Temperature-Dependent Propagation of Resonance Parameter Uncertainty

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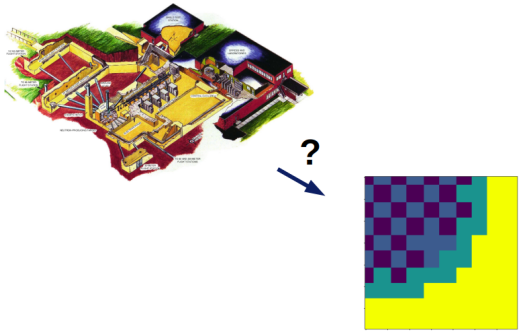
Neutronic simulation allows engineering of safe and economic systems

- Nuclear data alone can cause between 1% and 3% uncertainty on k_{eff} in criticality safety benchmarks [1]
- 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] Saylor, Ellen Marie, Marshall, William J., Clarity, Justin B., Clifton, Zia, and Rearden, Bradley T.. Criticality Safety Validation of SCALE 6.2.2. United States: N. p., 2018. Web. doi:10.2172/1479759.

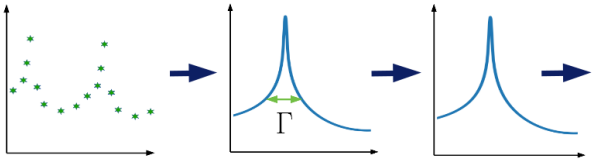
1 Uncertainty Quantification in the Resolved Resonance Region

2 One Group/One Resonance Model

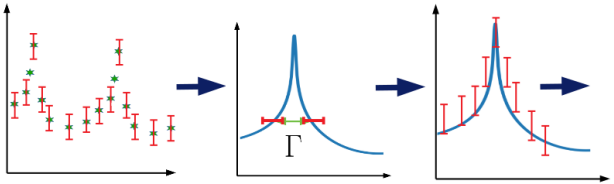
3 PUFF-IV Implementation

4 Benchmark

The path of resonance parameter data

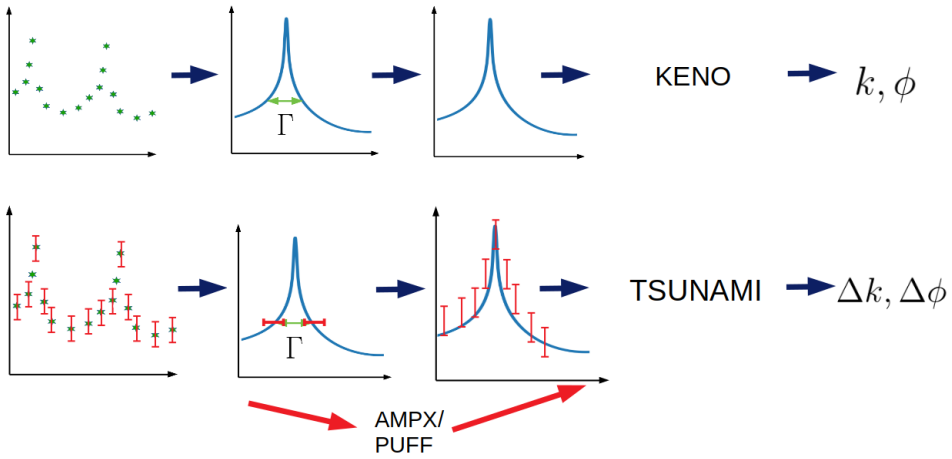


KENO → k, ϕ



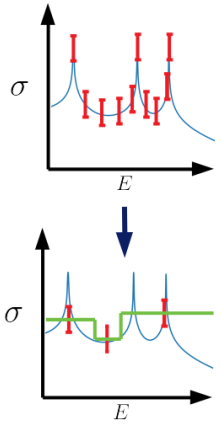
TSUNAMI → $\Delta k, \Delta \phi$

The path of resonance parameter data



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



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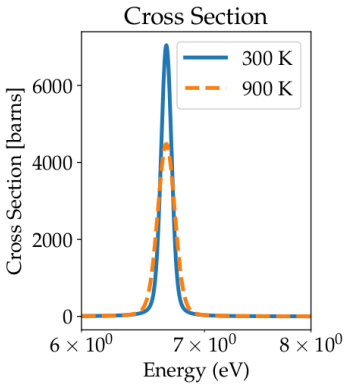
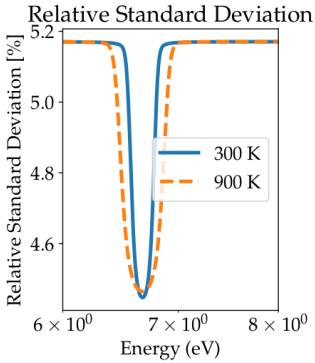
Capture Cross Section: continuous uncertainty from resonance parameters

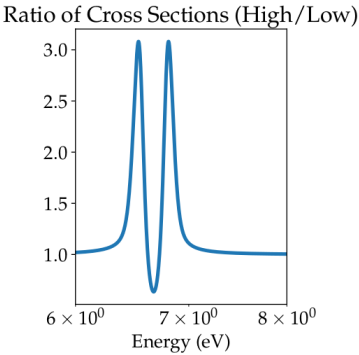
- Parameters were chosen such that the capture cross section relative error $\approx 5\%$ at 300 K

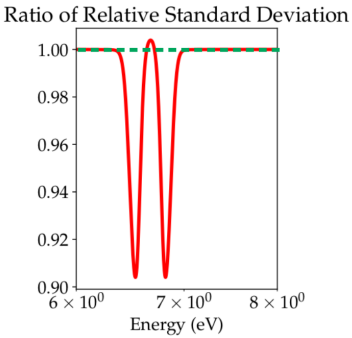




Capture Cross Section: continuous uncertainty from resonance parameters

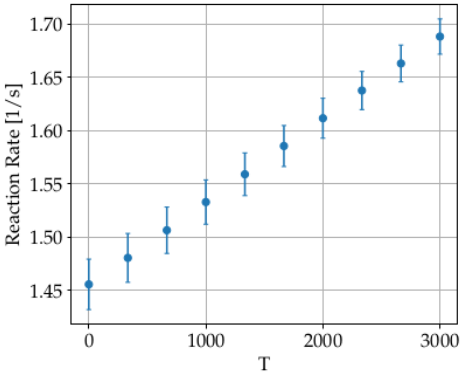
- The ratio between the relative standard deviations (red) shows that incorporating temperature effects causes a change in relative standard deviation across the energy range

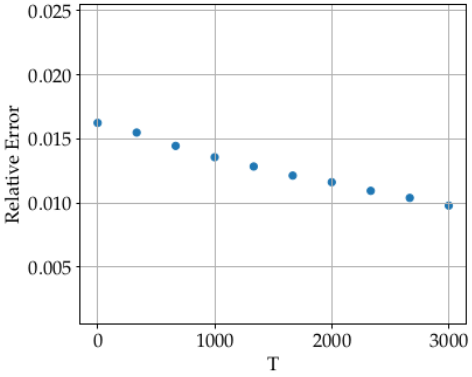




6-8 eV Capture Group Reaction Rate for single resonance

For a fixed dilution of $\sigma_d = 0$ barns





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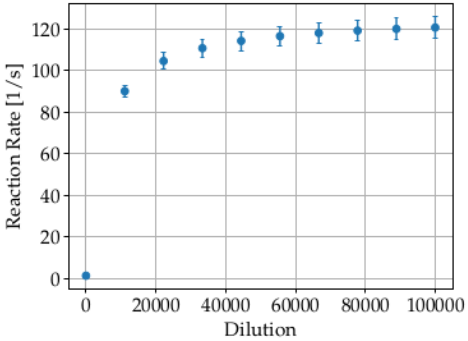
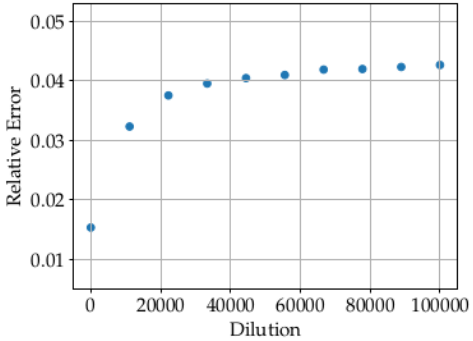
For a fixed temperature of 300 K





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Evaluating groupwise uncertainty from cross section parameters - temperature considerations

$$\mathrm{Cov}\left(x_I^m, x_J^l\right) =$$

$$\frac{1}{\Phi_I \Phi_J} \sum_{kn} \int_I \int_J \underbrace{\Phi(E,T)\Phi\left(E',T\right)}_{\text{Flux}} \overbrace{\frac{\partial \sigma_m(E,T)}{\partial P_k}}^{\text{RP Sensitivity}} \underbrace{\mathrm{Cov}\left(\delta P_k, \delta P_n\right)}_{\text{RP Covariance}} \frac{\partial \sigma_j(E',T)}{\partial P_n} dE dE'$$

Evaluating groupwise uncertainty from cross section parameters - temperature considerations

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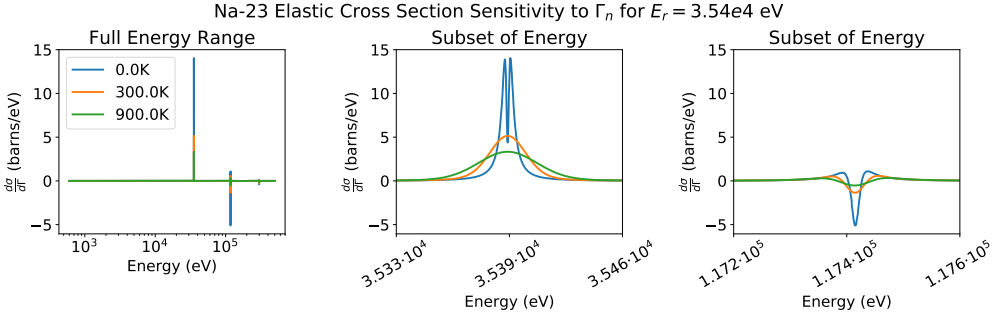
$\frac{\partial \sigma_m(E,T)}{\partial P_k}$ can be quite large: (Number of Resonance Parameters * Number of Reactions) continuous energy cross-section sized arrays

Calculating resonance parameter sensitivities in AMPX

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

Algorithm 1: PUFF-IV Pseudocode

Calculating resonance parameter sensitivities in AMPX



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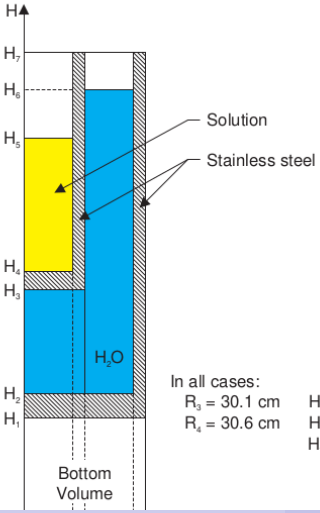
Application to HEU-SOL-THERM-016-03 ^{157}Gd Propagation



In all cases:

$R_3 = 30.1$ cm $\quad H_1 = 40.0$ cm

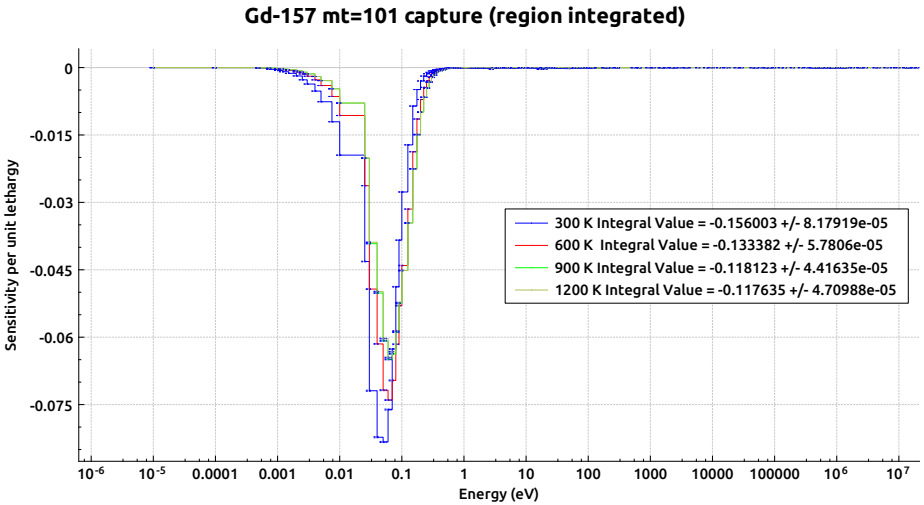
$R_4 = 30.6$ cm $\quad H_2 = 41.6$ cm

$H_7 = 160.0$ cm

Table 6. Solution Properties.

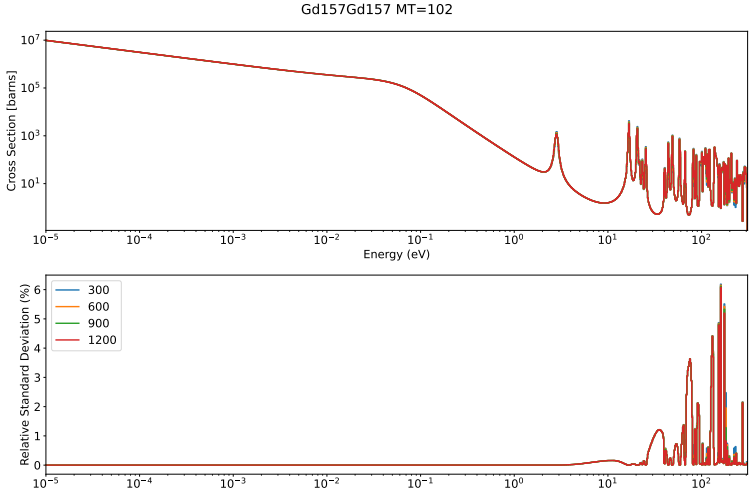
Case No.	Uranium Concentration (grams/liter)	Gadolinium Concentration (grams/liter)	Solution Density (g/cm^3)	Total NO_3^- Concentration (moles/liter)
1	156.5 ± 0.8	0.0	1.210 ± 0.001	1.57 ± 0.02
2	143.6 ± 0.7	0.300 ± 0.015	1.195 ± 0.001	1.44 ± 0.02
3	144.2 ± 0.7	0.525 ± 0.020	1.196 ± 0.001	1.46 ± 0.02

^{157}Gd Sensitivity from KENOV



Density of materials left constant across runs

^{157}Gd Multigroup Capture Cross Section Uncertainty (1000 Groups)



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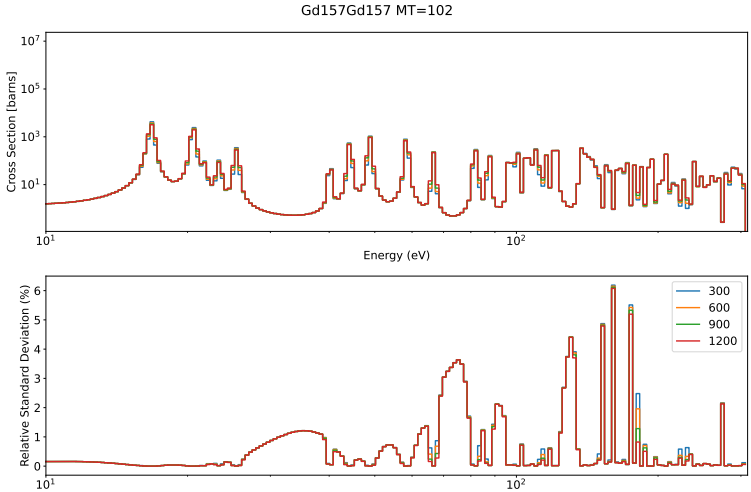
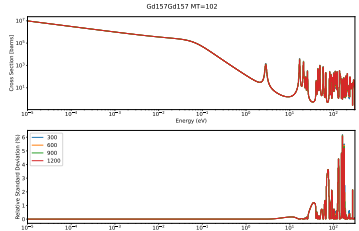
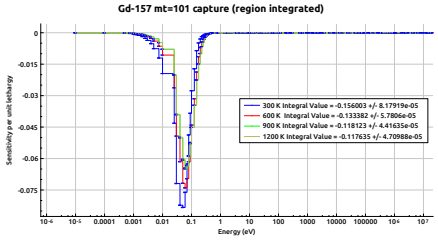


Temperature Impacts Both Reaction Sensitivities and Multigroup Uncertainties





k Uncertainty - ^{157}Gd Capture

		Temperature (K)			
	$\%dk/k$	300	600	900	1200
Groups	50	0.62398	0.53350	0.47246	0.47051
	100	0.62398	0.53350	0.47246	0.47051
	250	0.62399	0.53350	0.47246	0.47051
	500	0.62399	0.53350	0.47246	0.47051
	1000	0.62399	0.53351	0.47246	0.47051
	scale (252)	0.62504	0.53731	0.47601	0.47398

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}U, ^{238}U, ^{239}Pu

Acknowledgements

Thanks to

- My advisor: Ben Forget
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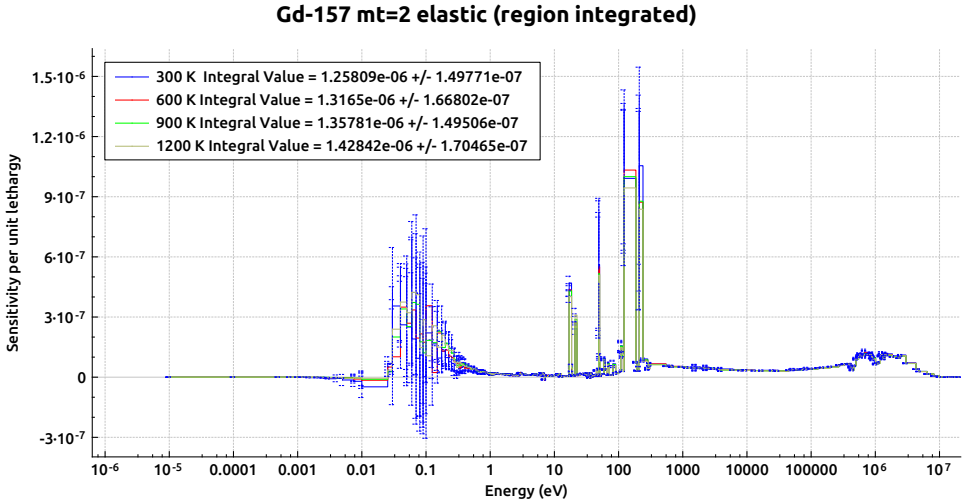
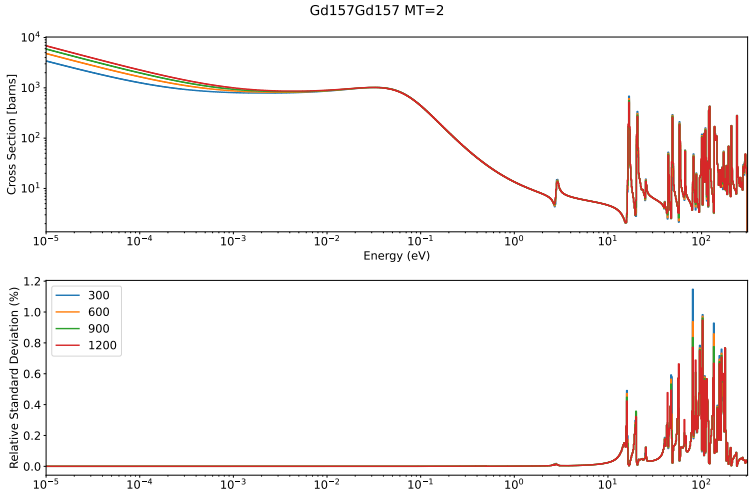
Backup slides

^{157}Gd Sensitivity from KENOV



Density of materials left constant across runs

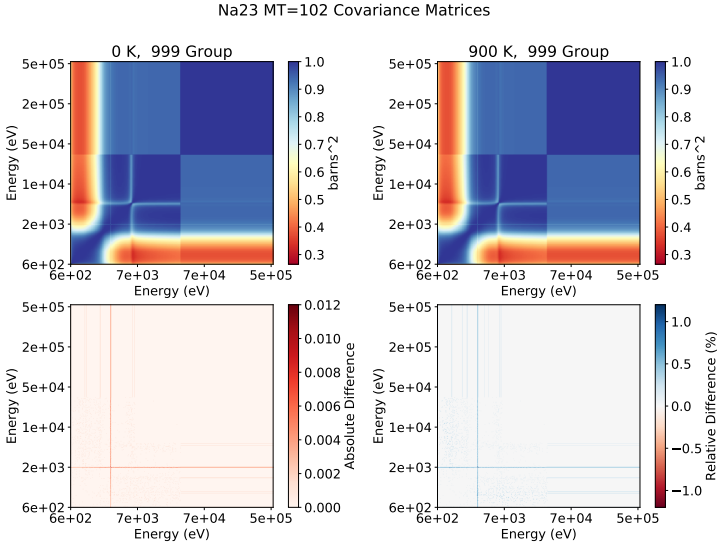
^{157}Gd MG Cross Section Uncertainty



k Uncertainty - ^{157}Gd Elastic

		Temperature (K)			
	$\%dk/k$	300	600	900	1200
Groups	50	0.000033	0.000032	0.000032	0.000031
	100	0.000033	0.000033	0.000033	0.000032
	250	0.000032	0.000032	0.000032	0.000031
	500	0.000031	0.000031	0.000031	0.000030
	1000	0.000028	0.000029	0.000028	0.000028
	scale (252)	0.000003	0.000003	0.000003	0.000004

Evaluation of groupwise covariance matrix



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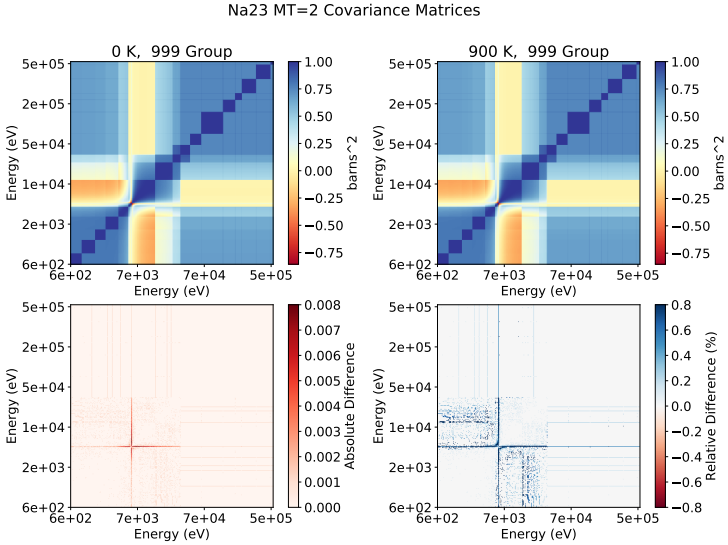


Uncertainty propagation with group condensation

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

Total Monte Carlo

- New flux evaluated for each set of sampled parameters

Sensitivity

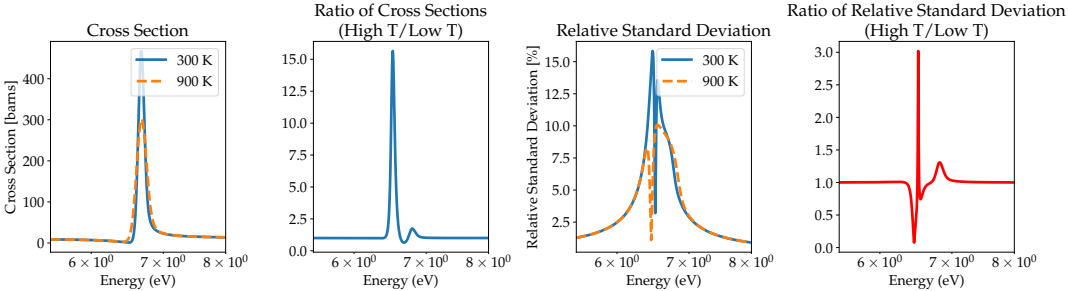
- Need to evaluate the influence of resonance parameters on the flux as well as the individual cross sections

$$\mathrm{Cov}(\Sigma_{g,\gamma}) = \frac{\partial\Sigma_{g,\gamma}}{\partial\sigma_\gamma}\mathrm{Cov}(\sigma_\gamma)\frac{\partial\Sigma_{g,\gamma}}{\partial\sigma_\gamma}^T + \frac{\partial\Sigma_{g,\gamma}}{\partial\sigma_s}\mathrm{Cov}(\sigma_s)\frac{\partial\Sigma_{g,\gamma}}{\partial\sigma_s}^T + \frac{\partial\Sigma_{g,\gamma}}{\partial\sigma_\gamma}\mathrm{Cov}(\sigma_\gamma,\sigma_s)\frac{\partial\Sigma_{g,\gamma}}{\partial\sigma_s}^T$$

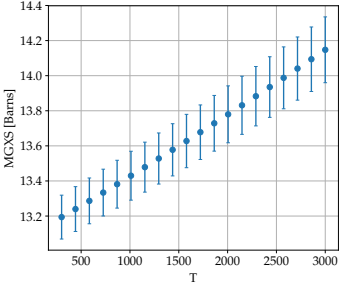
Parameter Values

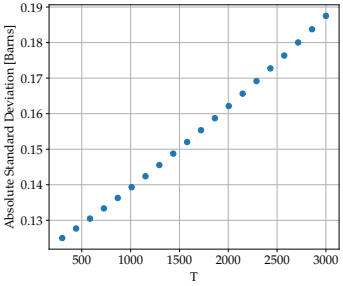
Parameter	Value	Manufactured Standard Deviation (%)
E	6.673491 eV	.0015
J	0.5	0.0
Γ_n	$1.475792\ 10^{-3}$ eV	4.79
Γ_γ	$2.30\ 10^{-2}$ eV	1.94
$\Gamma_{fission}$	$9.990\ 10^{-9}$ eV	0.0

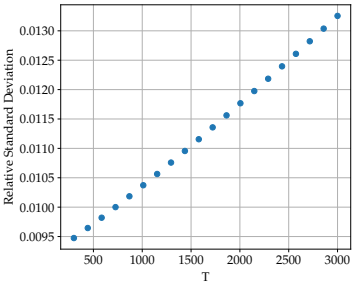
Scattering Cross Section: continuous uncertainty from resonance parameters



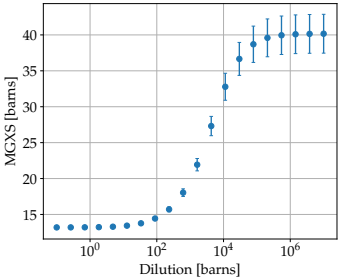
6-8 eV Group Scatter Cross Section: 0 barns dilution, Function of T

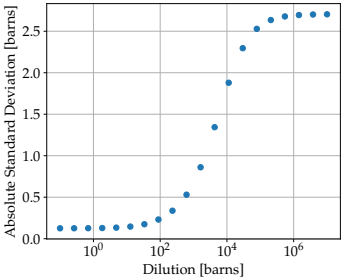


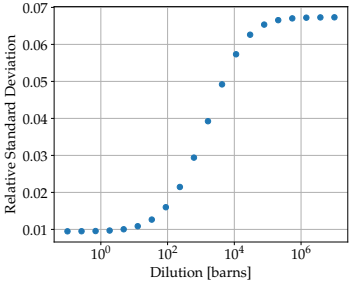




6-8 eV Group Scatter Cross Section: 300 K, Function of Dilution







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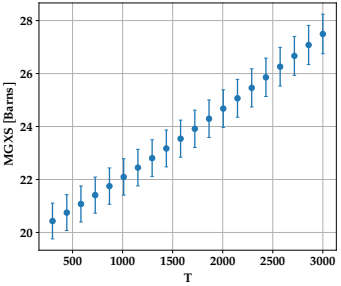

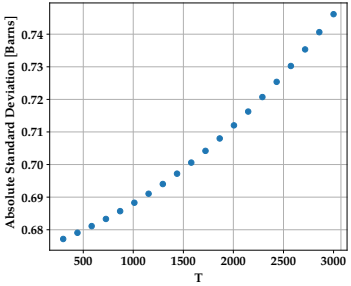

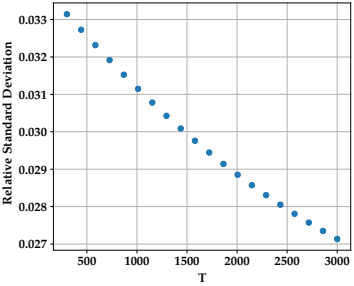

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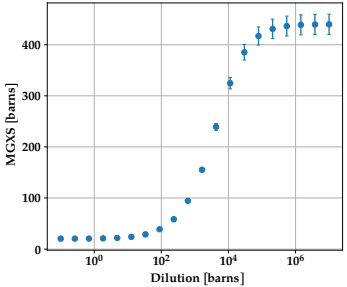
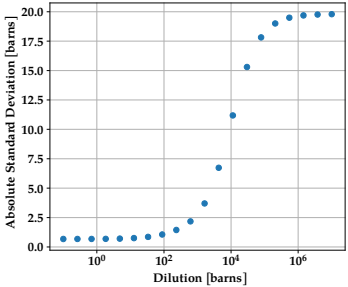
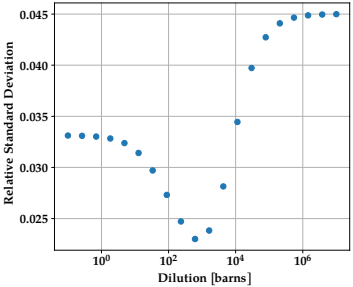
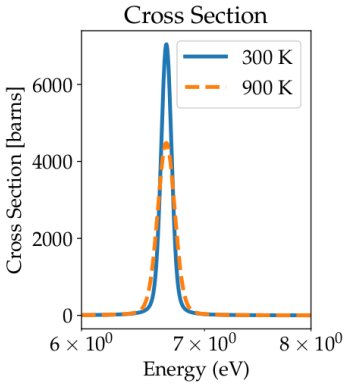
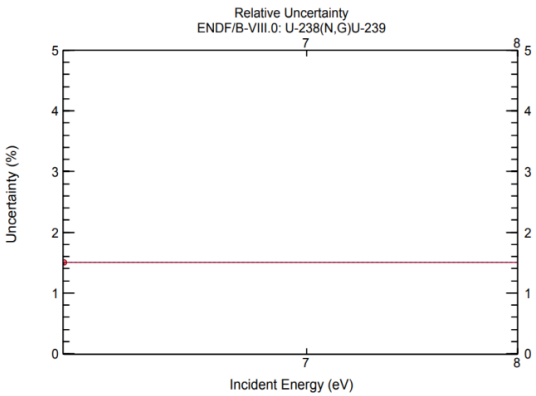
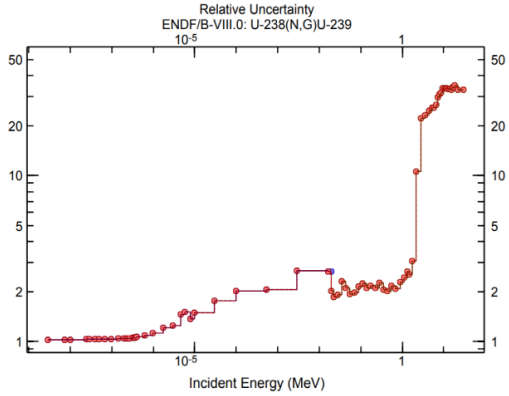






Capture Cross Section: continuous uncertainty from resonance parameters

- Doppler broadening performed using ψ/χ approximation



Comparison to real cross section data