A Markov Chain Monte Carlo Tool for Hauser-Feshbach Codes

O. C. Gorton[1] and J. E. Escher[2]

[1]San Diego State University
[2]Lawrence Livermore National Laboratory

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Cross sections are probabilities expressed as areas

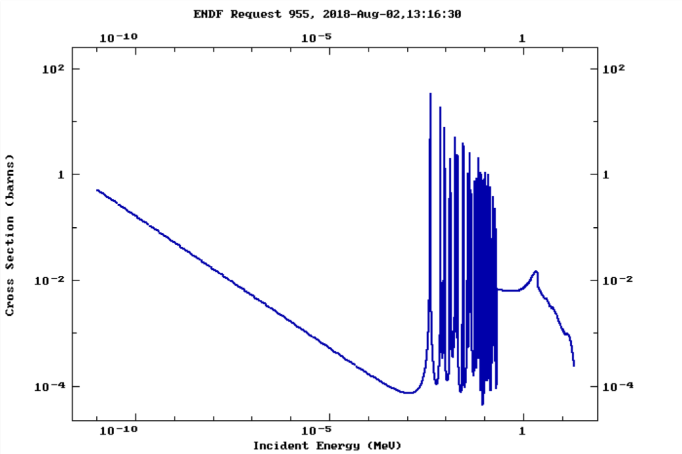


Figure 1: Neutron capture cross section $\sigma_{n\gamma}(E_n)$ for $^{90}Zr(n,\gamma)$ evaluated from experimental data.

Nuclear cross sections are important and data is not always available

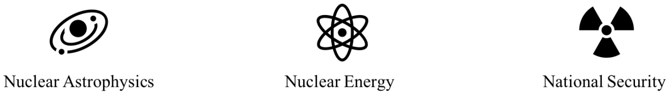


Figure 2: Nuclear cross sections have applications in nuclear astrophysics, nuclear energy, and national security.

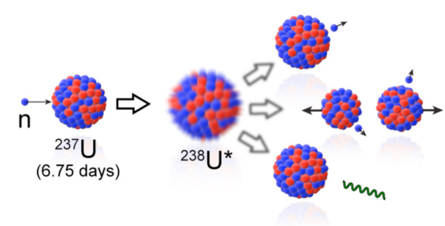


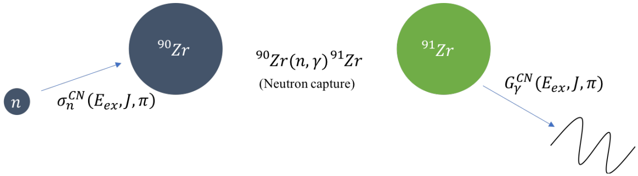
Figure 3: An important reaction with an unstable target.

Overview

1. Big Picture: Nuclear cross sections
2. Recent development: The Surrogate Method
3. This work: Markov Chain Monte Carlo tool for Hauser-Feshbach codes

The Surrogate Method is necessary because the microscopic theory of the compound nucleus cannot be computed accurately enough

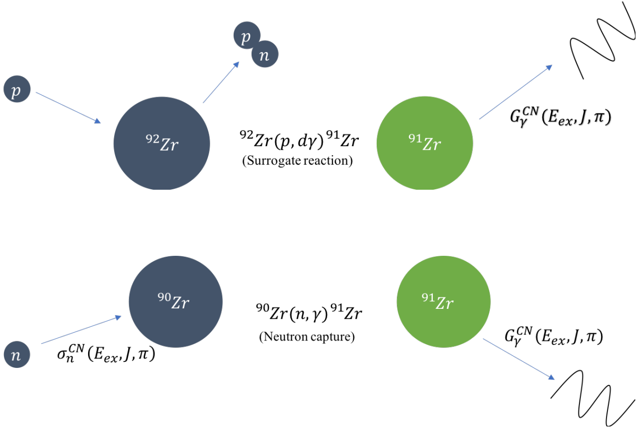
Let's consider neutron capture reactions:



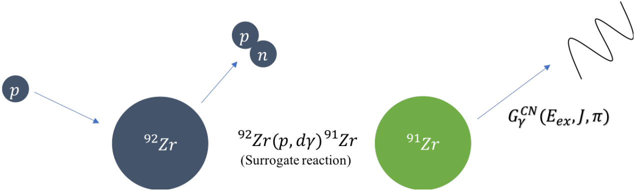
Hauser-Feshbach theory

$$\sigma_{n,\gamma}(E_n) = \sum_{J,\pi} \sigma_n^{CN}(E_{ex}, J, \pi) G_\gamma^{CN}(E_{ex}, J, \pi) \tag{1}$$

Surrogate reaction produces the compound nucleus whose γ-decay probability we need to compute the (n, γ) cross section



The decay model G_γ^{CN} is constrained by surrogate experimental data



$$P_{\delta\pi}(E_{ex}) = \sum_{J,\pi} F_\delta^{CN}(E_{ex},J,\pi)G_\gamma^{CN}(E_{ex},J,\pi) \tag{2}$$

$$\sigma_{n,\gamma}(E_n) = \sum_{J,\pi} \sigma_n^{CN}(E_{ex},J,\pi)G_\gamma^{CN}(E_{ex},J,\pi) \tag{3}$$

Recent publication demonstrated the Surrogate Method for neutron capture

Escher et al., "Constraining neutron capture cross sections for unstable nuclei with surrogate reaction data and theory" Phys. Rev. Lett. 121, 052501 – Published 31 July 2018.

- $^{90}Zr(n,\gamma)$ from $^{92}Zr(p,d\gamma)$ data test case
- $^{87}Y(n,\gamma)$ from $^{89}Y(p,d\gamma)$ data

- Approximate fitting method

Overview

1. Big Picture: Nuclear cross sections
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I developed an interactive Python code for the Surrogate Method

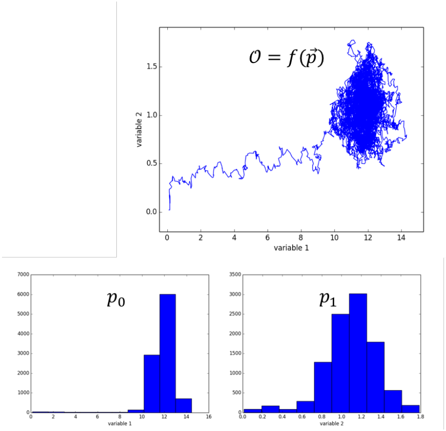
"A Markov Chain Monte Carlo Tool for Hauser-Feshbach Codes" (MCHF)

Two general functions:

1. Use Markov Chain Monte Carlo to constrain/fit parameters using (surrogate) data
2. Sample a distribution of parameters to calculate cross sections

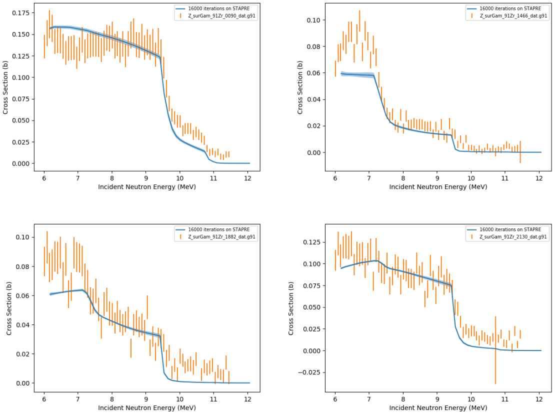
Markov Chain Monte Carlo (MCMC) and experimental data used to constrain parameters

Figure 4: MCMC applied to a simple two-parameter space. Sampling the parameter space with MCMC yields posterior distribution of parameters according to their χ^2 values.



The decay model G_γ^{CN} is constrained with MCMC by surrogate experimental data

Figure 5: Coincidence probabilities $P_{pd\gamma}(E) = \sum_{J\pi} F_{pd}^{CN} G_\gamma^{CN}$ vs projectile energy for $^{92}Zr(p,d)$ reactions.



We search for 5 level-density parameters and 9 gamma-ray strength function parameters to determine G_γ^{CN}

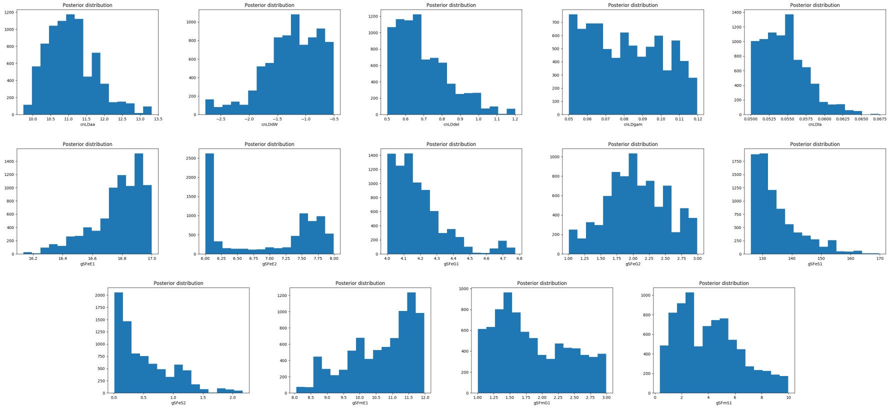


Figure 6: Posterior distribution of parameters from Markov Chain, which determine G_γ^{CN}.

By sampling the posterior parameter distribution we obtain constraints on the neutron capture cross section

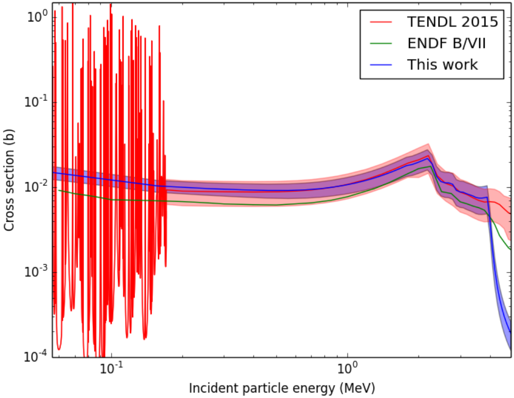


Figure 7: $^{90}Zr(n,\gamma)$ cross section $\sigma_{n\gamma}(E_n) = \sum_{J\pi} \sigma_n^{CN} G_\gamma^{CN}$ obtained using the MCMC parameter distribution for G_γ^{CN}.

We track a number of metrics to assess convergence

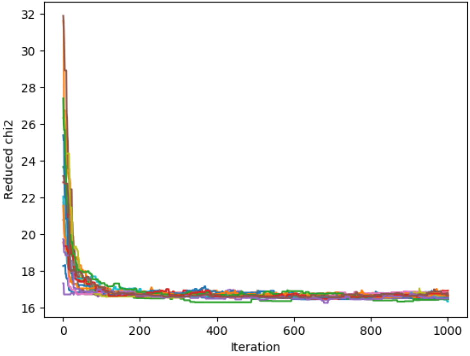


Figure 8: χ^2 as a function of iteration number for several initial conditions.

Other metrics we use: (1) Total distribution of χ^2 values. (2) Distribution of a MCMC random walk parameter. (3) Parameter covariances.

Summary

Importance of these calculations:

- Reactions where experimental data doesn't exist
- Experimentally constrained with uncertainties

"A Markov Chain Monte Carlo Tool for Hauser-Feshbach Codes" (MCHF)

Previous calculation*:	**This work:**
Bayesian Monte Carlo	Markov Chain Monte Carlo
Proof of concept	General purpose and interactive
STAPRE	STAPRE, (TALYS and EMPIRE)**
Serial	Parallel

*Escher et al., "Constraining neutron capture cross sections for unstable nuclei with surrogate reaction data and theory" Phys. Rev. Lett. 121, 052501 – Published 31 July 2018.

Extra slides

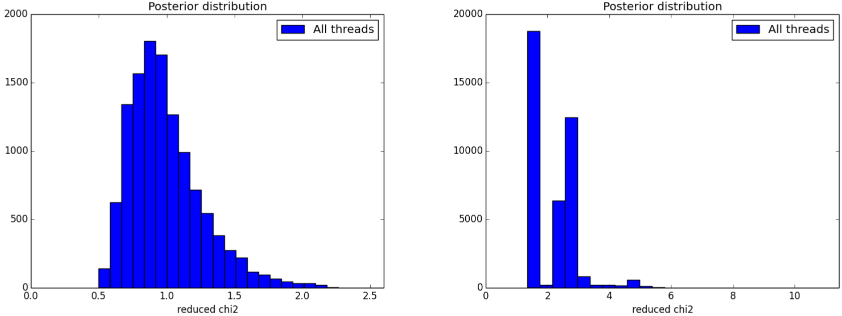
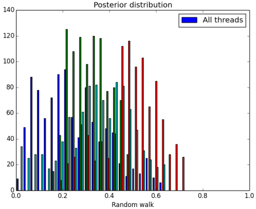


Figure 9: (Left) Smooth χ^2 distribution. (Right) Jagged χ^2 distribution, indicative of non-convergence and/or poor choice of step size.



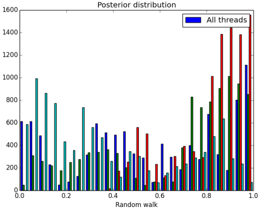


Figure 10: (Left) A random variable that appears to have structure. (Right) Another random variable with a greater number of iterations and a flatter distribution.

More recent and future work

- Robustness / sensitivity
- Is P-normalization necessary?
- Are all of the parameters important? Random?
- Parameter importance

Coincidence probability

$$P_{\delta\pi}(E_ex, \theta_d) = \frac{N_{d\gamma}(E_{ex}, \theta_d)}{\epsilon_\gamma N_d(E_{ex}, \theta_d)} \quad (4)$$

$$P_{\delta\pi}(E_{ex}) = \sum_{J,\pi} F_\delta^{CN}(E_{ex}, J, \pi) G_\gamma^{CN}(E_{ex}, J, \pi) \quad (5)$$

$$\sigma_{n,\gamma}(E_n) = \sum_{J,\pi} \sigma_n^{CN}(E_{ex}, J, \pi) G_\gamma^{CN}(E_{ex}, J, \pi) \quad (6)$$

Hauser-Feshbach formula

An energy averaged statistical approach to modeling compound nuclear reactions

$$\frac{d\sigma}{dE} = \frac{\pi}{k^2} \sum_{J\pi} \frac{T_{formation} T_{decay}}{\sum T_{discrete} + \sum \int T_{continuum} \rho dE} W \rho \tag{7}$$

T: Transmission coefficients for formation/decay of compound nucleus
ρ: Level densities in the compound nucleus
E: Energy of the incident particle
σ: Cross section for a particular reaction channel
W: 'Other statistical and correction factors'
J: Angular momentum of compound nucleus
π: Parity of compound nucleus

Program schematic