Standardizing a Renewed Fission Product Yield Library and Related Covariances

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Motivations

- Application to depletion perturbation theory
  - Recent extension (ORSEN) to TSURFER module to perform nuclear data adjustment for fixed-source problems[1]
- To establish methodology to generate evaluated fission product yield data with related covariances
  - Is a fission product yield covariance matrix, a matrix with prescribed row/column sum?
- To establish HFIR (High Flux Isotope Reactor) as a facility relevant for nuclear data measurements
- To improve the ENDF/B-VIII.0 fission product yield sub-library
- To consistently perform uncertainty quantification analysis for fuel decay heat, radio toxicity, burn up credit
  - Consistency between (cumulative and independent) product yield and decay sub-library
- Experimental database with consistently constrained correlated data

[1] Previously, TSURFER was only applicable to criticality problems

Independent Fission Product Yields (IFPY)

Definitions

Independent fission product yield y from the fission of a nucleus with mass number A_T and atomic number Z_f

$$I \equiv I(A,Z,M;\vec{x}) \qquad \text{with} \qquad \vec{x} \equiv \vec{x}(A_f,Z_f,E)$$

- For neutron-induced fission, $A_f = A_\mathrm{T}+1$ (compound nucleus undergoing fission). For spontaneous fission, $A_f = A_\mathrm{T}$
- For a semi-empirical model, the independent fission yield depends on a set of parameters:

$$\vec{x} \equiv \{\vec{\mu}(A_f,Z_f,E),\vec{\lambda}(A_f,Z_f,E)\}$$

$$I \equiv \underbrace{Y(A;\vec{\mu})}_{\text{Sum yield}} \times \underbrace{F(A,Z;\vec{\lambda})}_{\text{Fractional yield}} \times \underbrace{R(A,Z,M)}_{\text{Isomeric ratio}}$$

Constraints

- $\sum_Z F(A,Z;\vec{\lambda}) = 1 \ \ \forall A$
- $\sum_M R(A,Z,M) = 1 \ \ \forall A,Z$
- $Y(A) = \sum_{Z,M} I(A,Z,M;\vec{x}) \ \ \forall A$
- $\sum_{A,Z,M} I(A,Z,M;\vec{x}) = 2$
- $\sum_{A,Z,M} A \cdot I(A,Z,M;\vec{x}) = A_f - \bar{\nu}(E)$
- $\sum_{A,Z,M} Z \cdot I(A,Z,M;\vec{x}) = Z_f$
- $\sum_A Y(A;\vec{\mu}) = 2$
- $\sum_A A \cdot Y(A;\vec{\mu}) = A_f - \bar{\nu}(E)$
- $\sum_{A,Z,M} Z \cdot F(A,Z,M;\vec{\lambda}) \cdot Y(A;\vec{\mu}) = Z_f$

IFPY Uncertainties in ENDF/B-VIII.0

- ENDF/B-VIII.0 sum yield $Y_{\mathrm{E}}(A)$ calculated from one of the constraints $Y_{\mathrm{E}}(A) = \sum_{Z,M} I_{\mathrm{E}}(A,Z,M)$
- Sum yield uncertainty $\Delta Y_{\mathrm{E}}(A)$ calculated from quadratic summation $\Delta Y_{\mathrm{E}}(A) = \sqrt{\sum_{Z,M} [\Delta I_{\mathrm{E}}(A,Z,M)]^2}$
  - ENDF/B-VIII.0 IFPYs do not have correlations, therefore related covariance matrix is diagonal
- Strategy to generate a *constrained* fission product yield covariance matrix
  - Set of sum yields and related uncertainties, $Y_{\mathrm{E}}(A) \pm \Delta Y_{\mathrm{E}}(A)\ \forall A$, was used to generate randomly sampled and constrained sets of sum yields, $Y^k(A)\ \forall A$ ($k = 1, \ldots, N$)
  - Mean values $\langle Y(A) \rangle = \sum_{k=1}^{N} Y^k(A)/N\ \forall A$
  - Covariance matrix $\langle \Delta Y(A)\ \Delta Y(A') \rangle = \sum_{k=1}^{N} (Y^k(A) - \langle Y(A) \rangle)(Y^k(A') - \langle Y(A') \rangle)/N\ \forall A, A'$
- Consistency checks
  - The set of mean values $\langle Y(A) \rangle\ \forall A$ is constrained since the set of $Y^k(A)\ \forall A$ is constrained for each sweep $k = 1, \ldots, N$
  - $|\langle Y(A) \rangle - Y_{\mathrm{E}}(A)| << 1\ \forall A$

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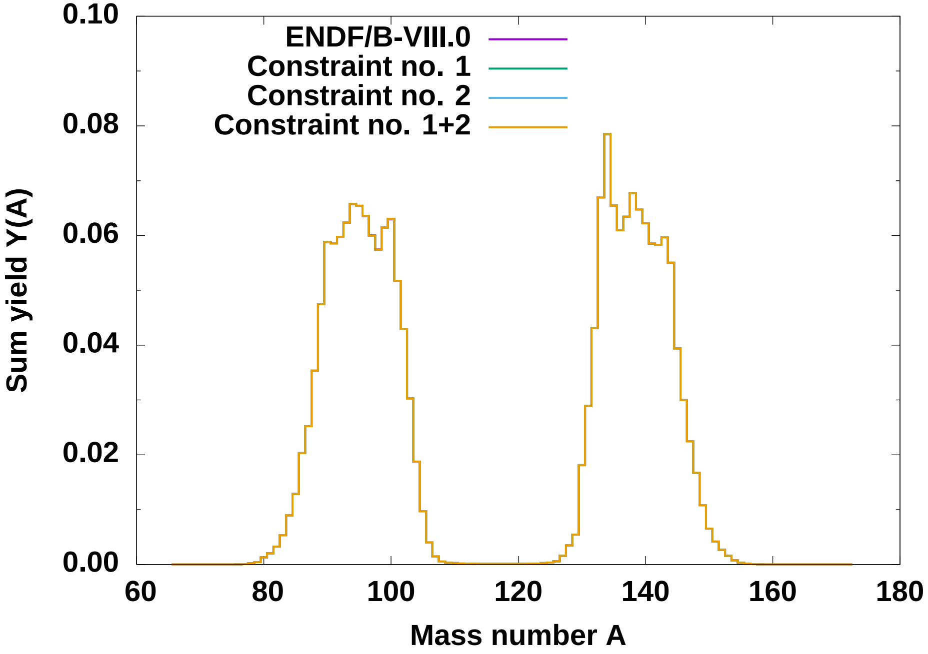
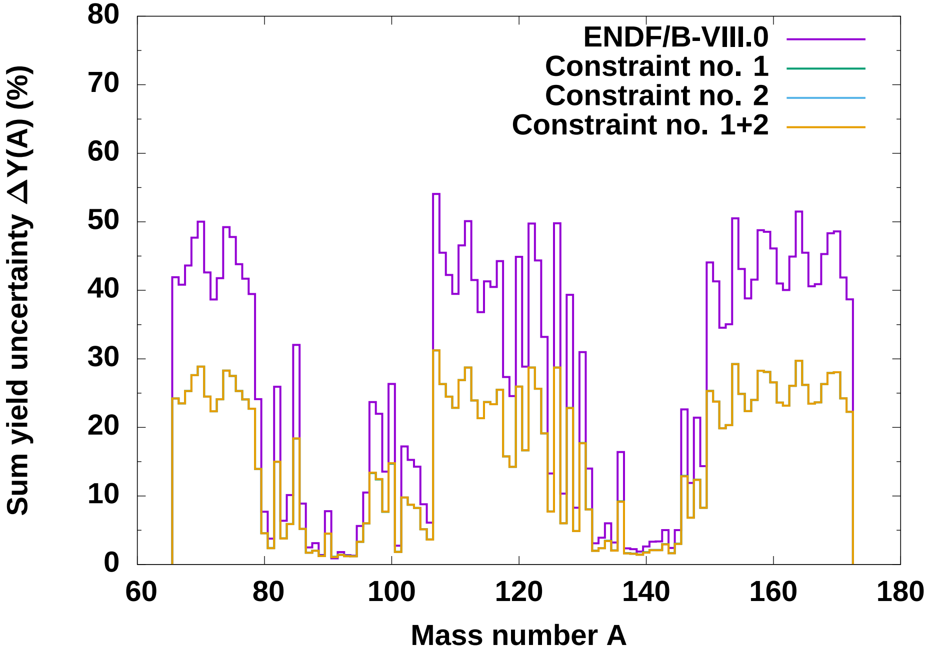
Sum Yield Uncertainty and Constraints on ^{235}U (thermal)

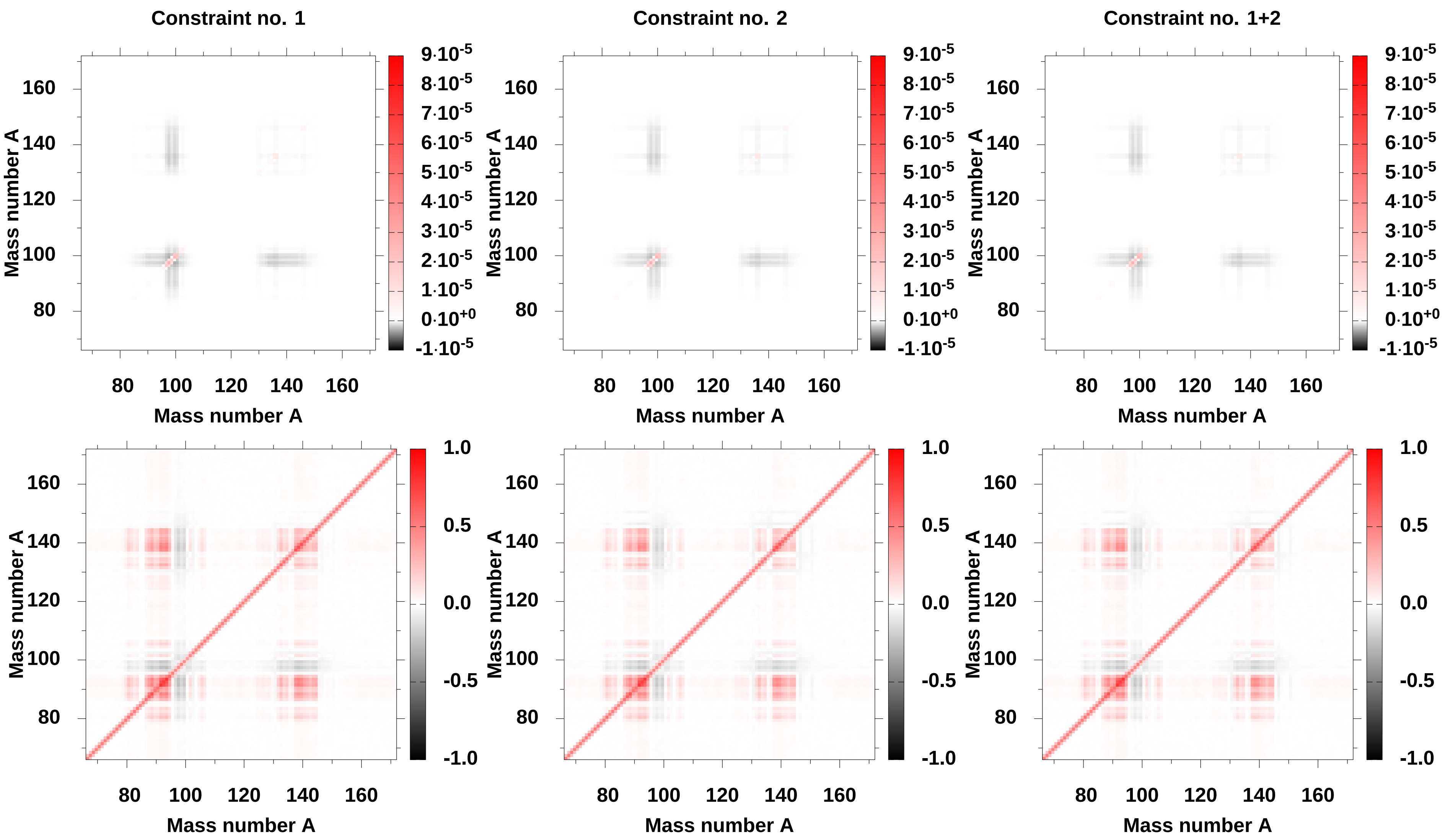
$\sum_A \langle Y(A)\rangle = 2$ (constraint no. 1) $\sum_A \langle Y(A)\rangle\, A = A_f - \bar{\nu}$ (constraint no. 2) $\sum_A \langle Y(A)\rangle\, (1+A) = 2 + A_f - \bar{\nu}$ (constraint no. 1+2)





- No meaningful differences (<0.5%) between ENDF/B-VIII.0 sum yields $Y_{\mathrm{E}}(A)$ and constrained $\langle Y(A)\rangle$ sampled within $Y_{\mathrm{E}}(A) \pm \Delta Y_{\mathrm{E}}(A)$
- Large reduction in the sum yield uncertainty ($\approx$ -40%) when constraints are applied to the sampled sum yields
- Rare cases where the uncertainty increased

Sum Yield Covariance/Correlation Matrices



Results of the Covariance Analysis

Impact of the Constraints to the Row/Column Sums

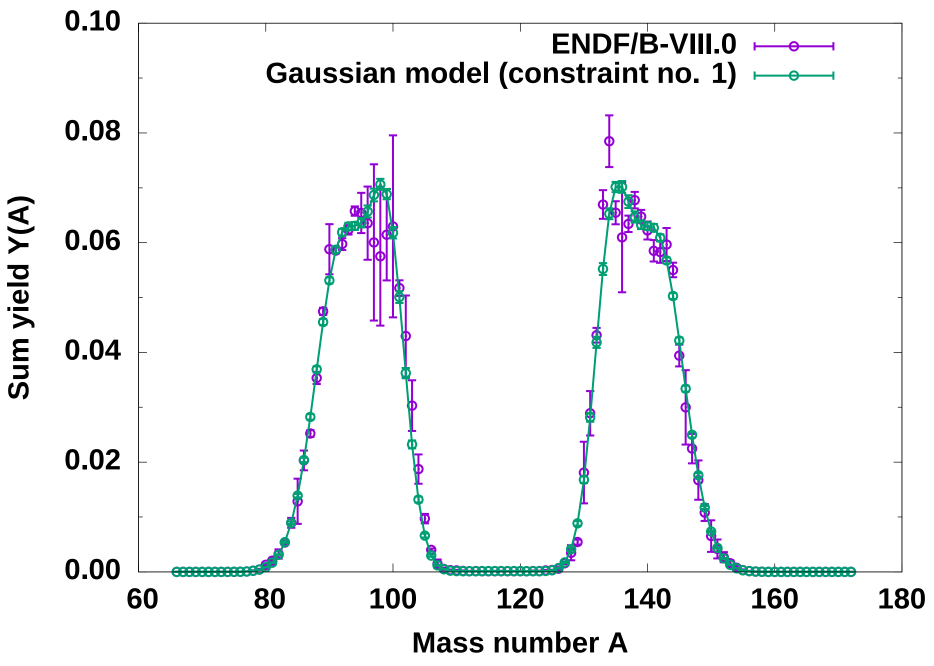
- Covariance/correlation matrices very sparse
- Short-range correlations mainly appearing between yields at the peaks of the mass distribution
- **Constraint no. 1**: the results of the constrain, $\sum_A \langle Y(A) \rangle = 2$, produces a covariance matrix having zero row/column sum
- **Constraint no. 2**: the constrain $\sum_A \langle Y(A) \rangle \, A = A_f - \bar{\nu}$ does not generate a prescribed row/column sum
- **Constraint no. 1+2**: as in constrain no. 2
- Note: A matrix with zero row/column sum is singular

Model for the Sum Yields

- Five Gaussian model: $Y(A;\vec{\mu}) = \sum_{i=1}^{5} N_i \psi_i$
- Gaussian curves: $\psi_i(A) = (\sqrt{2\pi}\sigma_i)^{-1} e^{-(A-A_i)^2/(2\sigma_i^2)}$
- Symmetry conditions: $A_1 = (A_f - \bar{\nu})/2$, $A_4 = 2A_1 - A_2$, $A_5 = 2A_1 - A_3$
- Symmetry conditions: $\sigma_2 = \sigma_4$, $\sigma_5 = \sigma_3$, $N_4 = N_2$, $N_5 = N_3$, $N_3 = 1 - N_2 - N_1/2$
- Energy-dependent parameters: $\vec{\mu} = \{N_1, \sigma_1, N_2, A_2, \sigma_2, A_3, \sigma_3\}$
  - $\sigma_i(E) = m_i(E - E_f)^{1/2}$ being $E = E_n + B_n$ the excitation energy and E_f the fission barrier
  - $A_1 = (A_f - \bar{\nu}_0)/2 - \beta E/2$ (energy dependence of the center)
  - $A_{i>1}(E) = A_i(E_f) + \alpha(E - E_f)^{-1/2}$
  - $N_1(E) = \sin^2\theta_1$ with $\tan\theta_1 = 2(E - E_1)/\Gamma_1$
  - $N_2(E) = \cos^2\theta_1 \cos^2\theta_2$ with $\tan\theta_2 = 2(E - E_2)/\Gamma_2$
  - $N_3(E) = (1/2)\sin^2\theta_1 + \cos^2\theta_1 \sin^2\theta_2$ (equivalent to N_3 above)
- Model parameters: $m_{i=1,2,3}$, $\Gamma_{i=1,2}$, $A_{i=2,3}$[2]
- Note: the mass distribution $Y(A;\vec{\mu})$ is normalized to 2 because of the condition on N_3

[2] In this work E_f=6.1 MeV, $\bar{\nu} = 2.4$, $\alpha = \beta = 0$, and the resonance energies E_1=4.6 MeV, E_2=17.3 MeV.

Fitting Sum Yield Data with a Gaussian Model (Normalized to 2)



Nonlinear least–squares (NLLS) Marquardt–Levenberg algorithm

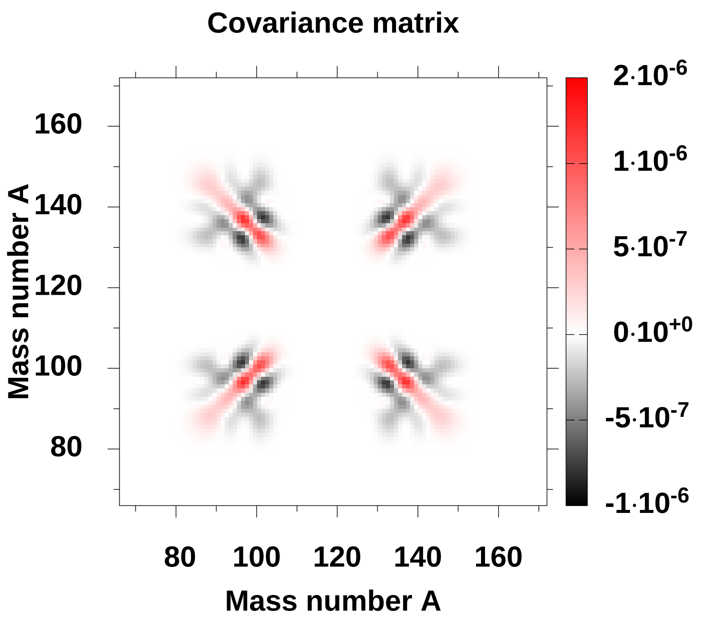
m_1	= 7.89369	+/– 0.1047	(1.326%)
m_2	= 3.40107	+/– 0.03528	(1.037%)
m_3	= 2.25366	+/– 0.05165	(2.292%)
a_2	= 141.489	+/– 0.1379	(0.09744%)
a_3	= 134.352	+/– 0.1298	(0.09664%)
Γ_1	= 102.018	+/– 8.371	(8.205%)
Γ_2	= 25.2895	+/– 0.8446	(3.34%)

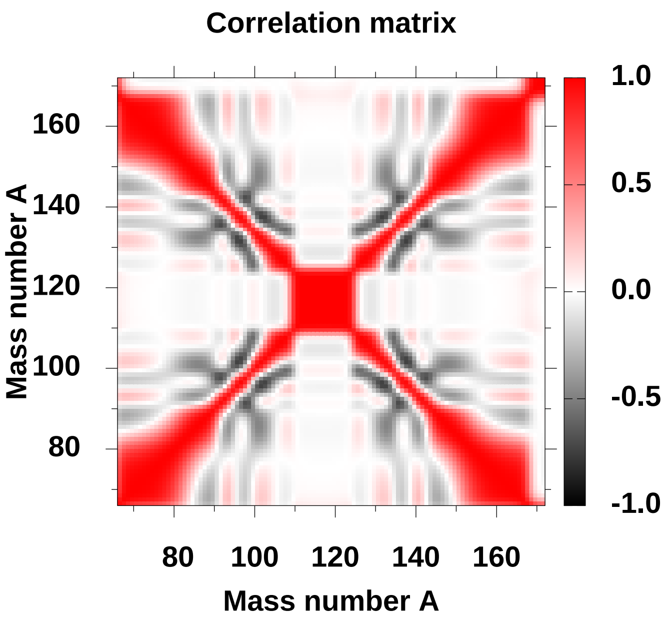
Correlation matrix of the fit parameters:

	m_1	m_2	m_3	a_2	a_3	Γ_1	Γ_2
m_1	1.000						
m_2	–0.061	1.000					
m_3	0.057	–0.564	1.000				
a_2	0.047	–0.879	0.685	1.000			
a_3	0.033	–0.656	0.760	0.787	1.000		
Γ_1	0.328	–0.020	0.106	0.034	0.024	1.000	
Γ_2	–0.057	0.829	–0.732	–0.910	–0.848	–0.060	1.000

- Small differences in the fitted model parameters when data sets with different uncertainty are used in the fit
- The theoretical sum yield uncertainties (obtained by the correlation matrix for the fitted parameters) are smaller than the fitted data

Fitting Sum Yield Data with Gaussian Model (Normalized to 2)





- Strong positive/negative correlations of the yields within the peaks and between the peaks
- Correlation matrix shows strong correlations for very small yields (valley and wings of the mass distribution)
- Covariance matrix has row/column with sum rule zero[3]
- Constraint of the sum yield produced a covariance matrix with prescribed row/column

[3] Deviations from zero can be seen for a few rows/columns related to very small yields of magnitude $\approx 10^{-11}$.

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Conclusions

- Numerical simulations to generate covariance matrices of constrained sum yield distributions were performed
- Monte Carlo simulations showed covariance matrices generated with sum yield distribution normalized to 2, have zero row/column sum
  - The correlations generated by applying the constraints to the sampled yields induced a reduction in the sum yield uncertainties
- When the constraints to the yield distribution are not a linear function of the distribution, the covariance matrices do not have zero row/column sum value
- The 5 Gaussian model implicitly defined to satisfy one of the constraints (normalized to 2) was used in a least-square procedure
- Calculated from the covariance matrix of 7 fitted parameters and related partial derivatives, the covariance matrix of the yield distribution obeyed the row-column sum zero rule (within numerical precision and except for very small yields)

Appendix : TSURFER Standard Methodology

The GLLS method in TSURFER is based on minimizing

$$\chi^2 = \Delta\alpha^{\mathsf{T}} C^{-1} \Delta\alpha + \Delta m^{\mathsf{T}} V^{-1} \Delta m \tag{1}$$

Indices : $\alpha \equiv$ nuclear data, $m \equiv$ measured integral quantities, $k \equiv k(\alpha)$ calculated integral quantities

- $\Delta\alpha = \frac{\alpha' - \alpha}{\alpha}$: $(n \times 1)$ vector of adjusted nuclear data with $(n \times n)$ relative covariance matrix C with elements $C_{ij} = \frac{\langle \delta\alpha_i \delta\alpha_j \rangle}{\alpha_i \ \alpha_j}$
- $\Delta m = \frac{m' - m}{m}$: $(s \times 1)$ vector of adjusted measured responses with $(s \times s)$ relative covariance matrix V with elements $V_{ij} = \frac{\langle \delta m_i \delta m_j \rangle}{m_i \ m_j}$

Eq. (1) is minimized subject to the linearity constraint $S\Delta\alpha - \Delta k = 0$ (with $S = (\partial k(\alpha)/\partial\alpha/(k/\alpha)) \equiv S(\alpha)$). To do this, one defines the Lagrangian function

$$\chi^2 = \Delta\alpha^{\mathsf{T}} C^{-1} \Delta\alpha + \Delta m^{\mathsf{T}} V^{-1} \Delta m + \lambda \left(S\Delta\alpha - \Delta k \right) \tag{2}$$

that, subject to the further constraint that adjusted responses must agree[4], i.e. $k(\alpha') = m'$, can be written as

$$\chi^2 = \Delta\alpha^{\mathsf{T}} C^{-1} \Delta\alpha + \Delta m^{\mathsf{T}} V^{-1} \Delta m + \lambda \left(S\,\Delta\alpha - F\,\Delta m + d \right). \tag{3}$$

Here the diagonal matrix F has matrix elements $F_{ii} = m_i/k_i$ of the ratio between measured and calculated responses and $d = \frac{k-m}{m}$ is the discrepancy vector. From the conditions $\partial\chi^2/\partial\Delta\alpha = 0$ and $\partial\chi^2/\partial\Delta m = 0$, one has

$$\Delta\alpha = -\lambda C S^{\mathsf{T}} \quad \text{and} \quad \Delta m = \lambda V F \tag{4}$$

with $\lambda = W^{-1} d$ obtained from the uncertainty of the discrepancy vector obtained by standard error propagation

$$W = SCS^{\mathsf{T}} + FVF^{\mathsf{T}} \tag{5}$$

[4] In TSURFER the integral quantity $k(\alpha')$ is calculated by first order approximation as $k(\alpha') = k(\alpha) + S(\alpha)(\alpha' - \alpha) = m'$ assuming $S(\alpha) \approx S(\alpha')$.

Appendix : TSURFER Enhanced Methodology

For the adjustment of nuclear data (such as fission product yields) subject to certain physical constraints (slide 3), the Lagrangian function is now defined by an additional term

$$\chi^2 = \Delta\alpha^{\mathsf{T}} C^{-1} \Delta\alpha + \Delta m^{\mathsf{T}} V^{-1} \Delta m + \lambda \left(S\Delta\alpha - F\,\Delta m + d \right) + \tilde{\lambda}\, h^{\mathsf{T}} \Delta\alpha \,. \tag{6}$$

From the constraint $h^{\mathsf{T}}\Delta\alpha = 0$ together with the conditions on the χ^2, the adjusted nuclear data vector is

$$\Delta\alpha = -C(\lambda S^{\mathsf{T}} + \tilde{\lambda} h) \tag{7}$$

and the adjusted measured responses vector Δm is as defined as in Eq. (4). Inserting $\Delta\alpha$, Δm in Eq. (5), the first Lagrangian multiplier λ is

$$\lambda = W^{-1}(d - Sh\tilde{\lambda})\,. \tag{8}$$

From $h^{\mathsf{T}}\Delta\alpha = 0$, the condition on the second Lagrangian multiplier is

$$h^{\mathsf{T}} C \left(-S^{\mathsf{T}} W^{-1} d + S^{\mathsf{T}} W^{-1} S h \tilde{\lambda} - h\tilde{\lambda} \right) = 0\,, \tag{9}$$

where, if $h^{\mathsf{T}}C = 0$ (meaning the zero row/column sum rule is satisfied), the TSURFER algorithm follows the standard methodology (slide 12) and, if $h^{\mathsf{T}}C \neq 0$, $\tilde{\lambda}$ is

$$\tilde{\lambda} = \left[(S^{\mathsf{T}} W^{-1} S - 1) h \right]^{-1} S^{\mathsf{T}} W^{-1} d\,, \tag{10}$$

where h is a vector with zero and one elements.

Acknowledgments

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