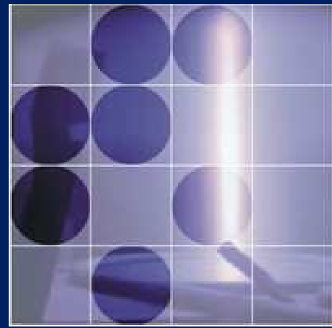
NUCLEAR DATA EVALUATION METHODOLOGY INCLUDING ESTIMATES OF COVARIANCE



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OUTLINE

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

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Definition of (ND) Evaluation

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

Bayesian approaches:

- ❑ "Non-model" GLSQ fit: standards
- ❑ Model prior + GLSQ fit

EFNUDAT workshop
Paris, France, 25-27 May 2010
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Nuclear Data Evaluation

Evaluated cross sections and covariance matrices

<u>Experimental Input</u>

Inter and -intra experiment correlations

Experimental cross sections

<u>Prior Knowledge</u>

Model Defects

Parameter Uncertainties

Model cross sections

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

Experimental uncertainties

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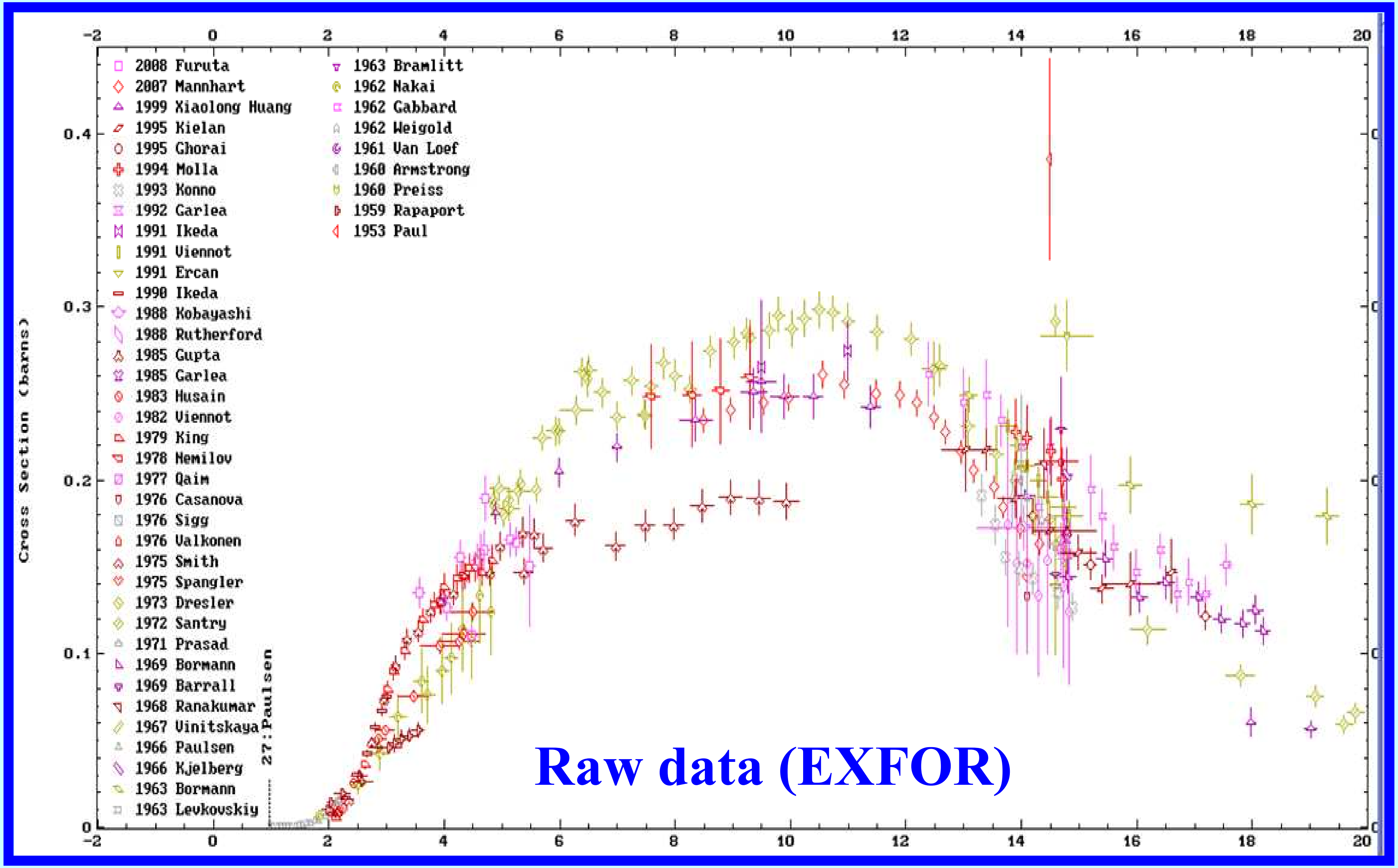
Selection of experimental data (1)



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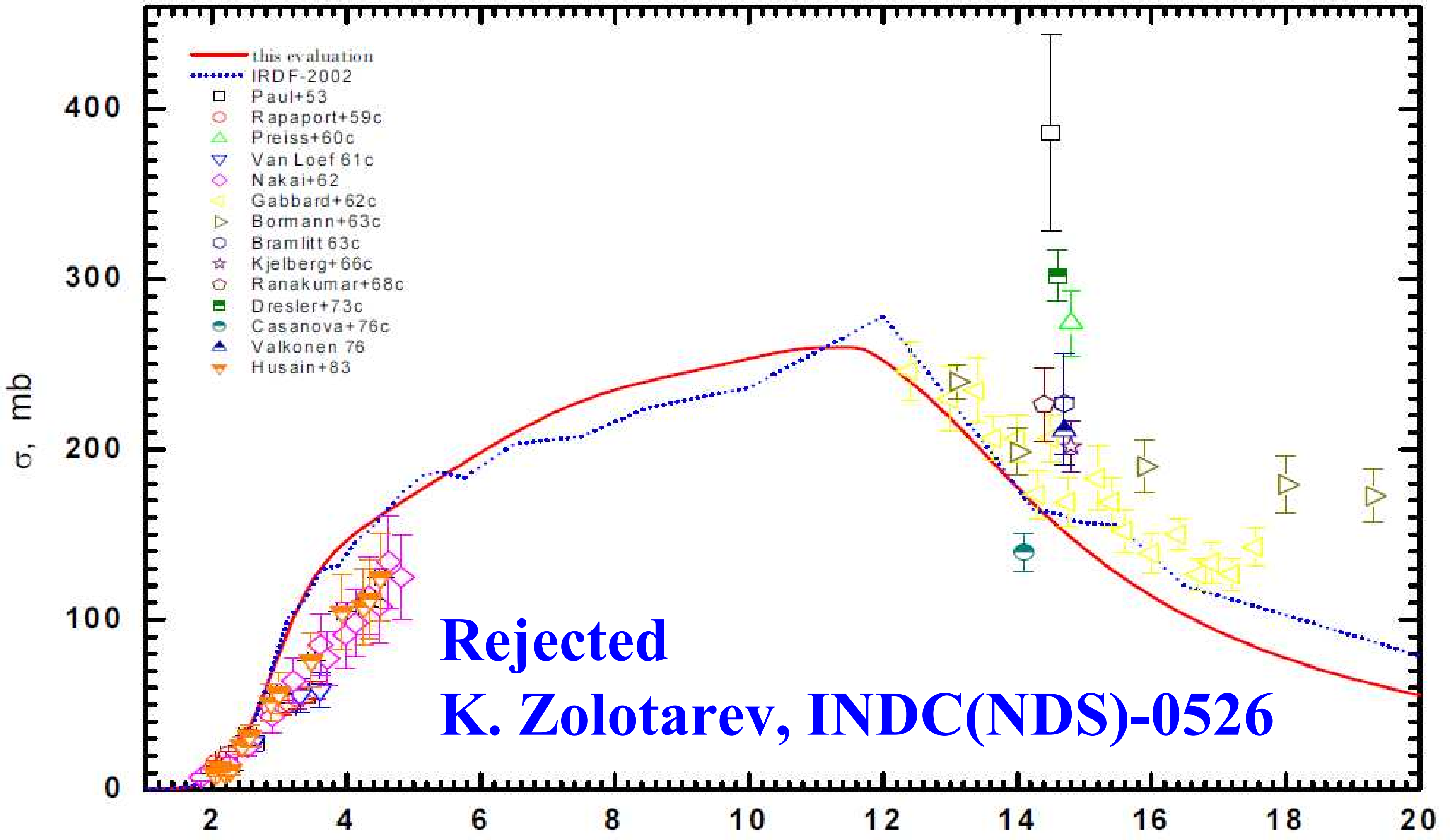
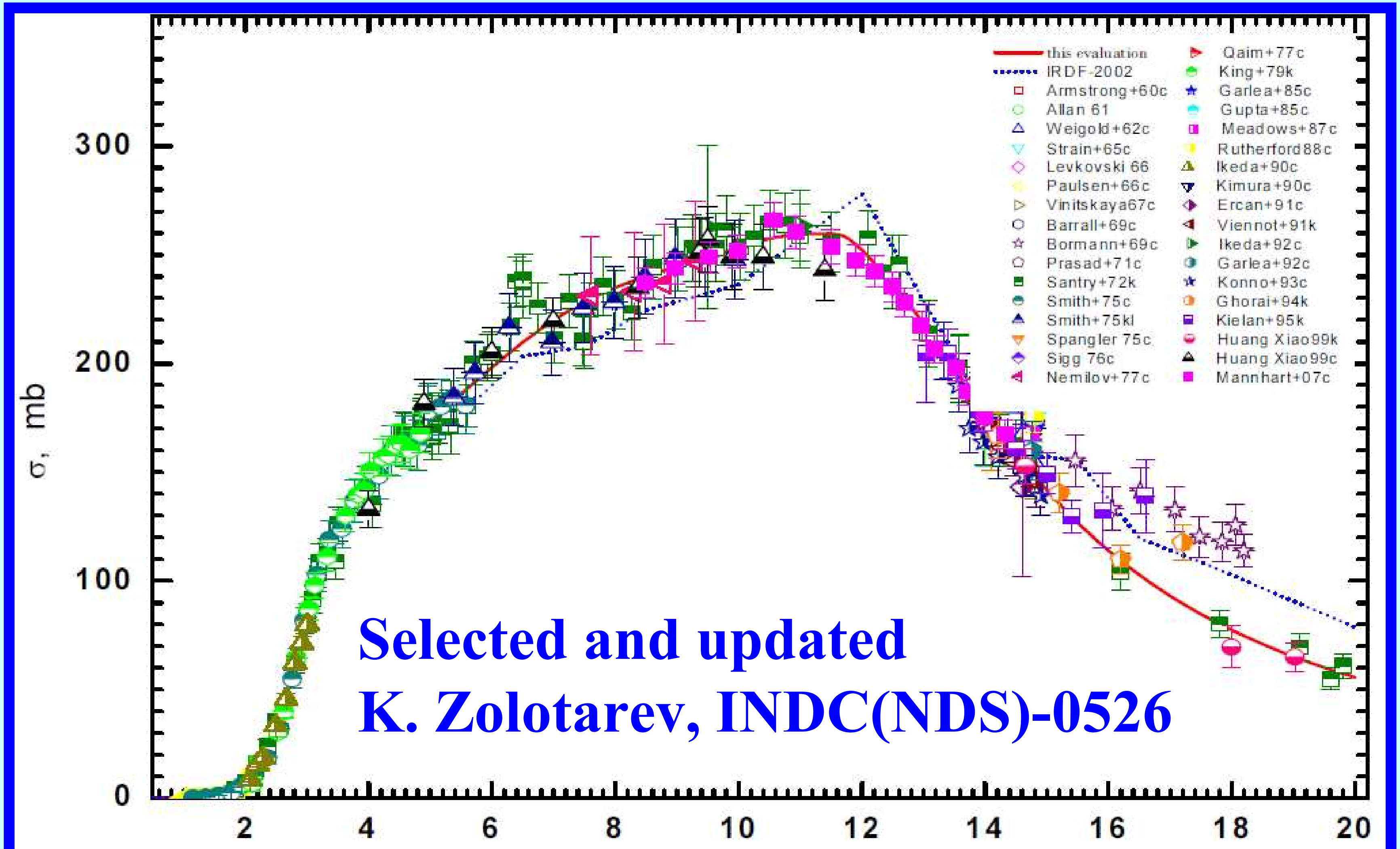
Selection of experimental data (2)



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

Selection of experimental data (3)



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

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 !!!)

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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

Model uncertainties

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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

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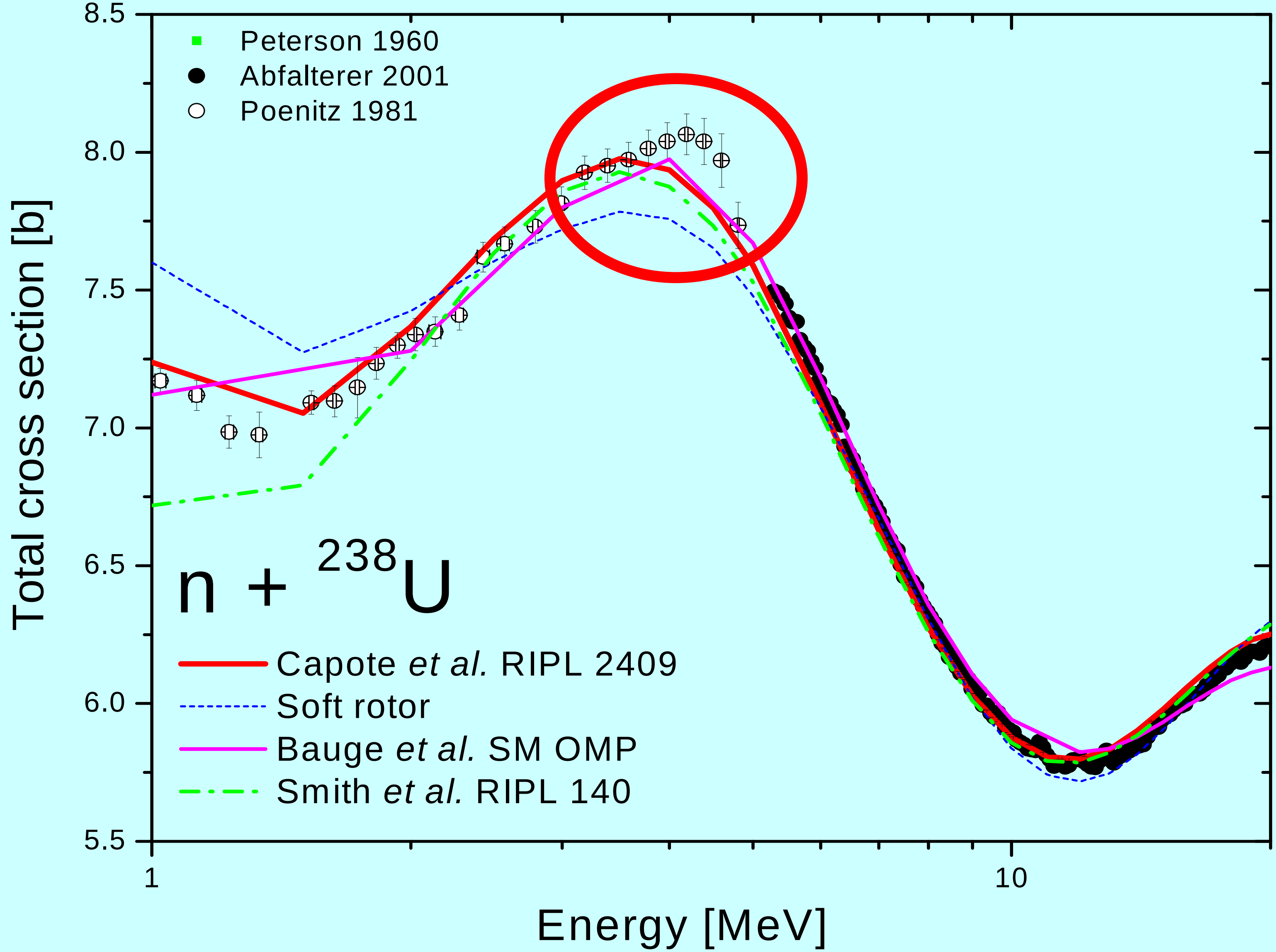
Model defects



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Evaluation methods

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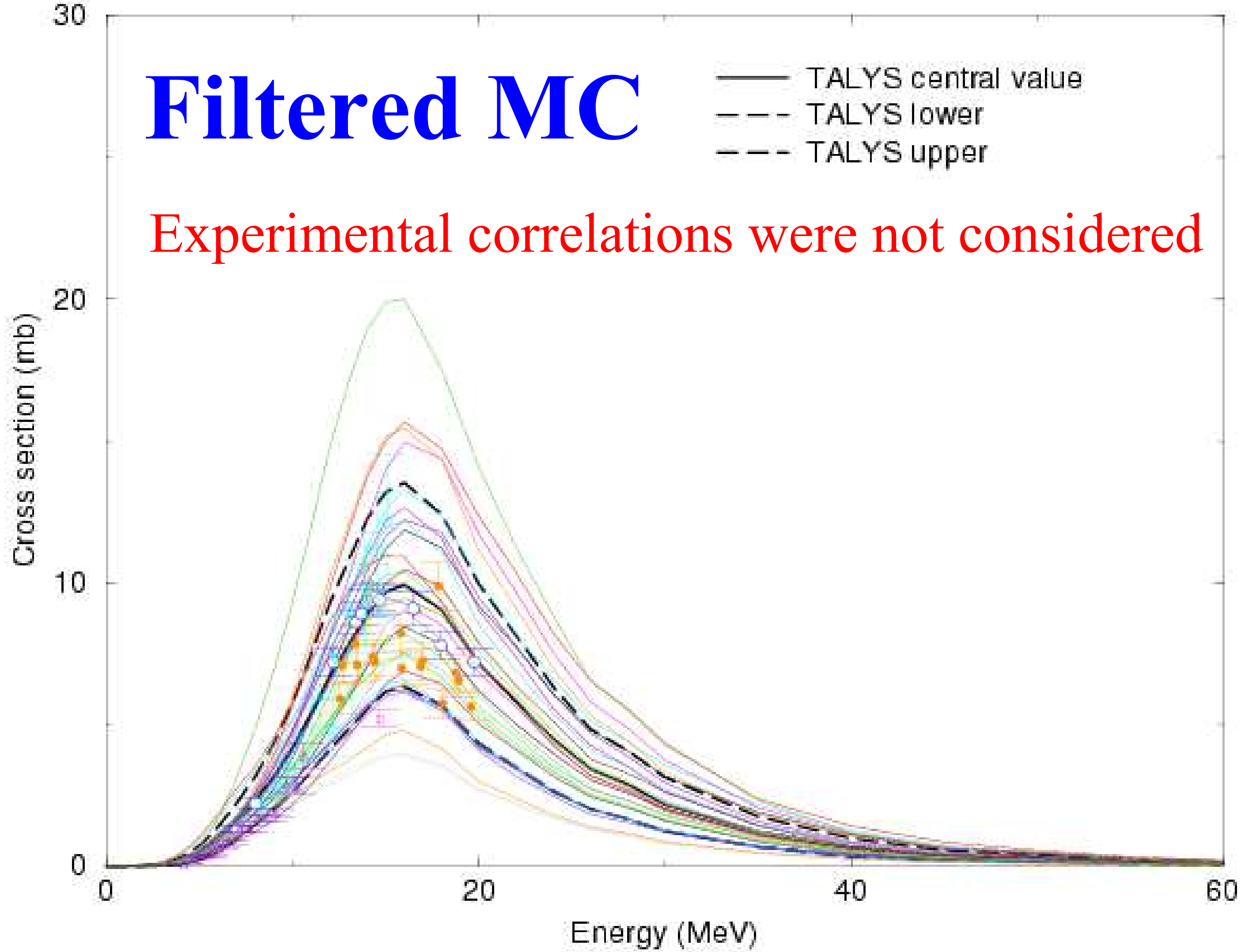
Model prior +GLSQ fit

Monte Carlo prior
+
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/.

Koning & Rochman approach: TENDL



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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

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

$$p_0(\boldsymbol{\sigma} \mid \boldsymbol{\sigma}_C, \mathrm{V}_C) \sim \exp\{-(½)[(\boldsymbol{\sigma}-\boldsymbol{\sigma}_C)^T \bullet (\mathrm{V}_C)^{-1} \bullet (\boldsymbol{\sigma}-\boldsymbol{\sigma}_C)]\}$$

$$\mathscr{L}(\mathrm{y}_E, \mathrm{V}_E \mid \boldsymbol{\sigma}) \sim \exp\{-(½)[(\mathrm{y}-\mathrm{y}_E)^T \bullet (\mathrm{V}_E)^{-1} \bullet (\mathrm{y}-\mathrm{y}_E)]\}, \; \mathrm{y}=f(\boldsymbol{\sigma})$$

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

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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

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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)

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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 (standards)
- Model prior + GLSQ fit (working horse)
- FMC (TENDL) ⇒ UMC(TENDL)
- TMC
- TMC + UMC (golden reference)

Experimental data and uncertainty analysis

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