



# Modern Structure-based Nuclear Data Evaluations for Basic Science, Nuclear Safety & Security

**“SBEND: Structure-based Evaluation of Nuclear Data”  
BNL/LANL/LLNL DOE Collaboration**

M. Paris (LANL/PI), D. Brown (BNL/co-PI), K. Kravvaris, I. Thompson (LLNL/co-PIs),  
G. Hale & A. Lovell (LANL/co-Invs)

**Workshop for Applied Nuclear Data Activities (WANDA 2024)  
Project Overview Session**

2024-02-29

LA-UR-24-21657



Managed by Triad National Security, LLC., for the U.S. Department of Energy's NNSA.



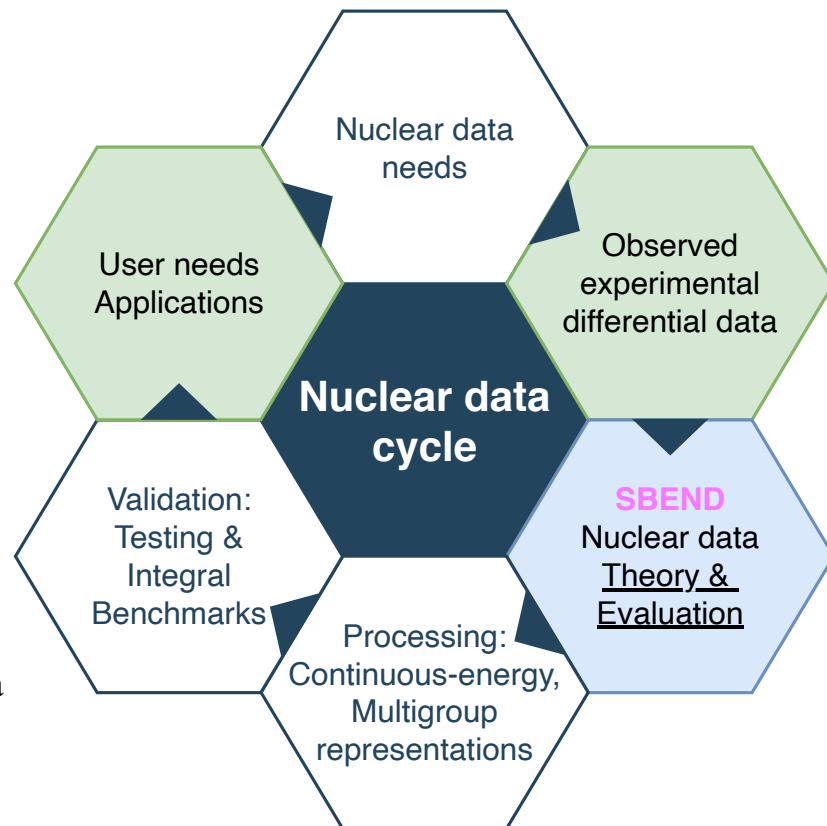
# Outline: SBEND project overview

- Collaboration
- Collaborative work overview
- Recent results



## The nuclear data cycle & SBEND

- Theory & evaluation (T&E) @ intersection
  - Observed differential, basic physics data
  - User needs/Applications
    - Basic science
    - Nuclear security
    - Nuclear energy
- T&E provides
  - Overarching: Technical/physics guidance
  - Concrete: Nuclear data parameters
    - Nuclear structure parameters
    - Smooth (differentiable) reaction cross section data
    - & these data should be consistent



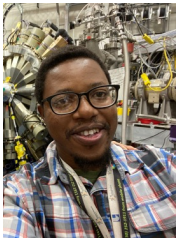
# SBEND Collaboration Project Overview



# Collaboration

## Key personnel

- M. Paris (PI, LANL)
  - Staff scientist Theoretical Division (T-2)
- D. Brown (co-PI, BNL)
  - Staff scientist Nucl. Science & Technology Dept.
- I. Thompson (co-PI, LLNL, Fellow APS/IoP)
  - Staff scientist Nuclear Data & Theory Group
- K. Kravvaris (co-PI, LLNL)
  - Staff scientist Nuclear Data & Theory Group
- G. Hale (co-Inv, LANL, Fellow APS)
  - Staff scientist T-Division (T-2)
- A. Lovell (co-Inv, LANL)
  - Staff scientist T-Division (T-2)
- L. Hlophe (MSU/FRIB visiting asst. prof.)
  - Joint position with LANL/T-2 (hired August '23)



# Collaboration

## *Synergistic activities*

- Experimentalist collaborators
  - **Univ. Notre Dame:** R.J. DeBoer, M. Wiescher, ...
  - **Ohio Univ:** C. Brune
  - **LANL:** M. Devlin, K. Kelly, S. Kuvin, H.Y. Lee, S. Paneru, ...
- Recent hires
  - Linda Hlophe (MSU/FRIB + LANL/T-2 joint position)
  - Hirokazu Sasaki (LANL/T-2 staff member)
- Graduate Student Employee
  - Joshua Adeleke (Ill. Inst. Tech, Physics & Math)
    - DOE Sustainable Research Pathways Program to build lasting collaborations
    - **Summer 2024** project: applications of deep neural networks to light-element evaluation
- Skills transfer (“training”) activities
  - Evaluation & data generation – current efforts
    - Som Paneru (LANL/P-3;  $^8\text{Be}$  system evaluation)
    - Hirokazu Sasaki (LANL/T-2:  $^{13}\text{C}$  system evaluation)
  - Theory
    - Linda Hlophe: breakup reactions in *ab initio* & Faddeev approaches
    - Hirokazu Sasaki: R-matrix methods
  - Aim to expand these skills-transfer/training efforts



# Objectives



NUCLEAR DATA INTERAGENCY WORKING GROUP  
(NDIAWG) RESEARCH PROGRAM

FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) NUMBER:  
DE-FOA-0002440

## I. Improve effectiveness of US Nuclear Data Program for broad community of ND users

- **improved analysis & computational techniques**
- **identification of high-priority needs**
- **support for experiment design, analysis & interpretation**
- **improve availability of data**
  - **online & published**
- **dissemination of nuclear reaction & structure data**

## II. Multi-use and/or high-impact nuclear

- NP basic science users
- Nuclear energy
- Non-proliferation
- Radiation & criticality safety; planetary & space science

## III. Support SC/NP funded research

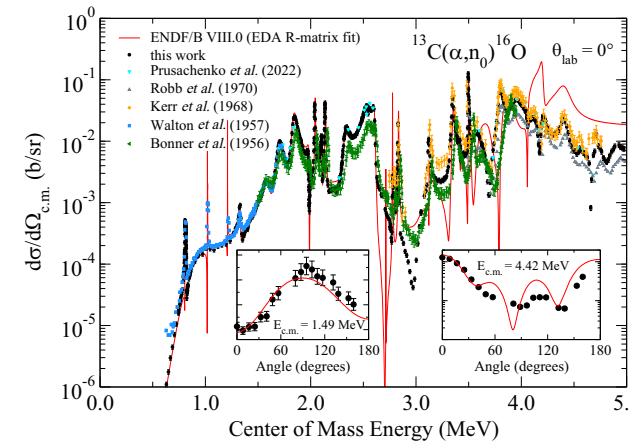
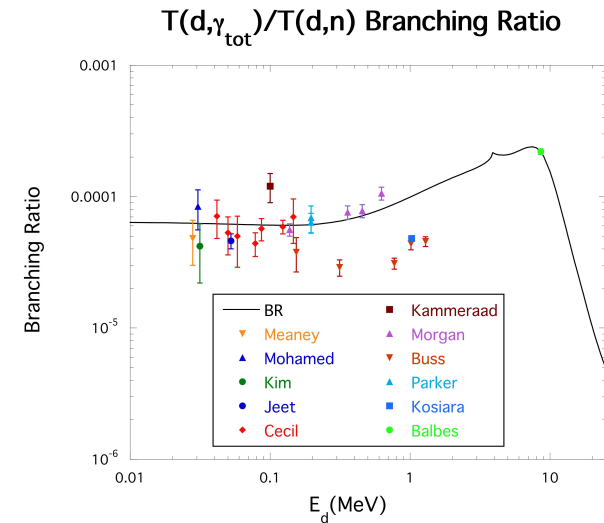
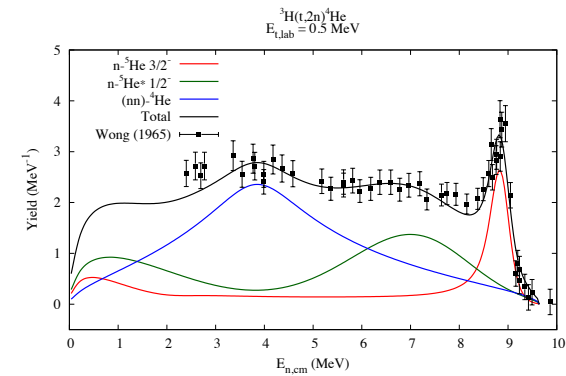
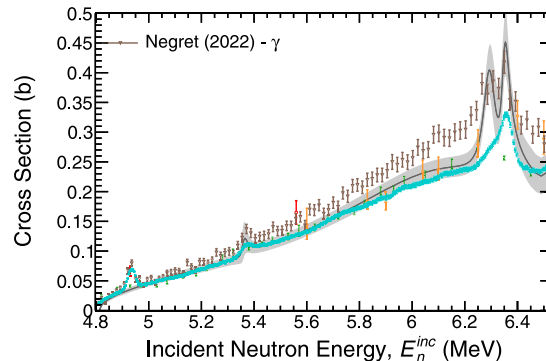
- Prioritize ND experiments in 2015 LRP for Nuclear Science
  - QCD, Nuclear Astro, Fundamental Symmetries &  $\nu$
- Elements of interest
  - Material categories: structural, controlled, intervening, detector, source



# Selected publications

## New/recent/upcoming SBEND and related work

- Resonant Faddeev-R-matrix theory for breakup reactions (LANL, Hale & Paris)
  - PHYSICAL REVIEW C (in preparation)
- Deuterium-Tritium Fusion  $\gamma$  Ray Spectrum at MeV Energies with Application to Reaction-in-Flight Inertial Confinement Fusion Measurements (LANL P-Division, w/Hale & Paris)
  - PHYSICAL REVIEW C (Accepted) (2024)
- Measurement  $^{13}\text{C}(\alpha, n_0)^{16}\text{O}$  diff. cross section from 0.8 MeV to 6.5 MeV (UND, w/Hale & Paris)
  - PHYSICAL REVIEW LETTERS 132, 062702 (2024)
- Measurement  $Q=4.4$  MeV  $^{12}\text{C}(n, n'\gamma)$  from threshold to 16.5 MeV (LANL P-Division, w/Paris)
  - PHYSICAL REVIEW C **108**, 014603 (2023)



# Caveats

## *R-matrix Evaluations compared to ENDF/B files*

### Long version

- This talk is focused on the (LANL) R-matrix evaluation capability
- These evaluations are (*should be*) consistent with ENDF/B library files
  - Up to the maximum energies in the R-matrix evaluation
    - Which may be less than 20 MeV (the ENDF mandated minimum highest energy)
  - With the MT (scattering or reaction designator)
    - There may be other final states/reactions/scatterings/processes in the ENDF/B files that did not come from our R-matrix evaluation

### Short version

- ENDF/B can (and usually does) contain scattering and reaction cross section data whose origin is not from the R-matrix analysis methodology





## **Collaborative Work Overview**

**i) Data efforts**

**ii) Light-element evaluation updates**

**Compound systems**

**${}^7\text{Li}$ ,  ${}^8\text{Be}$ ,  ${}^{10}\text{Be}$ ,  ${}^{13}\text{C}$ ,  ${}^{15}\text{N}$ ,  ${}^{17}\text{O}$**



# Collaborative work

## Broad overview

- Materials of interest

- First priority

- H, C, N, O

- Follow-up

- He, Li, Be, B

Category	Material	SBEND Elements
Structural	Al, steel, AM material	H, C, N, O
Controlled substances	Conventional explosives, pharmaceuticals, chemical agents, SNM	H, C, N, O, F, P
Intervening (shielding)	Poly, H <sub>2</sub> O, <i>n</i> abs, Pb, W	H, Li, Be, B, C, O
Detector	Org & inorg scint, semicon, housings, PMT	He, He, C, O
Source	Detector housing, source reactions	Li, Be

- Elemental processes of interest

- SBEND initial prioritization

- subject to need

- DOE/SC & NNSA motivation

Priority evaluations	DOE-SC user interest	NNSA user interest
$^1\text{H}(n, n)^1\text{H}$ ; $^1\text{H}(n, \gamma)^2\text{H}$ ; $^2\text{H}(\gamma, n)^1\text{H}$	Reference/monitor cross section; BBN	Reference/monitor for various actinides, <i>e.g.</i> $^{235}\text{U}(n, f)$ ; Non-proliferation/interrogation
$^6\text{Li}(d, \alpha)^4\text{He}$ ; $^7\text{Li}(p, \gamma/\gamma^*)^8\text{Be}$	BSM physics; BBN	Nuclear security
$^{12}\text{C}(n, n'\gamma)^{12}\text{C}$ ; $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$ ; $^{12}\text{C}(\alpha, \alpha'\gamma)^{12}\text{C}$	Stellar nucleosynthesis; nuclear structure	Secondary $\gamma$ -rays non-proliferation/interrogation
$^{13}\text{C}(\alpha, \gamma)^{17}\text{O}$ ; $^{13}\text{C}(\alpha, \gamma)^{16}\text{O}$ ; $^{13}\text{C}(\alpha, \alpha'\gamma)^{13}\text{C}$	Stellar nucleosynthesis; nuclear structure; Neutrino-detection backgrounds	Secondary $\gamma$ -rays non-proliferation/interrogation
$^{14}\text{N}(n, n)^{14}\text{N}$ ; $^{14}\text{N}(n, p)^{14}\text{C}$ ; $^{14}\text{N}(n, \alpha)^{11}\text{B}$ ; $^{14}\text{N}(n, n'\gamma)^{14}\text{N}$	Stellar nucleosynthesis; nuclear structure	Secondary $\gamma$ -rays non-proliferation/interrogation
$^{15}\text{N}(n, n'\gamma)^{15}\text{N}$ ; $^{15}\text{N}(p, \alpha'\gamma)^{12}\text{C}$ ;	Stellar nucleosynthesis; nuclear structure	Secondary $\gamma$ -rays non-proliferation/interrogation
$^{16}\text{O}(n, \alpha)^{13}\text{C}$ ; $^{16}\text{O}(\gamma^*, \alpha)^{12}\text{C}$ ; $^{16}\text{O}(n, n')^{16}\text{O}^*$ ; $^{16}\text{O}(n, n'\gamma)^{16}\text{O}$ ;	Stellar nucleosynthesis; nuclear structure; Neutrino-detection backgrounds	Secondary $\gamma$ -rays non-proliferation/interrogation



# Data effort: planned improvements to x4i

## EXFOR interface; python (<https://github.com/brown170/x4i.git>)

- Developed at LLNL by D. Brown as a lightweight API for EXFOR.
- GPL release in 2010 when D. Brown transitioned to BNL; pip install and Python3 update in 2022
- Used by FUDGE & ADVANCE for ENDF V&V
- Modest use in SG-30 for checking EXFOR
- Used in two papers

### More updates needed:

- New EXFOR coding (e.g. “PAR”)
- Ensure levels in EXFOR match RIPL
- Sync with new EXFOR Master file locations, new EXFOR Dicts
- Implement EXFOR checking
- Compatibility with PANDAS DataFrames
- Improve database indexing

Available online at [www.sciencedirect.com](http://www.sciencedirect.com)  
**ScienceDirect**  
 Nuclear Data Sheets  
 Nuclear Data Sheets 131 (2016) 377–399  
[www.elsevier.com/locate/ndst](http://www.elsevier.com/locate/ndst)

Identifying Understudied Nuclear Reactions by Text-mining the EXFOR Experimental Nuclear Reaction Library

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 (Received 28 April 2015; revised received 27 June 2015; accepted 22 August 2015)

The EXFOR library contains the largest collection of experimental nuclear reaction data available as well as the data's bibliographic information and experimental details. We text-mined the REACTION and REACTION fields of the EXFOR in the EXFOR library in order to identify understudied reactions and quantities. Using the results of the text mining, we created an undirected graph from the EXFOR datasets with each graph node representing a single reaction and quantity and graph links representing the various types of connections between those reactions and quantities. This graph is an abstract representation of the connections in EXFOR, similar to graphs of social networks, authorship networks, etc. We use various graph theoretical tools to identify important yet understudied reactions and quantities in EXFOR. Although we identified a few cross sections relevant for shielding applications and isotope production, mostly we identified charged particle transfer nuclear cross sections. As a side effect of this work, we learn that our abstract graph is typical of other real-world graphs.

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www.nature.com/scientificreports

## SCIENTIFIC REPORTS

**OPEN** Nuclear Physics Meets the Sources of the Ultra-High Energy Cosmic Rays

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Denise Boncioli, Anatoli Fedynitch & Walter Winter

The determination of the injection composition of cosmic ray nuclei within astrophysical sources requires sufficiently accurate descriptions of the source physics and the propagation – apart from concealing astrophysical uncertainties. We therefore study the implications of nuclear data and models for cosmic ray astrophysics, which involves the photo-disintegration of nuclei up to iron in astrophysical environments. We demonstrate that the impact of nuclear model uncertainties is potentially larger in environments with non-thermal radiation fields than in the cosmic microwave background. We also study the impact of nuclear models on the nuclear cascades in a gamma-ray burst radiation field, simulated at a level of complexity comparable to the most precise cosmic ray propagation code. We conclude with an isotopic chart describing which information is in principle necessary to describe nuclear interactions in cosmic ray sources and propagation.

Particles from space reaching the Earth with energies higher than  $10^{19}$  GeV are detected by ultra-high energy cosmic ray (UHECR) observatories such as the Pierre Auger Observatory<sup>1</sup> and the Telescope Array (TA) experiment<sup>2</sup>. UHECRs are expected to be accelerated in astrophysical sources and to travel through extragalactic space before they hit the Earth's atmosphere; they can interact with photons in both environments. The primary composition of UHECRs is still unknown; however, the main composition measured by the Auger Observatory indicates heavier elements at the highest energies beyond  $10^{19}$  GeV<sup>3,4</sup>, i.e., significantly heavier than helium and a most as heavy as iron. The study of interactions of nuclei is therefore critical for our understanding of cosmic ray astrophysics both within sources and during propagation.<sup>5</sup>

Most of interactions, as for example<sup>6,7</sup>, involve the breaking the right cosmic ray composition injected from the sources into the intergalactic medium, propagating it through the cosmic microwave background (CMB) and the extragalactic background light (EBL), which are thermal target photon fields, i.e., relatively strongly peaked. The

Help EXFOR modernization project and NRDC

Enable SBEND data extraction

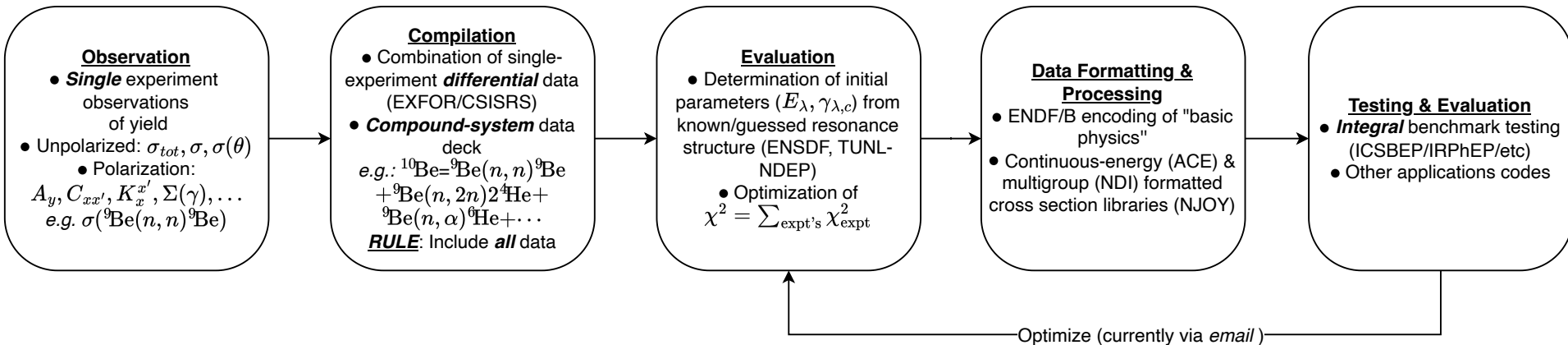


# Evaluation pipeline

## EDA R-matrix procedure

### Nuclear Data Evaluation Pipeline

#### EDA cross section evaluation



1. **EDAf90** code handles all types of data [*EXFOR/CSISRS; publications; priv. comm.*]
  - total, integrated, diff'l, polarized, unpolarized; neutron-, CP-induced, photon: (n,X), (p,X), (d,X), (t,X), ( $\gamma$ ,X), ...
2. **EDAf90** handles all the compound system (here:  $^{10}\text{Be}$ ) data **simultaneously**
3. Optimization over parameters simultaneously fits all the data with the same parameters
4. **EDAf90**  $\rightarrow$  ENDF-6 formatted ENDF/B libraries for processing to CE & MG libraries
5. Testing & evaluation by hand; future: automate



# Evaluation updates/publications

## \*Accepted ENDF/B-VIII.1

\*<sup>7</sup>Li system:  $n+^6\text{Li}$ ,  $t+^4\text{He}$ ,  $n_1+^6\text{Li}^*$ ,  $n_2+^6\text{Li}^{**}$

\* To appear Nucl. Data Sheets ENDF/B-VIII.1

•<sup>8</sup>Be system:  $\alpha+^4\text{He}$ ,  $p+^7\text{Li}$ ,  $p_1+^7\text{Li}^*$ ,  $n+^7\text{Be}$ ,  $n_1+^7\text{Be}^*$ ,  $d+^6\text{Li}$

– Work with Som Paneru & Hye Young Lee

▪ Include inelastic channels

– Improve <sup>8</sup>Be system evaluation

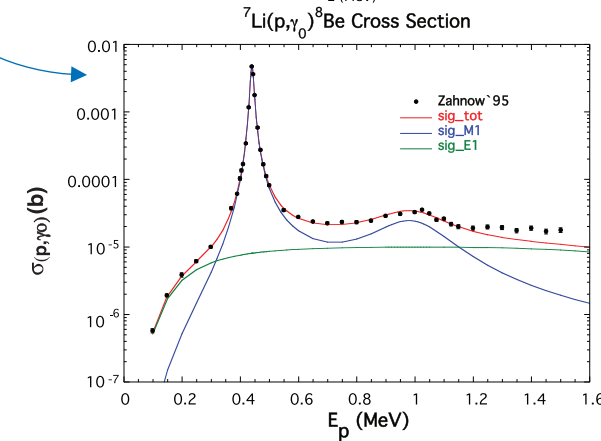
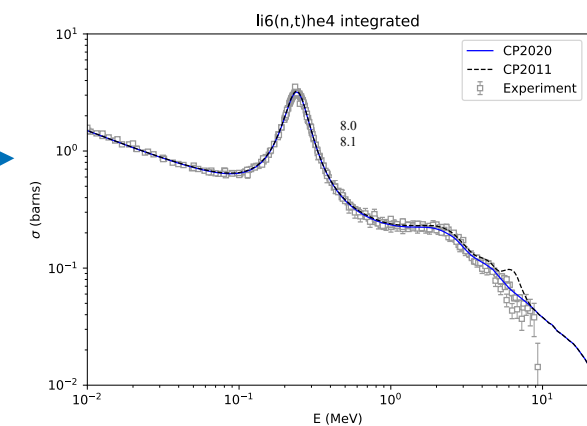
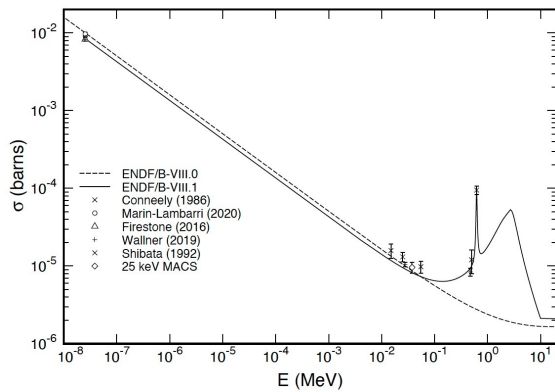
▪ Include electromagnetic channels:  $\gamma+^8\text{Be}$

– Follow-up work on "X17" anomaly

▪ Hayes, Friar, Hale & Garvey PRC105, 2023

\*<sup>10</sup>Be system:  $n+^9\text{Be}$ ,  $\alpha+^6\text{He}$ ,  $(nn)+^8\text{Be}^*$ ,  $n_1+^9\text{Be}^*$ ,  $\gamma+^{10}\text{Be}$

\* To appear Nucl. Data Sheets ENDF/B-VIII.1



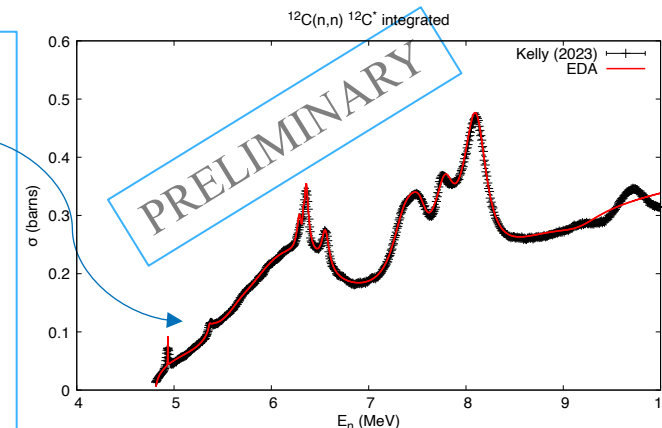
•<sup>13</sup>C system:  $n+^{12}\text{C}$ ,  $n_1+^{12}\text{C}^*$ ,  $\alpha+^9\text{Be}$ ,  $\gamma+^{13}\text{C}$

– Work with Hiro Sasaki

– Goal: increase max  $E_n$  from 8 MeV to 20 MeV

– Good description of new LANL inelastic data

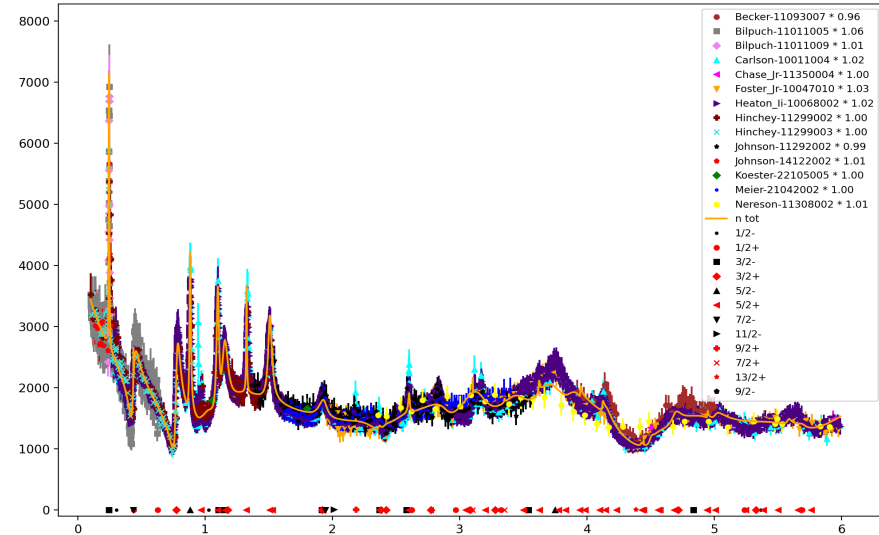
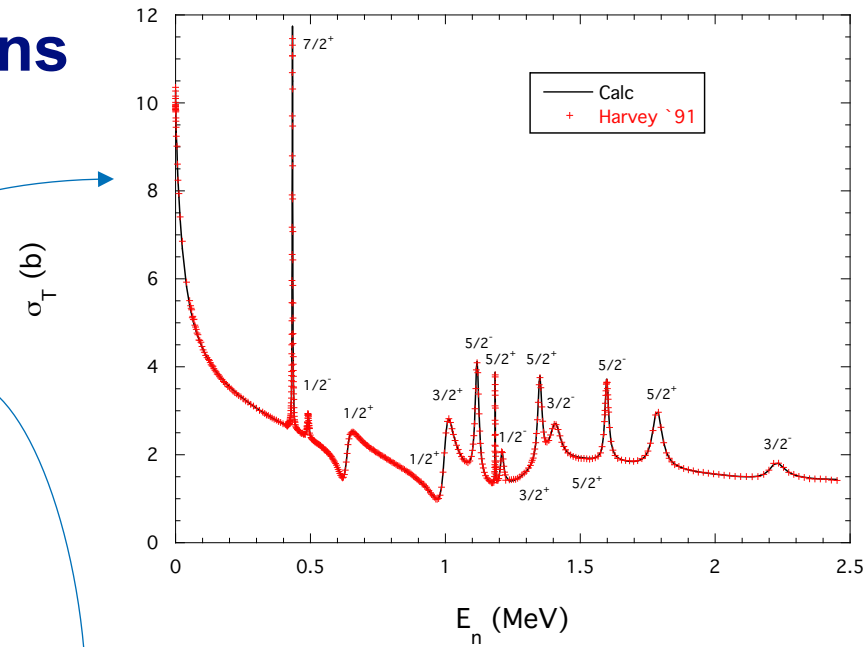
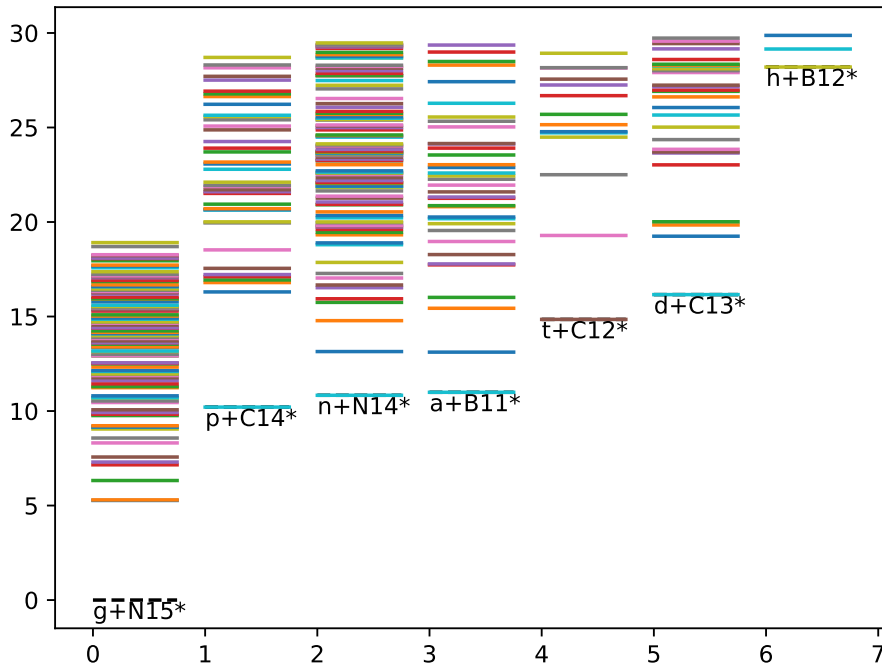
– Phys. Rev. C 108, 014603 (2023)



# Evaluation updates/publications

*LLNL/LANL joint effort;*

- LANL evaluation
  - $^{15}\text{N}$  system:  $n+^{14}\text{N}$ ,  $p+^{14}\text{C}$ ,  $\alpha+^{11}\text{B}$
- LLNL evaluation (RFLOW)
  - $^{15}\text{N}$  system:  $n_{0,1}+^{14}\text{N}$ ,  $p+^{14}\text{C}$ ,  $\alpha_{0,1}+^{11}\text{B}$
  - To higher energies
  - RFLOW: TensorFlow based R-matrix code



# Evaluation updates/publications

**\*Accepted ENDF/B-VIII.1**

**\* $^{17}\text{O}$  system:  $n+^{16}\text{O}$ ,  $\alpha+^{13}\text{C}$ ,  $n_1+^{16}\text{O}^*$ ,  $n_1+^{16}\text{O}^{**}$**

**\* To appear Nucl. Data Sheets ENDF/B-VIII.1**

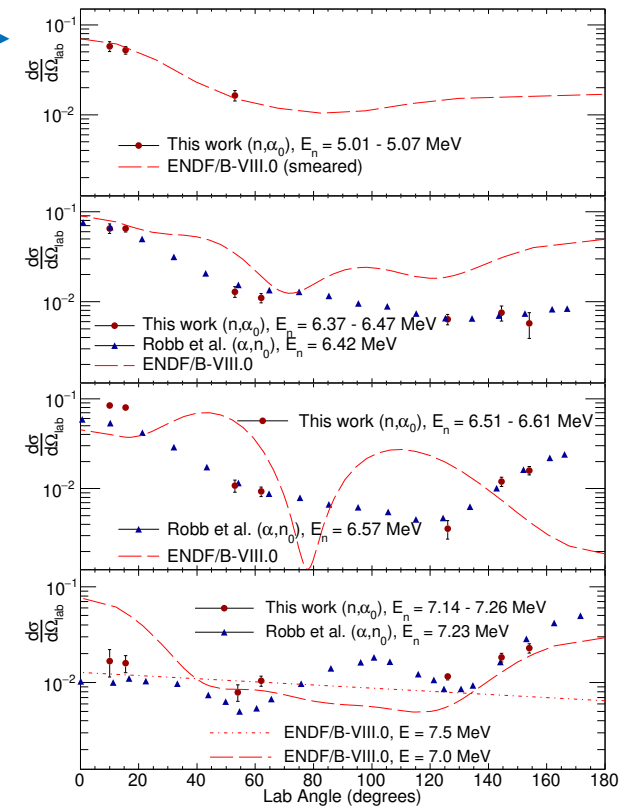
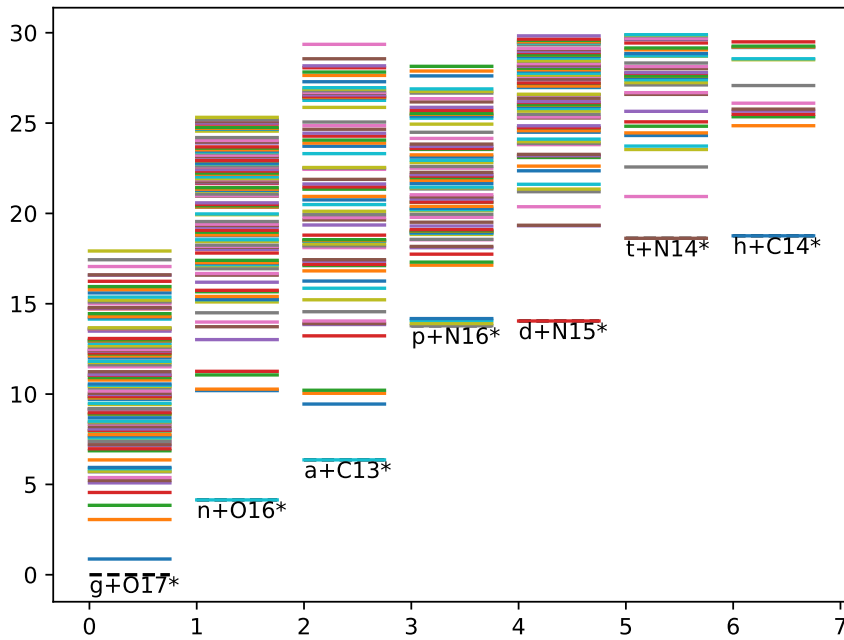
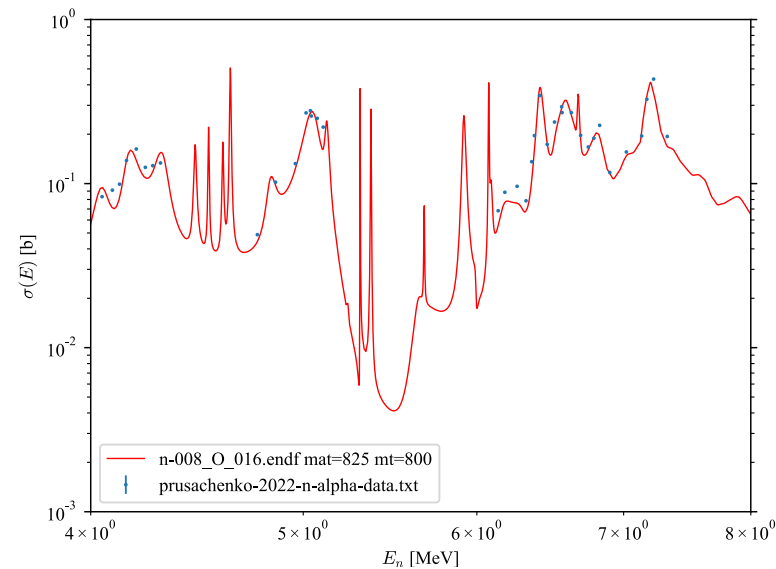
**\* New data**

**\* Prusachenko (IPPE, 2022)**

**\* Lee (LANL, 2023)**

**• LLNL evaluation (code: RFLOW)**

**– Will take into account more channels**



# Recent theoretical work

*With applications*





# Recent work

## Theoretical modeling

T2: Improved physics modeling and theoretical work

- Objective:**
- predictive model for breakup
  - use existing R-matrix parameters

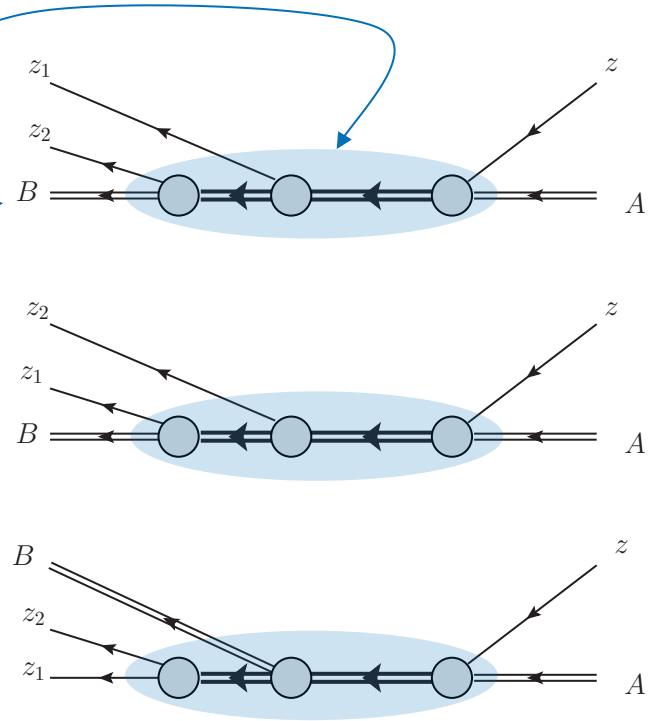
### Breakup Reactions

$$\begin{aligned}
 & A(z, z_1 z_2) B \\
 &= A(z, (z_2 B)) z_1 \\
 &+ A(z, (z_1 B)) z_2 \\
 &+ A(z, (z_1 z_2)) B
 \end{aligned}$$

$$|\psi_{\mathbf{k}_0}^+\rangle = |\chi_{\mathbf{k}_0}\rangle + \mathcal{G}_i^+ H'_i |\psi_{\mathbf{k}_0}^+\rangle.$$

$$\mathcal{G}_i^+(E) = \frac{1}{2\pi i} \int_C dz G_i^{(x)+}(z) G_{0,i}^{(r)+}(E - z).$$

$$\begin{aligned}
 |\psi_{\mathbf{k}_0}^+\rangle &\doteq - \left( \frac{2\pi\bar{\mu}_i}{\hbar^2} \right)^{1/2} \int_0^\infty dE_{\mathbf{q}_i} \frac{e^{ik_i r_i}}{r_i \sqrt{k_i}} |\phi_{\mathbf{q}_i}^-\rangle \langle \phi_{\mathbf{q}_i}^- | H'_i | \psi_{\mathbf{k}_0} \rangle, \\
 &= \int_0^\infty dE_{\mathbf{q}_i} \sqrt{\frac{2\bar{\mu}_i}{\pi \hbar^2 k_i}} \frac{e^{ik_i r_i}}{r_i} |\phi_{\mathbf{q}_i}^-\rangle \tilde{T}_{\mathbf{q}_i \mathbf{k}_i, \mathbf{k}_0}^{(2)},
 \end{aligned}$$



# Recent work

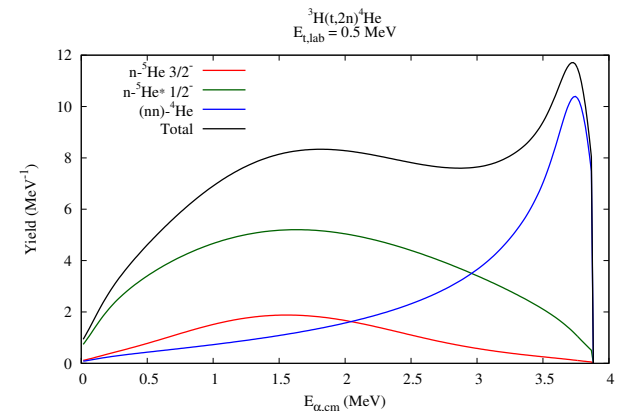
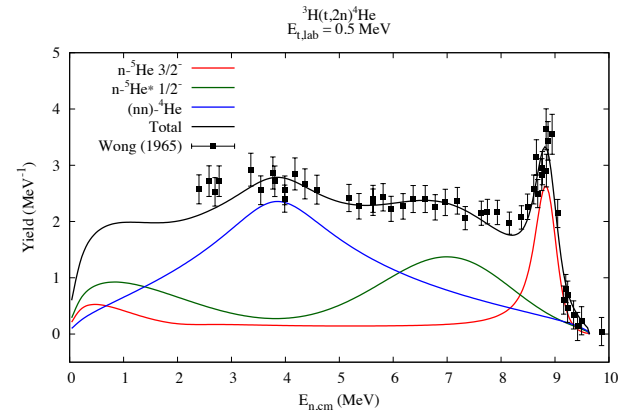
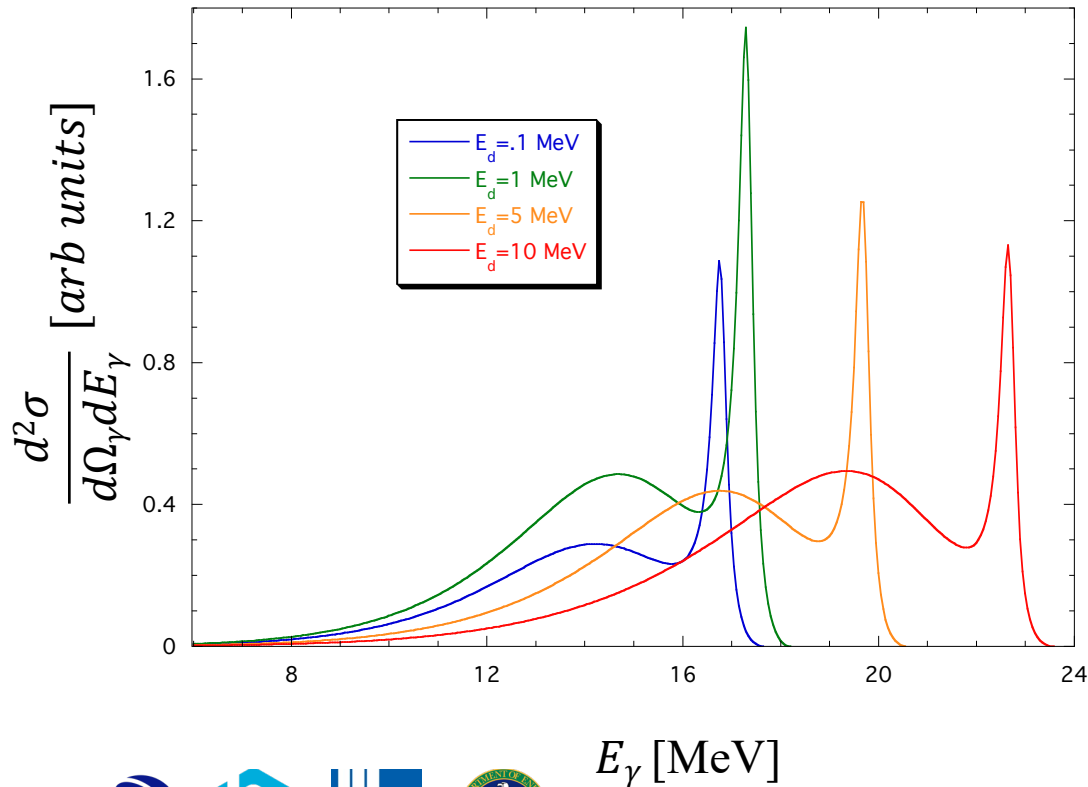
## Theoretical modeling & Applications

- Applications
  - ${}^3\text{H}(d, n\gamma){}^4\text{He}$
  - ${}^3\text{H}(t, 2n){}^4\text{He}$

## SPECT code calculation

- Employs state-of-the-art Faddeev-like resonance model
- Relativistic kinematics necessary for  $\gamma$  production

${}^3\text{H}(d, n\gamma){}^4\text{He}$  spectrum @  $90^\circ$



# SBEND collaboration

## Conclusion & Outlook

- Sustaining current momentum
  - Close collaboration and interface with experimentalist colleagues
  - New personnel represents a significant expansion of our efforts
    - Hlophe, Sasaki, summer GRA
    - Skills transfer/training efforts
  - New work on data management and handling
    - x4i/EXFOR
    - Clarification of inelastic observed data (PAR)
- Maintain new initiatives
  - Experimental database
  - Evaluations (to higher energy)
  - Theory
  - Algorithms (ML, TensorFlow)
  - Data generation
- Address data needs
  - Fusion energy, nuclear safety, security & basic science
  - **Source priority needs list from these communities**

Tell us what your needs are!



**Thanks in advance for your questions  
& support**



# Collaboration work: methods & approach

- Multi-channel R-matrix
- Coupled-channel approach
- Machine learning algos
  - BRR, MDN, QUILTR

EDA<sub>f90</sub>



R-matrix

Exterior region

$$|\Psi_c\rangle = |\mathcal{I}_c\rangle - \sum_{c'} |\mathcal{O}_{c'}\rangle S_{c'c}$$

$$S_{cc'} = \delta_{cc'} + 2i T_{cc'}$$

$r \rightarrow \infty$

Channel surface

$$\mathcal{I}_c \in \mathbb{R}^{3A-4}$$



Interior region

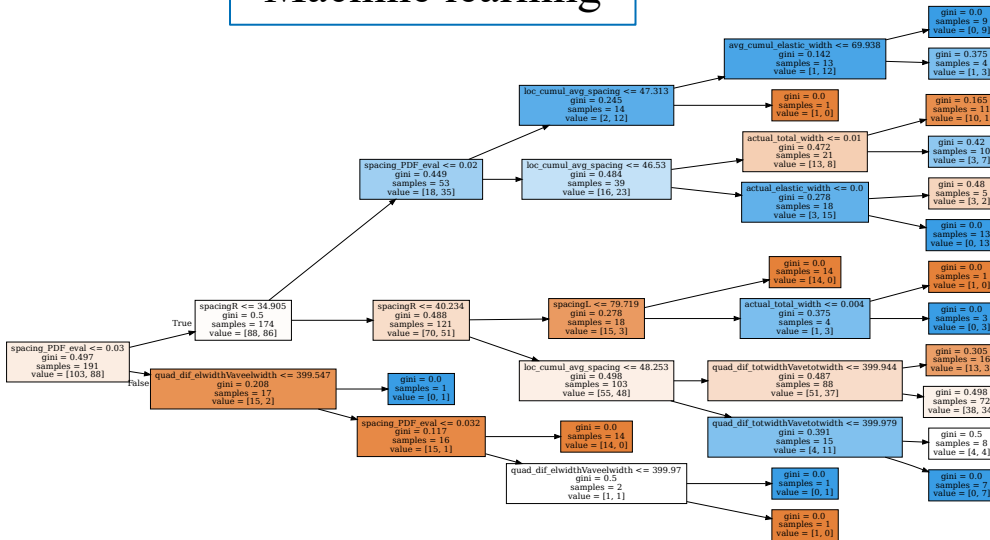
$$[H + \mathcal{L}_B] |\lambda\rangle = E_\lambda |\lambda\rangle$$

$$|\Psi\rangle = [H + \mathcal{L}_B - E]^{-1} \mathcal{L}_B |\Psi\rangle$$

$$\mathcal{L}_B = \sum_c \frac{ia_c}{2m_c} |a_c\rangle \langle a_c| (\hat{p}_r + iB_c)$$

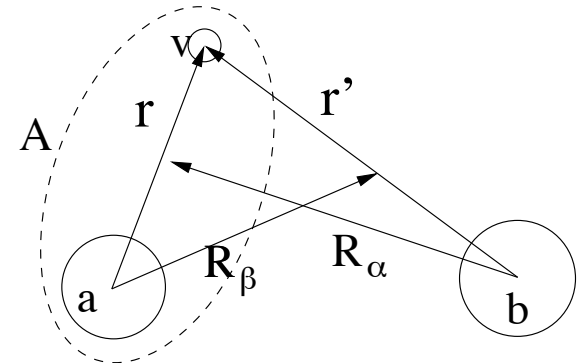
$$R_{B,c'c} = \langle c' | [H + \mathcal{L}_B - E]^{-1} |c\rangle = \sum_\lambda \frac{\langle c' | \lambda \rangle \langle \lambda | c \rangle}{E_\lambda - E}$$

Machine learning



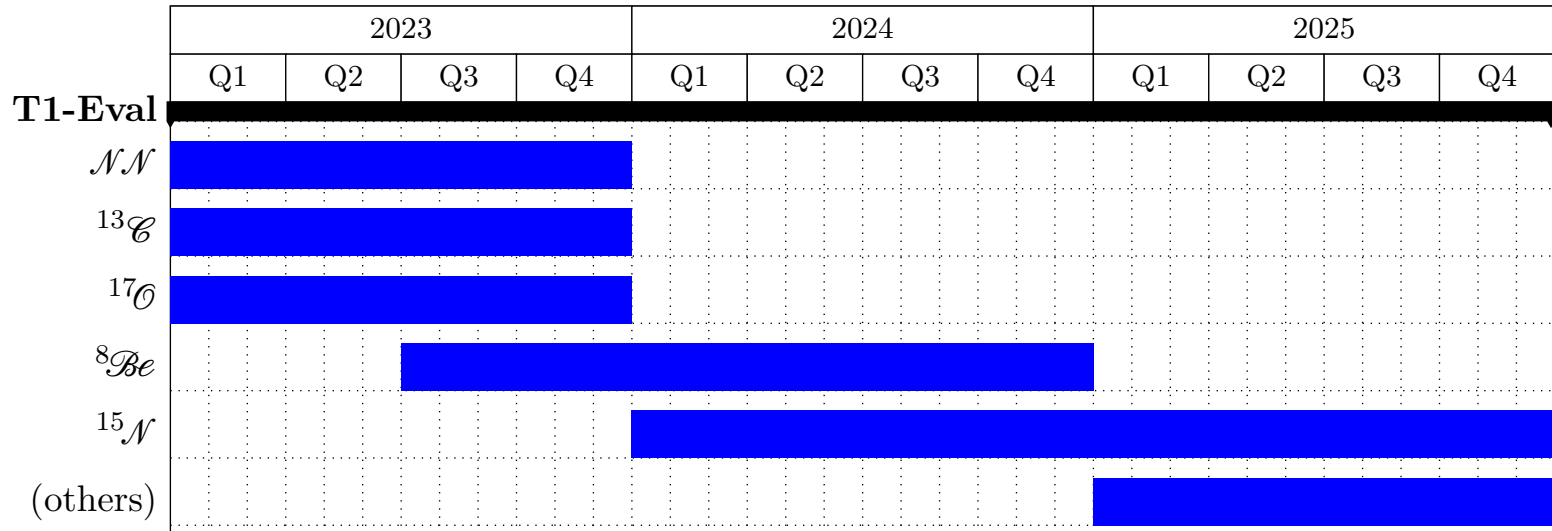
Decision tree @ 5 nodes

Coupled-channel methods



# Deliverables: Tasking

- T1: New evaluation work



$$\mathcal{NN} \sim (\gamma + {}^2\text{H}) + (n + p) + (p + p) + (n + n),$$

$$^8\mathcal{Be} \sim (\gamma/\gamma^* + {}^8\text{Be}) + (n + {}^7\text{Be}) + (p + {}^7\text{Li}) + (d + {}^6\text{Li}),$$

$$^{13}\mathcal{C} \sim (\gamma + {}^{13}\text{C}) + (n + {}^{12}\text{C}) + (n + {}^{12}\text{C}^*(E_j)) + (\alpha + {}^9\text{Be}) + (p + {}^{12}\text{B}) + (d + {}^{11}\text{B}),$$

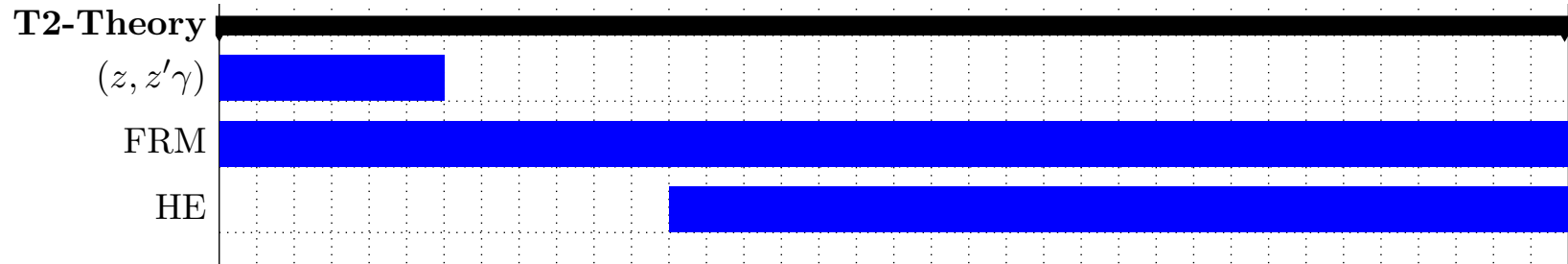
$$^{15}\mathcal{N} \sim (\gamma + {}^{15}\text{N}) + (n + {}^{14}\text{N}) + (p + {}^{14}\text{C}) + (n + {}^{14}\text{N}^*(E_k)) + (\alpha + {}^{11}\text{B}) + (d + {}^{13}\text{C}),$$

$$^{17}\mathcal{O} \sim (\gamma + {}^{17}\text{O}) + (n + {}^{16}\text{O}) + (\alpha + {}^{13}\text{C}) + (n + {}^{16}\text{O}^*(E_l)) + (\alpha + {}^{13}\text{C}^*(E_m)) \\ + (p + {}^{16}\text{N}) + (d + {}^{15}\text{N}),$$



# Deliverables: Tasking

T2: Improved physics modeling and theoretical work



- $(z, z' \gamma)$ ,  $z, z' = n, p, d, t, \alpha$ 
  - Rapid progress in basic theory; implementation needs more effort
- FRM: Feshbach-Reich-Moore
- HE: High-energy evaluations
  - Theoretical framework to join the R-matrix approach with Coupled-Channel methods
  - Continuous effort on these exploratory works



# Deliverables: Tasking

T3: Numerical code development and implementation



- C1: Data formatting, storage, and transmission
- ML1: Extend BRR code to address optimization of spin-group parameters
- ML2: Bayesian optimization to improve search algo
- C2: Backend code development for generating data in GNDS & ENDF-6 formats





# Deliverables: Code development

## FIII. Data formatting, storage, and transmission

- Code capabilities & development driven by
  - FOA objectives
  - Evaluation needs: higher  $A, E$  (number of nucleons, reaction energies)

Code name	Purpose	Language	Improvements
EDA <sub>f90</sub>	R-matrix calc/fitting	Fortran90/95	Full $(z, z'\gamma)$ ; integration
RESPAR	Resonance parameters	Fortran77	Python/ENDFtk/FERDINAND
FRESCO	Coupled-channel/R-matrix	Fortran90/95	GPU
RFLOW	GPU/fast optimization R-matrix	Python/TensorFlow	Multi-GPU
FERDINAND	R-matrix parameter handler	Python	Concurrent covariance matrix
SPECT	$(z, z'\gamma)$	Fortran77	Full theory; Fortran2008
STEEP	$\langle\sigma v\rangle$	Fortran77	NJOY module/Python
NDIOUT	Multigroup $\sigma$	Fortran77	NJOY module/Python
COVAR/ANGCOV	$\langle\rho_i(E)\rho_j(E')\rangle$	Fortran77	NJOY module/Python
QUILTR	MCMC parameter optimization	Python	Integration with R-matrix
BRR [scikit-learn]	Resonance classification and optimization	Python	Integration with R-matrix, CC, for global optimization



# Collaborative work targeting objectives

I. Effectiveness USNDP

II. Multi-user

III. SC/NP support

• T1: Evaluations

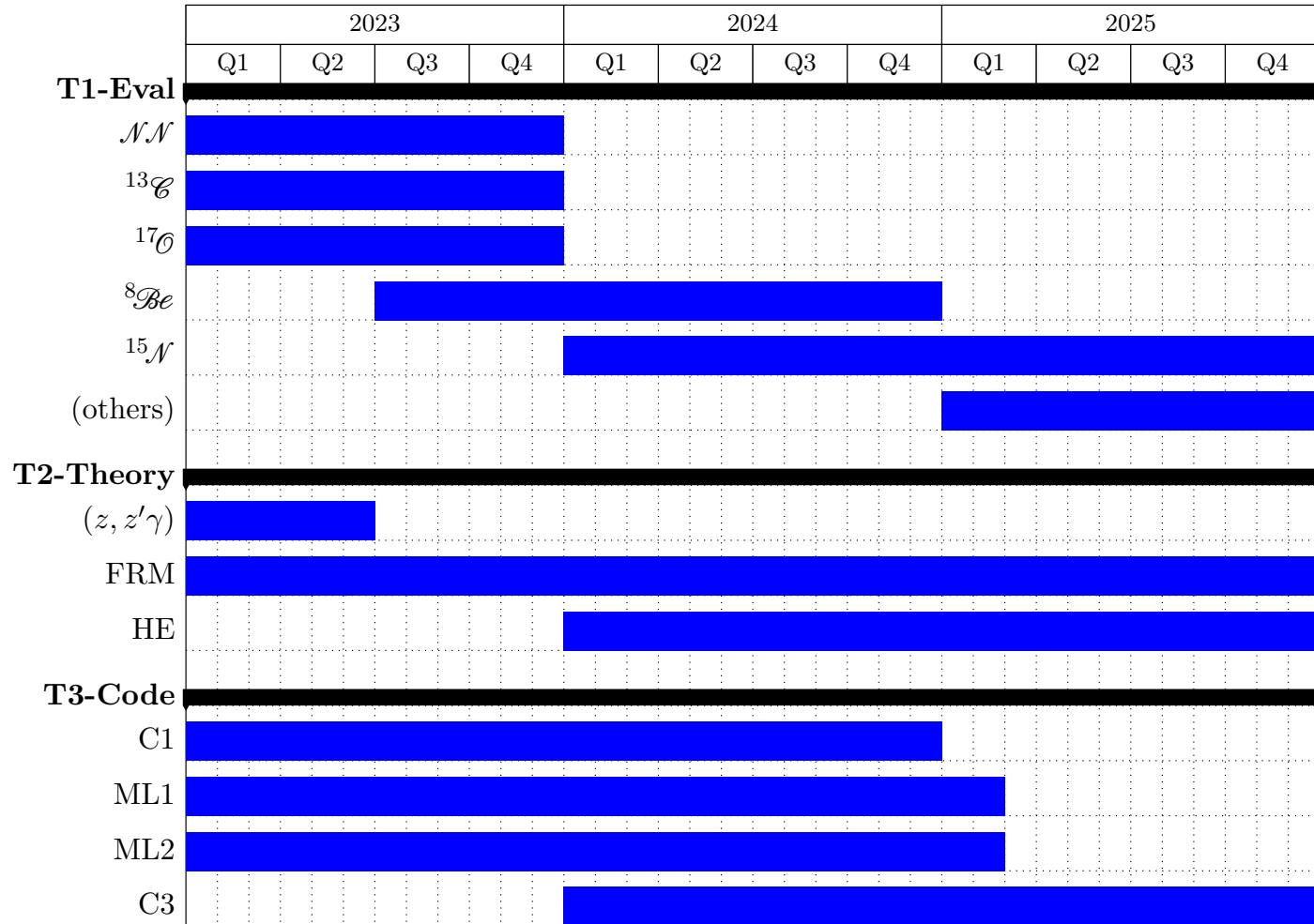
• T2: Theory

• T3: Codes

– analysis

– development

Fiscal Years



# Collaboration work

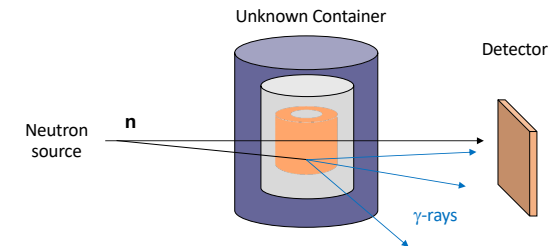
## Recent evaluations

- Neutrino detection:  $^{13}\text{C}(\alpha, n_x)^{16}\text{O}$   $x = 0, \dots, 3$ 
  - KamLAND detector neutrino spectrum
    - Phys. Rev. Lett. 125, 062501 (2020) [Febbraro *et al.*]
      - agrees well with ENDF/B-VII.1 & ENDF/B-VIII.0 based on LANL R-matrix evaluations
    - “we encourage the KamLAND collaboration to assess the impact of these new results.”
- Beyond standard-model (BSM) physics
  - putative BSM candidate  $X17$ 
    - $^7\text{Li}(p, e^+e^-)\alpha\alpha$
    - require better determinations of isovector & isoscalar  $MI$  transitions  $^8\text{Be}$  system
  - Sterile neutrinos and other exotica
    - use Big Bang nucleosynthesis as precision probe [PRD 93, 083522 (2016)]
    - requires  $\sim 1\%$  accuracy in light-element cross sections
- Nuclear science & engineering
  - Traditional reactors – BW, PWR, CANDU, ...
    - H, C, N & O neutron moderators
  - Next generation reactors
    - Coolant: FLiBe
    - Molten salt: F, Cl, Na



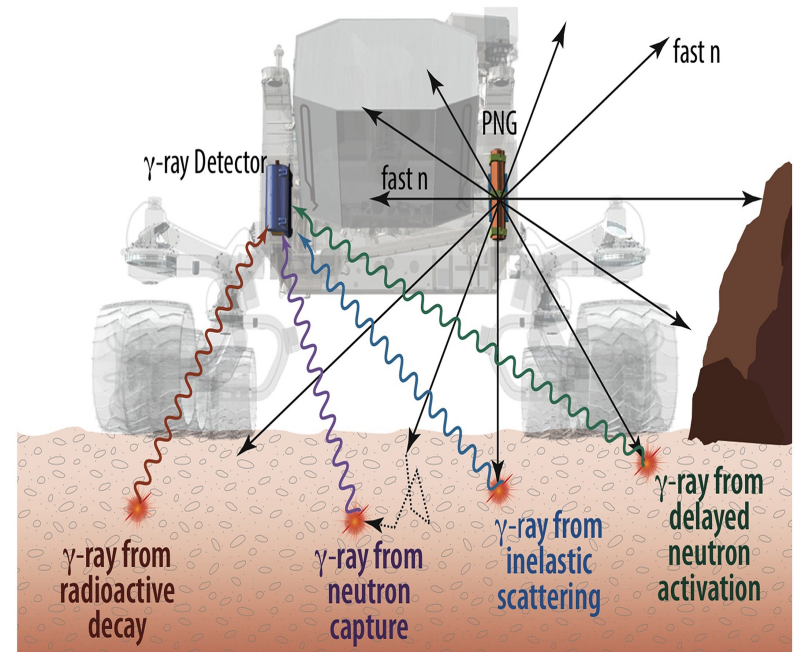
# Overlap with other NDIAWG funded work

- AIACHNE (PI: Denise Neudecker LANL)
  - Explore systematic bias in differential ND databases; design experiments ( $^{252}\text{Cf}(\text{sf})$ )
  - Use ML methods to search large number of differential data features
    - We, too, are interested in systematics in differential data for light elements
  - Light-elements are often monitor reactions for relative measurements
- White-Source n- $\gamma$  Coincidence Measurements (PI: Keegan Kelly LANL)
  - Non-destructive active interrogation for non-proliferation
  - M. Paris co-investigator
  - $^{16}\text{O}(n, n'\gamma)^{16}\text{O}$
- GRIN [next slide]



# Gamma-rays Induced by Neutrons (GRIN) to address $(n,n'\gamma)$ and $(n,\gamma)$ gamma data deficiencies [PI: D. Brown]

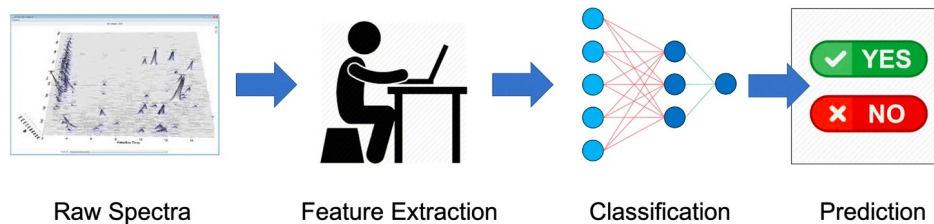
- Outgoing gamma data needed for active interrogation applications in non-proliferation, safeguards, space exploration, soil science, etc.
- Worlds most reliable source of gamma branching ratios, primary gammas is ENSDF
  - This data not reflected in ENDF
  - GRIN project will fix!
  - ENSDF is only experiment, so must “complete” with simulations
  - Leverage modernized ENSDF format & API (SC NP funded)
- Enable event-by-event gamma cascades
- Funded by NDWIAG process (NA-22)
- Gamma data needed also by SBEND evaluations, is out of scope of conventional R-matrix approaches



# Collaboration work: Machine Learning

Address task of determining resonance parameters (spin, parity, couplings)

- Resonance *classification* problem
  - spin, parity, other quantum numbers
  - *expert knowledge* reliant
- The *Atlas Neutron Res* has many misclassified resonances!
- *Classification* well suited for ML



BRR uses a Machine Learning approach

## ML-algo code tools

- **BRR simple and robust method**
  - Resonance spin group assignment is label
  - Use out-of-distribution metrics as ML features
  - Train on high-fidelity evaluations
  - extend other compound systems, higher energies
- **MDN (Mixture Density Network)**
  - probabilistic ML for uncertainty quantification
- **QUILTR (Quantified Uncertainties in Low-energy Theory for Reactions)**
  - Bayesian Markov Chain Monte Carlo for FRESCO
  - quantifies parametric uncertainties on model parameters

Employ lightweight scikit-learn classifiers and clever problem design



BRR reclassified 17% of  $^{52}\text{Cr}$  resonances

