# Neutron capture cross sections from surrogate reaction data and theory: connecting the pieces with a Markov-Chain Monte Carlo approach


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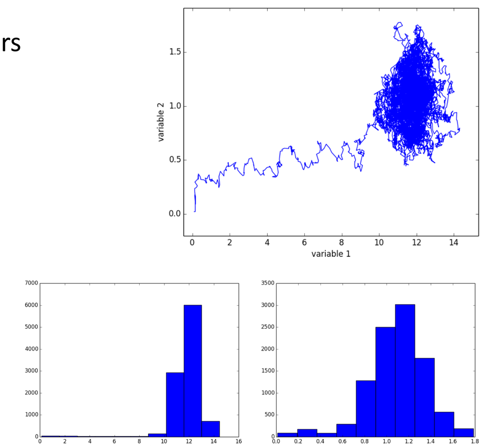
## What is Markov Chain Monte Carlo (MCMC)?

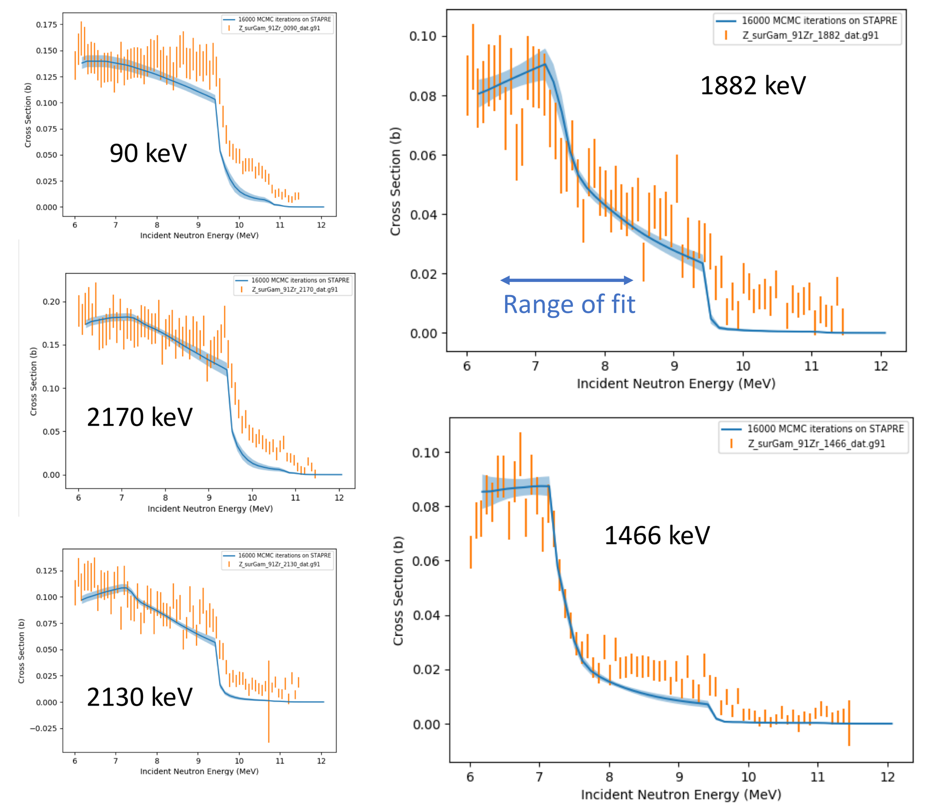
A method for obtaining best-fit parameters and their uncertainties by a `censored' random walk in a parameter space [4].

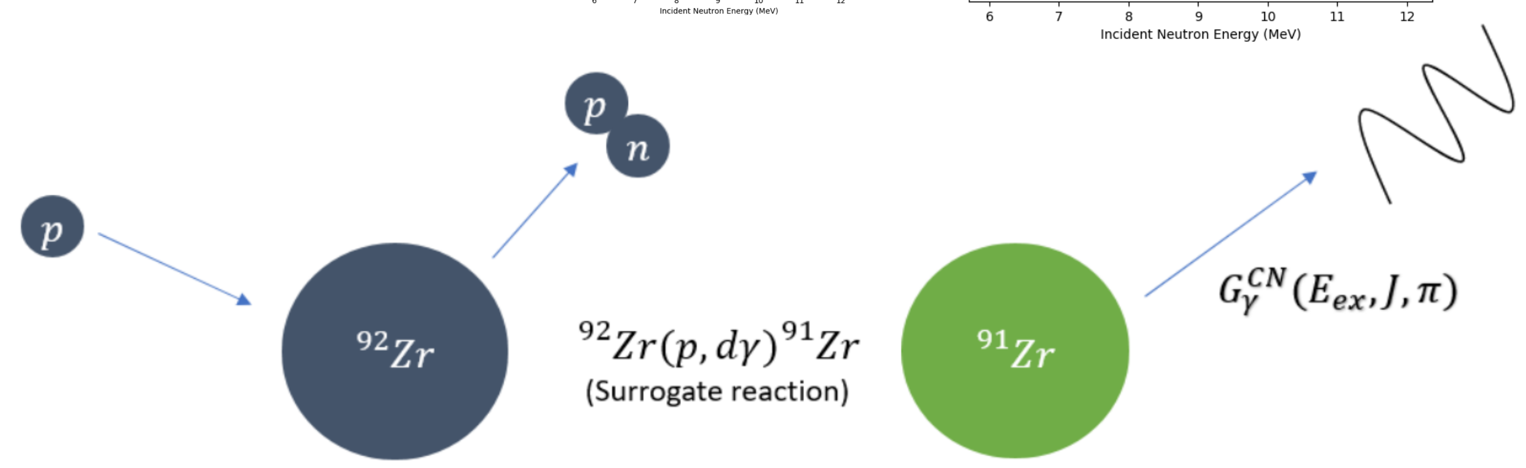
Shown here is MCMC applied to a simple two-parameter space. Sampling the parameter space with MCMC yields a posterior distribution of parameters according to their $\chi^2$ values.




## Fit to surrogate data

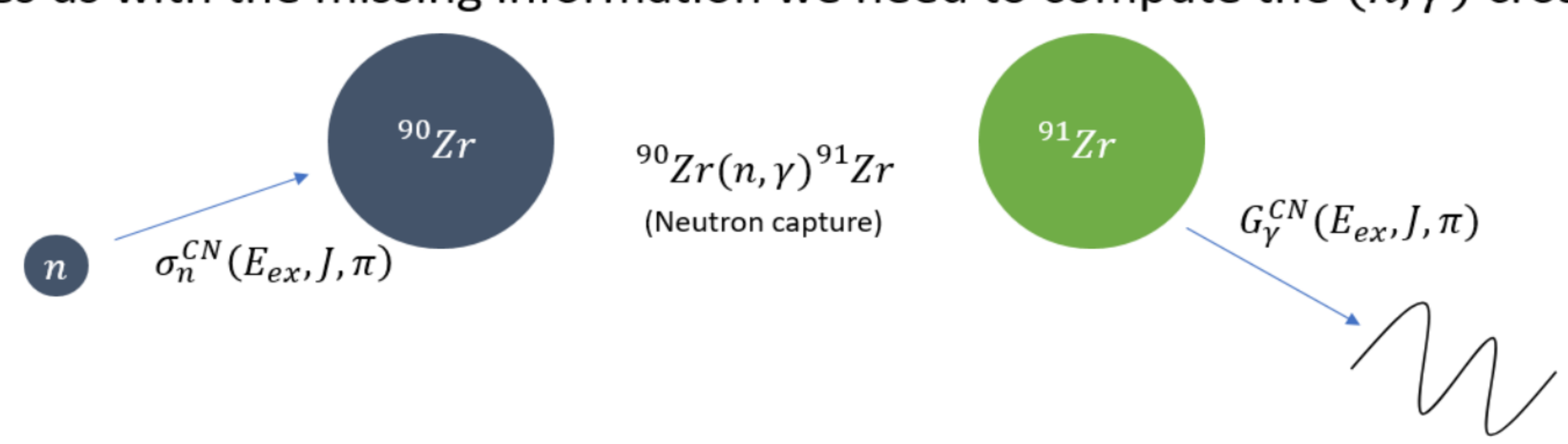
We use MCMC to fit parameters in a nuclear reaction model code to experimentally available $^{92}Zr(p,d\gamma)^{91}Zr$ data

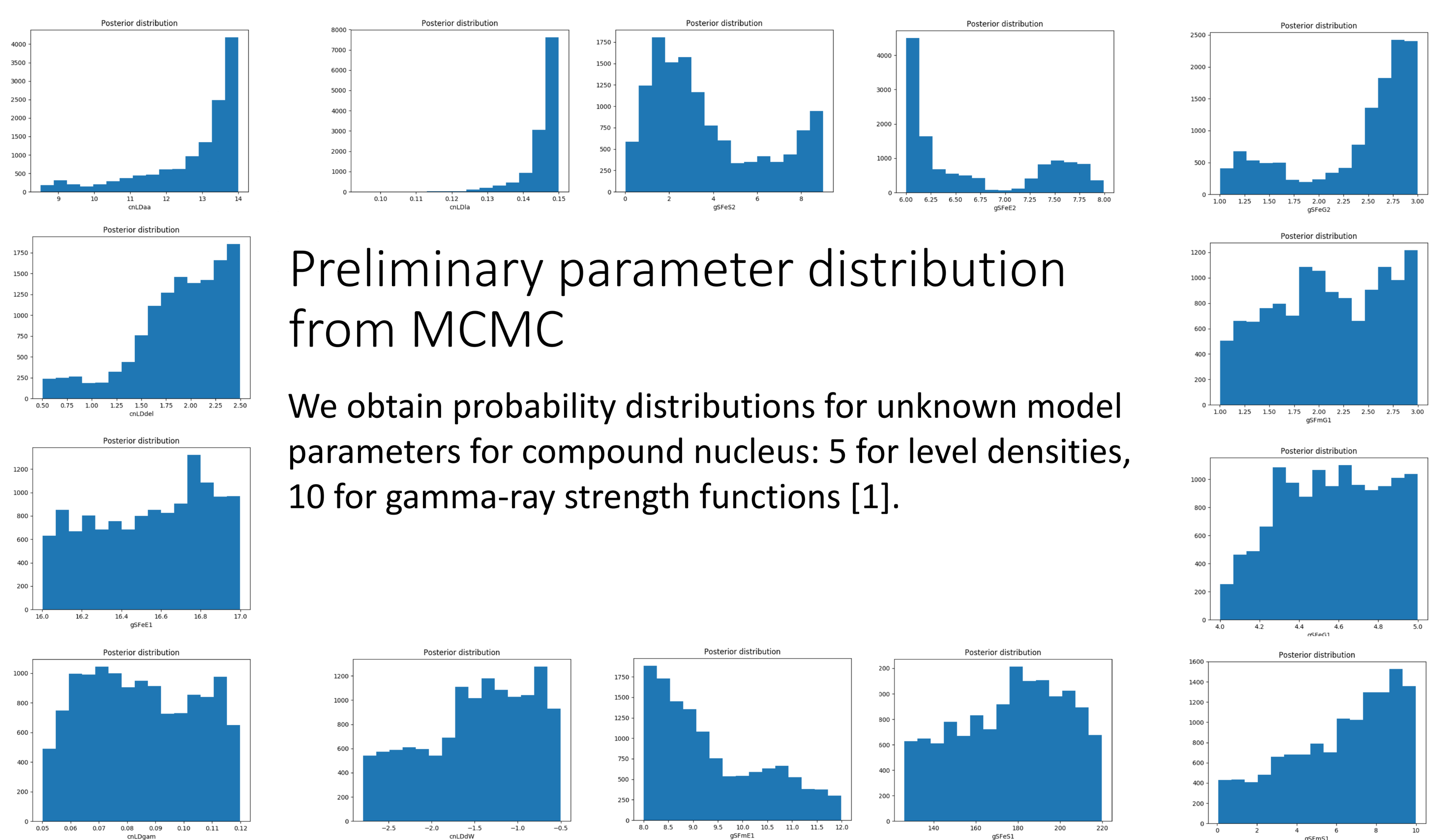



Surrogate reaction produces the compound nucleus whose $\gamma$-decay we are interested in.

This provides us with the missing information we need to compute the $(n,\gamma)$ cross section.




## Preliminary parameter distribution from MCMC

We obtain probability distributions for unknown model parameters for compound nucleus: 5 for level densities, 10 for gamma-ray strength functions [1].

## How do we calculate the cross sections?

**Surrogate experiment** measures: $P_{\delta\pi}(E_{ex},\theta_d) = \frac{N_{d\gamma}(E_{ex},\theta_d)}{\epsilon_\gamma N_d(E_{ex},\theta_d)}$.

**Fit decay parameters** in $G_\gamma^{CN}(E_{ex},J,\pi)$ to reproduce $P_{\delta\pi}(E_{ex},\theta_d)$:

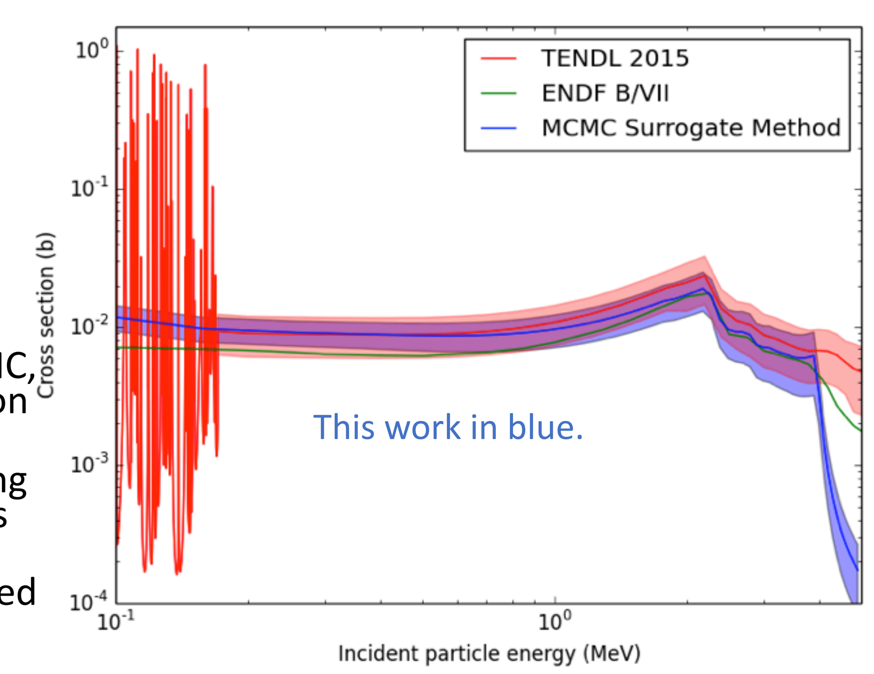
$$P_{\delta\pi}(E_{ex},\theta_d) = \sum_{J,\pi} F_\delta^{CN}(E_{ex},J,\pi,\theta_d) G_\gamma^{CN}(E_{ex},J,\pi).$$

**Calculate** Hauser-Feshbach cross section:

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

## Preliminary $(n,\gamma)$ Neutron Capture Cross Section with Statistical Uncertainties

- We sample the parameter distribution, found using MCMC, to compute the desired neutron capture cross section
- Reproduces cross sections using well known statistical methods
- Method can be applied to unstable nuclei where measured values do not exist





## Abstract

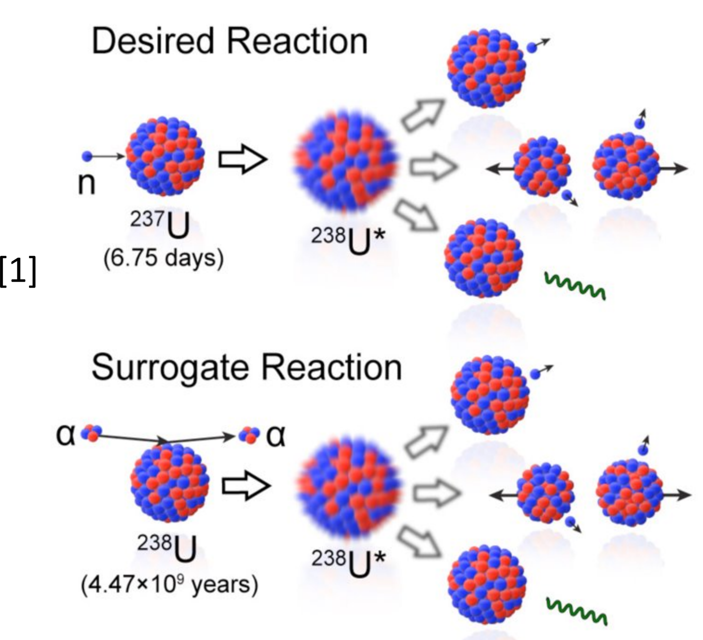
Neutron capture cross sections can be measured by bombarding a sample of target nuclei with neutrons and detecting decay products. Such measurements cannot be completed in the laboratory when the target isotopes have half-lives which are small compared to timescales relevant to the experiment. This leaves critical gaps in libraries of nuclear data. To predict the missing data, nuclear cross section calculations for neutron capture reactions are carried out using statistical Hauser-Feshbach models [1]. These models depend on a number of nuclear structure inputs including nuclear level densities, and gamma-ray strength functions. Each of these depend on some model for which the input parameters are not well constrained. The `surrogate reaction method' [2] allows us to obtain statistical constraints on model parameters by fitting to experimentally accessible cross sections involving the same compound nucleus. These experimental constraints are then used to predict cross sections which are not directly measured.

The 90Zr(n,γ) cross section has recently been determined from 92Zr(p,dγ) data [3]. That calculation used an approximate fitting method based on Bayesian Monte Carlo sampling. We now employ a Markov Chain Monte Carlo (MCMC) [4] sampling to produce our probability distribution of parameters: the statistical constraints we need to predict neutron capture cross sections in the surrogate method. This approach is statistically rigorous, and this work represents a reusable structure for future applications of the surrogate method. Here we recompute the same benchmark case, 90Zr(n,γ) from 92Zr(p,dγ) data and report preliminary results.


## Surrogate Method

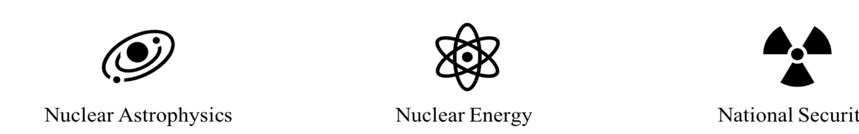
**Experimental constraints** from indirect measurements are used to **predict cross sections** which are not directly measured.

- Uses statistical Hauser-Feshbach models [1] and requires:
  - nuclear level densities
  - gamma-ray strength functions
- Obtain statistical constraints on model parameters by fitting to experimentally accessible cross sections involving the same compound nucleus [3].




## Big Picture and Motivation

**Applications** of neutron capture reactions include [5][6]:




**Need** indirect measurements to determine the desired reactions. This requires fitting procedures/parameter searches.

- Direct experimental data is not always available or even possible to obtain
- Uncertainty quantification is crucial for error propagation here and in data evaluations

## Summary

The importance of these calculations is that we can use experimental data to constrain neutron capture cross sections for reactions where experimental data does not exist.

| Previous work [3]: | This work: |
|---|---|
| Bayesian Monte Carlo | Markov Chain Monte Carlo |
| Proof of concept | General purpose and reusable |
| STAPRE | STAPRE, (potentially TALYS and EMPIRE) |
| Serial | Parallel |


[1] Capote et al., "RIPL - Reference Input Parameter Library for Calculation of Nuclear Reactions and Nuclear Data Evaluations" NDS 110, 3107 (2009). [2] Escher et al., "Compound-nuclear reaction cross sections from surrogate measurements" RMP 84, 353 (2012). [3] Escher et al., "Constraining neutron capture cross sections for unstable nuclei with surrogate reaction data and theory" Phys. Rev. Lett. 121, 052501 (2018). [4] Hastings, "Monte Carlo sampling methods using Markov chains and their applications" Biometrika 57, 97 (1970). [5] N. Colonna, et al., Energy and Environmental Science 3, 1910 (2010). [6] F. N. Mortensen, J. M. Scott, and S. A. Colgate, Los Alamos Science 28 38 (2003).



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