Description and usage of experimental data for evaluation in the resolved resonance region

Subgroup - 36

EC – JRC – IRMM
Standards for Nuclear Safety, Security and Safeguards (SN3S)
1) Status

2) EXFOR reporting, Meeting 8 – 10 October 2013, IAEA

3) Activities at IRMM in 2013 – 2014, B. Becker
   • AGS, Manual + distribution (OECD/NEA)
   • Full Bayesian analysis

4) Preparation Final report
Objective

Produce accurate cross section data together with reliable covariance information in the resonance region

⇒ Reduce bias effects
⇒ Produce reliable and realistic covariance data
Activities

The main task:

identify and quantify the metrological parameters involved in each step of the evaluation process, starting from the production of experimental data.

Activities:

(1) Identify the uncertainty components
(2) Identify methods for evaluating uncertainties in the resonance region using experimental covariance information
(3) Define and analyse case studies
(4) Provide recommendations for reporting and usage of experimental details and uncertainty components

Status: finalised

(1-3) Nuclear data sheets, 113 (2012) 3054 – 3100
ND2013, Becker et al.

(2-3) Additional studies at IRMM: contribution to CW2014, Santa Fe

(4) Consultants meeting at IAEA
AGS, will be distributed by OECD/NEA
EXFOR, Reporting

Consultants' Meeting, 8 to 10 October 2013, IAEA Headquarters, Vienna, Austria
"EXFOR Data in Resonance Region and Spectrometers' Response Function"
https://www-nds.iaea.org/index-meeting-crp/CM-RF-2013/

Summary
- Report TOF- response function
- Report full experimental details
- Recommendation to report data in TOF
- AGS concept recommended to process TOF-data
- Templates to report TOF-data

Examples
- RPI
- GELINA
Methods to account for all uncertainty components

- **Conventional uncertainty propagation (CUP)** Fröhner, NSE 126 (1997) 1 – 18
- **Monte Carlo (MC)** De Saint Jean et al., NSE 161 (2009) 363 - 370
- **Marginalization (MA)** Habert et al., NSE 166 (2010) 276 - 287

Differ in the way the uncertainty of experimental parameters are taken into account

⇒ Application: NDS 113 (2012) 3054 – 3100 + Becker et al. (ND2013)
⇒ Problems in understanding results: more studies required
results reported at CW2014, Santa Fe
Unresolved resonance region

\[ \chi^2(\hat{\theta}) = (Z_{\text{exp}} - Z_M(t, \hat{\theta}))^T V^{-1}_{Z_{\text{exp}}} (Z_{\text{exp}} - Z_M(t, \hat{\theta})) \]

\[ \hat{\theta} = (G_{\hat{\theta}}^T V_{Z_{\text{exp}}}^{-1} G_{\hat{\theta}})^{-1} (G_{\hat{\theta}}^T V_{Z_{\text{exp}}}^{-1} Z_{\text{exp}}) \]

\[ V_{\hat{\theta}} = (G_{\hat{\theta}}^T V_{Z_{\text{exp}}}^{-1} G_{\hat{\theta}})^{-1} \]

Conventional uncertainty propagation (CUP)

\[ Z_{\text{exp}} = \begin{cases} <\sigma_{\text{tot,exp}} > \\ <\sigma_{\gamma,\text{exp}} > \\ <\sigma_{\text{tot,M}} > = \frac{1}{N_{\sigma_{\text{tot}}}} f(R_{\ell}, S_{\ell}, T_{\gamma,\ell}) \\ <\sigma_{\gamma,M} > = \frac{1}{N_{\sigma_{\gamma}}} g(R_{\ell}, S_{\ell}, T_{\gamma,\ell}) \end{cases} \]

- Include normalization as fit parameter
  ⇒ avoids PPP
  in URR due to limitations of the model!
PPP in URR for $^{103}\text{Rh}(n,\gamma)$
Example URR: $\sigma(n,\text{tot})$ and $\sigma(n,\gamma)$ for $^{197}\text{Au}$

- **Transmission at 50 m (GELINA)**: $T_{\exp}$ with $u_{N\sigma_{\text{tot}}}/N_{\sigma_{\text{tot}}}=2.0\%$ (normalization)
  

- **Capture at 12.5 m (GELINA)**: $Y_{\exp}$ with $u_{N\sigma_{\gamma}}/N_{\sigma_{\gamma}}=1.5\%$ (normalization)
  
  Massimi et al., submitted to Eur. J. Phys. A

- **Hauser – Feshbach + WF**: $(R_\ell, S_\ell, T_{\gamma, \ell})$

---

![Graph 1](image1.png)

![Graph 2](image2.png)
### Parameter covariance matrix (GLSQ + CUP)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>100 x (uθ/θ)</th>
<th>ρ(θ,θ') x 100</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NT</td>
<td>Nc</td>
</tr>
<tr>
<td>N_{σtot}</td>
<td>1.00</td>
<td>2.0 → 1.9</td>
</tr>
<tr>
<td>N_{σγ}</td>
<td>1.00</td>
<td>1.5 → 1.5</td>
</tr>
<tr>
<td>R∞ / fm</td>
<td>-0.163</td>
<td>10.1</td>
</tr>
<tr>
<td>S0 / 10^{-4}</td>
<td>1.89</td>
<td>1.8</td>
</tr>
<tr>
<td>S1 / 10^{-5}</td>
<td>2.84</td>
<td>10.8</td>
</tr>
<tr>
<td>Tγ^2+/ 10^{-2}</td>
<td>3.44</td>
<td>2.8</td>
</tr>
<tr>
<td>Tγ^2-/ 10^{-2}</td>
<td>1.62</td>
<td>7.8</td>
</tr>
</tbody>
</table>
Cross Section Uncertainty

\[ \frac{u_{N_{\sigma_{\text{tot}}}}}{N_{\sigma_{\text{tot}}}} = 2.0\% \]

\[ \frac{u_{N_{\sigma_{\gamma}}}}{N_{\sigma_{\gamma}}} = 1.5\% \]

CUP: normalization uncertainties \( u_{N_T} \) and \( u_{N_c} \) propagate to

- reaction model parameters and
- evaluated cross sections

Monte Carlo + LSQ: De Saint Jean et al., NSE 161 (2009) 363 – 370
GLSQ : Resolved resonance region

\[ \chi^2(\vec{\theta}) = (Z_{\text{exp}} - Z_M(t, \vec{\theta}))^T V_{Z_{\text{exp}}}^{-1} (Z_{\text{exp}} - Z_M(t, \vec{\theta})) \]

\[ \vec{\theta} = (G_{\vec{\theta}}^T V_{Z_{\text{exp}}}^{-1} G_{\vec{\theta}})^{-1} (G_{\vec{\theta}}^T V_{Z_{\text{exp}}}^{-1} Z_{\text{exp}}) \]

\[ V_{\vec{\theta}} = (G_{\vec{\theta}}^T V_{Z_{\text{exp}}}^{-1} G_{\vec{\theta}})^{-1} \]

Conventional uncertainty propagation (CUP)

\[ T_{\text{exp}} \]

\[ Y_{\text{exp}} \]

\[ Z_{\text{exp}} = \begin{cases} T_{\text{exp}} \\ Y_{\text{exp}} \end{cases} \]

\[ \eta \]

\[ k \]

\[ \begin{align*} T_M(t, \vec{\theta}) &= \frac{1}{N_T} \int R(t, E) T'(E) \, dE \\ Y_M(t, \vec{\theta}) &= \frac{1}{N_c} \int R(t, E) Y'(E) \, dE \end{align*} \]

\[ T'(E) = e^{-\sum_k \eta_k \sigma_{\text{tot},k}} \]

\[ Y'(E) = (1 - e^{-\sum_k \eta_k \sigma_{\text{tot},k}}) \frac{\bar{\sigma}_{\gamma,k}}{\sigma_{\text{tot},k}} + \ldots \]
GLSQ: include $\kappa$ as adjustable parameter

$$\chi^2(\hat{\theta}) = (Z_{\text{exp}} - Z_M(t, \hat{\theta}))^T V_{Z_{\text{exp}}}^{-1} (Z_{\text{exp}} - Z_M(t, \hat{\theta}))$$

JEFF Report 18

$$\hat{\theta} = (G^{-T}_{\hat{\theta}} V^{-1}_{Z_{\text{exp}}} G_{\hat{\theta}})^{-1} (G^{-T}_{\hat{\theta}} V^{-1}_{Z_{\text{exp}}} Z_{\text{exp}})$$

$$V_{\hat{\theta}} = (G^{-T}_{\hat{\theta}} V^{-1}_{Z_{\text{exp}}} G_{\hat{\theta}})^{-1}$$

Conventional uncertainty propagation (CUP)

- Consider prior as experimental data ($\theta \in Z_{\text{exp}}$)
  - allows correlation between prior and new (updating) data
  (not possible in Bayesian updating fitting approach)
- Include experimental parameters as fit parameter ($\equiv$ including $u_N$ in $V_{Z_{\text{exp}}}$)
  - avoids PPP
  - allows full correlation between updating experimental data
  - verify the influence of $u_\kappa$ on nuclear model parameters
Normalization uncertainty: RP from $Y_{\text{exp,}\gamma}$

Normalization capture data (external)

$Y_{\text{exp}}$ with $u_N / N \approx 2\%$

$^{197}\text{Au} + n$

$E_r = 4.9 \text{ eV}$

$\Gamma_n = 0.015 \text{ eV}$

$\Gamma_\gamma = 0.122 \text{ eV}$

<table>
<thead>
<tr>
<th>Peak uncertainty (counts)</th>
<th>10 %</th>
<th>1%</th>
<th>0.1 %</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_N/N$</td>
<td>0.019</td>
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</tr>
<tr>
<td>$u_{\Gamma_n}/\Gamma_n$</td>
<td>0.025</td>
<td>0.022</td>
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</tr>
<tr>
<td>$u_{\Gamma_\gamma}/\Gamma_\gamma$</td>
<td>0.018</td>
<td>0.003</td>
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</tr>
<tr>
<td>$\rho(N,\Gamma_n)$</td>
<td>-0.90</td>
<td>-1.00</td>
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<td>0.15</td>
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</table>

$Y_M \approx n \sigma_\gamma$

$\Rightarrow$ normalization uncertainty $u_N / N \approx 2\%$ remains independent of counting statistics

$\Rightarrow$ $u_N$ propagates fully to the uncertainty of $\Gamma_n$
Normalization uncertainty: RP from $Y_{\text{exp,}\gamma}$

Normalization capture data (external)

$Y_{\text{exp}}$ with $u_{N}/N \approx 2\%$

$^{197}\text{Au} + n$

$E_r = 4.9 \text{ eV}$

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Sample thickness: 0.01 mm

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<td>$\rho(N,\Gamma_\gamma)$</td>
<td>0.50</td>
<td>0.94</td>
<td>0.96</td>
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<td>$\rho(\Gamma_n,\Gamma_\gamma)$</td>
<td>-0.67</td>
<td>-0.96</td>
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$Y_M \approx (1 - e^{n\sigma_{\text{tot}}}) \frac{\sigma_\gamma}{\sigma_{\text{tot}}}$

⇒ normalization uncertainty $u_{N}$ decreases with increasing counting statistics

⇒ $u_{N}$ has no impact on $\Gamma_n$ in case of high precision data
Normalization uncertainty : RP from $Y_{\text{exp},\gamma}$

Normalization capture data (external)
$Y_{\text{exp}}$ with $u_N/N = 2\%$

**CUP + GLSQ**

Final normalization uncertainty and its impact on nuclear model parameters depend on:
- on the precision of the data
- target thickness

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Sample thickness : 0.010 mm

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Normalization uncertainty : RP from $Y_{\text{exp},\gamma}$

Normalization capture data (external)
$Y_{\text{exp}}$ with $u_N / N = 2\%$

**CUP + GLSQ**
Final normalization uncertainty and its impact on nuclear model parameters depend on:
- on the precision of the data
- target thickness

**Monte Carlo + GLSQ**
De Saint Jean et al., NSE 161 (2009) 363 – 370

Normalization
- Is not updated (by constraint)
- Has a direct impact on $u_{\Gamma_n}$ and $u_{\Gamma_\gamma}$ also in case of high precision data

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Uncertainty on $\sigma(n, \gamma)$: $Y_{\text{exp}}$

$Y_{\text{exp}}$ with $u_N / N = 2$

$Y_\gamma = n \sigma$

0.1 % at peak

$100 \times (u_{\sigma_\gamma} / \sigma_\gamma)$

Neutron energy / eV

$10^2$

$10$

$1$

$0.1$

$0.01$

CUP : $Y_{\text{exp}}$

MC : $Y_{\text{exp}}$

$n = 4 \times 10^{-5}$ at/b

0.1 % at peak

$10^2$

$10$

$1$

$0.1$

$0.01$

CUP : $Y_{\text{exp}}$

MC : $Y_{\text{exp}}$
Full Bayesian statistical analysis

- **Bayes' theorem:**
  \[ P(\theta | Z) = \frac{P(Z | \theta) P(\theta)}{P(Z)} \]
  - \( P(\theta) \) : Prior probability distribution gets updated
  - \( P(Z | \theta) \) : Likelihood of acquired additional data \( Z \) (transmission, yield, …)
  - \( P(\theta | Z) \) : Updated posterior probability distribution \( P(\theta) \) and \( P(Z | \theta) \) based on maximum entropy

- **Example: RP derived from \( Y_{\text{exp}} \) for \( E_r = 4.9 \text{ eV} \) of \(^{197}\text{Au}, \) (0.02 mm thick sample)**
  - \( P(\theta) \) prior for \( \theta = (\eta, \kappa) \)
    - \( N_c = 1.00 \pm 0.02 \) : normal distribution
    - \( (\Gamma_n, \Gamma_y) \) : non-informative prior \((\Gamma_n & \Gamma_y > 0)\), Jeffrey's prior
  - \( P(Y_M | \theta) \) likelihood of yield
    - \( (Y_{\text{exp}}, V_{y_{\text{exp}}}) \) : normal distribution
      \[ P(Y_M | \theta) = \frac{1}{\sqrt{\det(2\pi V_Y)}} e^{-\frac{1}{2}(Y_{\text{exp}} - Y_M(\theta))^T V_Y^{-1} (Y_{\text{exp}} - Y_M(\theta))} \]
Capture measurements for $^{197}$Au

$^{197}$Au + $n$

- $E_r = 4.9$ eV
- $\Gamma_n = 0.015$ eV
- $\Gamma_\gamma = 0.122$ eV

Generated test case:
- Large yield with extreme small counting statistics uncertainties (0.2% in the peak)
- Randomized data points
Posterior distributions $P(N, \Gamma_n, \Gamma_\gamma)$

\[
\begin{align*}
1^{97}\text{Au} + n \\
E_r &= 4.9 \text{ eV} \\
\Gamma_n &= 0.015 \text{ eV} \\
\Gamma_\gamma &= 0.122 \text{ eV}
\end{align*}
\]

1\text{st} and 2\text{nd} moment of marginalized distribution:
\[
\begin{align*}
N &= 1.0001 \pm 0.0009 \\
\Gamma_n &= 0.0151 \pm 0.0001 \text{ eV} \\
\Gamma_\gamma &= 0.1233 \pm 0.0010 \text{ eV}
\end{align*}
\]

GLSQ + CUP
\[
\begin{align*}
N &= 1.0000 \pm 0.0008 \\
\Gamma_n &= 0.0151 \pm 0.0001 \text{ eV} \\
\Gamma_\gamma &= 0.1233 \pm 0.0010 \text{ eV}
\end{align*}
\]

$\neq$ MC
Capture measurements for $^{197}$Au

$^{197}$Au + n

$E_r = 4.9$ eV

$\Gamma_n = 0.015$ eV

$\Gamma_\gamma = 0.122$ eV

Generated test case:
- Large yield with relatively large counting statistics uncertainties
- Randomized data points
Posterior distributions $P(N, \Gamma_n, \Gamma_\gamma)$

$^{197}\text{Au} + n$

$E_r = 4.9\text{ eV}$

$\Gamma_n = 0.015\text{ eV}$

$\Gamma_\gamma = 0.122\text{ eV}$

$1^{\text{st}}$ and $2^{\text{nd}}$ moment of marginalized distribution:

$N = 1.00 \pm 0.018$

$\Gamma_n = 0.016 \pm 0.003\text{ eV}$

$\Gamma_\gamma = 0.126 \pm 0.022\text{ eV}$

GLSQ + CUP

$N = 1.00 \pm 0.019$

$\Gamma_n = 0.013 \pm 0.002\text{ eV}$

$\Gamma_\gamma = 0.143 \pm 0.017\text{ eV}$

Max. likelihood
Resonance parameters + covariances in RRR

\[ \chi^2(\vec{\theta}) = (Z_{\text{exp}} - Z_M(t, \vec{\theta}))^T V_{Z_{\text{exp}}}^{-1} (Z_{\text{exp}} - Z_M(t, \vec{\theta})) \]

\[ \vec{\theta} = (G_{\vec{\theta}}^T V_{Z_{\text{exp}}}^{-1} G_{\vec{\theta}})^{-1} (G_{\vec{\theta}}^T V_{Z_{\text{exp}}}^{-1} Z_{\text{exp}}) \] (LSQ)

\[ V_{\vec{\theta}} = (G_{\vec{\theta}}^T V_{Z_{\text{exp}}}^{-1} G_{\vec{\theta}})^{-1} \] (CUP)

\[ Y_M(t, \vec{\theta}) = \frac{1}{N_c} \int \frac{R(t, E) Y'(E) dE}{R(t, E) dE} \]

\[ Y'(E) = (1 - e^{-\sum_k n_k \bar{\sigma}_{\text{tot},k}} \sum_k \frac{\bar{\sigma}_{\gamma,k}}{\bar{\sigma}_{\text{tot},k}}) + \ldots \]

- No direct measurement of the cross section
- Interpretation model depends on RP and experimental parameters
- GLSQ + CUP relies on a perfect model (reaction + experiment)

\[
P(\theta|Z,M) \propto P(Z|\theta,M) P(\theta)\]
Validation of resonance parameters by NRTA

- **Covariances for W isotopes** (NDS, various publications)

- **Validation experiment: determine areal density by NRTA**
  
  - **Sample: metallic disc of $^{nat}W$**
    - Homogeneous sample
    - Areal density $n$: from weight and area
    \[ \Rightarrow u_n/n < 0.1 \%
  
  - **Transmission: absolute measurement**
    - Absolute measurement
    - Methodology well understood (background, dead time correction, …)
    
    \[ \Rightarrow u_{T_{exp}}/T_{exp} < 0.3 \%
  
  \[ \Rightarrow \text{One of the most accurate integral experiment to validate resonance parameters} \]
Validation of resonance parameters by NRTA

Transmission measurements
- a 25 m station of GELINA
- $^6$Li detector

$Y_M : $ REFIT

Least squares adjustment (REFIT)

$$ T_M(t, \hat{\theta}) = \frac{-\sum n_k \sigma_{tot,k}}{\int R(t,E) e^{-\theta} dE} $$

$$ \hat{\theta} = (\eta, \kappa) $$

- $\eta$: resonance parameters
- $\kappa$: experimental parameters

$$ \hat{\theta} = (G^T_{\hat{\theta}} V^{-1}_{T_{\exp}} G_{\hat{\theta}})^{-1} (G^T_{\hat{\theta}} V^{-1}_{T_{\exp}} T_{\exp}) $$

$$ V_{\hat{\theta}} = (G^T_{\hat{\theta}} V^{-1}_{T_{\exp}} G_{\hat{\theta}})^{-1} $$

$G_{\hat{\theta}}$: partial derivatives

(non-linear model: solved by iteration)
Validation of resonance parameters by NRTA

<table>
<thead>
<tr>
<th>Reference</th>
<th>$E_R = 46.26 \text{ eV}$</th>
<th>$E_R = 47.80 \text{ eV}$</th>
<th>$100 \times n_{\text{FIT}}/n$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\Gamma_n / \text{meV}$</td>
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<td>$\Gamma_n / \text{meV}$</td>
</tr>
<tr>
<td>ENDF/B - VI.8</td>
<td>154</td>
<td>115</td>
<td>109.7 (0.5)</td>
</tr>
<tr>
<td>JENDL - 3.3</td>
<td>154</td>
<td>119</td>
<td>111.3 (0.5)</td>
</tr>
<tr>
<td>ENDF/B - VII.1</td>
<td>154 (0.8)</td>
<td>119 (1.2)</td>
<td>111.3 (1.1)</td>
</tr>
<tr>
<td>JEFF - 3.2</td>
<td>163.4</td>
<td>120.8</td>
<td>100.2 (0.5)</td>
</tr>
</tbody>
</table>

Overestimation of $n$ compensates for underestimation of $\Gamma_n$
Impact of sample characteristics

Declared: \( n_W = (1.084 \pm 0.014) \times 10^{-3} \text{ at/b} \)

\( T_M \) (hom.): \( n_W = (0.939 \pm 0.003) \times 10^{-3} \text{ at/b} \)

Heterogeneous sample:

\[
\bar{T} = \int T(n') p(n') dn' = \int e^{-n'} \sigma_{\text{tot}} p(n') dn'
\]

\( \neq \)

\[
T(\bar{n}) = e^{-\bar{n}} \sigma_{\text{tot}}
\]

Similar bias effects:

- when determining RP from such samples (\( \Gamma_n \) underestimated)
- integral reactor experiments with powder samples

\( \text{natW}-\text{powder mixed with natS-powder} \)

(80 cm diameter, 14 g \( \text{natW} \), 3.5 g \( \text{natS} \))
Impact of sample characteristics

Declared: \( n_W = (1.084 \pm 0.014) \times 10^{-3} \text{ at/b} \)

\( T_M \) (hom.): \( n_W = (0.939 \pm 0.003) \times 10^{-3} \text{ at/b} \)

\( T_M \) (inhom.): \( n_W = (1.096 \pm 0.003) \times 10^{-3} \text{ at/b} \)

\[ \overline{T} = \int T(n')p(n')dn' = \int e^{-n'} \sigma_{\text{tot}} p(n')dn' \]

LP Model

Levermore, Pomraning et al., J. Math. Phys. 27, 2526, 1986

Implemented in REFIT


\( T_M \): REFIT + JEFF 3.2

\( \text{nat} W \)-powder mixed with \( \text{nat} S \)-powder

(80 cm diameter, 14 g \( \text{nat} W \), 3.5 g \( \text{nat} S \))
Summary & conclusions

- Methods to produce and report \((Z_{\text{exp}}, V_{Z_{\text{exp}}})\) well established

- \((RP ,V_{RP})\) in URR: well understood

- \((RP ,V_{RP})\) in RRR:
  - Covariances (including correlations) depend on the experimental conditions!
  - Main problem: propagate the covariance of experimental parameters
  - GLSQ + CUP: relies on a perfect model (reaction and experiment)
    - Requires verification of the quality of the model
  - GLSQ + MC: conservative
    - Recommended when quality of the experimental model cannot be verified

- Transmission measurements on homogeneous well-characterized samples can be considered as one of the most accurate integral experiments to validate cross data in the RRR.

- Data obtained with powder samples might be strongly biased!