Fission Products Off Stability

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2024 CSEWG Meeting

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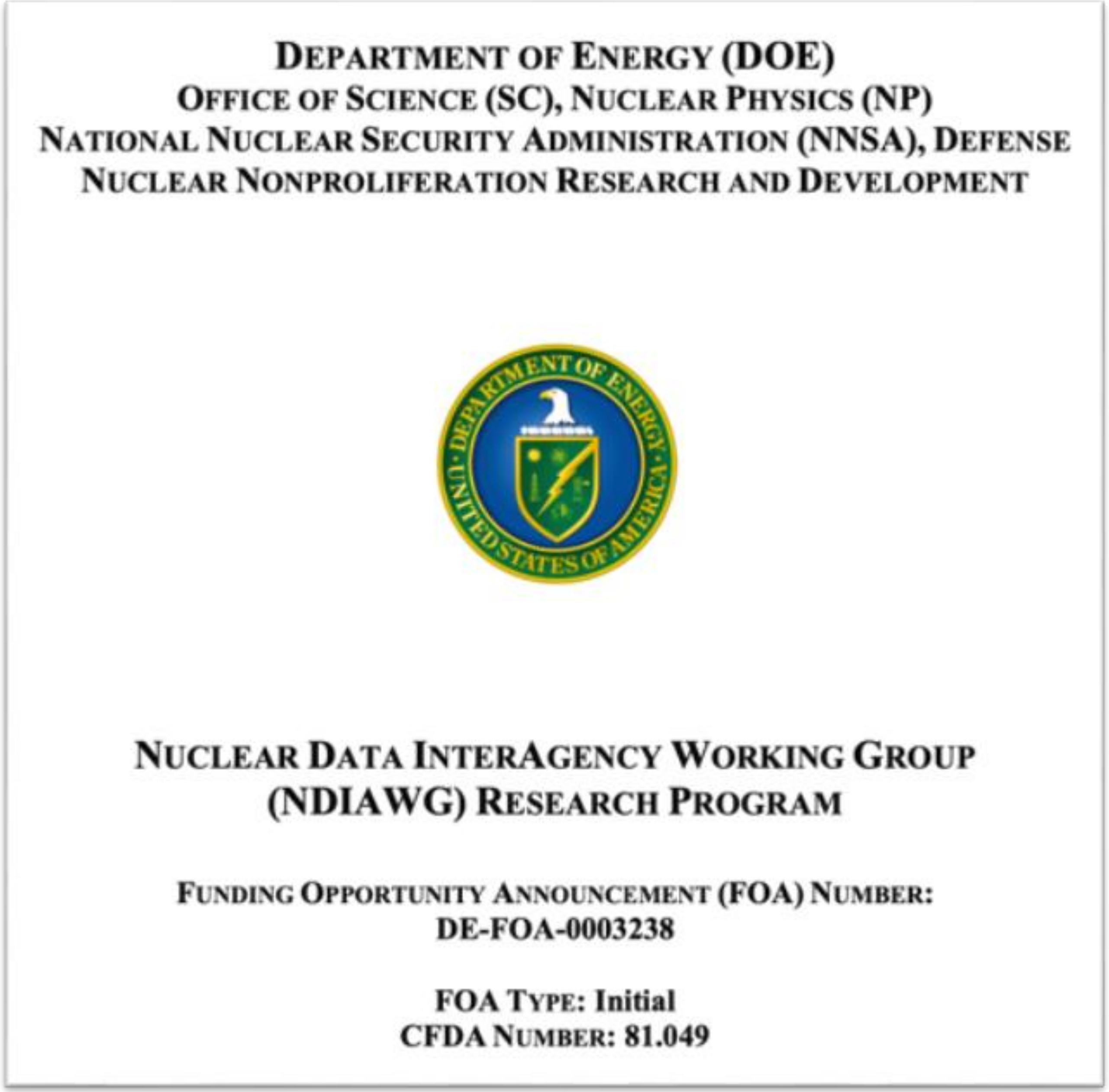
Outline

- Project Goals and Objectives
- Approach
- Project Description

The project has just begun, so this talk reports on the planned evaluation efforts, not work already performed!



DEPARTMENT OF ENERGY (DOE)
OFFICE OF SCIENCE (SC), NUCLEAR PHYSICS (NP)
NATIONAL NUCLEAR SECURITY ADMINISTRATION (NNSA), DEFENSE NUCLEAR NONPROLIFERATION RESEARCH AND DEVELOPMENT

NUCLEAR DATA INTERAGENCY WORKING GROUP (NDIAWG) RESEARCH PROGRAM

FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) NUMBER:
DE-FOA-0003238

FOA TYPE: Initial
CFDA NUMBER: 81.049

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Project Goals and Objectives

Goals:

- To develop a reproducible method to produce realistic evaluations for nuclei off-stability
- Apply the method to produce new evaluations of fission products off stability

Key Objectives:

- To provide evaluated files for the main off-stability fission products of ^{235}U and submit them to the ENDF/B nuclear data library
- Develop a robust and reproducible method for such evaluations
- Stretch goal: develop evaluated files for all off-stability fission products from ^{235}U, ^{239}Pu, ^{252}Cf

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Project Goals and Objectives

The **core-goal nuclei** (mostly produced by ^{235}U fission):

- <u>1st Fission yield bump</u>: $^{87-89}$Br, $^{88-92}$Kr, $^{91-94}$Rb, $^{92-97}$Sr, $^{95-99}$Y, $^{97-102}$Zr, $^{101-103}$Nb
- <u>2nd Fission yield bump</u>: $^{131-133}$Sb, $^{132-136}$Te, $^{135-138}$I, $^{136-141}$Xe, $^{139-143}$Cs, $^{141-146}$Ba, $^{144-145}$La, $^{147-148}$Ce

Secondary goal (main fission products from ^{239}Pu and ^{252}Cf):

- <u>1st Fission yield bump</u>: ^{94,100}Y, ^{96,103}Zr, ^{99,100,104,105}Nb, $^{102-108}$Mo, $^{105-110}$Tc, $^{107-112}$Ru, $^{110-114}$Rh, $^{112-116}$Pd, ^{114}Ag
- <u>1st Fission yield bump</u>: ^{131}Te, ^{134}I, ^{135}Xe, ^{137,138,144}Cs, ^{140}Ba, $^{143,146-148}$La, ^{145,146,149,150}Ce, $^{149-152}$Pr, $^{151-153}$Nd

Stretch goal (whole isotopic chain of fission products from ^{235}U, ^{239}Pu, and ^{252}Cf):

- ^{66}V, $^{66-67}$Cr, $^{66-71}$Mn, $^{66-75}$Fe, $^{66-77}$Co, $^{66-80}$Ni, $^{66-82}$Cu, $^{66-85}$Zn, $^{68-87}$Ga, $^{70-90}$Ge, $^{72-92}$As, $^{75-95}$Se, $^{77-98}$Br, $^{79-101}$Kr, $^{81,83-103}$Rb, $^{83-106}$Sr, $^{87-109}$Y, $^{88-112}$Zr, $^{91-114}$Nb, $^{93-117}$Mo, $^{97-119}$Tc, $^{98-121,124}$Ru, $^{101-125}$Rh, $^{103-126,128}$Pd, $^{106-132}$Ag, $^{108-134}$Cd, $^{111-137}$In, $^{113-139}$Sn, $^{118-140}$Sb, $^{120-143}$Te, $^{123,125,126,128-145}$I, $^{125,128,130-148}$Xe, $^{131-151}$Cs, $^{132-153}$Ba, $^{135,137-155}$La, $^{137-157}$Ce, $^{139-159}$Pr, $^{142-161}$Nd, $^{144-163}$Pm, $^{147-165}$Sm, $^{149,151-168}$Eu, $^{152-170}$Gd, $^{155-172}$Tb, $^{157-172}$Dy, $^{161-172}$Ho, $^{162-172}$Er, $^{165-172}$Tm, $^{168-172}$Yb, $^{171-172}$Lu

<u>Project will be successful if core-goal is achieved</u>. *However*, when the methods are well-stablished, generalization to secondary and stretch goals should be possible with relative low effort.

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Project impact on the program

- Applications such **nonproliferation, post-detonation forensics, spent-fuel assay, reactor burnup and design**, as well as **astrophysics**, rely on the accurate description of the neutron interaction with unstable fission products.
- Current cross-section descriptions of these nuclei are either non-existent or based on simplified assumptions, leading to unquantified impacts on predicted cross-sections.
- By project completion, more **predictive/realistic** new nuclear data will be produced, improving the **reliability** of applications involving **fission products off stability!**

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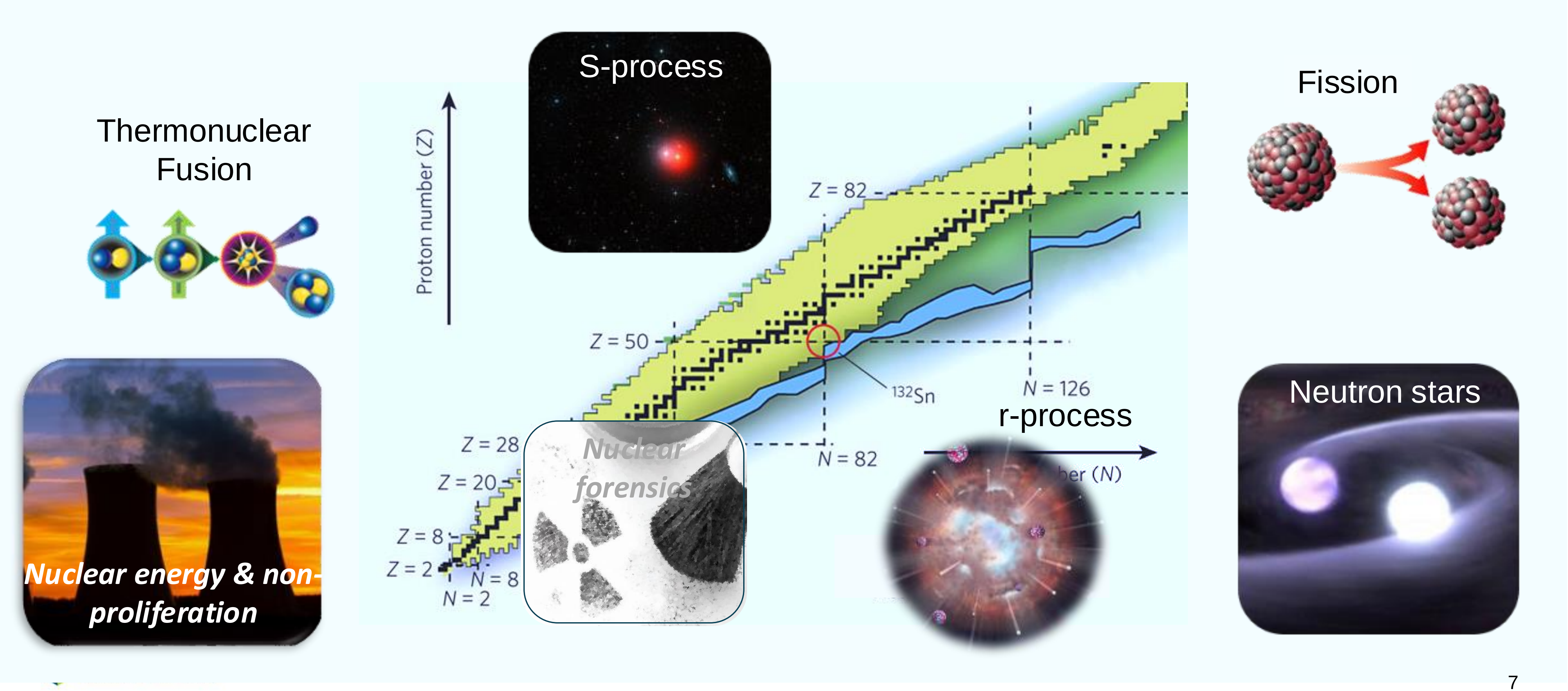
Approach

Approach:

- Resonance region:
  - Treat whole resonance region as unresolved, leveraging machine-learning (ML) and stochastic methods to estimate cross-section probabilities
- Fast region:
  - Employ more predictive and realistic reaction models
  - Leverage ML approach to extrapolate threshold reactions to be used as priors for parameter fitting
  - Experimental component to measure nuclear level densities of neighboring nuclei to further constrain models.

Nuclear Data is the interface between nuclear physics and science and technical application that depend nuclear physics



Many software packages use embedded ENDF/B data

PHITS — Particle and Heavy Ion Transport code System

FLUKA

MCNP6

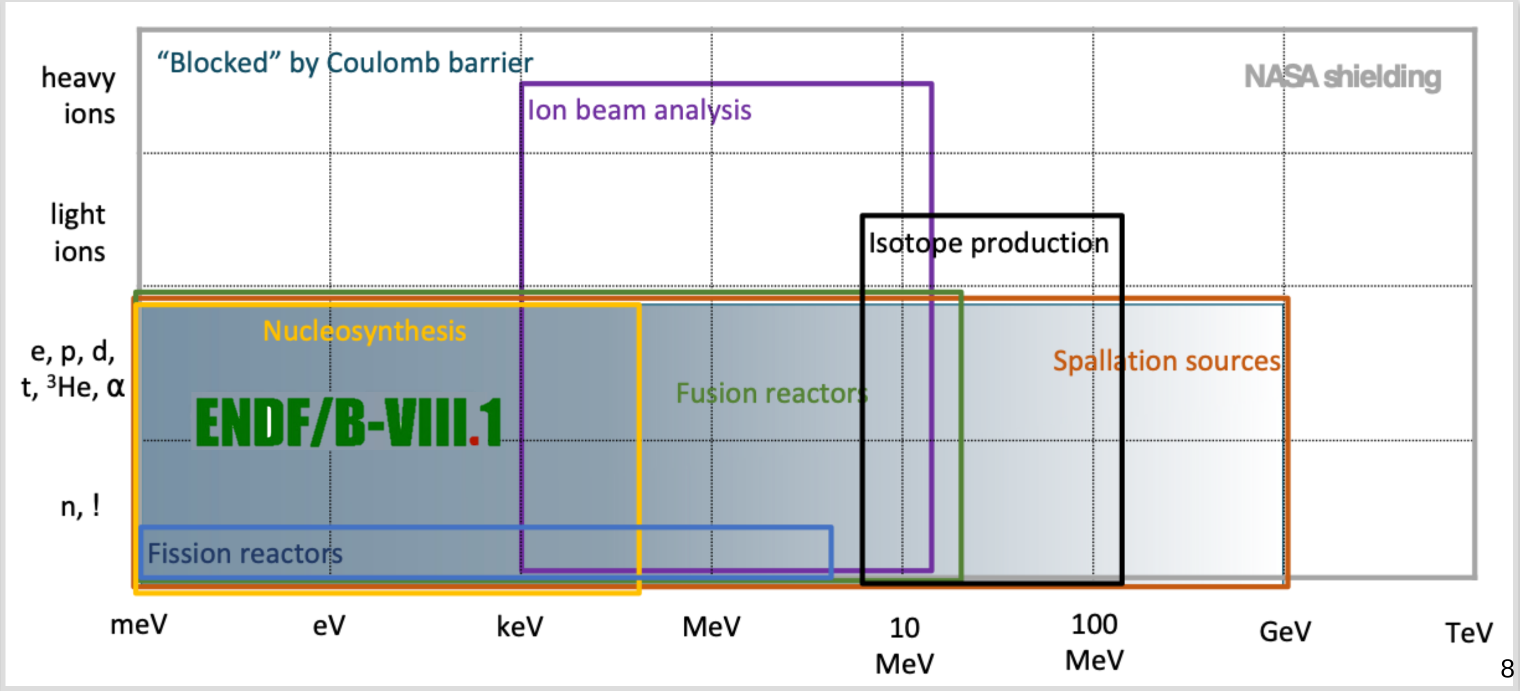
scale — Nuclear Systems Modeling & Simulation

GEANT4 — A SIMULATION TOOLKIT

OpenMC

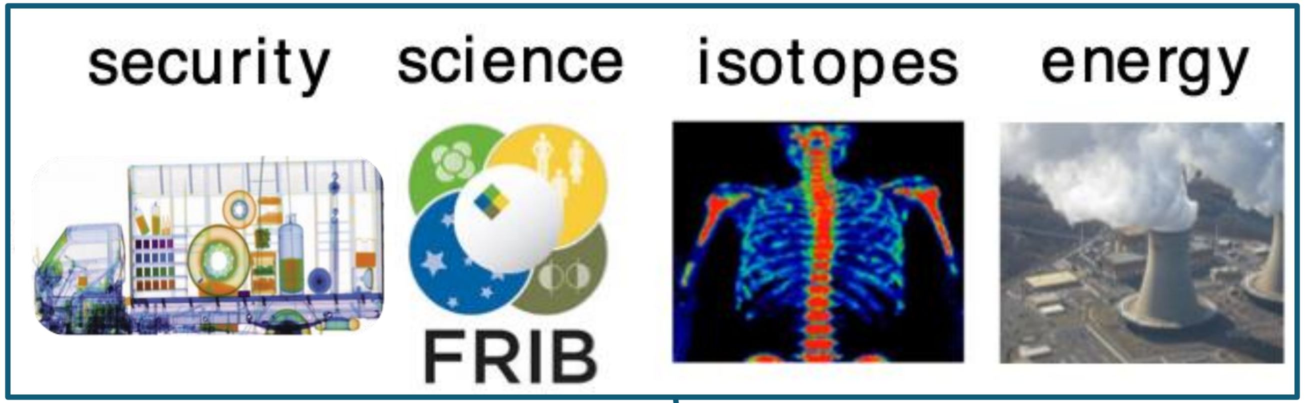
GENIE 2000 — Applications Software

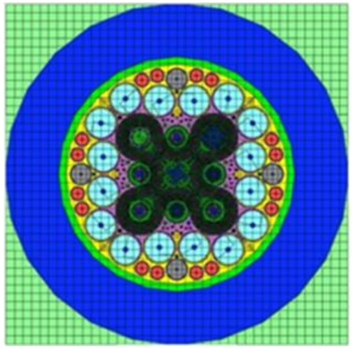
- Reactor design, simulation and licensing codes.
- Nuclear waste and repositories.
- Radiation spectroscopy, dose, detectors and shielding.
- Defense and CTBTO.

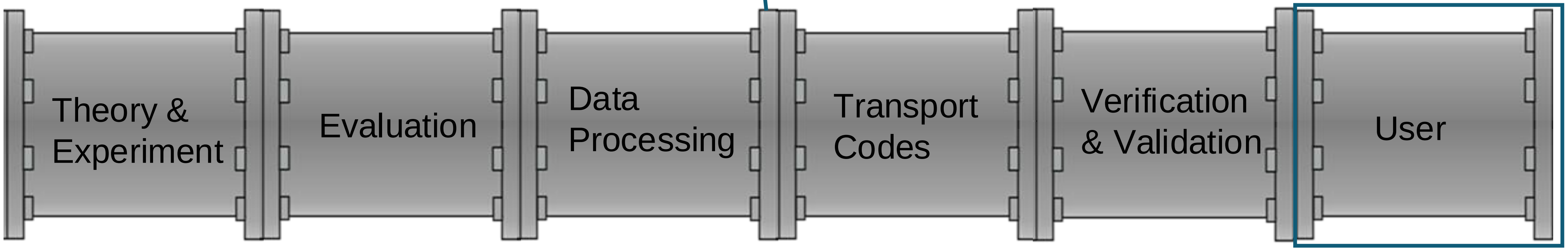


The Nuclear Data Pipeline

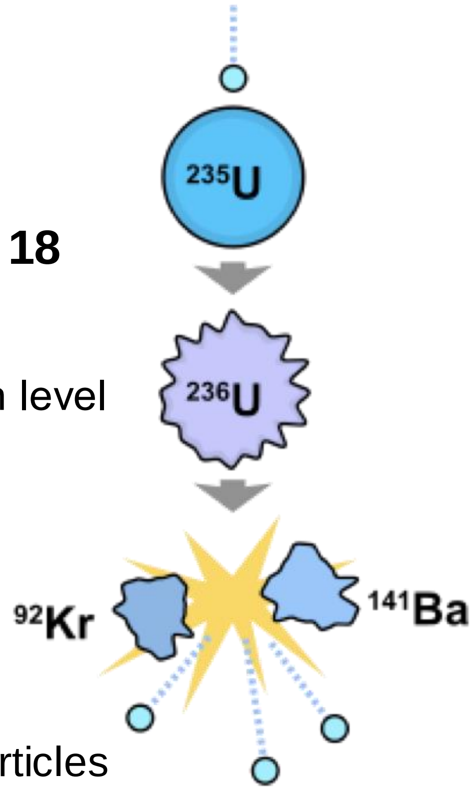
Our goal is to get the highest quality data to users





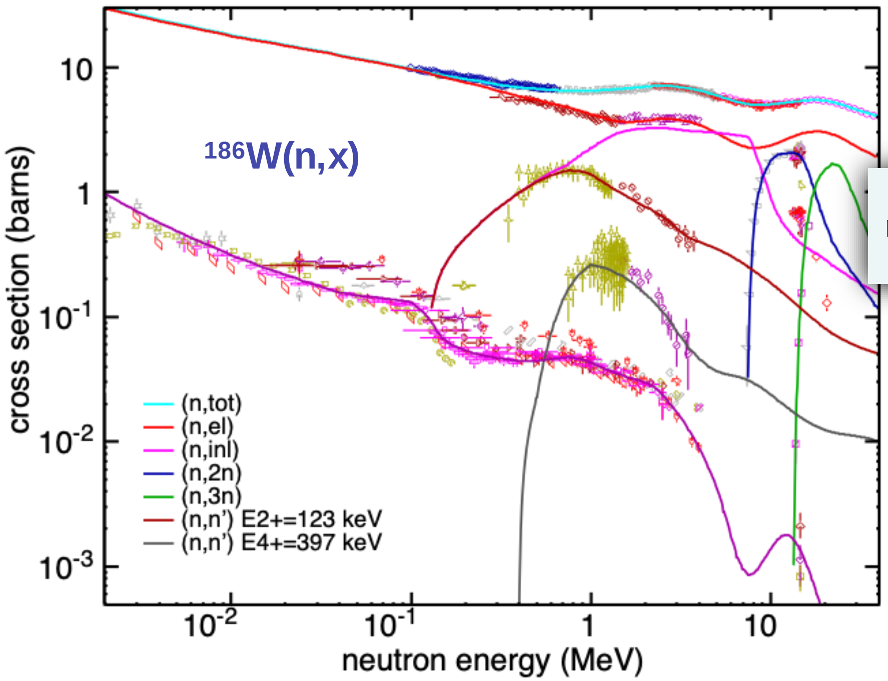


Evaluated Nuclear Data File: Nuclear reactions

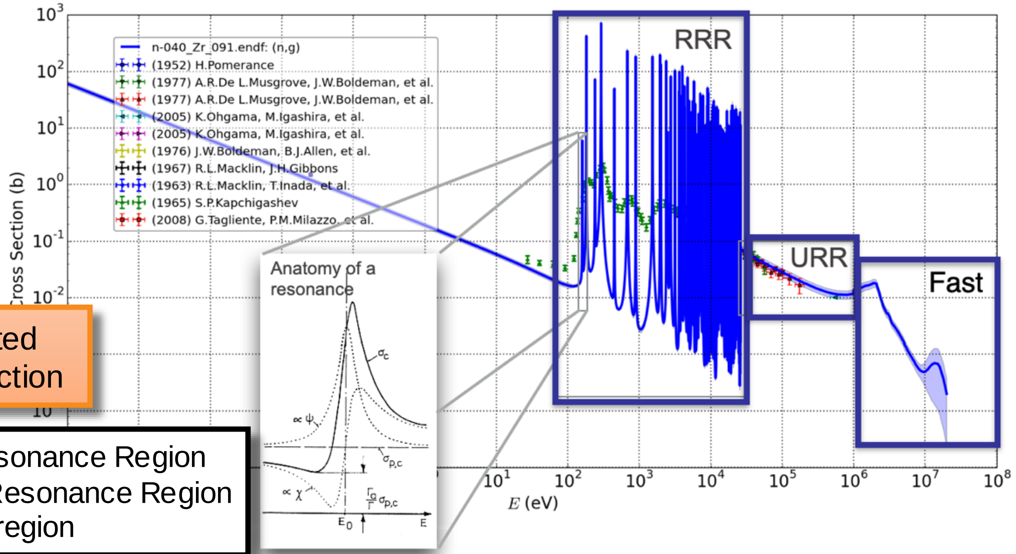


A **reaction evaluation** is the description of **everything** that can happen from the nuclear reaction between a **projectile** and a **target**

- **Typical neutron incident on non-actinide has ~ 18 relevant reactions**
  - ~ 5 threshold reactions: (n,2n), (n,3n), (n,p), etc.
  - ~ 10 discrete level excitation reactions: (n,n') for each level in residual nucleus
  - 3 non-threshold reactions: (n,tot), (n,el), (n,γ)
- **Actinides add fission, (n,f)**
- **For transport studies, need:**
  - Cross sections
  - Multiplicities of all emitted particles
  - Outgoing energy-angle distributions for all emitted particles



Experimental data never enough: need theory to fill in gaps



Typical evaluated capture cross section

RRR: Resolved Resonance Region
URR: Unresolved Resonance Region
Fast: Fast-neutron region

Which nuclei are we focusing on in this project?

- 1st Bump: $^{87-89}$Br, $^{88-92}$Kr, $^{91-94}$Rb, $^{92-97}$Sr, $^{95-99}$Y, $^{97-102}$Zr, $^{101-103}$Nb
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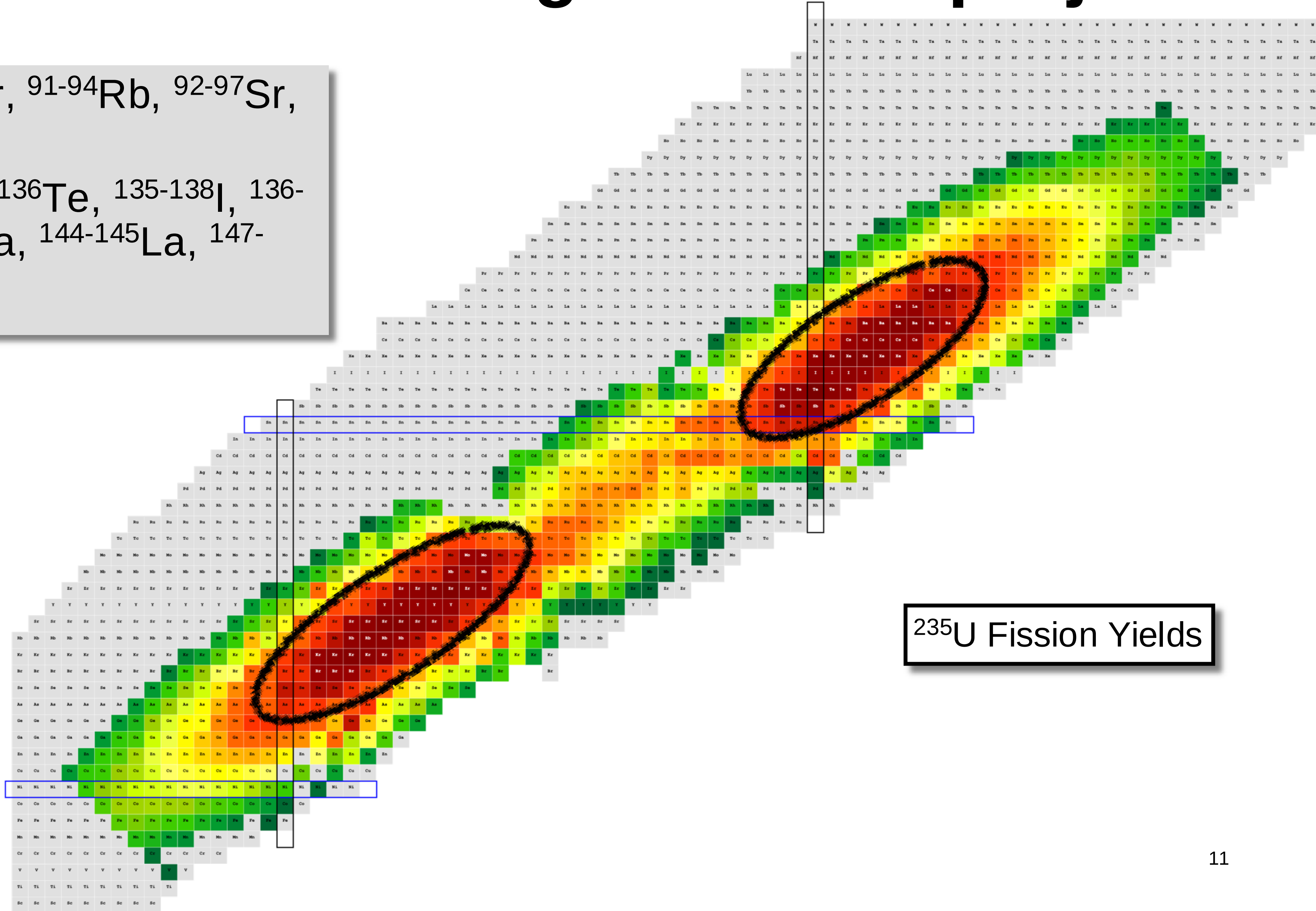

^{235}U Fission Yields

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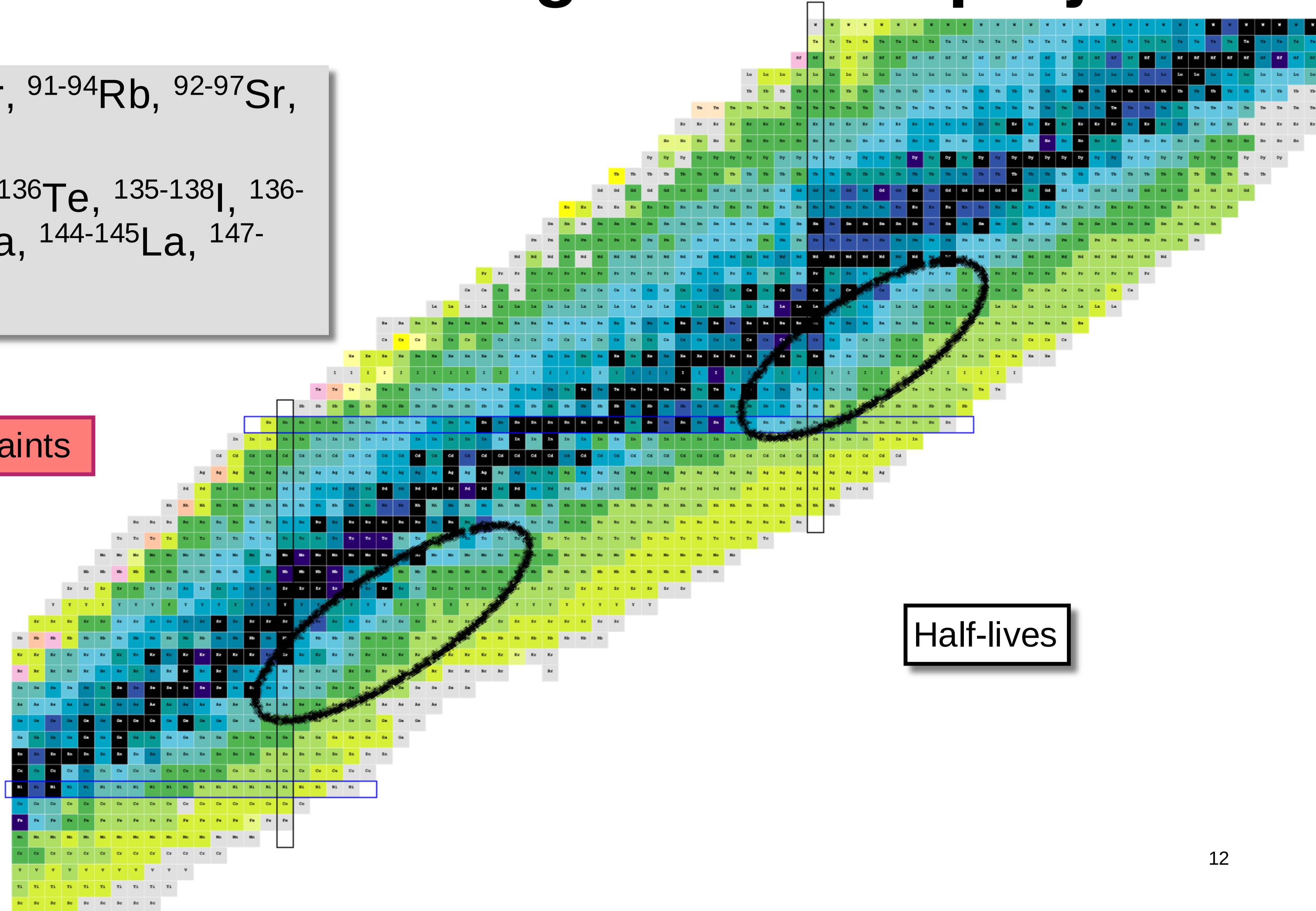
Off-stability = few data constraints



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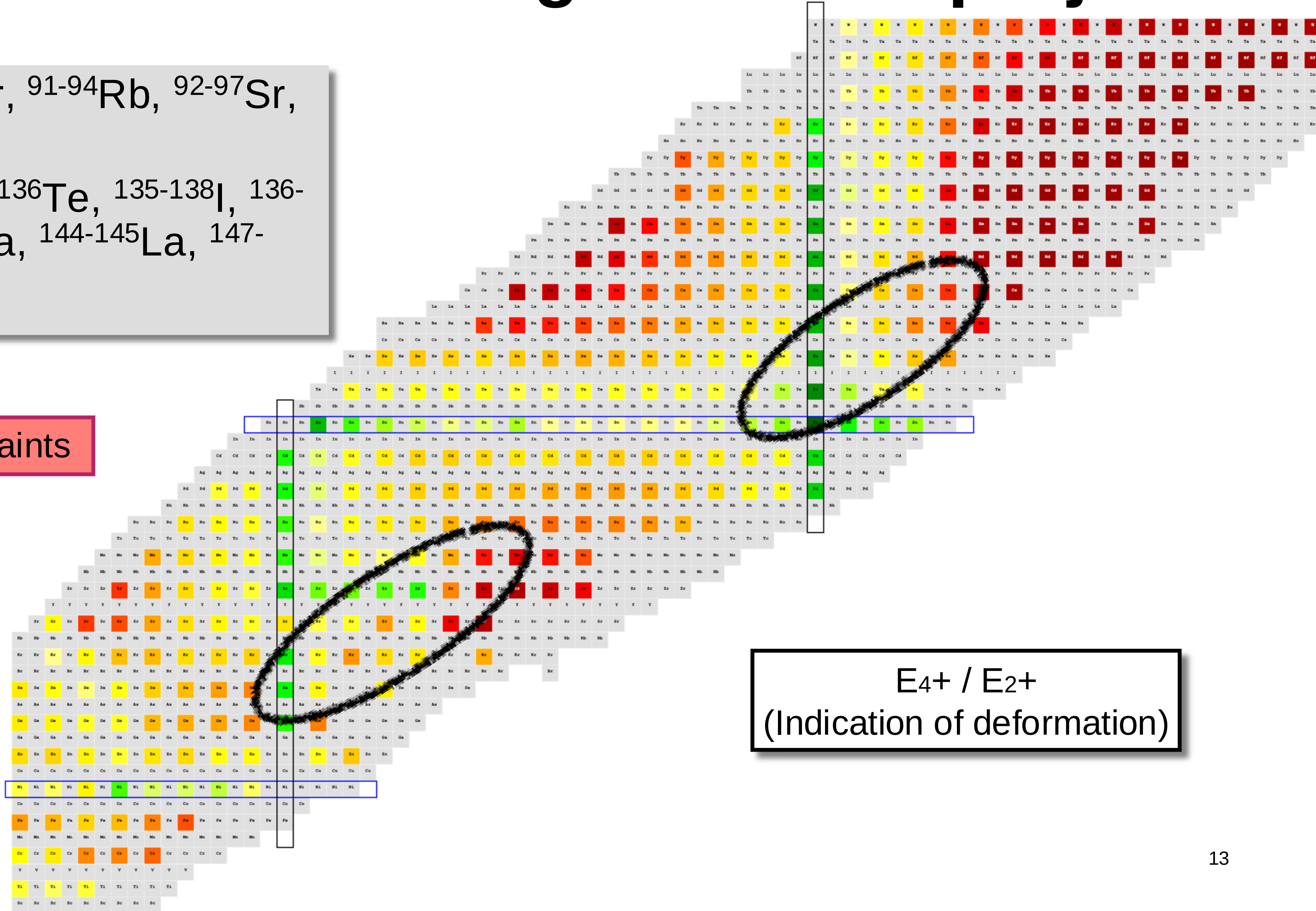
Off-stability = few data constraints

Many are (highly-)deformed!



E_{4+} / E_{2+}
(Indication of deformation)

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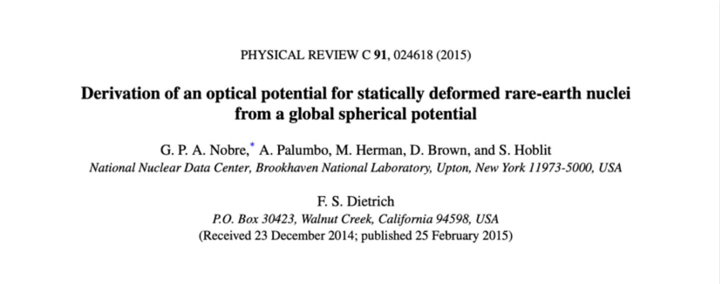
Fast region: We will leverage previous experience with deformed nuclei


PHYSICAL REVIEW C 91, 024618 (2015)

Derivation of an optical potential for statically deformed rare-earth nuclei from a global spherical potential

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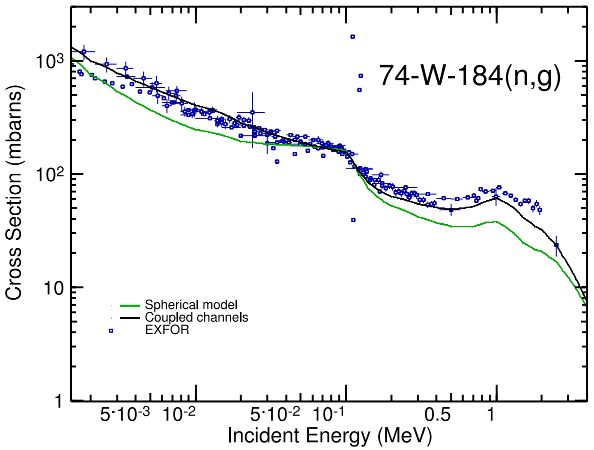
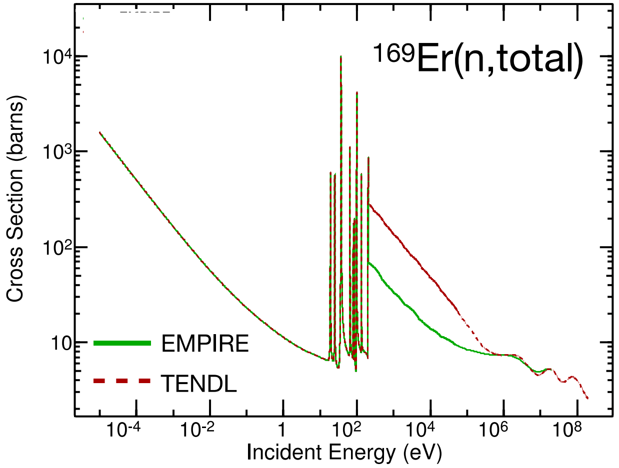
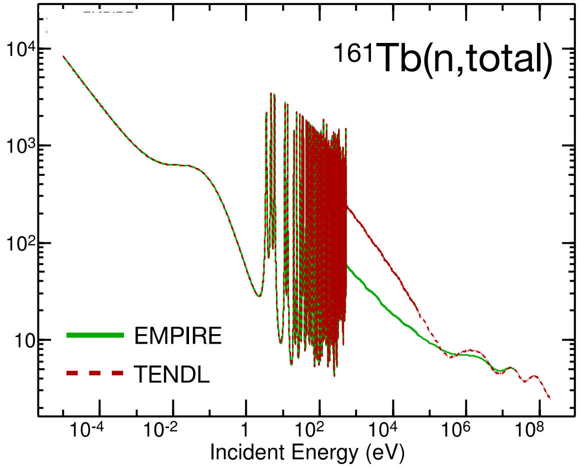
- Predictive adiabatic model for deformed nuclei
- Proper treatment changes cross sections by orders of magnitude







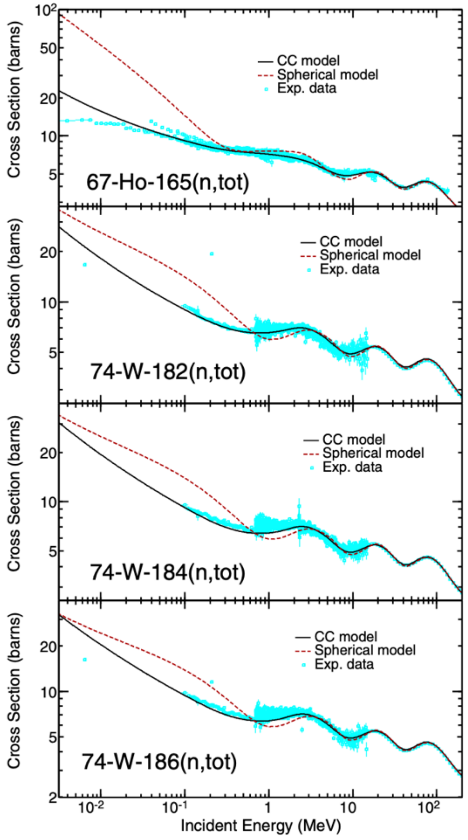
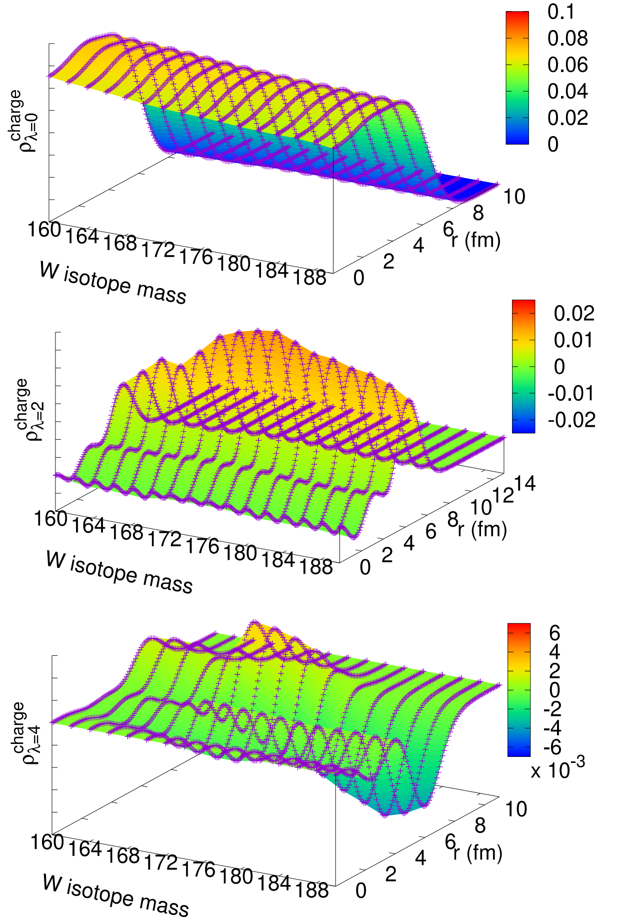
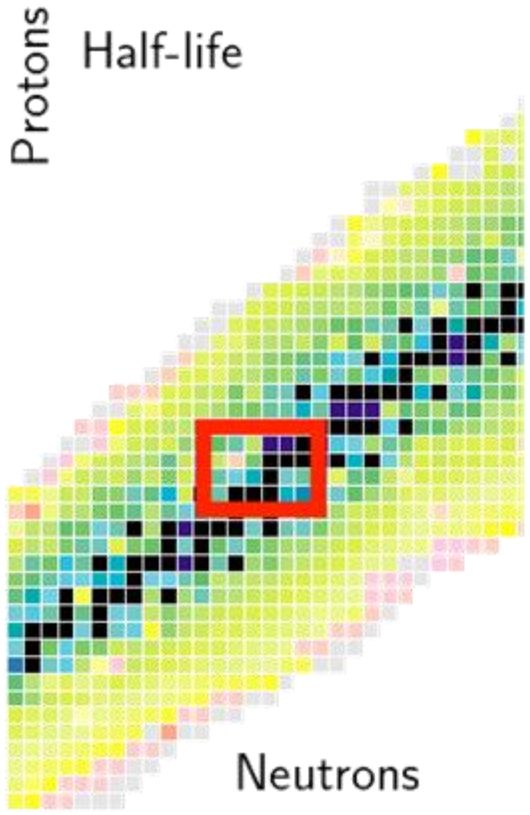


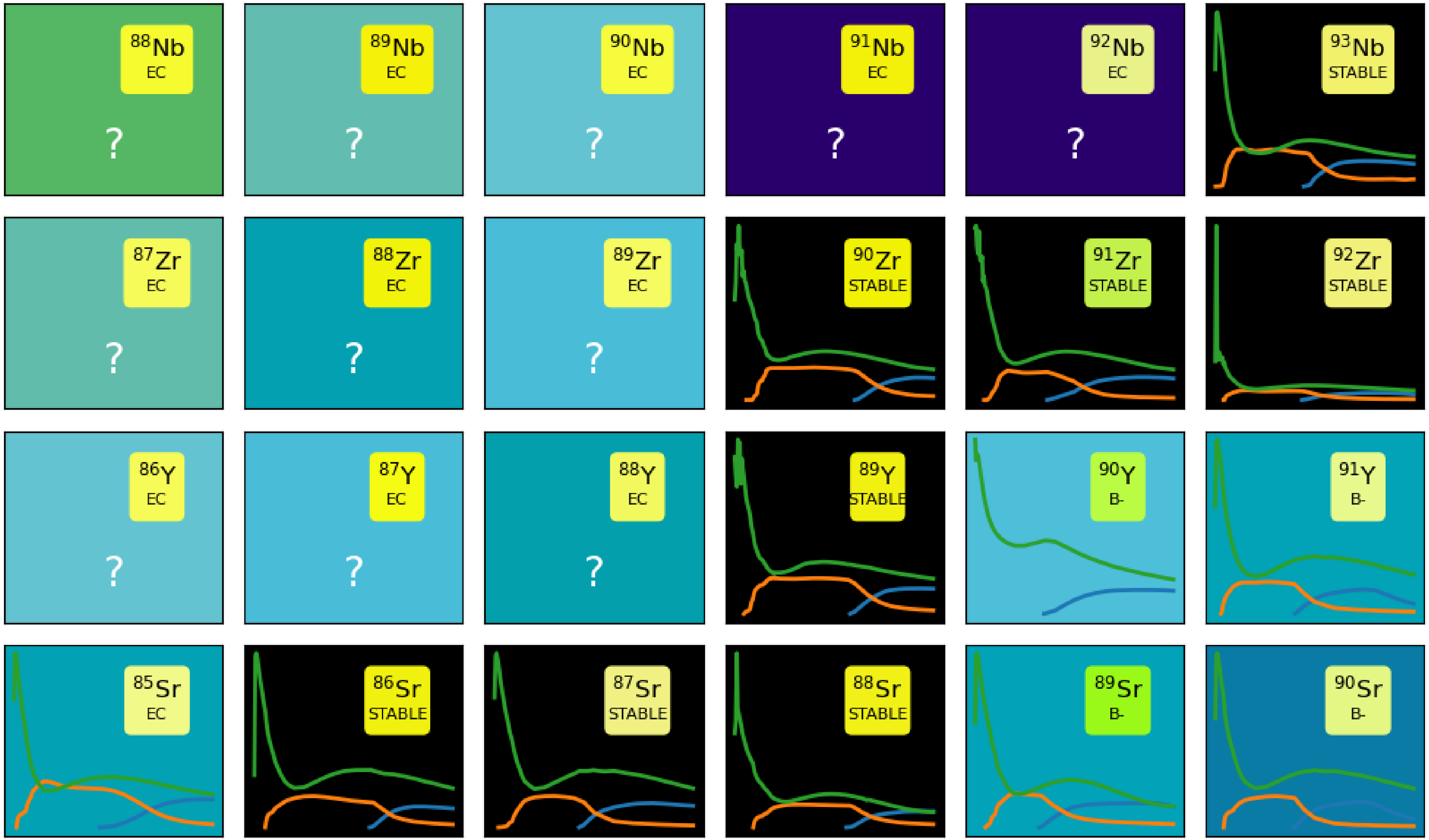
FIG. 1. (Color online) Total cross sections for neutrons scattered by a ^{165}Ho and ^{182,184,186}W targets for incident energies ranging from as low as ≈3 keV to as high as 200 MeV, which is the upper limit of validity for the KD optical potential [2]. The solid black curves correspond to the predictions of our CC model, while the dashed red curves are the results of calculations within the spherical model. The experimental data were taken from the EXFOR nuclear data library [39].



Nuclear density of charge for $^{160\text{-}188}$W calculated within a microscopic HFB model.

Under LDRD at LLNL, we are using existing calculations and measurements to learn how cross sections transform across the nuclear chart





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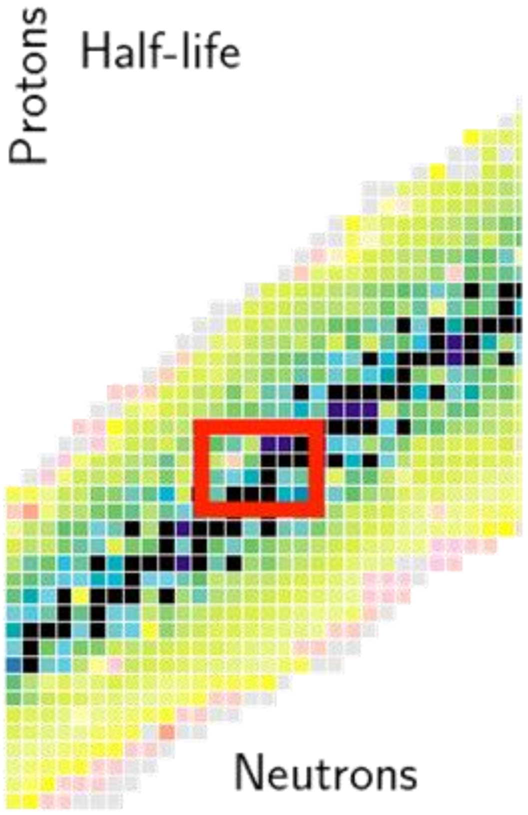

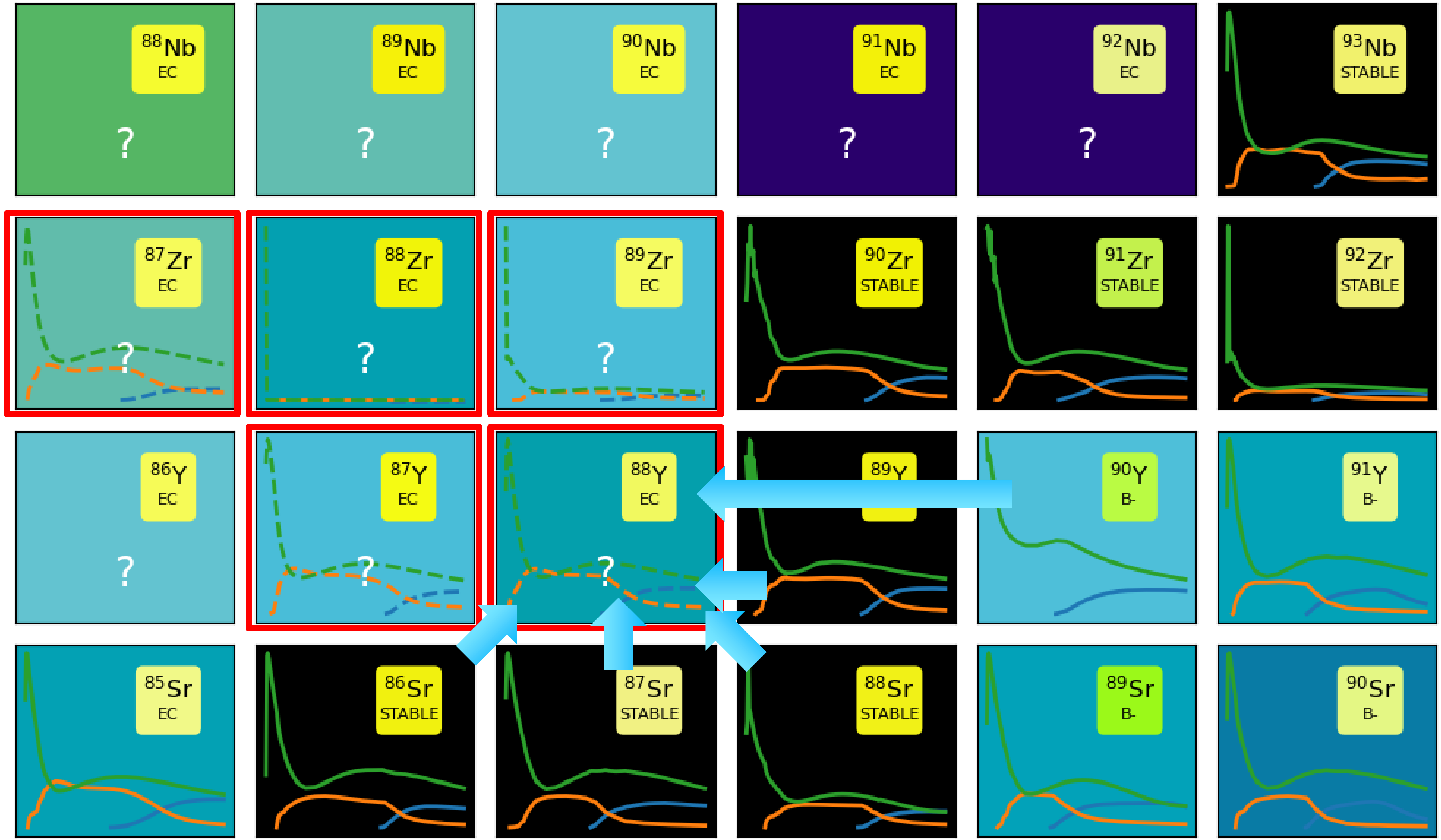

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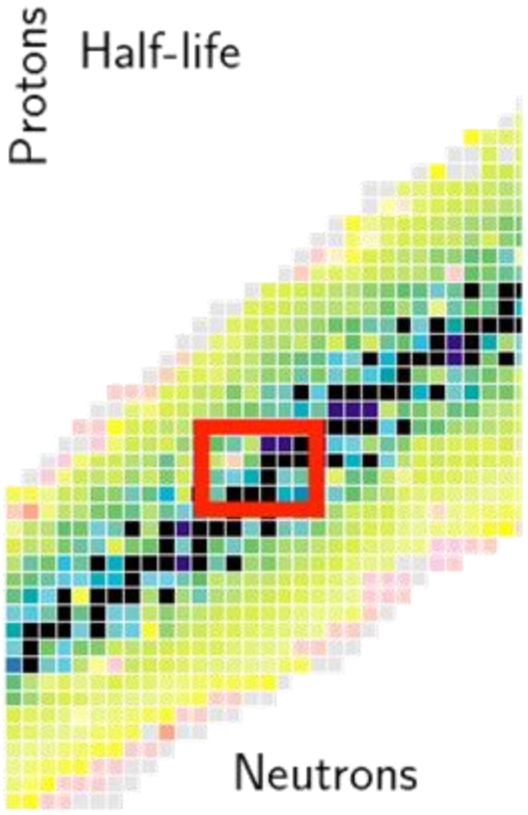
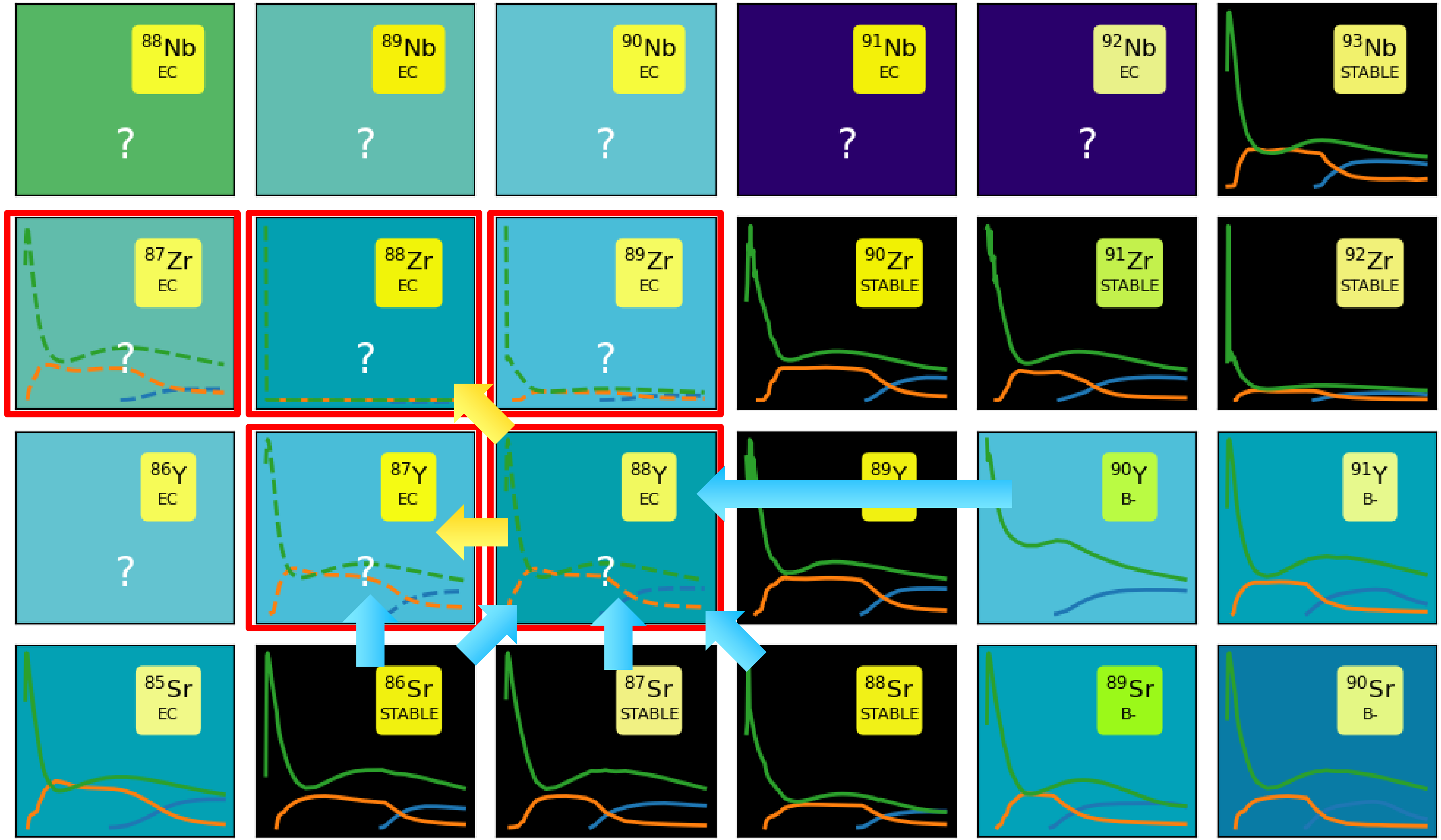
We will leverage the tools from this LDRD to provide "systematic" priors for evaluations on unstable nuclei.





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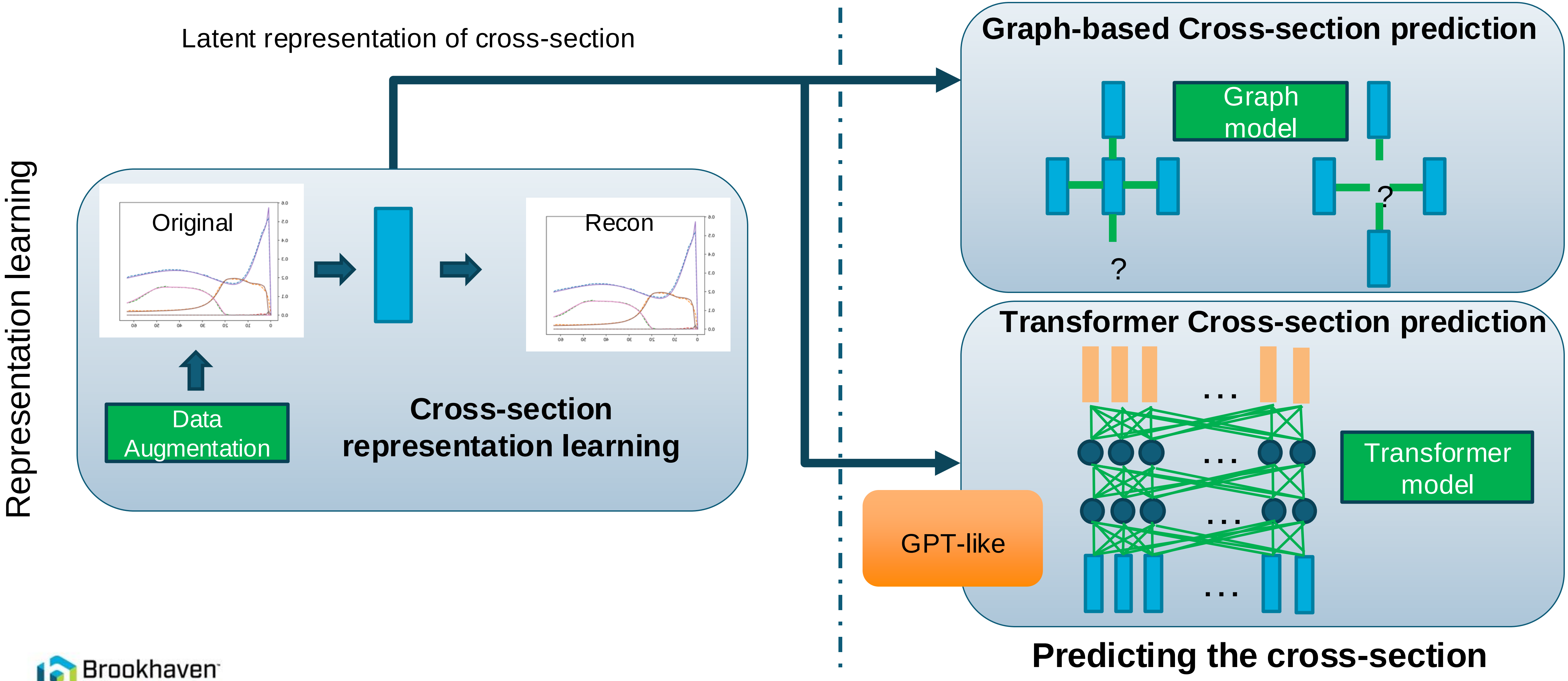
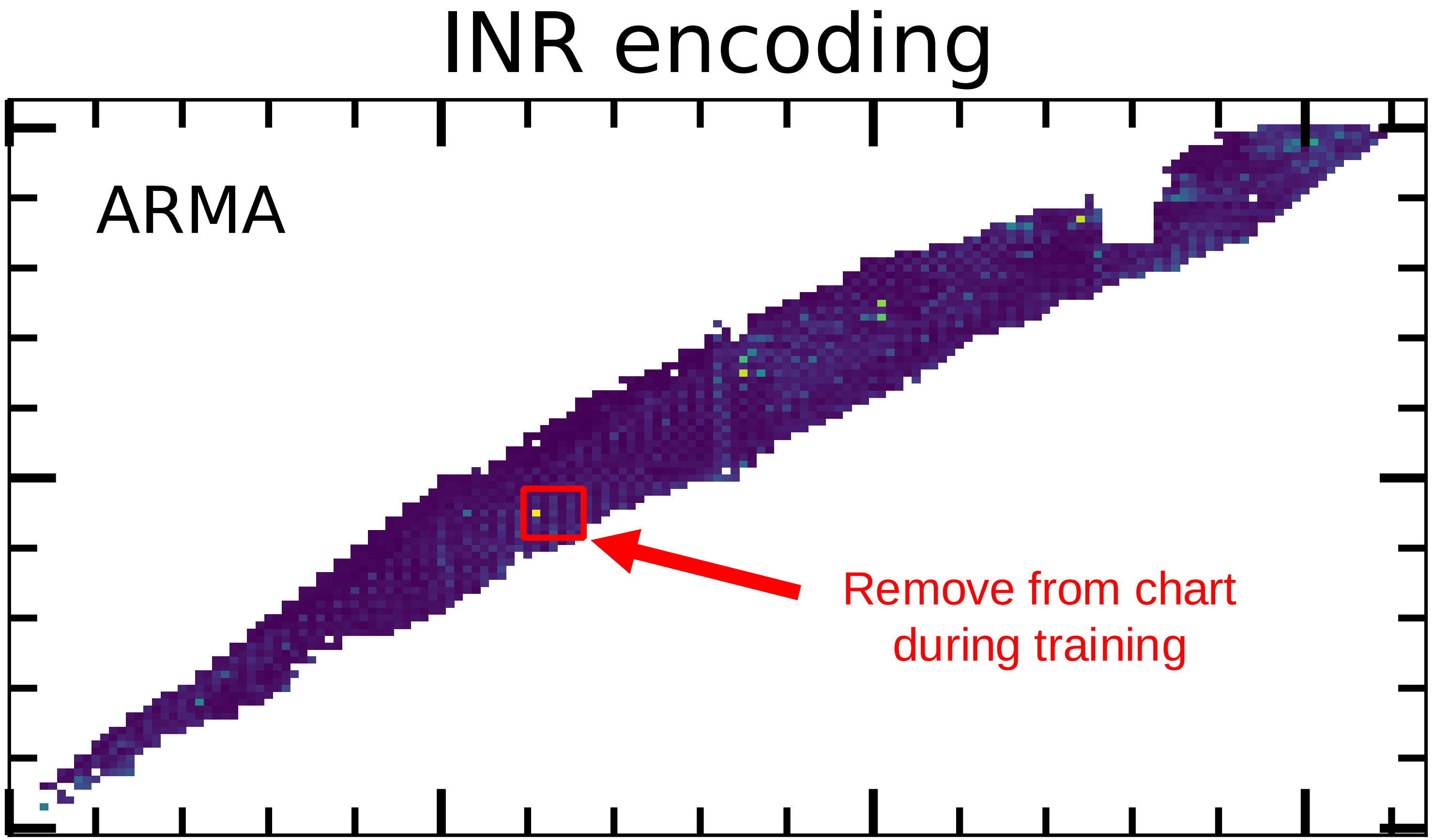
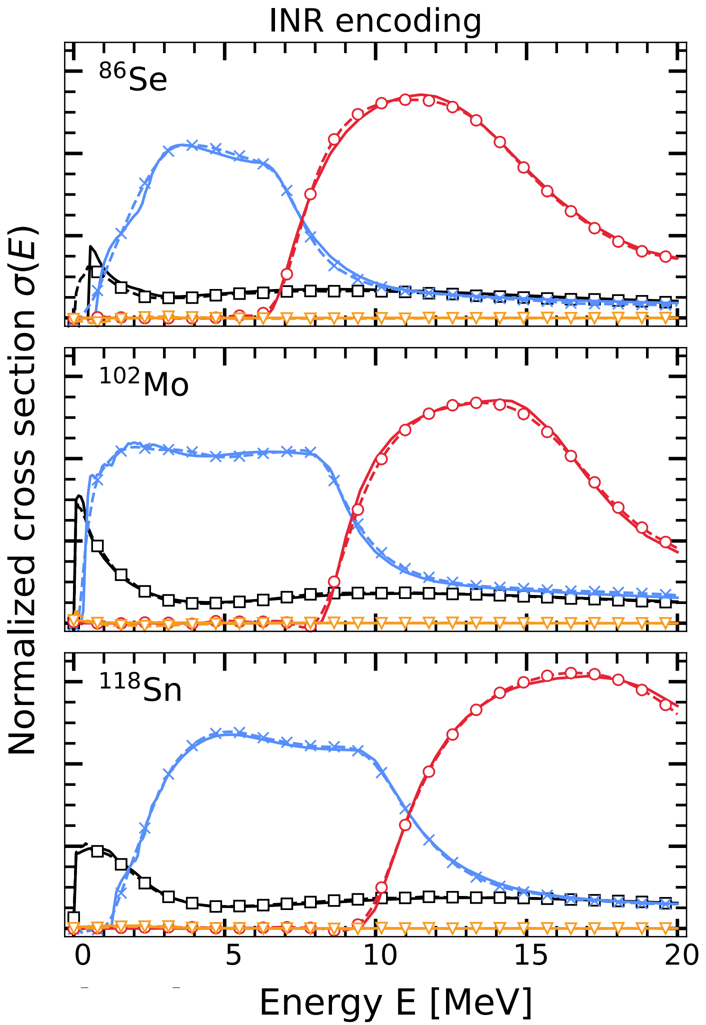
We have developed a framework for learning and predicting cross sections across the chart.

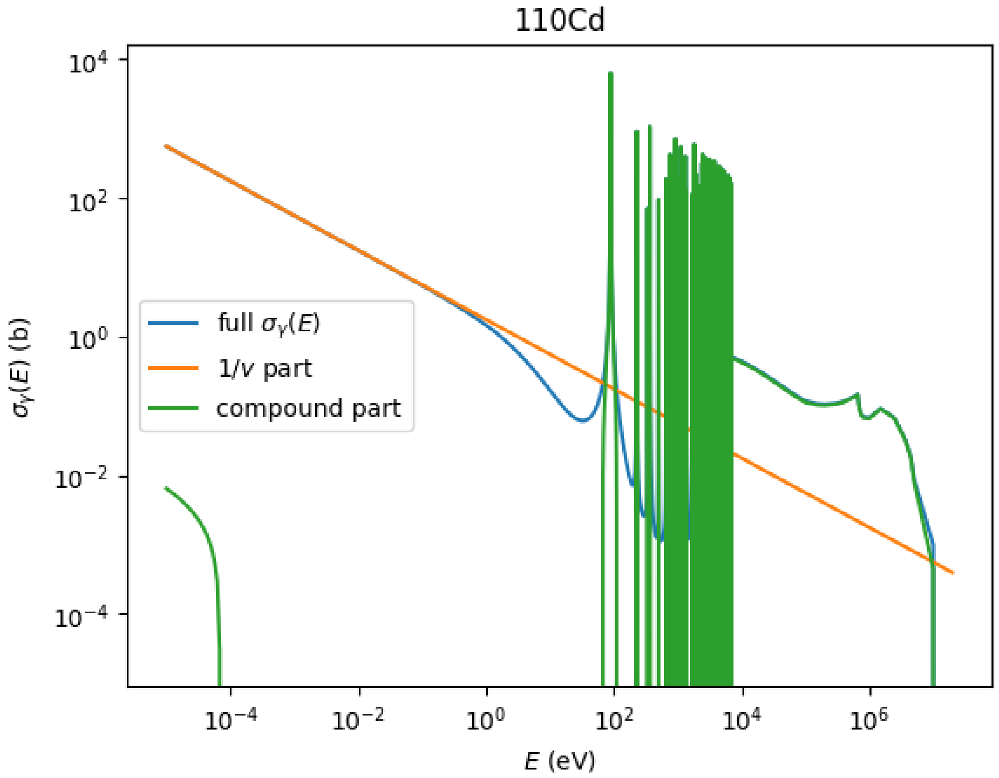


Graph framework can precisely infer missing data





Capture cross-sections at low energies



Capture cross-sections have

- A 1/v part – the shape is analytic, the magnitude must be measured
- A compound nuclear part consisting of many resonances
- A smooth high-energy part that peaks around 14 MeV with σ~100 mb

Practical division:

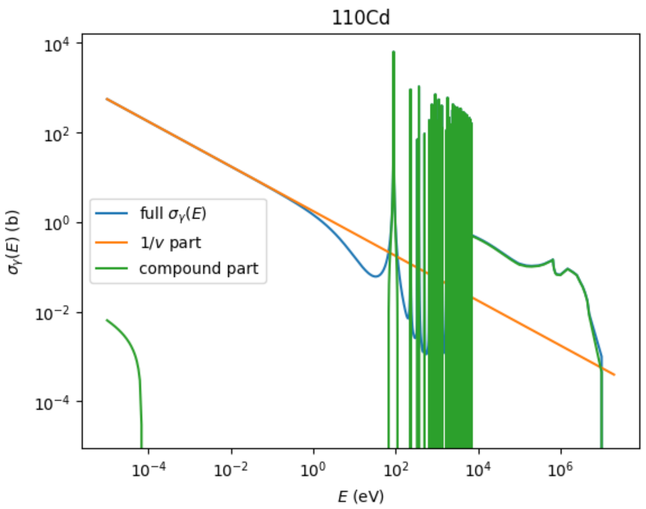
$$\sigma_\gamma(E) = \sigma_{th}\sqrt{\frac{E_{th}}{E}} + \sigma_{CN}(E)$$

Thermal component

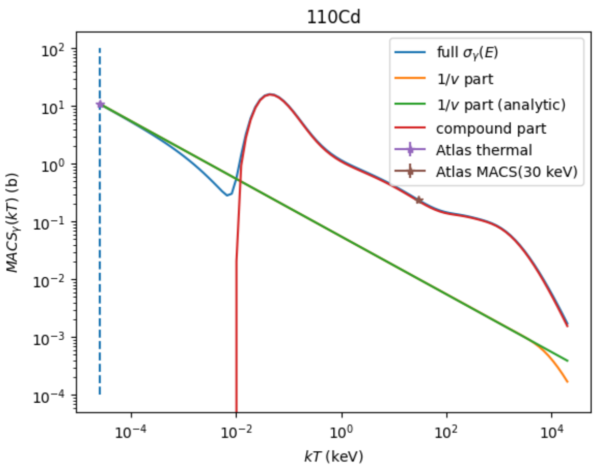
Compound nucleus component

- There are **too many** resonances.
- It is not possible to predict their position or width
- We focus on an "*average*" cross section and some *probability distribution* that captures the size of fluctuations

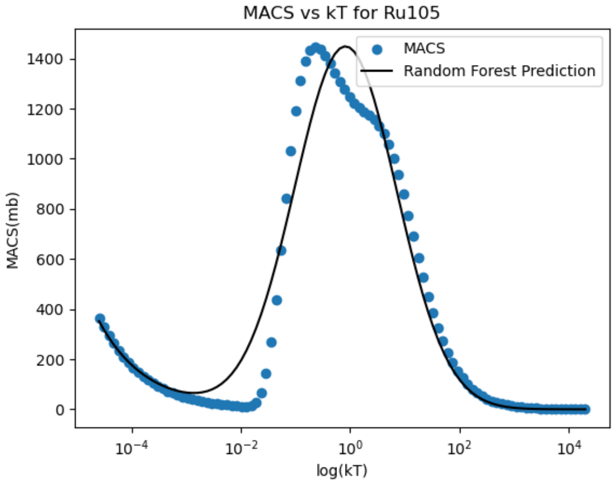
Capture cross-section average values



Build reduced order model of MACS



Learn parametric (Z,A) dependence of reduced order model



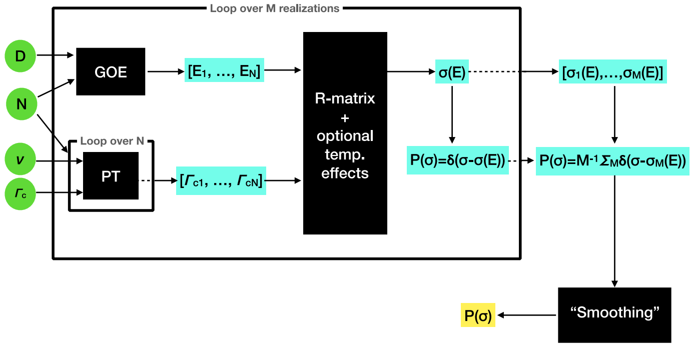
Transform model back to cross-section space

"magic" function $\sigma_\gamma(Z,A,E)$

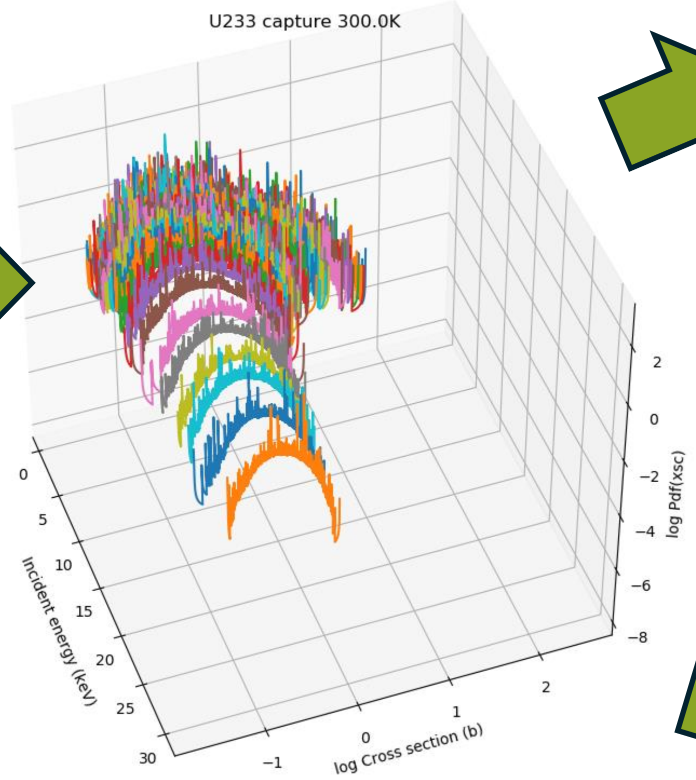
Test against original cross-sections or MACS

Leveraging preliminary work under NA-22 Intentional Forensics Venture

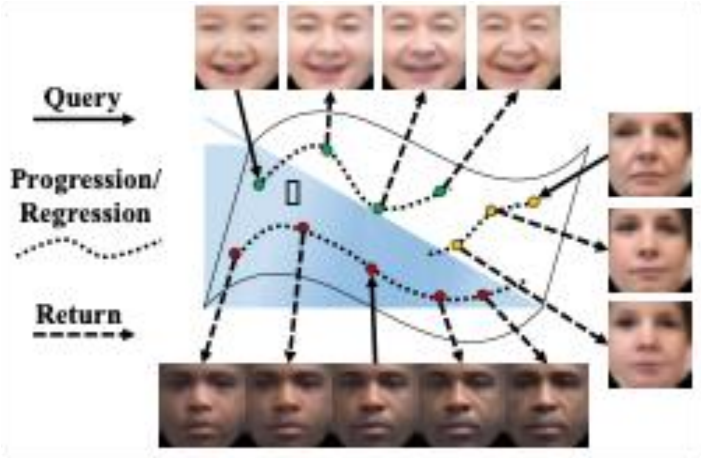
Capture cross-section fluctuations



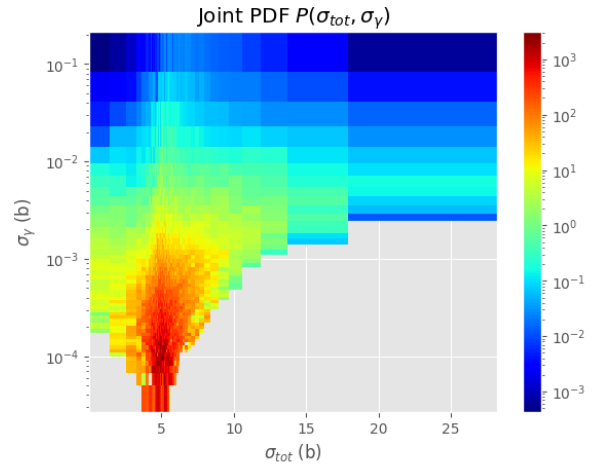
Use FUDGE as a generative model to simulate cross-section probability distribution function (PDF)



^{238}U(n,g) cross-section PDF



Use age-progression software to learn the temperature (and energy?) dependence of the cross-section PDF

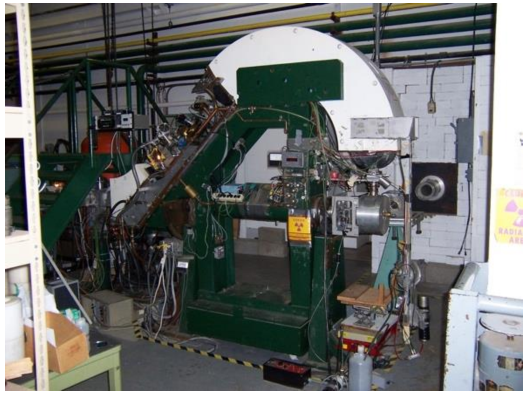


Alternatively, we can use the PDFs directly with estimates of RRR spacings & widths

Leveraging preliminary work under NCSP AM-6

Experimental level density constraints at Edwards lab, Ohio University

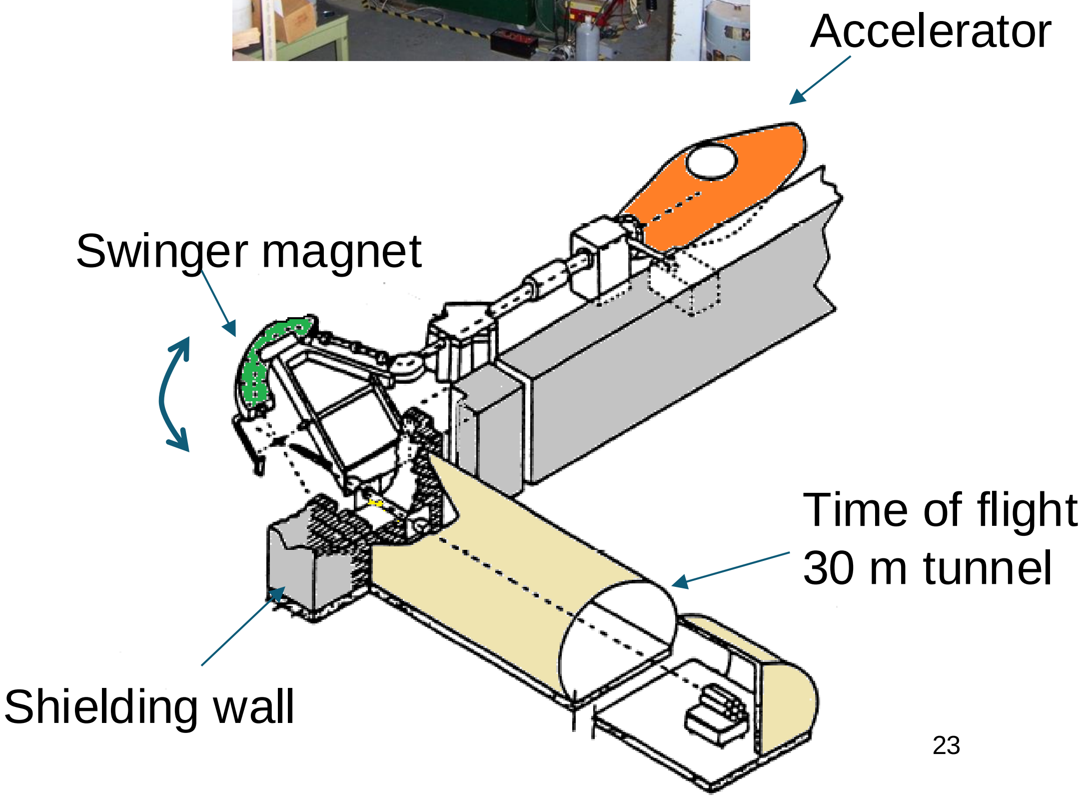
Swinger magnet



Goal: to improve systematics of the level density model parameters in the mass region of fission products thereby enhancing the **predictive power** of level density models for nuclear data evaluations when **extrapolating to nuclei off stability**.

Method:

- to review and validate available literature data on level densities measured with the different techniques over the mass range of the fission products (about 20 data sets are available).
- to address gaps in level density systematics by conducting targeted experiments at the Edwards Lab and benchmark models against experimental data



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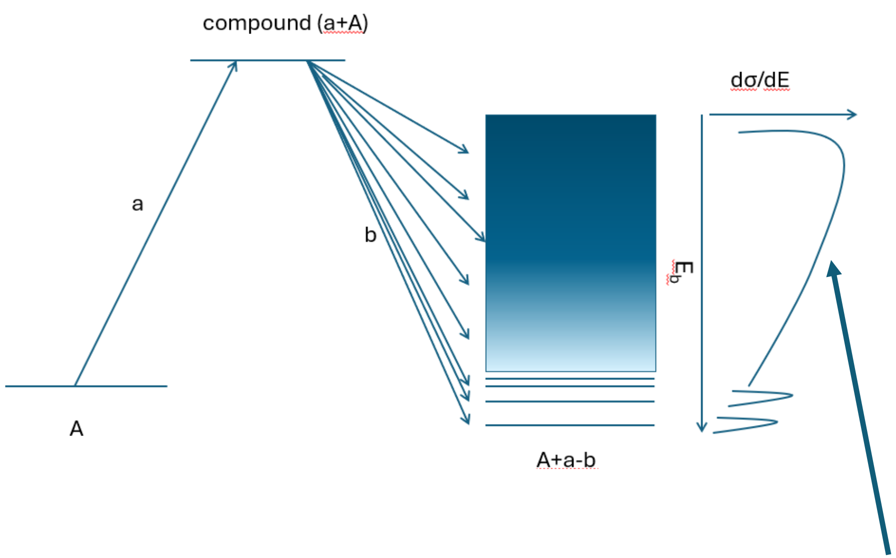
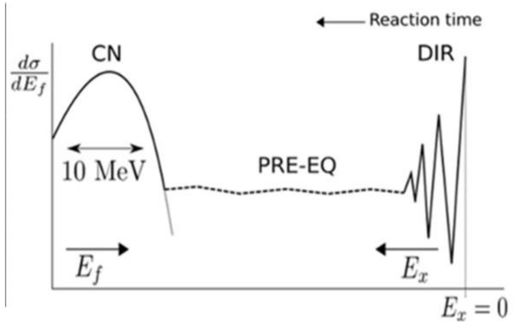
Particle evaporation technique to study level densities at the Edwards Lab

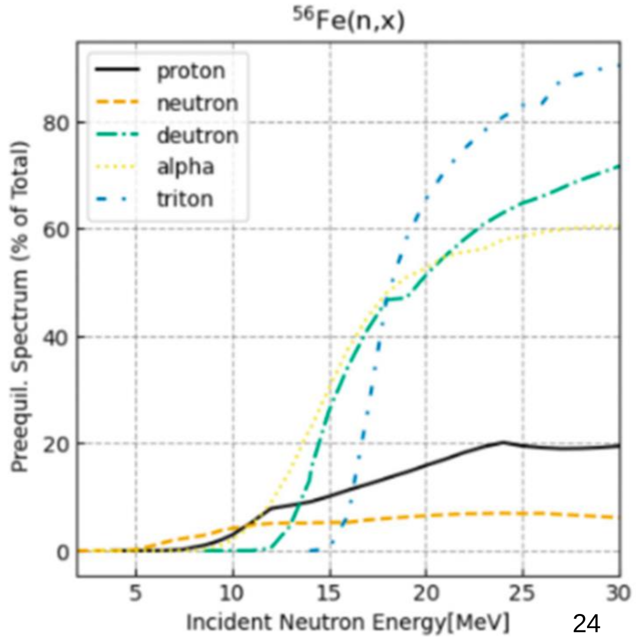
1. Create a reaction which proceeds through the compound reaction mechanism. This implies selecting appropriate beam species and energies.
2. Differential spectra of particles emitted from compound reactions depends on level density of nuclei populated.



- **Preequilibrium** emissions become dominant **at high energies**
- We will use experimental information to constrain microscopic PE models
- Increase confidence in the description at stable isotopes before applying to unstable ones

We will use (p,n) reactions to measure neutron dσ/dE spectra





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Validation…?

- Validation is challenging
- Seeking feedback from CSEWG
  - Depletion?
  - Spent fuel?
  - Nuclear waste?
  - ??

Acknowledgements

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