Temperature-Dependent Propagation of Resonance Parameter Uncertainty

Isaac Meyer\textsuperscript{a}
Advisor: Benoit Forget\textsuperscript{a}
Lab Mentor: Andrew Holcomb\textsuperscript{b}

\textsuperscript{a} Massachusetts Institute of Technology
\textsuperscript{b} Oak Ridge National Laboratory

Nuclear Criticality Safety Program Technical Program Review
February 15, 2022
Neutronic simulation allows engineering of safe and economic systems

- Nuclear data alone can cause between 1% and 3% uncertainty on $k_{eff}$ in criticality safety benchmarks.

- Accurately assessing the uncertainty from nuclear data is essential for both safety and improving nuclear data libraries.

- Nuclear systems in general span a broad range of temperatures which can affect neutron behavior.

---

1 Uncertainty Quantification in the Resolved Resonance Region

2 One Group/One Resonance Model

3 PUFF-IV Implementation

4 Benchmark
The path of resonance parameter data

KENO $\rightarrow k, \phi$

TSUNAMI $\rightarrow \Delta k, \Delta \phi$
The path of resonance parameter data

KENO $\rightarrow k, \phi$

TSUNAMI $\rightarrow \Delta k, \Delta \phi$

AMPX/PUFF
Propagation of nuclear data uncertainty with coarse groups makes approximations

- Uncertainties are subject to the same limitations as continuous energy cross sections when formed into groups
- Evaluation at a single temperature and use at higher temperatures
- Requires knowledge of a flux for condensing cross sections
1 Uncertainty Quantification in the Resolved Resonance Region

2 One Group/One Resonance Model

3 PUFF-IV Implementation

4 Benchmark
Parameters were chosen such that the capture cross section relative error $\approx 5\%$ at 300 K.
The ratio between the relative standard deviations (red) shows that incorporating temperature effects causes a change in relative standard deviation across the energy range.
6-8 eV Capture Group Reaction Rate for single resonance

For a fixed dilution of $\sigma_d = 0$ barns
6-8 eV Capture Group Reaction Rate for single resonance

For a fixed temperature of 300 K
1 Uncertainty Quantification in the Resolved Resonance Region

2 One Group/One Resonance Model

3 PUFF-IV Implementation

4 Benchmark
Evaluating groupwise uncertainty from cross section parameters - temperature considerations

\[
\text{Cov} (x^m_I, x^l_J) = \frac{1}{\Phi_I \Phi_J} \sum_{kn} \int_I \int_J \Phi(E, T) \Phi(E', T) \left( \frac{\partial \sigma_m(E, T)}{\partial P_k} \right) \text{Flux} \left( \text{Flux} \right) \left( \text{RP Sensitivity} \right) \left( \text{RP Covariance} \right) \text{Cov} (\delta P_k, \delta P_n) \frac{\partial \sigma_j(E', T)}{\partial P_n} dEdE'
\]
Evaluating groupwise uncertainty from cross section parameters - temperature considerations

\[
\text{Cov} (x^m_I, x^l_J) = \frac{1}{\Phi_I \Phi_J} \sum_{kn} \int_I \int_J \Phi(E, T) \Phi(E', T) \underbrace{\frac{\partial \sigma_m(E, T)}{\partial P_k}}_{\text{RP Sensitivity}} \underbrace{\text{Cov}(\delta P_k, \delta P_n)}_{\text{RP Covariance}} \underbrace{\frac{\partial \sigma_j(E', T)}{\partial P_n}}_{\text{RP Sensitivity}} dEdE'
\]

\[
\frac{\partial \sigma_m(E, T)}{\partial P_k}
\]

can be quite large: (Number of Resonance Parameters * Number of Reactions) continuous energy cross-section sized arrays
Calculating resonance parameter sensitivities in AMPX

Algorithm 1: PUFF-IV Pseudocode

1: for Energy Region $E$ do
2:   Calculate extension of energy region
3:   Calculate 0K $\frac{d\sigma}{dT}$
4:   Broaden to $T$ and store
5:   Integrate over original energy region (recently improved)
6:   Discard $\frac{d\sigma}{dT}(T)$
7: end for
Calculating resonance parameter sensitivities in AMPX

Na-23 Elastic Cross Section Sensitivity to $\Gamma_n$ for $E_r = 3.54 \times 10^4$ eV

Meyer
1 Uncertainty Quantification in the Resolved Resonance Region

2 One Group/One Resonance Model

3 PUFF-IV Implementation

4 Benchmark
Table 6. Solution Properties.

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Uranium Concentration (grams/liter)</th>
<th>Gadolinium Concentration (grams/liter)</th>
<th>Solution Density (g/cm³)</th>
<th>Total NO₃⁻ Concentration (moles/liter)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>156.5 ± 0.8</td>
<td>0.0</td>
<td>1.210 ± 0.001</td>
<td>1.57 ± 0.02</td>
</tr>
<tr>
<td>2</td>
<td>143.6 ± 0.7</td>
<td>0.300 ± 0.015</td>
<td>1.195 ± 0.001</td>
<td>1.44 ± 0.02</td>
</tr>
<tr>
<td>3</td>
<td>144.2 ± 0.7</td>
<td>0.525 ± 0.020</td>
<td>1.196 ± 0.001</td>
<td>1.46 ± 0.02</td>
</tr>
</tbody>
</table>

In all cases:
- $R_3 = 30.1$ cm
- $H_1 = 40.0$ cm
- $R_4 = 30.6$ cm
- $H_2 = 41.6$ cm
- $H_r = 150.0$ cm

Meyer
Gd Sensitivity from KENOV

G-157 mt=101 capture (region integrated)

Density of materials left constant across runs
157 Gd Multigroup Capture Cross Section Uncertainty (1000 Groups)

The graph shows the cross-section in barns for 

\[ \text{Gd}_{157} \text{Gd}_{157} \text{ MT}=102 \]

as a function of energy (eV) with relative standard deviation (%). The graph includes data points for different energies and shows the cross-section variation over a range of energies from \(10^{-5} \text{ eV} \) to \(10^2 \text{ eV} \).
157 Gd Multigroup Capture Cross Section Uncertainty (1000 Groups)
Temperature Impacts Both Reaction Sensitivities and Multigroup Uncertainties
Uncertainty - $^{157}$Gd Capture

<table>
<thead>
<tr>
<th>Groups</th>
<th>Temperature (K)</th>
<th>300</th>
<th>600</th>
<th>900</th>
<th>1200</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td></td>
<td>0.62398</td>
<td>0.53350</td>
<td>0.47246</td>
<td>0.47051</td>
</tr>
<tr>
<td>100</td>
<td></td>
<td>0.62398</td>
<td>0.53350</td>
<td>0.47246</td>
<td>0.47051</td>
</tr>
<tr>
<td>250</td>
<td></td>
<td>0.62399</td>
<td>0.53350</td>
<td>0.47246</td>
<td>0.47051</td>
</tr>
<tr>
<td>500</td>
<td></td>
<td>0.62399</td>
<td>0.53350</td>
<td>0.47246</td>
<td>0.47051</td>
</tr>
<tr>
<td>1000</td>
<td></td>
<td>0.62399</td>
<td>0.53351</td>
<td>0.47246</td>
<td>0.47051</td>
</tr>
<tr>
<td>scale (252)</td>
<td></td>
<td>0.62504</td>
<td>0.53731</td>
<td>0.47601</td>
<td>0.47398</td>
</tr>
</tbody>
</table>
Conclusion

A demonstration of a single resonance shows variation of uncertainty over temperature and dilution.

The proper accounting of temperature in resonance parameter uncertainty propagation may increase or reduce integral parameter error.

Assessing whether or not the temperature approximation of multigroup data conservative is important for safety calculations.

Future Work

Gauge the impact of this treatment on actinides and other benchmarks: $^{235}\text{U}$, $^{238}\text{U}$, $^{239}\text{Pu}$.
Acknowledgements

Thanks to

- My advisor: Ben Forget
- My lab mentor: Andrew Holcomb

This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.
$^{157}Gd$ Sensitivity from KENOV

Gd-157 mt=2 elastic (region integrated)

Density of materials left constant across runs
157 Gd MG Cross Section Uncertainty

![Graph showing the cross section of 157 Gd as a function of energy (eV) with relative standard deviation (%). The graph displays data at different energies (10^3, 10^4, 10^5, 10^6, 10^7) and cross sections (10^1, 10^2, 10^3, 10^4). The graph includes a legend for different energy levels (300, 600, 900, 1200) and a key for cross section values.]
<table>
<thead>
<tr>
<th>Groups</th>
<th>%(dk/k)</th>
<th>Temperature (K)</th>
<th>300</th>
<th>600</th>
<th>900</th>
<th>1200</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>0.000033</td>
<td>0.000032</td>
<td>0.000032</td>
<td>0.000031</td>
<td></td>
<td></td>
</tr>
<tr>
<td>100</td>
<td>0.000033</td>
<td>0.000033</td>
<td>0.000033</td>
<td>0.000032</td>
<td></td>
<td></td>
</tr>
<tr>
<td>250</td>
<td>0.000032</td>
<td>0.000032</td>
<td>0.000032</td>
<td>0.000031</td>
<td></td>
<td></td>
</tr>
<tr>
<td>500</td>
<td>0.000031</td>
<td>0.000031</td>
<td>0.000031</td>
<td>0.000030</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1000</td>
<td>0.000028</td>
<td>0.000029</td>
<td>0.000028</td>
<td>0.000028</td>
<td></td>
<td></td>
</tr>
<tr>
<td>scale (252)</td>
<td>0.000003</td>
<td>0.000030</td>
<td>0.000030</td>
<td>0.000040</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Evaluation of groupwise covariance matrix

Na23 MT=102 Covariance Matrices

0 K, 999 Group

900 K, 999 Group

Energy (eV)

Absolute Difference

Relative Difference (%)
Evaluation of groupwise covariance matrix

Na23 MT=2 Covariance Matrices

0 K, 999 Group

900 K, 999 Group

Meyer

30
Uncertainty propagation with group condensation

\[ \Sigma_{g,r}(\sigma_\gamma, \sigma_s) = \frac{\int_I \phi(E) \sigma_r(E) dE}{\int_I \phi(E) dE} \quad \phi_{NR}(E_i) = \frac{1}{E_i} \frac{\sigma_p + \sigma_d}{\sigma_{\gamma,i} + \sigma_{s,i} + \sigma_p + \sigma_d} \]

**Total Monte Carlo**

- New flux evaluated for each set of sampled parameters

**Sensitivity**

- Need to evaluate the influence of resonance parameters on the flux as well as the individual cross sections

\[ \text{Cov}(\Sigma_{g,\gamma}) = \frac{\partial \Sigma_{g,\gamma}}{\partial \sigma_\gamma} \text{Cov}(\sigma_\gamma) \frac{\partial \Sigma_{g,\gamma}}{\partial \sigma_\gamma}^T + \frac{\partial \Sigma_{g,\gamma}}{\partial \sigma_s} \text{Cov}(\sigma_s) \frac{\partial \Sigma_{g,\gamma}}{\partial \sigma_s}^T + \frac{\partial \Sigma_{g,\gamma}}{\partial \sigma_\gamma} \text{Cov}(\sigma_\gamma, \sigma_s) \frac{\partial \Sigma_{g,\gamma}}{\partial \sigma_s}^T \]
## Parameter Values

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Manufactured Standard Deviation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>6.673491 eV</td>
<td>0.0015</td>
</tr>
<tr>
<td>$J$</td>
<td>0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>$\Gamma_n$</td>
<td>$1.475792 \times 10^{-3}$ eV</td>
<td>4.79</td>
</tr>
<tr>
<td>$\Gamma_\gamma$</td>
<td>$2.30 \times 10^{-2}$ eV</td>
<td>1.94</td>
</tr>
<tr>
<td>$\Gamma_{\text{fission}}$</td>
<td>$9.990 \times 10^{-9}$ eV</td>
<td>0.0</td>
</tr>
</tbody>
</table>
Scattering Cross Section: continuous uncertainty from resonance parameters

**Cross Section**

Cross Section [barns]

**Ratio of Cross Sections (High T/Low T)**

**Relative Standard Deviation**

**Ratio of Relative Standard Deviation (High T/Low T)**

Meyer

33
6-8 eV Group Scatter Cross Section: 0 barns dilution, Function of T
6-8 eV Group Capture Cross Section: 0 barns dilution, Function of T
6-8 eV Group Capture Cross Section: 300 K, Function of Dilution
Capture Cross Section: continuous uncertainty from resonance parameters

- Doppler broadening performed using $\psi/\chi$ approximation
Comparison to real cross section data

![Graphs showing relative uncertainty vs incident energy for ENDF/B-VIII.0: U-238(N,G)U-239]