# Indirect measurements of nuclear cross sections: tempering experimental results with theory

Oliver Gorton<sup>1</sup>, Jutta Escher<sup>2</sup>, Orlando Olivas-Gomez<sup>3</sup>

<sup>1</sup>Computational Science (PhD) San Diego State University | UC Irvine

<sup>2</sup>Lawrence Livermore National Laboratory Nuclear Data & Theory PLS/NACS

<sup>3</sup>University of Notre Dame

September 9, 2019



IM RELEASE: LLNL-PRES-789322

Lawrence Livermore National Laboratory

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

# I will give a summary of the major results of my summer projects

### PART 1:

- Use of in inverse-reactions for <u>indirect measurements</u> at University of Notre Dame
- Applying our theory capabilities to improve predictive power of indirect measurements

### PART 2:

- Sensitivity of an approximation method used for <u>indirect</u> <u>measurements</u>
- Applying this surrogate method to recent data

# All of the elements in the universe came from a handful of astrophysical processes



groups.nscl.msu.edu/SuN/

# **Proton-rich elements formed in p-process**



Images: Anna Simon, SuN GROUP @ NSCL

groups.nscl.msu.edu/SuN/

# The details of the p-process(es) remain a mystery: unable to predict abundances

z					103Sb	104Sb	105Sb	106Sb	107Sb	108Sb	109Sb	110Sb	111Sb	112Sb	113Sb	114Sb	115Sb
		99Sn	100Sn	101Sn	102Sn	103Sn	104Sn	105Sn	106Sn	107Sn	108Sn	109Sn	110Sn	111Sn	112Sn	113Sn	114Sn
49	97In	98In	99In	100In	101In	102In	103In	104In	105In	106In	107In	108In	109In	110In	111In	112In	113In
	96Cd	97Cd	98Cd	99Cd	100Cd	101Cd	102Cd	10201 (γ,	101Cd n)	105Cd	106Cd	107Cd	108Cd	109Cd	110Cd	111Cd	112Cd
47	95Ag	96Ag	97Ag	98Ag	99Ag	100Ag	101Ag	102Ag	103Ag	104Ag	105Ag	106Ag	107Ag	108Ag	109Ag	110Ag	111Ag
	94Pd	95Pd	96Pd	97Pd	98Pd	99F (	γ, α)	1017 d	102Pd		ro iPd	105Pd	106Pd	107Pd	108Pd	109Pd	110Pd
45	93Rh	94Rh	95Rh	96Rh	97Rh	98Rh	99Rh	100Rh	101Rh	102Rh	103Rh	104Rh	105Rh	106Rh	107Rh	108Rh	109Rh
	92Ru	93Ru	94Ru	95Ru	96Ru	97Ru	98Ru	99Ru	100Ru	101Ru	102Ru	103Ru	104Ru	105Ru	106Ru	107Ru	108Ru
43	91Tc	92Tc	93Tc	94Tc	95Tc	96Tc	97Tc	98Tc	99Tc	100Tc	101Tc	102Tc	103Tc	104Tc	105Tc	106Tc	107Tc
	48		50		52		54		56		58		60		62		N

Images: NNDC chart of nuclides

# Measuring $(p,\gamma)$ can tell us about $(\gamma,p)$

- Astrophysics application need better cross sections
- Orlando Olivas-Gomez from University of Notre Dame
- <u>Indirect measurement</u> of (γ,p) cross sections from (p,γ) experiment

 $(p,\gamma)$  = Proton capture  $(\gamma,p)$  = photo-disintegration of a photon

# UND group measured proton capture cross sections

- Original idea:
  - Find the best theoretical model to describe (p,  $\gamma$ ) data
  - Use that model to predict ( $\gamma$ ,p) cross sections



# I wrote a code for this!

#### My work with the theory side of indirect measurements

- Fit nuclear reaction model parameters with MCMC
- Indirect measurement

   > data
  - -> parameter estimation
  - -> predict desired reaction
- Surrogate method

#### Tech specs

 Python, multiple Hauser-Feshbach reaction codes, multiple observables, simultaneous fitting, parallel sampling, 2000+ LOC

#### Notable improvements this summer

- Ability to include prior distributions for parameters
- Compatibility with open-source Hauser-Feshbach model code, EMPIRE

# **Applying MCMC to linear regression**



# I can improve the resulting theory with MCMC

- Original idea:
  - Find the best theoretical model to describe (p,  $\gamma$ ) data
  - Use that best model to predict ( $\gamma$ ,p) cross sections



## From nearest-facsimile to probability distribution



Selecting the best 'default' option

Tuning a model to constraints given by the data

# I examined nuclear structure model parameters

- Gamma-ray strength functions
- Nuclear level densities
- Priors mostly from Reference Input Parameter Library (RIPL-3)

## **Nuclear reaction model parameter estimation**

Parameter distributions from the 102Pd cross section fitting





# With parameters that reflect the data, now we can find the desired cross sections

Steps

- 1. Find the best theoretical model to describe (p,  $\gamma$ ) data
- 2. Use that model to predict ( $\gamma$ ,p) cross sections

 $^{102}$ Pd(p, $\gamma$ ) Cross Sections  $10^{3}$ NON-SMOKER  $(p, \gamma)$ Our Results Dillmann 2011 Ozkan 2002  $10^{2}$ -3 Best Global -1-2 Best 102Pd 1-5-5 Best 108Cd 0-5-5 Best 110Cd 10 σ (mb)  $10^{-1}$ Figure: O. Gomez preliminary analysis  $10^{-2}$ 3 4 5 8 6  $E_{CM}$  (MeV)

# Ag103 ( $\gamma$ ,p) cross section from (p, $\gamma$ )-constrained parameters



# Improved cross sections means improved astrophysics models

#### <u>Take aways</u>

- Re-evaluated cross sections may change understanding of the p-process
- Error bars tell us how much we can infer from the new measurements



Images: Anna Simon, SuN GROUP @ NSCL

groups.nscl.msu.edu/SuN/

### p + 108Cd $\rightarrow$ 109In + $\gamma$



### $p + 110Cd \rightarrow 111ln + \gamma$



### **Hauser-Feshbach Model**

Full Hauser-Feshbach formulation:

$$\frac{d\sigma_{\alpha\chi}^{HF}(E_{\alpha})}{dE_{\chi'}} = \pi \frac{\lambda_{\alpha}^2}{2\pi} \sum_{J\pi} \omega_{\alpha}^J \sum_{lsl's'I'} \frac{T_{\chi''l''s''}^J T_{\chi''l''s''}^J (E_{\alpha}) T_{\chi'l's'}^J (E_{\chi'}) \rho_{I'}(U')}{\sum_{\chi''l''s''}^{'} T_{\chi''l''s''}^J (E_{\chi''}) + \sum_{\chi''l''s''I''} \int T_{\chi''l''s''}^J (E_{\chi''}) \rho_{I''}(U'') dE_{\chi''}}$$
(8)



### **Gamma-ray strength functions**

$$f_{E1}^{EGLO}(E_{\gamma}) = 8.674 \times 10^{-8} \left\{ \sum_{i=1}^{2} \Gamma_{E1i} \sigma_{E1i} \frac{E_{\gamma} \bar{\Gamma}(E_{\gamma}, T)}{(E_{E1i}^2 - E_{\gamma}^2)^2 + (E_{\gamma} \bar{\Gamma}(E_{\gamma}, T))^2} + \frac{0.7}{E_{E1i}^3} \bar{\Gamma} \right\}$$

The energy dependent width is

$$\bar{\Gamma}(E_{\gamma},T) = \left[k_0 + (1-k_0)\frac{(E_{\gamma}-\epsilon)}{(E_{E1i}-\epsilon)}\right] \frac{\Gamma_{E1i}(E_{\gamma}^2 + 4\pi T^2)}{E_{E1i}^2}.$$



### **Nuclear level density**

$$\rho(E_x) = \begin{cases} \rho^{CT}(E_x) = \frac{1}{T} \exp\left(\frac{E_x - E_0}{T}\right) & E_x \ge U_x \\ \rho^{FG}(E_x) \propto \frac{1}{\sigma^{3/2} a^{1/4} U^{5/4}} \exp\left(2\sqrt{aU} - \frac{(J + 1/2)^2}{2\sigma^2}\right) & E_x > U_x \end{cases}$$

where

$$\sigma^2 = \lambda \sqrt{aU} A^{2/3} = 0.146 \sqrt{aU} A^{2/3}$$
$$\boldsymbol{a} = \tilde{\boldsymbol{a}} [1 + (1 - \exp(-\gamma U)) \delta W / U] = E_x / T^2$$
$$U = E_x - \Delta$$



### PART 1:

- Collaboration with University of Notre Dame experimentalists using in inverse-reactions for <u>indirect measurements</u>
- Applying our theory capabilities to improve predictive power of their measurements

### PART 2:

- Sensitivity of an approximation method used for <u>indirect</u> <u>measurements</u>
- Applying this surrogate method to recently new data

# Indirect Measurements are Necessary for Radioactive Target Measurements



Reactions on *radioactive targets* are difficult or impossible to measure.



Theory of compound nuclear reactions limited by available nuclear structure.



*The Surrogate Method* allows indirect measurements of cross sections by combining surrogate data and theory.

# Hauser-Feshbach Theory models compound nuclear reactions in two stages

- 1. Formation of the compound nucleus (CN)
- 2. Decay of the CN



\* Conservation of energy, spin and parity

$$\sigma_{\alpha\beta}(E) = \sum_{J\pi} \sigma_{\alpha}^{CN}(E, J\pi) G_{\beta}^{CN}(E, J\pi)$$

# The Surrogate Idea: requires a lot of theory



# The Weiskopf-Ewing Limit applies under special conditions

$$\sigma_{\alpha\beta}(E) = \sum_{J\pi} \sigma_{\alpha}^{CN}(E, J\pi) G_{\beta}^{CN}(E, J\pi)$$

*E* (CN) must be high -> decay into continuum of states

- Works for neutron induced fission (n,f)
- Fails for neutron capture

 $\sigma_{\alpha\beta}^{WE}(E) = \sigma_{\alpha}^{\prime CN}(E) G_{\beta}^{CN}(E)$ 

# The Weiskopf-Ewing Limit Greatly Simplifies the Surrogate Method



# Does the Weisskopf-Ewing approximation work? Yes, for fission (n,f), not for gamma decay (n,g).



# What about other neutron induced reactions?

- Remains untested for (n,n') and (n,2n) reactions
- We can test the model sensitivity to Spin and Parity



# I tested the Weisskopf-Ewing approximation for the (n,n') reaction on 90Zr targets



# I tested the Weisskopf-Ewing approximation for the (n,2n) reaction on 90Zr targets



## A reaction produces nuclei with a range of spins and parities!



Escher, Dietrich, Phys. Rev. C 74, 054601 (2006)

## I chose an analytic distribution with two parameters to occupy the compound nucleus



# Full picture: Weisskopf-Ewing approximation



# The tests I preformed suggest that the WE approximation is valid for these reactions



# The tests I preformed suggest that the WE approximation is valid for these reactions



# Variance of the predictions fall within current experimental error



# I tested the WE approximation for (n,n) and (n,2n) on 90Zr

- Generate artificial spin and parity distributions
- 2. Create simulated surrogate data
- Compute the WE limit using the simulated surrogate data

The simulated predictions  $\sigma_{\alpha\beta}^{WE}$ are sufficiently similar for reasonable  $F(J, \pi)$   $F(J,\pi)$ 

$$P_{d\beta}^{WE}(E) = G_{\beta}^{CN}(E)$$

$$\sigma_{\alpha\beta}^{WE}(E) = \sigma_{\alpha}^{\prime CN}(E) P_{d\beta}^{CN}(E)$$

The WE limit is valid

# **Results are promising**

Conclusions:

- (n,n') and (n,2n) reactions on Zr are much less sensitive to spin and parity than capture reactions
- Whether this is sufficient depends on the application
- Further investigations are required, but results are promising

Next steps:

- Investigate effects of pre-equilibrium
- Apply this theory to new Gadolinium data













2.0















5.0











0.14 0.16 LDIa1

























Posterior distributio

Prior All threads

0.0030 -

0.002

0.0020

0.2

3.0



Posterior distribution

32.0

3175

215

212

0100

1075

2050

3025

1000

Prior All threads



3.5 4.0 E1g2

4.5











44

## **The Surrogate Idea**



# The (General) Surrogate Method Combines Surrogate Data and Theory

