NUCLEAR DATA EVALUATION METHODOLOGY INCLUDING ESTIMATES OF COVARIANCE

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Thanks to my collaborators

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OUTLINE

- Overview of (Nuclear) Data Evaluation Methods
- Selection of experimental data
- Experimental uncertainties and correlations (covered by N. Otsuka)
- Modelling uncertainties
  - Model defects
  - Model parameters
- Evaluation methods: GLSQ & UMC

BAYES THEOREM (1763)

\[ p(\sigma) = C \times \mathcal{L}(y_E, V_E \mid \sigma) \times p_0(\sigma \mid \sigma_C, V_C) \]
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
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

Unified Monte Carlo

From D. Neudecker, S. Gundacker, H. Leeb et al., ND2010, Jeju Isl., Korea
Experimental uncertainties
Selection of experimental data (1)

Raw data (EXFOR)
Selection of experimental data (3)

Selected and updated
K. Zolotarev, INDC(NDS)-0526

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 !!!)*
Model uncertainties
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

\[
\bar{\sigma}_i = \frac{1}{K} \sum_{k=1}^{K} \sigma_{ik} \quad V_{ij} = \sigma_i \sigma_j - \bar{\sigma}_i \times \bar{\sigma}_j \quad i, j - \text{indexes}
\]

Monte Carlo calculation of covariance first tested by A. Koning
Model defects

\[ \text{n} + ^{238}\text{U} \]

Total cross section [b] vs. Energy [MeV]

- Peterson 1960
- Abfalterer 2001
- Poenitz 1981
- Capote et al. RIPL 2409
- Soft rotor
- Bauge et al. SM OMP
- Smith et al. RIPL 140

Data Centres Network Network Meeting, IAEA HQ, Vienna, Austria, 4-6 Sept. 2013

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Evaluation methods
“Non model” GLSQ fit : STDs

U-235(n,f) STD

Incident Energy (MeV)
Typical situation (see above 21 MeV)
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

\[
\overline{\sigma_i} = \frac{1}{K} \sum_{k=1}^{K} \sigma_{ik} \quad V_{ij} = \sigma_i \sigma_j - \overline{\sigma_i} \times \overline{\sigma_j} \quad i, j - energy indexes
\]

Monte Carlo calculation of covariance first tested by A. Koning

Monte Carlo prior

\[ GANDR \ (GLS) \]

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

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.
Uncertainty (%) vs Incident Energy (MeV)

- Monte Carlo prior (EMPIRE)
- Final evaluation (GANDR)
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 (1763) & PRINCIPLE OF MAXIMUM ENTROPY**

\[
p(\sigma) = C \times \mathcal{L}(y_E, V_E | \sigma) \times p_0(\sigma | \sigma_C, V_C)
\]

\[
p_0(\sigma | \sigma_C, V_C) \sim \exp\{-\frac{1}{2}[(\sigma - \sigma_C)^T \cdot (V_C)^{-1} \cdot (\sigma - \sigma_C)]\}
\]

\[
\mathcal{L}(y_E, V_E | \sigma) \sim \exp\{-\frac{1}{2}[(y - y_E)^T \cdot (V_E)^{-1} \cdot (y - y_E)]\}, \; y = f(\sigma)
\]

\(y_E, V_E\): measured quantities with “n” elements

\(y_C, V_C\): calculated using nuclear models with “m” elements

UMC based on \(p(\sigma)\), GLS on the peak of the distribution
Unified Monte Carlo (UMC-B)

1) MC modeling (EMPIRE, TALYS, CCONE, CoH,…) \( \{\sigma_i\} \)

2) For each random set \( \{\sigma_i\} \) we calculate \( \mathcal{L}(y_E, V_E | \sigma_i) \)

\[
\mathcal{L}(y_E, V_E | \sigma_i) = \exp\{ -\frac{1}{2} [(f(\sigma_i) - y_E)^T \cdot (V_E)^{-1} \cdot (f(\sigma_i) - y_E)] \}
\]

\[
\langle \tilde{\sigma} \rangle = \frac{\sum_{i=1}^{N} W_{\text{exp}}(\tilde{\sigma}_i) \tilde{\sigma}_i}{\sum_{i=1}^{N} W_{\text{exp}}(\tilde{\sigma}_i)}, \quad \text{cov}(\tilde{\sigma}_i, \tilde{\sigma}_j) = \langle \tilde{\sigma}_i \tilde{\sigma}_j \rangle
\]

OUTPUT: 1) \( \langle \tilde{\sigma} \rangle \), \( \text{cov}(\tilde{\sigma}_i, \tilde{\sigma}_j) = \langle \tilde{\sigma}_i \tilde{\sigma}_j \rangle \)

2) Stochastic set \( \{\sigma_i\} \) (e.g. to be used in TMC)
Selection of experimental data (1)

Raw data (EXFOR)

Incident Energy (MeV)

Cross Section (barns)

10^{-2}

10^{-3}

1978 Garg
1976 Le Rigoleur
1990 Gautam
1990 Gautam
1987 Trofimov
1987 Trofimov
1980 Magnusson
1979 Budnar
1977 Manjushree
1976 Schwerer
1974 Vuletin
1969 Dovbenko
1968 Stupegia
1968 Colditz
1967 Menlove
1967 Peto
1967 Csinkai
1967 Csinkai
1961 Stavisskiy
1959 Johnsrud
1959 Bostrom
1958 Leipunskiy
1958 Perkin
1949 Beghian
Selection of experimental data (2)

Accepted and renormalized

Cross Section (barns)

Incident Energy (MeV)

10^{-2}

10^{-3}

1978 Garg
1976 Le Rigoleur
1990 Gautam,*
1987 Trofimov*
1987 Trofimov*
1980 Magnusson,*
1979 Budnar
1976 Schwerer
1974 Vuletin,*
1969 Dovbenko,*
1968 Stupegia,*
1967 Peto
1967 Menlove,*
1967 Csikai,*
1961 Stavisskiy
1959 Bostrom,*
1958 Perkin,*
RIPL – Reference Input Parameter Library for Calculation of Nuclear Reactions and Nuclear Data Evaluations

R. Capote, M. Herman, P. Obložinský, P.G. Young, S. Goriely, T. Belgya, A.V. Ignatyuk, A.J. Koning, S. Hilaire, V.A. Plujko, M. Avrigeanu, O. Bersillon, M.B. Chadwick, T. Fukahori, Zhigang Ge, Yinlu Han, S. Kailas, J. Kopecky, V.M. Maslov, G. Reffo, M. Sin, E.Sh. Soukhovitskii, and P. Talou

EMPIRE: Nuclear Reaction Model Code System for Data Evaluation

M. Herman, R. Capote, B.V. Carlson, P. Obložinský, M. Sin, A. Trkov, H. Wienke, and V. Zerkin

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Available online at www.sciencedirect.com

Nuclear Data Sheets 108 (2009) 2655

www.elsevier.com/locate/nds
UMC vs GLSQ: a real evaluation

$^{55}\text{Mn}(n,\gamma)$

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Take home message

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

Bayesian approaches
- “Non-model” GLSQ fit (standards)
- Model prior + GLSQ fit (working horse)
- UMC (golden reference)

Experimental data and uncertainty analysis