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Finalise methodology studies to avoid compensation, to point out to systematic effects, etc.

Methodology studies: summary

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Outline

- Parameters/indices for assessing adjustments
- Premises for valid adjustments
- Assessment of adjustments
- Compensation effects
- Avoiding compensation effects
- Use of “a posteriori” covariance matrix
- Appendix
  - Common nomenclature
  - Adjustment formulas

Parameters for Assessing Adjustments

- Representativity factor between two experiments, E and E' (= correlation factor):

$$f_{EE'} \equiv \frac{(S_{E'} M_\sigma S_E^T)}{[(S_{E'} M_\sigma S_{E'}^T)(S_E M_\sigma S_E^T)]^{1/2}}$$

- Individual chi-value measured in sigmas (= ratio of |C/E -1| to the total uncertainty):

$$\chi_{ind,i} \equiv \frac{|E_i - C_i|}{\sqrt{S_i M_\sigma S_i^T + (M_{EC})_{ii}}} = \sqrt{(E_i - C_i)^2 (G_{ii})^{-1}}$$

- Ishikawa factor:

$$IS_i \equiv \frac{S_i M_\sigma S_i^T}{(M_{EC})_{ii}}$$

Parameters for Assessing Adjustments (contd.)

- Initial chi-square value:

$$\chi^2_{init} \equiv (\sigma - \tilde{\sigma})^T M_\sigma^{-1} (\sigma - \tilde{\sigma}) + (E - C(\tilde{\sigma}))^T M_{EC}^{-1} (E - C(\tilde{\sigma}))\Big|_{\tilde{\sigma}=\sigma}$$

$$= (E - C)^T M_{EC}^{-1} (E - C)$$

- Contribution to chi-square value:

$$\chi^2_{con,i} \equiv \frac{(E - C)^T (G^{-1})_{i\bullet} (E_i - C_i)}{N_E}$$

- Diagonal chi-value measured in sigmas:

$$\chi_{diag,i} \equiv \sqrt{(E_i - C_i)^2 (G^{-1})_{ii}} = \frac{|E_i - C_i|}{\sqrt{((SM_\sigma S + M_{EC})^{-1})_{ii}}} \neq \chi_{ind,i}$$

Indices for Interpreting Adjustments

- Square root of mobility (= pseudo standard deviation including correlations):

$$\sqrt{D_j} = \mathrm{sgn}(M_{\sigma,j}J)\sqrt{\left|M_{\sigma,j}\right|} \quad \text{where} \quad J = [1,1,..,1]^T$$

- Adjustment motive force:

$$F_{i,j} = \frac{\left\|(\Delta\sigma/\sigma)_{i,j}\right\|}{\left\|J\right\|}\cos\theta \quad \text{where} \quad (\Delta\sigma/\sigma)_{i,j} = M_{\sigma,j}S_{i,j}^T G_{i,j}^{-1}(J - C_i/E_i)$$

$$\cos\theta = \frac{(\Delta\sigma/\sigma)_{i,j}\cdot J}{\left\|(\Delta\sigma/\sigma)_{i,j}\right\|\cdot\left\|J\right\|}$$

$(\Delta\sigma/\sigma)_{i,j}$ is a special adjustment result, in which only one cross section j is adjusted by using only one integral experiment i

- Adjustment potential
  - This index is calculated with averaged C_I/E_I over a set of core parameters I, which is related to the core parameter i

Premises of Valid Adjustment

- No missing/underestimation of uncertainty
  - Valid nuclear data covariance: M_σ
  - Valid experiment covariance: M_E
  - Valid calculation covariance: M_C
- Consistency of C/E values and covariance matrices (=chi-square test)

$$\chi^2_{min}/N_E \approx 1$$

- Note:
  - If there are missing isotopes and reactions in nuclear data covariance (i.e. extreme underestimation), variations of some other cross sections could be unreliable due to compensations
  - Both underestimation and overestimation of experiment and/or calculation uncertainty could give unreliable results as well
  - Overestimation of experiment and/or calculation uncertainty does not affect adjustment results because it is equivalent to elimination of the experiment

Assessment of Adjustment

- Before adjustments
  - Some assessments can be performed before adjustments
  - The assessments before adjustment are independent from the set of experiments
- After adjustments
  - Others are done after adjustments with referring to the adjustment results
  - The assessments after adjustment depend on the set of experiments

Assessment of Adjustment (before)

- Selection of experiments
  - Representativity factor: $f_{EE'} << 1$
    - The complementarity of the experiments can be established by looking at the factor among the selected experiments
  - Individual chi-value: $\chi_{ind,i} >> 1$
    - Inconsistency between $|C - E|$ and covariance matrices, $SM_\sigma S$, M_E and M_C
  - Ishikawa factor: IS_i
    - If $IS_i >> 1\ (S_i M_\sigma S_i^T << (M_{EC})_{ii})$, then $\sigma_j' \approx \sigma_j$ and $S_i M_\sigma' S_i^T \approx S_i M_\sigma S_i^T$
    - If $IS_i << 1\ (S_i M_\sigma S_i^T >> (M_{EC})_{ii})$, then $S_i M_\sigma' S_i^T \approx (M_{EC})_{ii}$
    - If $IS_i << 1\ (S_i M_\sigma S_i^T \approx (M_{EC})_{ii})$, then $S_i M_\sigma' S_i^T \approx \frac{1}{2} S_i M_\sigma S_i^T$

Assessment of Adjustment (after)

- Detection of unreliable adjustments
  - Rejection of the associated experiment is suggested
    - Cross section variation is larger than one sigma of the “a priori” standard deviation, and no abnormality is observed in covariance matrix
  - Physical mechanism should be investigated
    - Large variations of the cross sections are observed in energy ranges, isotopes or reactions that are not the main target
    - Large variations of the cross sections are produced but the “a posteriori” associated standard deviation reductions are small
  - Recommended checks
    - Comparison of adjusted results with existing validated nuclear data files and/or reliable differential measurements

Assessment of Adjustment (after) (contd.)

- After adjustment if chi-square value is not satisfactory (> 1), experiments can be removed (chi-filtering) based either on diagonal chi-square value (ORNL) or chi-square contribution (INL).
- For instance the "a posteriori" (=minimum) chi-square contribution indicates the integral parameters that contribute more to the final $\chi_{min}{}^2$. In this way, it is possible to classify in a hierarchical way which experiment should be discarded or reconsidered. It has to be noted that an experiment can give a negative contribution, which means that the corresponding integral parameter is very effective in the adjustment.

Compensation Effects

- Examples
  - Pu-239 χ and inelastic in general
    - Equivalent effect through neutron spectrum changes
  - Capture and (n,2n) for irradiation experiments
    - Same impact of disappearing the associated isotope
  - Capture and fission for spectral indices
    - e.g. U-238 capture and Pu-239 fission for C28/F49
    - Compensation between numerator and denominator
  - Many reactions for criticalities
    - Capture, fission, ν, χ, inelastic, elastic, …

Avoiding Compensation Effects (Static method)

- Use of specific experiments
  - "Flat" or "steep" adjoint flux reactivity experiments
    - To separate inelastic from absorption cross sections
  - Neutron transmission of leakage experiments
    - Sensitive mostly for inelastic
  - Reaction rate distribution
    - Sensitive mostly for elastic and inelastic
  - Reaction rate ratio
    - Sensitive mostly for specific reactions
  - Sample oscillations (maybe we can find more …)

Avoiding Compensation Effect (Dynamic method)

- Physical interpretation of adjustments
  - To understand the mechanism of adjustments
    - If the compensation effect is reasonable and physical, we may rely on the adjustment results
  - One possible way is to use the adjustment motive force and adjustment potential
  - It works for limited cases, for example, a small case which uses a few of experiments
  - More sophisticated method is needed to settle this issue

Use of "A Posteriori" Covariance Matrix

- Not only the standard deviation of the "a priori" covariance matrix, but also the correlations significantly affect the adjustment results
- The "a posteriori" correlation matrix is full and have a significant impact in reducing the "a posteriori" uncertainty

The "a posteriori" correlations are useful and physical since they come from combination of two physical data, i.e. differential and integral experiments

- Once the adjustment is utilized, the "a posteriori" correlations should be reflected to the nuclear data evaluation, otherwise it might be unphysical

APPENDIX

Common Nomenclature

- $E_i(i=1, \ldots, N_E)$: experimental value of measured integral parameter i
- $C_i(i=1, \ldots, N_E)$: "a priori" calculated value of integral parameter i
- $C_i'(i=1, \ldots, N_E)$: "a posteriori" calculated value of integral parameter i
- $\sigma_j\ (j=1, \ldots, N_\sigma)$: "a priori" cross sections
- $\sigma_j'\ (j=1, \ldots, N_\sigma)$: "a posteriori" cross sections
- S_{ij}: sensitivity coefficients for integral parameter i and cross section j
- $M_{EC}=(M_E+M_C)$: integral parameter covariance matrix
- M_E: integral parameter covariance matrix due to experiment covariance
- M_C: integral parameter covariance matrix due to calculation covariance
- M_σ: " a priori" cross section covariance matrix
- M_σ': "a posteriori" cross section covariance matrix
- $\chi^2(\tilde{\sigma})$: chi-square function to be minimized in the adjustment
- χ^2_{min} : minimized chi-square value
- $G=(M_{EC}+S\ M_\sigma S^T)$: total integral-parameter covariance matrix (to be inverted in adjustment formulas)

Common Nomenclature (contd.)

- Matrix indexing:

$$A_{ij} = (A)_{ij} = a_{ij}$$

$$A_{i\bullet} = (A)_{i\bullet} = \begin{pmatrix} a_{i1} & a_{i2} & \cdots & a_{in} \end{pmatrix}$$

$$A_{\bullet j} = (A)_{\bullet j} = \begin{pmatrix} a_{1j} \\ a_{2j} \\ \vdots \\ a_{mj} \end{pmatrix}$$

$$\text{where } A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix}$$

Adjustment Formulas

- "A posteriori" cross sections:

$$\sigma' = \sigma + M_\sigma S^T G^{-1}(E - C)$$

- "A posteriori" cross section covariance matrix:

$$M'_\sigma = M_\sigma - M_\sigma S^T G^{-1} S M_\sigma$$

- Chi-square function to be minimized:

$$\chi^2(\tilde{\sigma}) = (\sigma - \tilde{\sigma})^T M_\sigma^{-1}(\sigma - \tilde{\sigma}) + (E - C(\tilde{\sigma}))^T M_{EC}^{-1}(E - C(\tilde{\sigma}))$$

- Minimized chi-square value:

$$\begin{aligned} \chi^2_{min} &= (E - C)^T G^{-1}(E - C) \\ &= (\sigma - \sigma')^T M_\sigma^{-1}(\sigma - \sigma') + (E - C')^T M_{EC}^{-1}(E - C') \end{aligned}$$