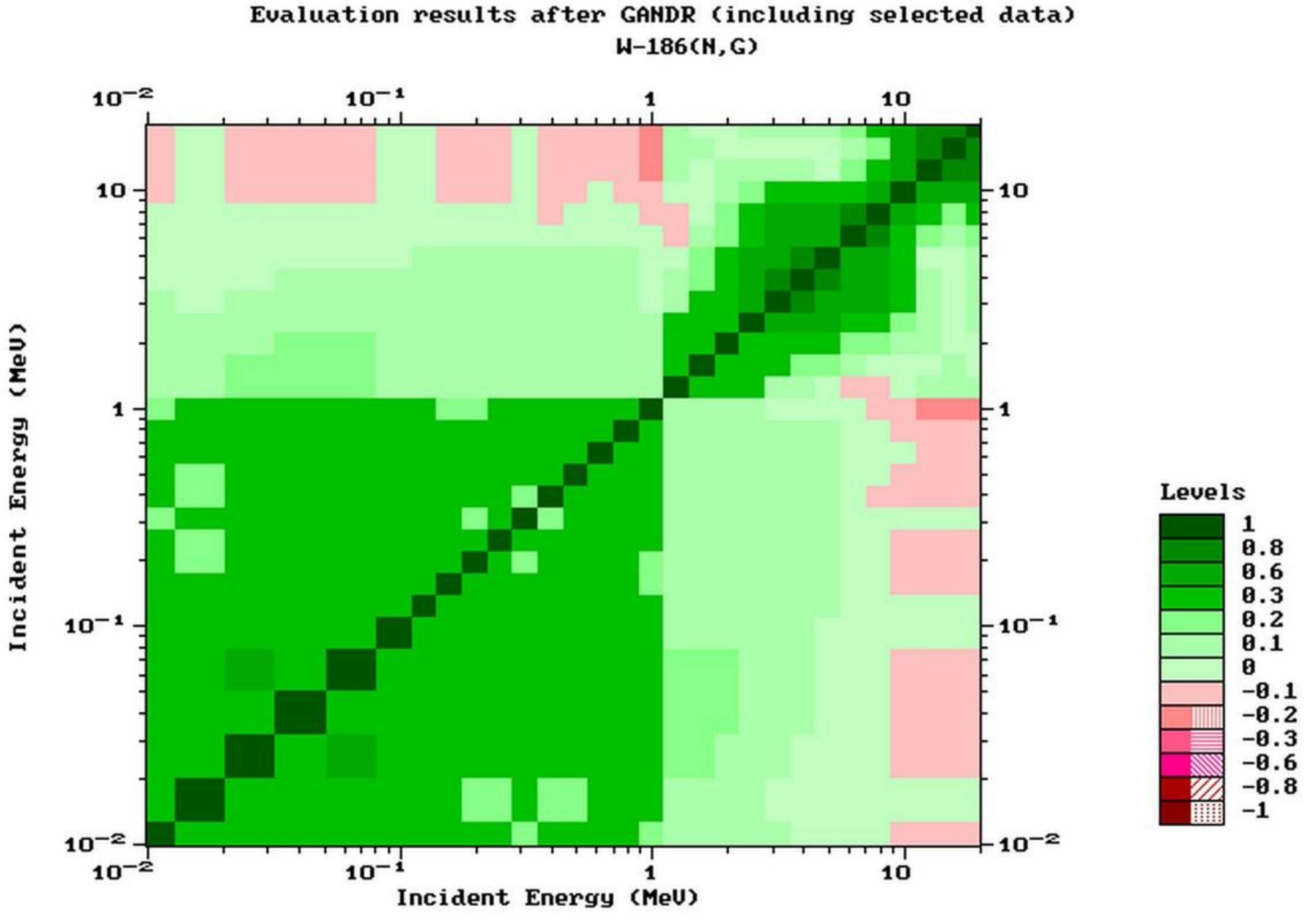
Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Model prior correlations



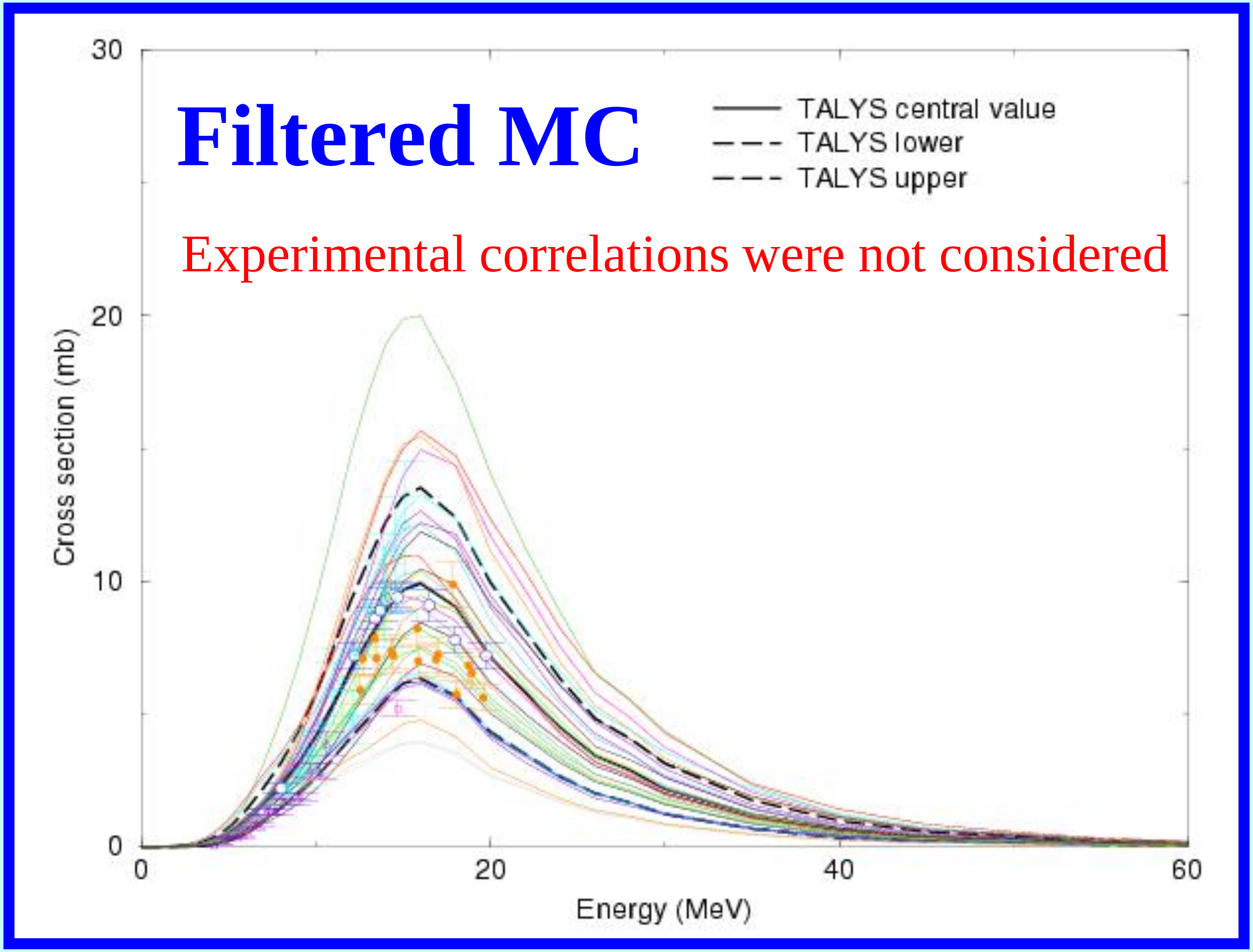
Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Final evaluation correlations



Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Koning & Rochman approach: TENDL



Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Take home message

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

Bayesian approaches

- ❑ "Non-model" GLSQ fit (e.g. standards & monitor reactions)
- ❑ Model prior + GLSQ fit (incomplete exp. database)
- ❑ FMC (TENDL)

Experimental data and uncertainty analysis

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Unified Monte Carlo (UMC)

D.L. Smith, "A Unified Monte Carlo Approach to Fast Neutron Cross Section Data Evaluation," *Proceedings of the 8th International Topical Meeting on Nuclear Applications and Utilization of Accelerators*, Pocatello, July 29 – August 2, 2007, p. 736.

BAYES THEOREM & PRINCIPLE OF MAXIMUM ENTROPY

$$p(\boldsymbol{\sigma}) = \mathrm{C} \times \mathscr{L}(\mathbf{y}_{\mathrm{E}},\mathbf{V}_{\mathrm{E}} \mid \boldsymbol{\sigma}) \times p_0(\boldsymbol{\sigma} \mid \boldsymbol{\sigma}_{\mathrm{C}},\mathbf{V}_{\mathrm{C}})$$

$$p_0(\sigma \mid \sigma_C,V_C) \sim \exp\{-(½)[(\sigma-\sigma_C)^T \bullet (V_C)^{-1} \bullet (\sigma-\sigma_C)]\}$$

$$\mathscr{L}(y_E,V_E \mid \sigma) \sim \exp\{-(½)[(y-y_E)^T \bullet (V_E)^{-1} \bullet (y-y_E)]\},\ y=f(\sigma)$$

y_E, V_E: measured quantities with "n" elements

y_C, V_C: calculated using nuclear models with "m" elements

UMC based on p(σ), GLS on the peak of the distribution

1st RCM, IAEA CRP on Nuclear Data for charged-particle monitor reactions …", 3-7 December 2012, Vienna, Austria

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

Total Monte Carlo (TMC)

- Propagating covariance data is an approximation of true uncertainty propagation (especially regarding ENDF-6 format limitations)
- Covariance data requires extra processing and "satellite software" for application codes
- Alternative: Create an ENDF-6 file for each random sample and finish the entire physics-to-application loop.

Koning and Rochman, Ann Nuc En **35**, 2024 (2008)

Experimental data was included via Filtered MC

Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org

TMC+UMC

- MC model uncertainties (param + model defects)
- Experimental uncertainties and correlations
- Uses **UMC** **(instead of FMC)** to produce samples according to the combined "a posteriori" PDF
- Create an ENDF-6 file for each random sample and finish the entire physics-to-application loop (**TMC**).

  Koning and Rochman, Ann Nuc En **35**, 2024 (2008)

UMC could be also used to produce covariance matrix to be stored in ENDF format (approximate treatment)

1st RCM, IAEA CRP on Nuclear Data for charged-particle monitor reactions …", 3-7 December 2012, Vienna, Austria
Roberto Capote, IAEA NAPC/NDS
R.CapoteNoy@iaea.org