Uncertainty quantification for activation cross sections

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Cross section evaluations

Region	Knowledge	Approach
Stable and very long-lived isotopes	Direct measurements of cross–sections, all structure details	Direct fit to measurements, R-matrix fits, fine-tuned models
Intermediate region, $T_{1/2}$ ~ seconds, minutes	Masses, lifetimes, some excited states, average level spacings	"Regional evaluations"
Very exotic, very short-live nuclei	Z,A, theoretical binding energies	Global systematics, global structure models (RPA, DFT)

ENDF, JEFF, JENDL …
s-process, reactors

Well-defined uncertainties, detailed covariances

Supernovae, neutron-bursts, Material activation

?

Astrophysics libraries
R-process nucleosynthesis

Strong model dependence, many parameters

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Very exotic, very short-live nuclei	Z,A, theoretical binding energies	Global systematics, global structure models (RPA, DFT)

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Update existing evaluations with robust UQ

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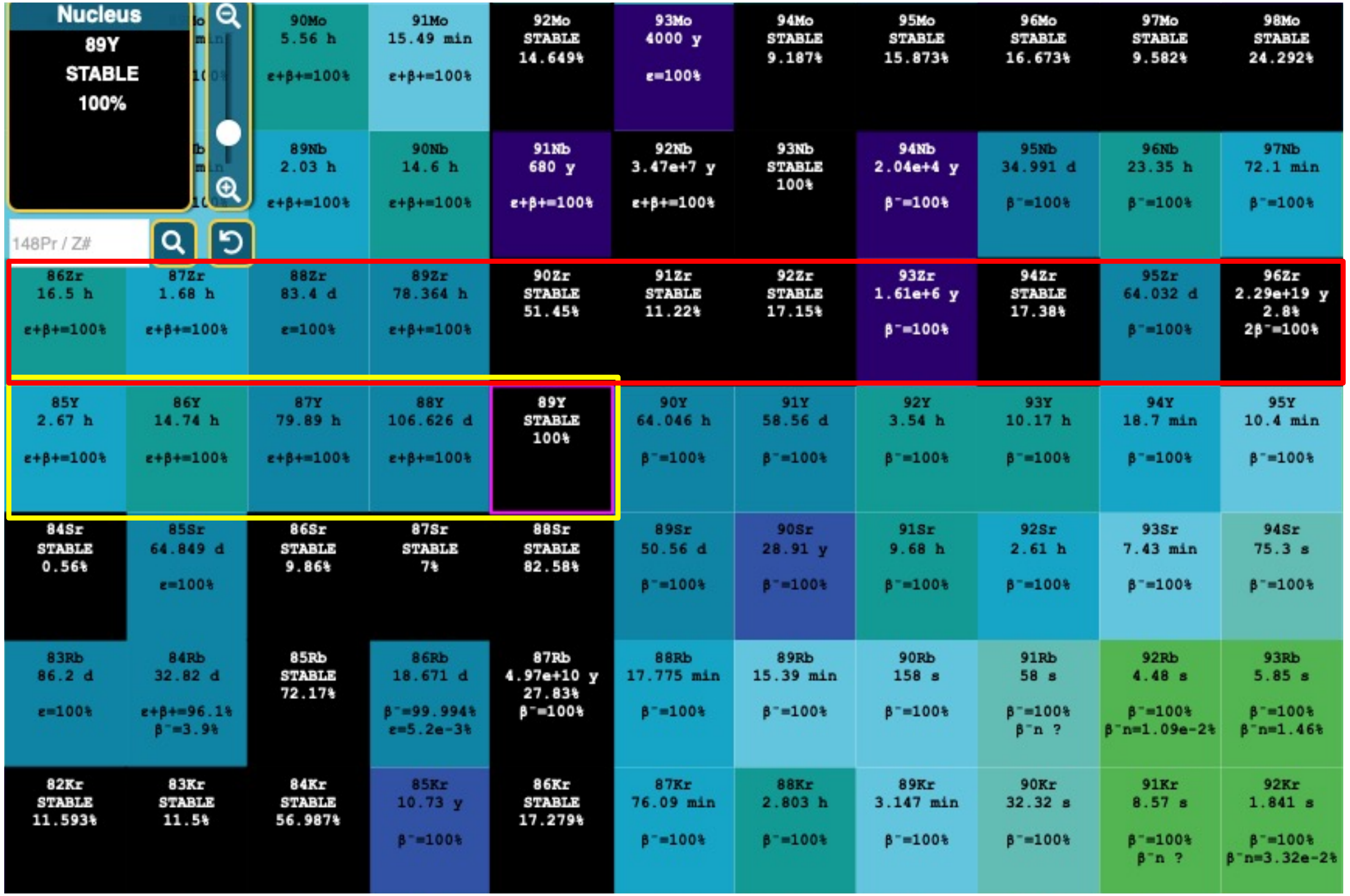
R-process nucleosynthesis

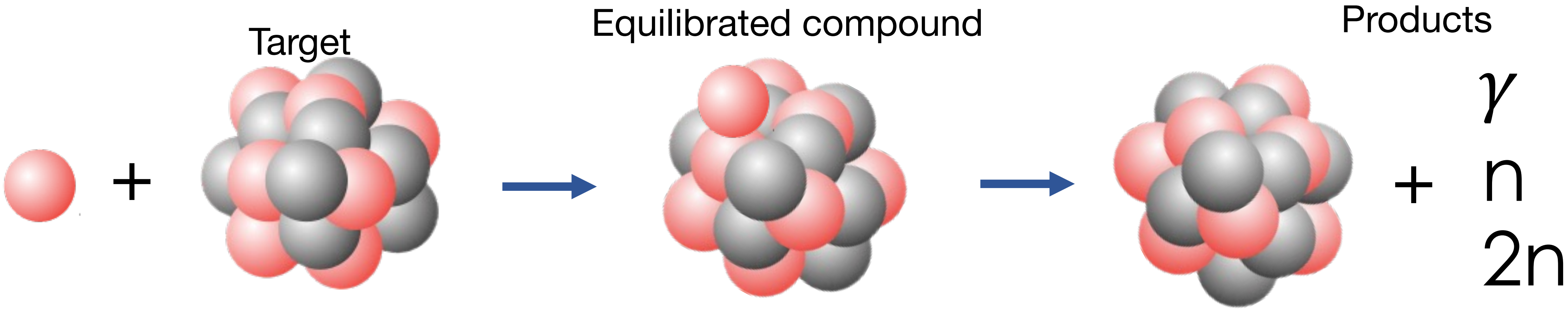
Strong model dependence, many parameters

Model parameters are experimentally determined for stable targets

- *Focus on transmutation (activation) cross sections for fast neutrons*
- Using Hauser-Feshbach statistical model (YAHFC)
- Experimental data (RIPL-3) that constrains model input:
  - Average level spacings D_0
  - Average radiative widths $\langle\Gamma_\gamma\rangle$
- Develop systematic trends of reaction model parameters
- measured cross sections for validation



The Hauser-Feshbach statistical model (HF)



$$\sigma_{jk} \sim \Sigma \frac{T_j \, T_k}{T_{tot}}$$

Model inputs can combine

- Experimental data
- Microscopic models
- Parameterizations

We use YAHFC *[E. Ormand et al.]*

https://github.com/LLNL/Yet-Another-Hauser-Feshbach-Code

- Experimental data (RIPL-3) that constrains model input:
  - Average level spacings D_0
  - Average radiative widths $\langle \Gamma_\gamma \rangle$
- Optical model with UQ: KDUQ

Nuclear Level Densities – low energy

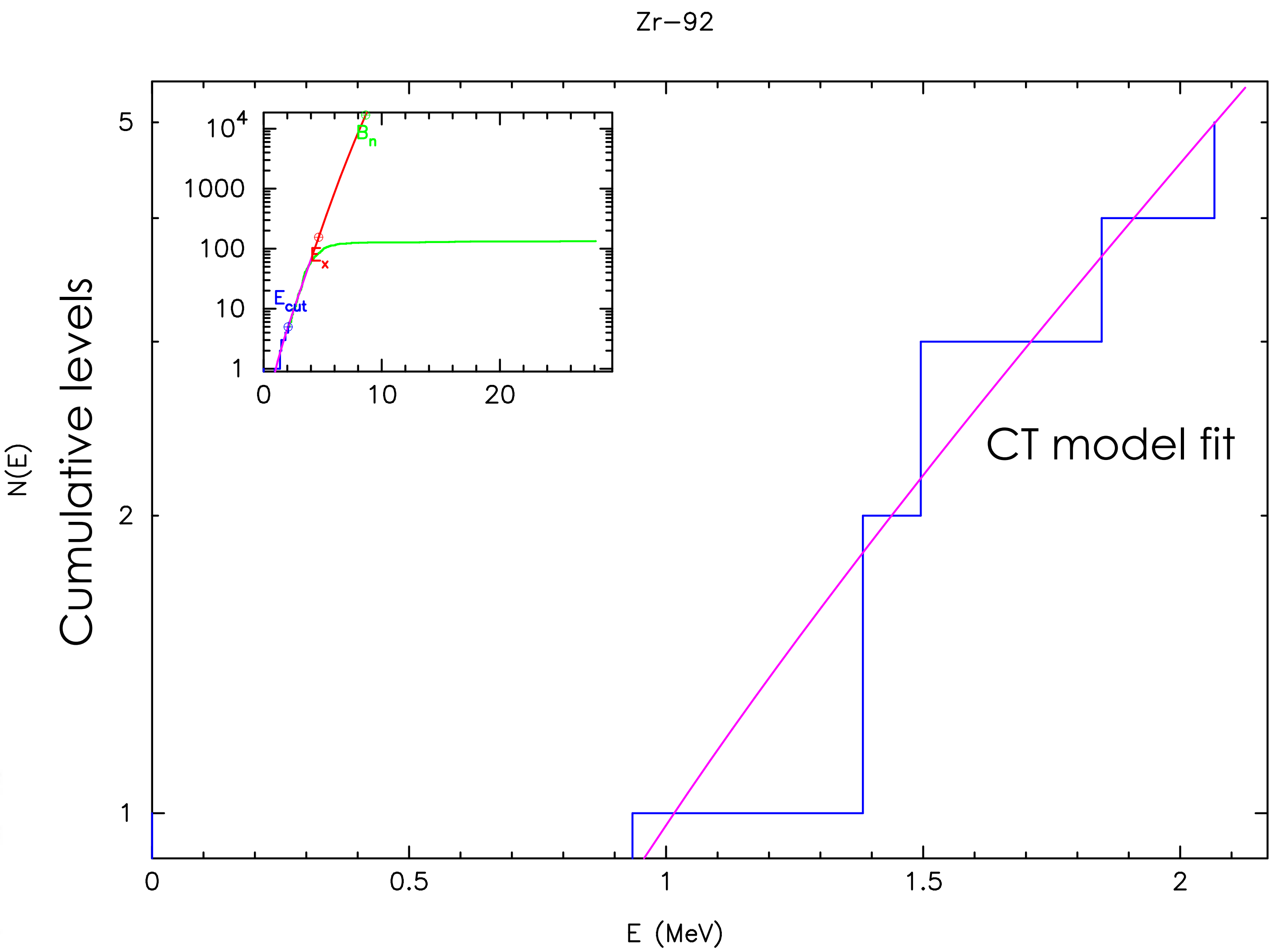
- At low incident particle energy the LD is calculated from the know spectroscopic levels, which increase exponentially.

- A constant temperature model is fit to these levels

$$N(E) = \exp\left[\frac{E - E_0}{T}\right]$$

- Observable level density is

$$\rho_2(E) = \frac{dN(E)}{dE} = \frac{1}{T}\exp\left[\frac{E - E_0}{T}\right]$$



Level densities: Back-shifted Fermi gas model

$$\rho_{FG}(E_x, J^\pi) = \frac{1}{12\sqrt{2}\sigma}\frac{\exp\left[2\sqrt{a\,U}\right]}{a^{1/4}U^{5/4}}P_J(E_x)P_\pi(E_x), \quad (2)$$

where $U = E_x - \Delta$ and $a = a(E_x)$ are functions of the excitation energy with the backshift Δ and *sigma* is the spin cutoff parameter. The latter also enters in in the angular momentum distribution

$$P_J(E_x) = \frac{2J+1}{2\sigma^2}\exp\left[-\frac{(J+1/2)^2}{2\sigma^2}\right]. \quad (3)$$

The spin cutoff σ is in principle a free parameter. However, in YAHFC, we assume the following relationship

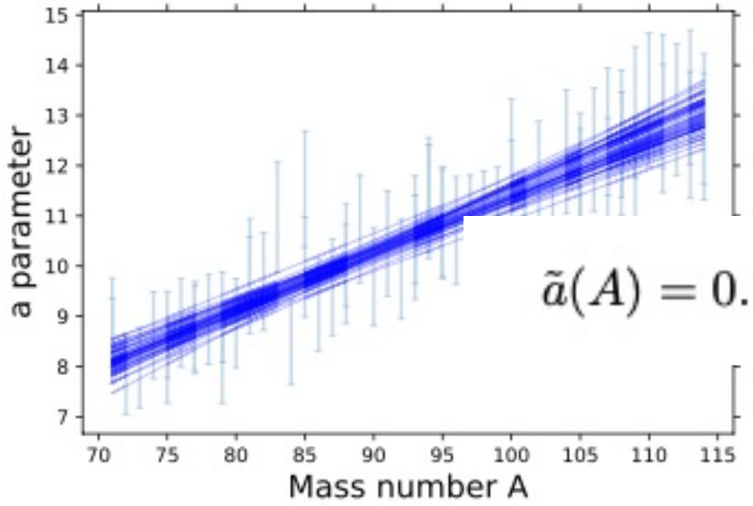
$$\sigma(E_x) = XA^{5/3}\sqrt{\frac{U}{a(U)}\frac{a(U)}{\tilde{a}}} \quad (4)$$

$$a(U,Z,N) = \tilde{a}(A)\left[1 + \delta W(Z,N)\frac{f(U)}{U}\right]$$

with

$$f(U) = 1 - \exp(-\gamma U)$$

- Back-shifted Fermi gas description:
  - Multiple parameters ($\Delta, \delta W, \tilde{a}, \sigma, \gamma$) are constrained by one experimental quantity: D_0
  - Keep fixed: σ, γ
  - Δ from comparison to mass formula
  - Parmetrized $\tilde{a}$
  - Fit δW to known D_0



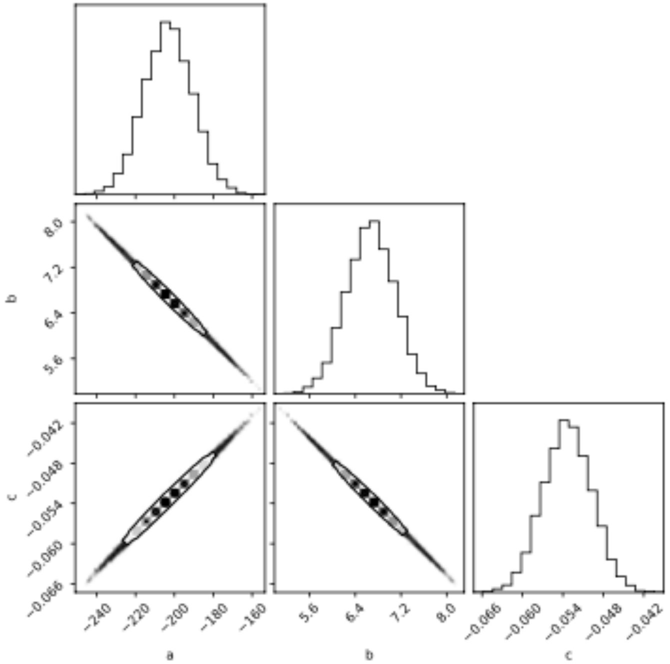
$$\tilde{a}(A) = 0.1744 + 0.11258 * A$$

Level Densities – shell corrections

- The fitted systematic is similar to hoffman:

N <= 50	N > 50
$c_0 = -364 \pm 70$	$c_0 = -202 \pm 12$
$c_1 = 17.2 \pm 3.0$	$c_1 = 6.67 \pm 0.43$
$c_2 = -0.20 \pm 0.03$	$c_2 = -0.053 \pm 0.004$

- Uncertainties represent the 1σ quantile of the distributions that results from the MC fitting procedure. Close to normal distributions.



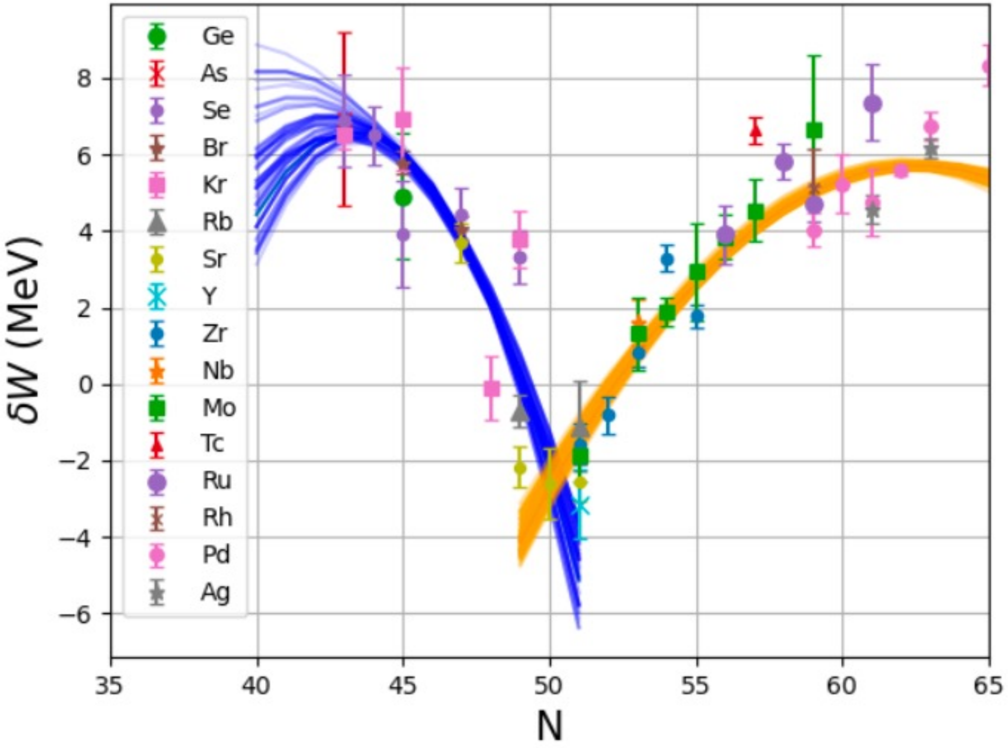


Figure 2: Results of the Monte-Carlo fitting procedure for the shell correction parameter δW.

Gamma-ray Transmission Coefficients

- γ-transmission coefficients calculated with a model that depends on multi-pole type (XL) and transition energy (ε) related to the γ-ray strength function

$$T^{\gamma}_{XL}(\epsilon) = 2\pi\epsilon^{2L+1} f^{\gamma}_{XL}(\epsilon)$$

- GDR model with enhanced generalized Lorentzian line shape

$$f^{\gamma}_{E1}(\epsilon) = \mathcal{N}\frac{4}{3\pi}\frac{e^2}{\hbar c}\frac{1}{M_p c^2} \times \left[\frac{\epsilon\Gamma_{GDR}(\epsilon, T_f)}{(\epsilon^2 - E^2_{GDR})^2 + (\Gamma_{GDR}(\epsilon, T_f)\epsilon)^2} + 0.7\frac{\Gamma_{GDR}(0, T_f)}{\epsilon^3}\right]$$

$$\langle\Gamma_\gamma\rangle_0 = \frac{J+1}{2J+1}\left\langle\Gamma_\gamma\left(B_n, J+\frac{1}{2}\right)\right\rangle + \frac{J}{2J+1}\left\langle\Gamma_\gamma\left(B_n, J-\frac{1}{2}\right)\right\rangle$$

$$\Gamma_\gamma(E, J) = \frac{T_\gamma(E, J)}{2\pi\rho(E, J)} \text{ (meV)}$$

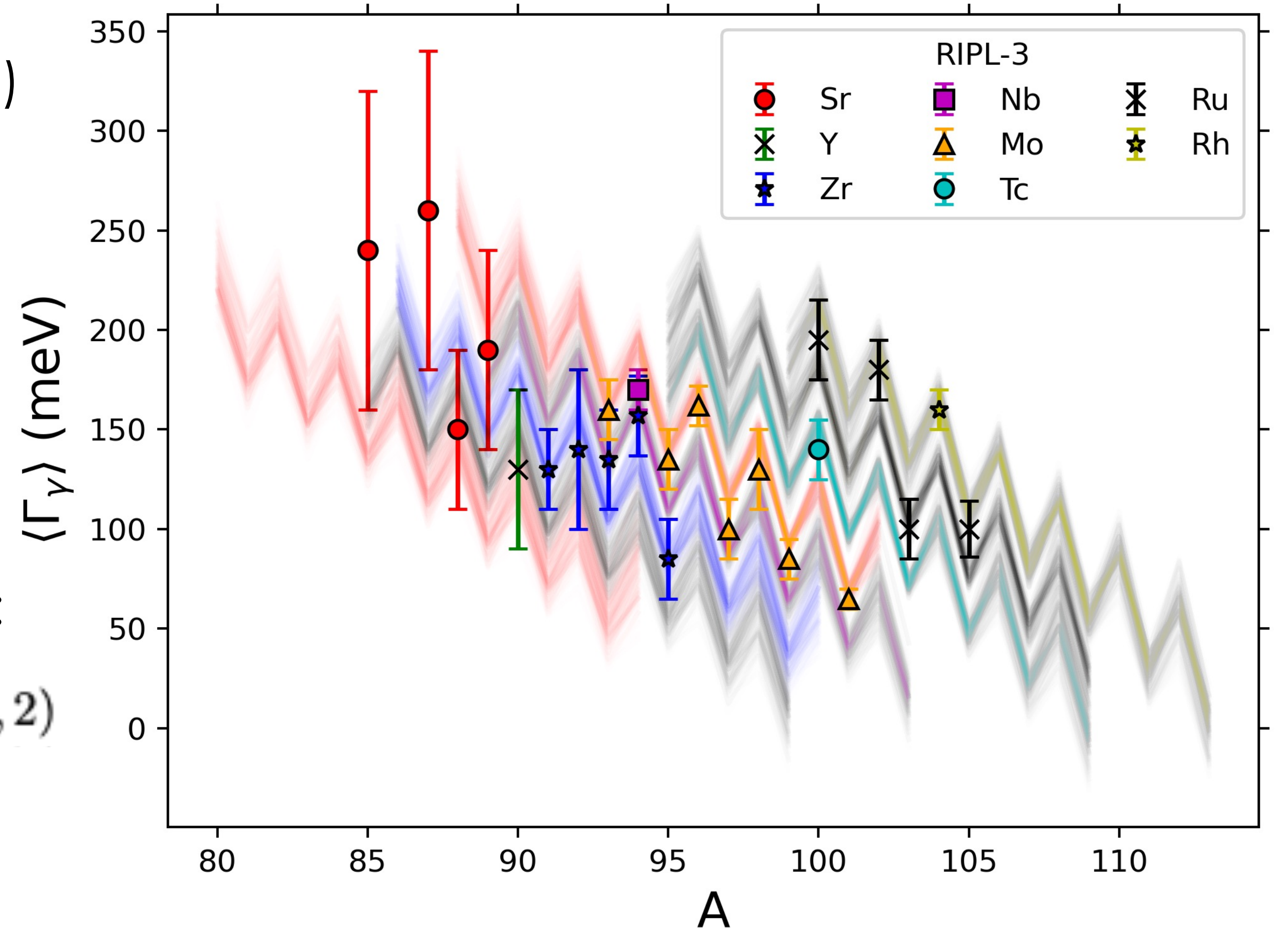
- Overall GSF is fitted to the measured $\langle\Gamma_\gamma\rangle_0$ by adding a E1 resonance

- **Sensitivity to GDR parameters is strongly reduced**

Gamma-ray Transmission Coefficients

- Average radiative width trends:
- $<\Gamma_\gamma>_0$ increases with charge number (Z)
- $<\Gamma_\gamma>_0$ generally decreases with mass number along an isotopic chain (N)
- $<\Gamma_\gamma>_0$ shows an odd-even staggering in A, only observable for even-Z nuclei
- We choose to fit with an empirical form:

$$\langle\Gamma_\gamma\rangle_0(Z, A) = c_0 + c_1 A^2 + c_2 Z^2 + c_3 Z \bmod(\mathrm{A}, 2)$$



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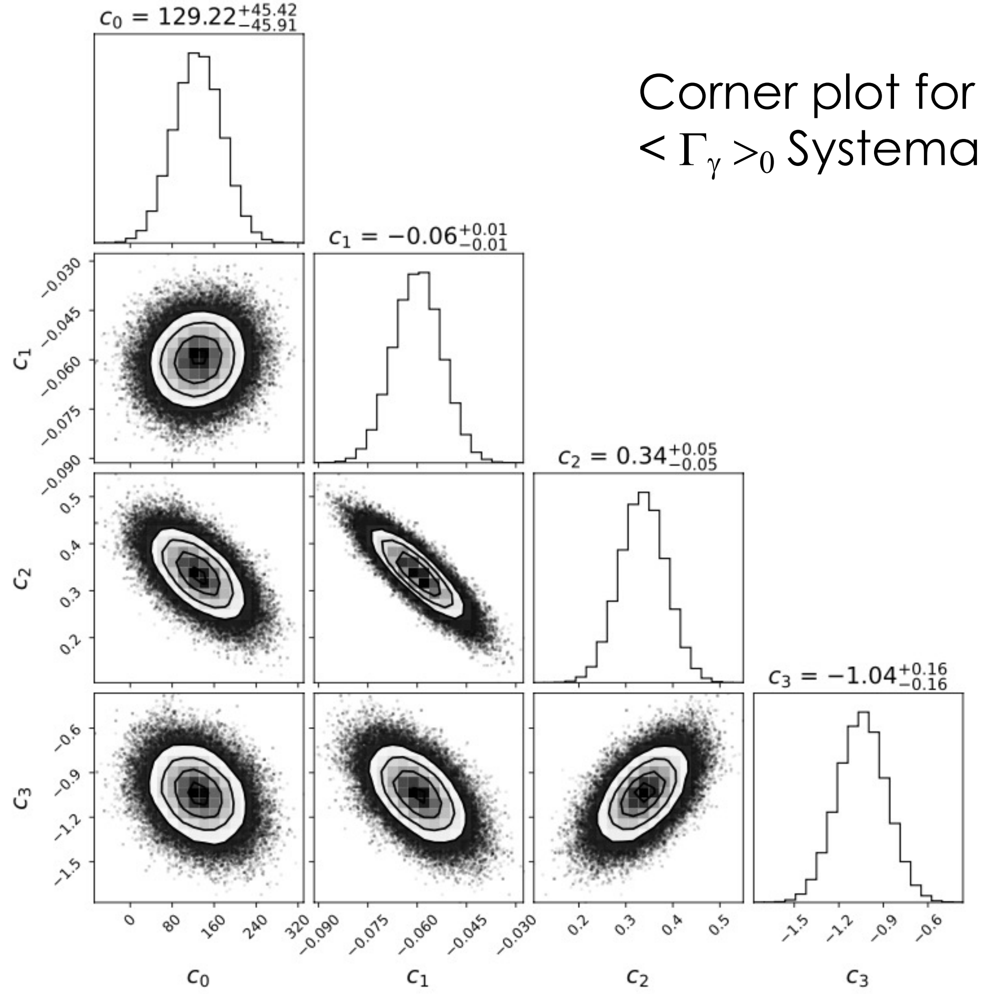
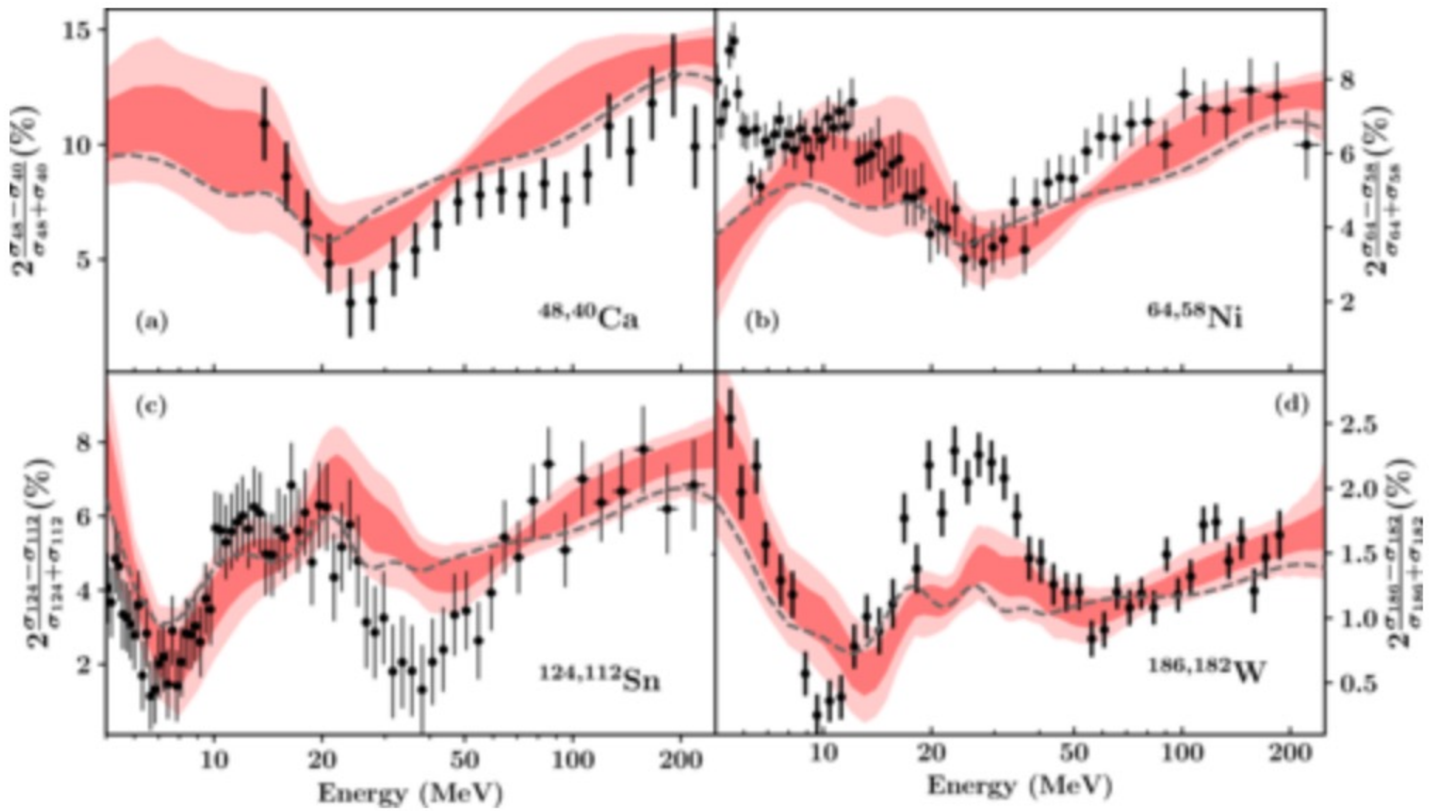


Corner plot for $<\Gamma_\gamma>_0$ Systematic

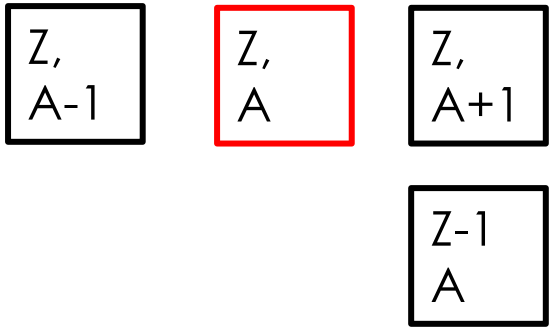
Neutron Transmission Coefficients

- Pruitt & Escher have re-evaluated the parameters of the Koning-Delaroche optical model
- Including MCMC UQ
- We consider a subset of 50 samples (out 400+) of pre-calculated neutron transmission coefficients



Sampling Procedure

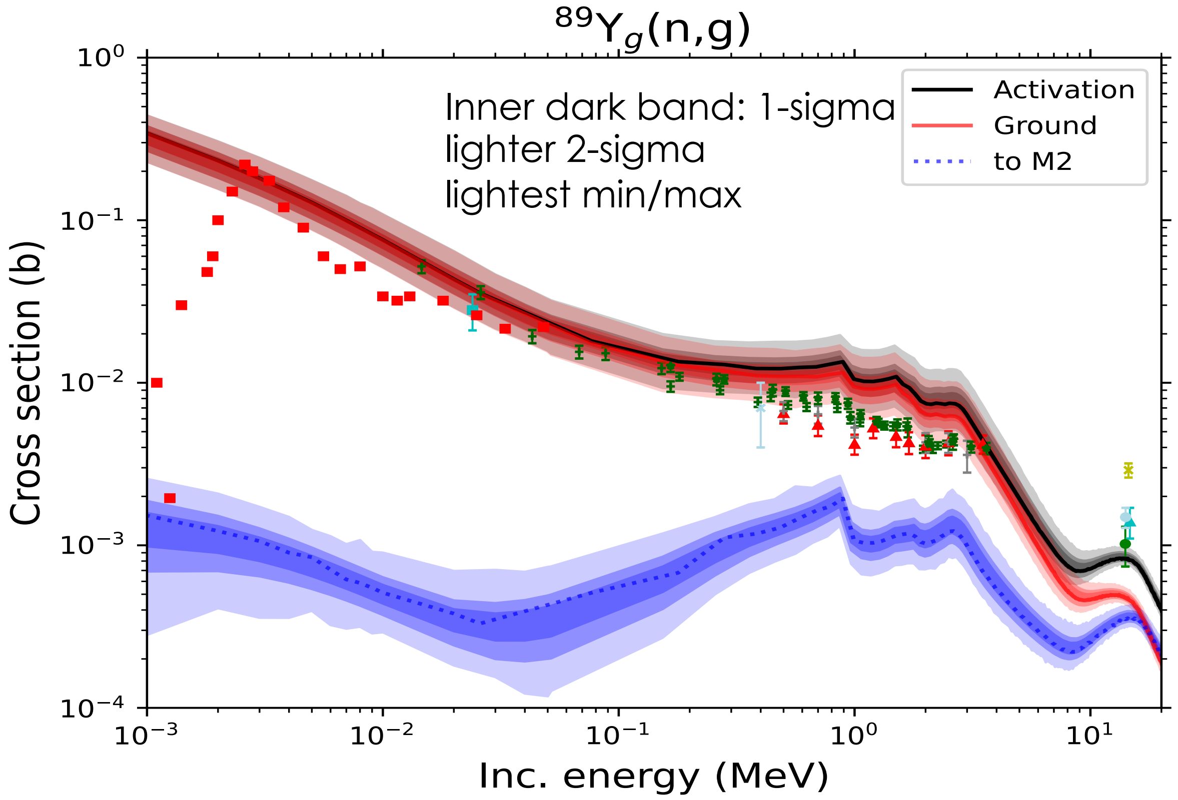
- For neutron-induced reactions on target (Z,A), vary of δW, $<\Gamma_\gamma>_0$ parameters **independently** (for now) for three compound nuclei
- Variation of the OMP is **correlated** between all compound nuclei

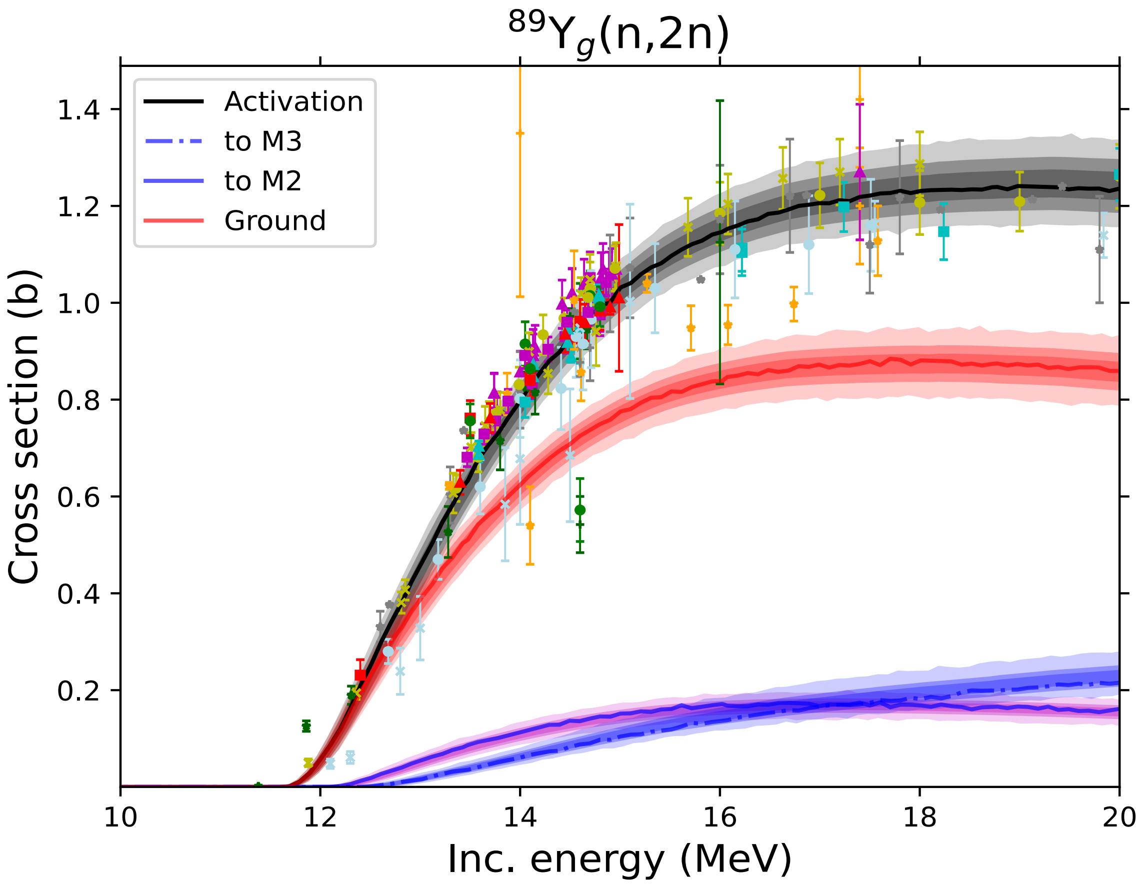


- Using the LLNL developed COMMCAS framwork by Oliver Gorton (using python emcee)
- Draws random samples from specified distributions and sets up input decks, then submits these for parallel on LC machines.
- About 15,000 calculations for each target nucleus.

Validation with measured cross sections

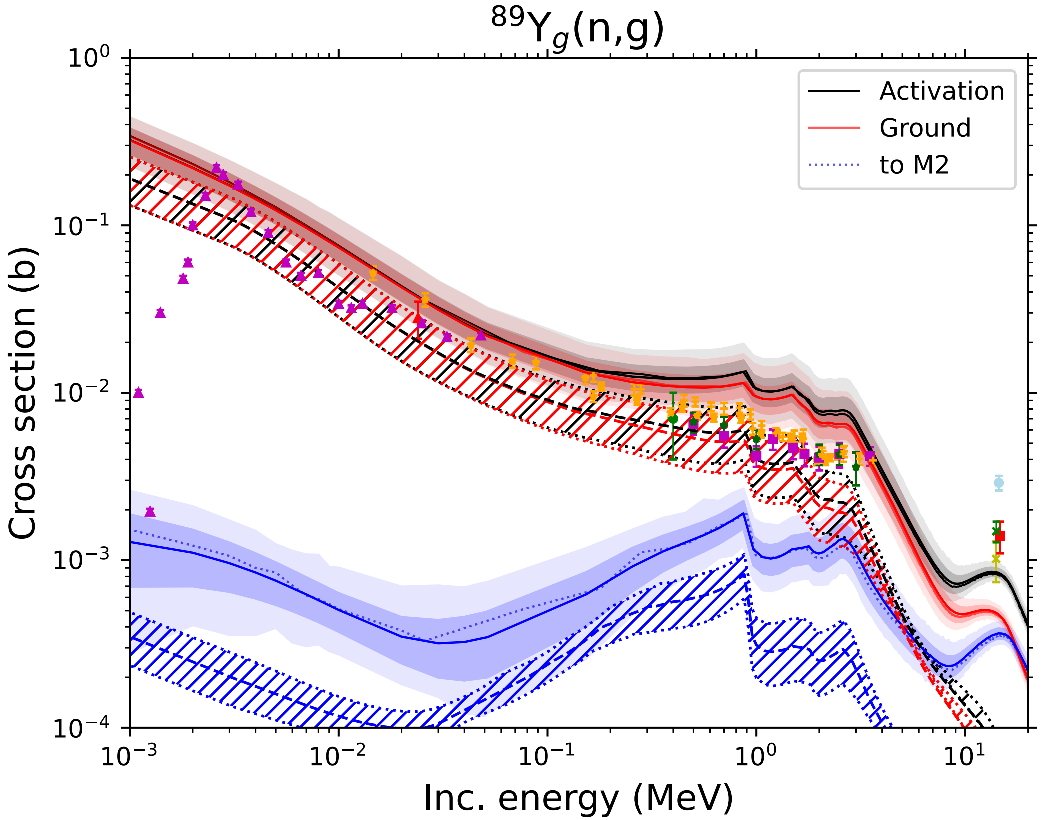
Calculations use the parameter systematics:
No fit to the measured cross section

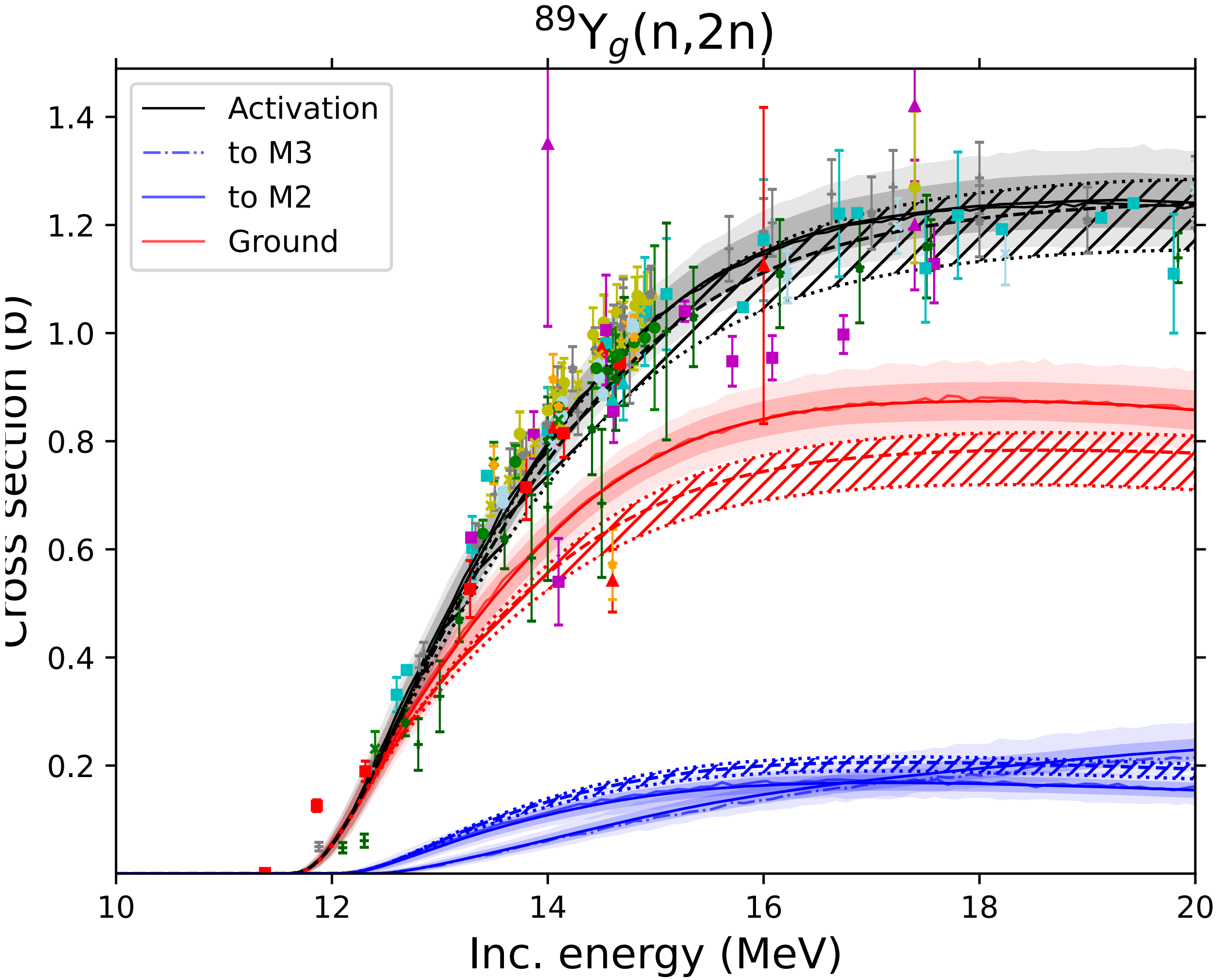




Comparison to previous evaluation

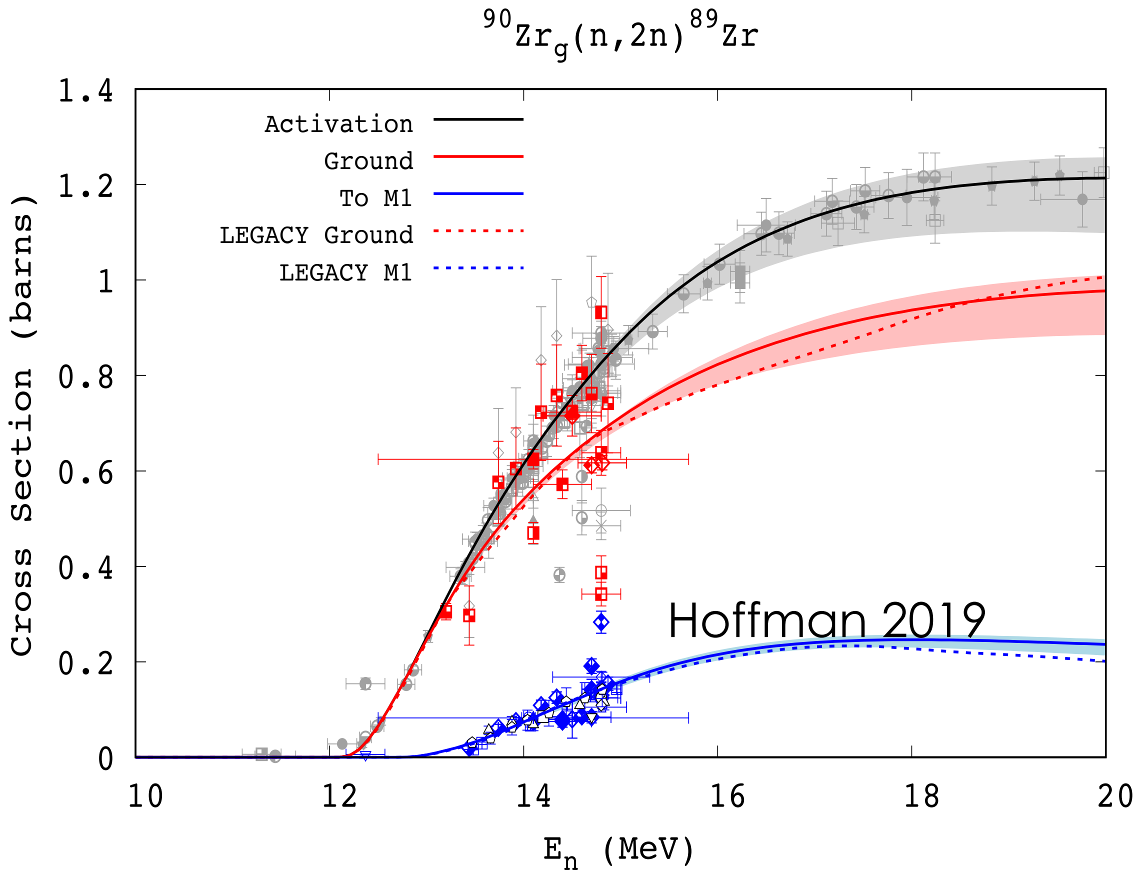
Hoffman et al. 2019, *LLNL-TR-737934*

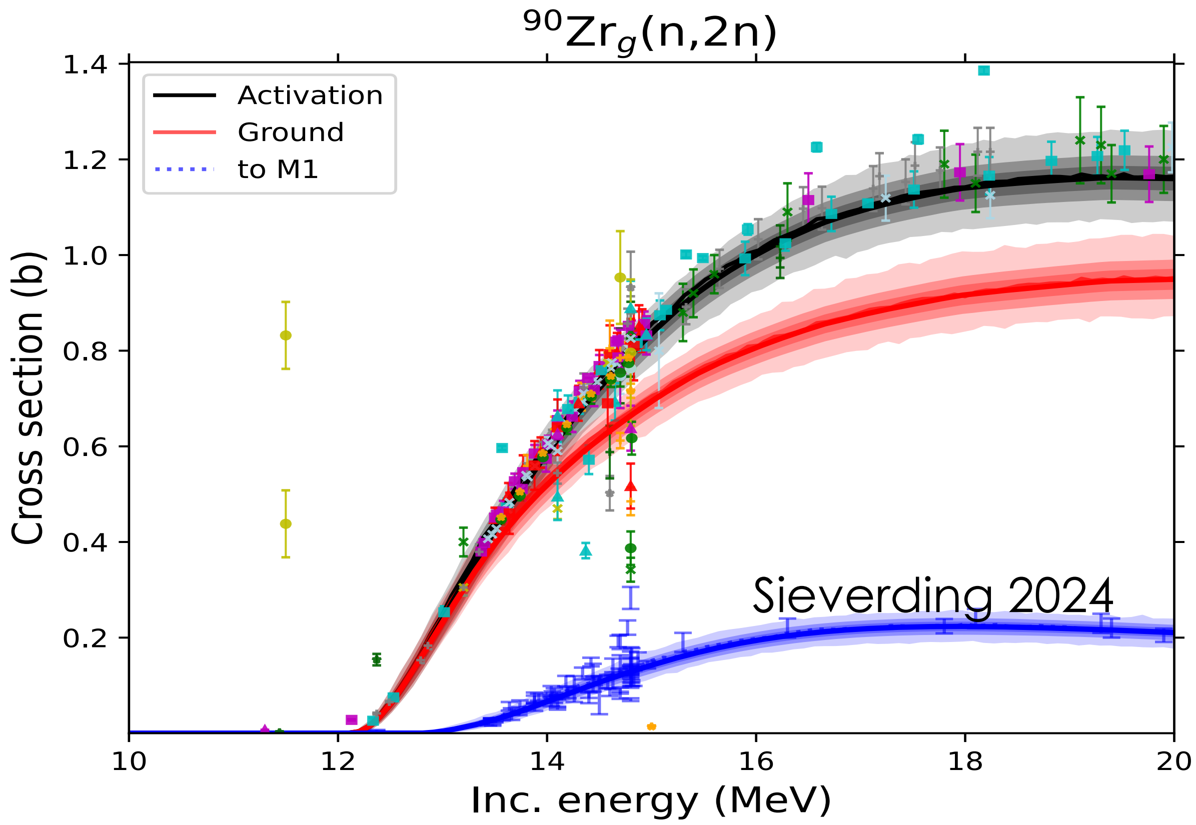




Cross Section comparison: vs UQ

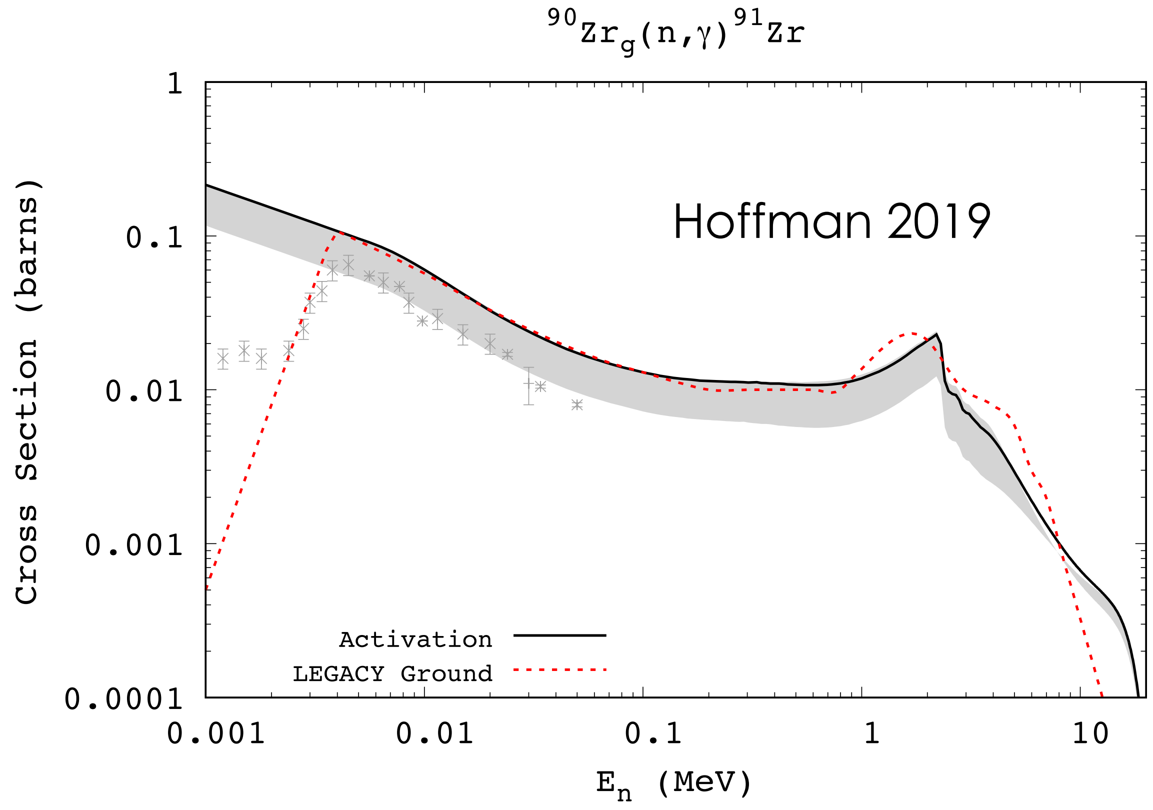
Inner dark band: 1-sigma, lighter 2-sigma, lightest min/max

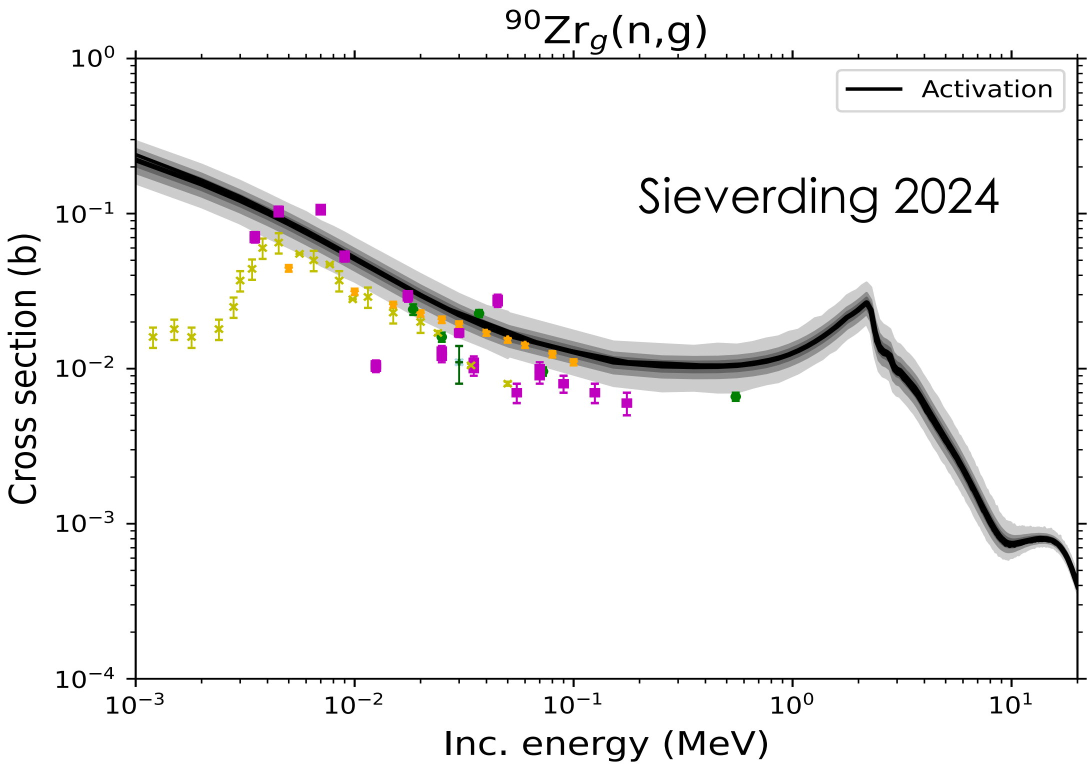




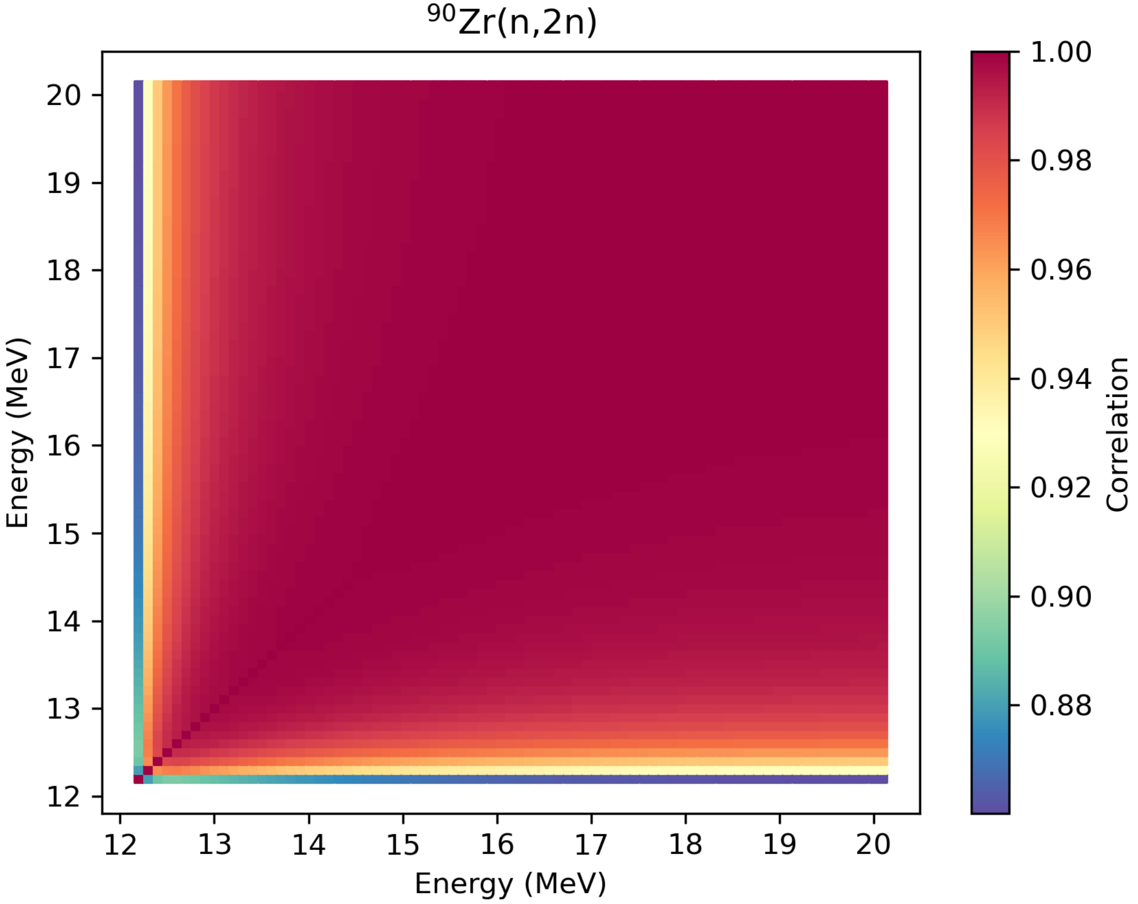
Cross Section comparison: HILO vs UQ

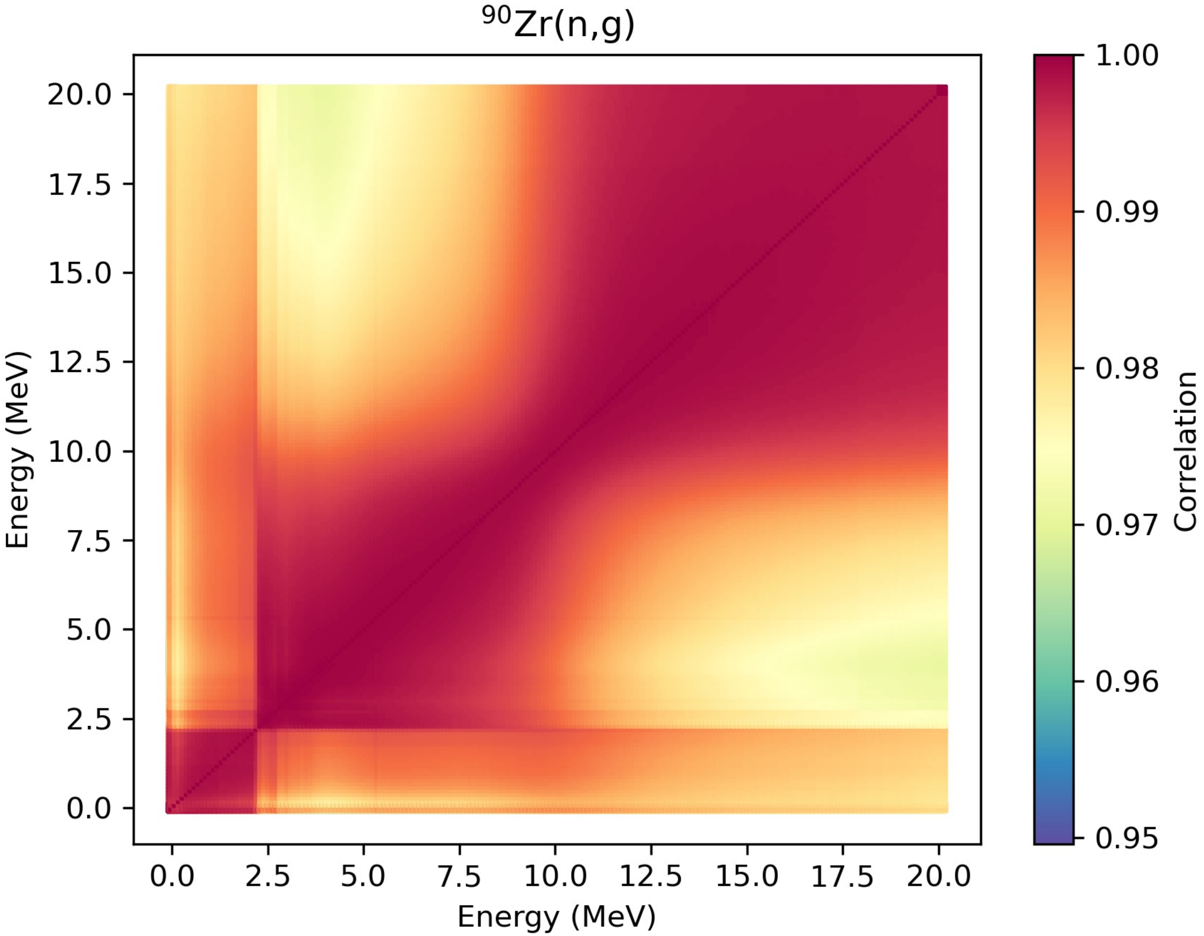
Inner dark band: 1-sigma, lighter 2-sigma, lightest min/max





MCMC approach provides covariance data





- Reaction model induces very strong correlations across all energies

Summary and outlook

- Developed ”regional systematics” based on MCMC fits of model parameters to a limited dataset
- The relevant parameters are specific to a region
- Allows systematic UQ including covariance information
- Correlations between cross sections and channels could be extracted
- Reaction model and parameter choice induce very strong correlations across energies
- Possible improvements with advanced data analysis tools:
  - GP or ML for parameters instead of functional form?
  - Emulators for faster sampling
  - Model mixing for some model choices: e.g. GSF model and NLD model
  - Robust UQ for optical model for deformed nuclei

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