Los Alamos NATIONAL LABORATORY

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)

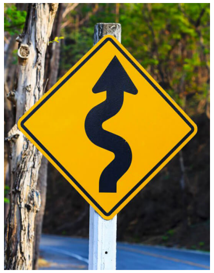
Workshop for Applied Nuclear Data Activities (WANDA 2024)
Project Overview Session

2024-02-29

LA-UR-24-21657

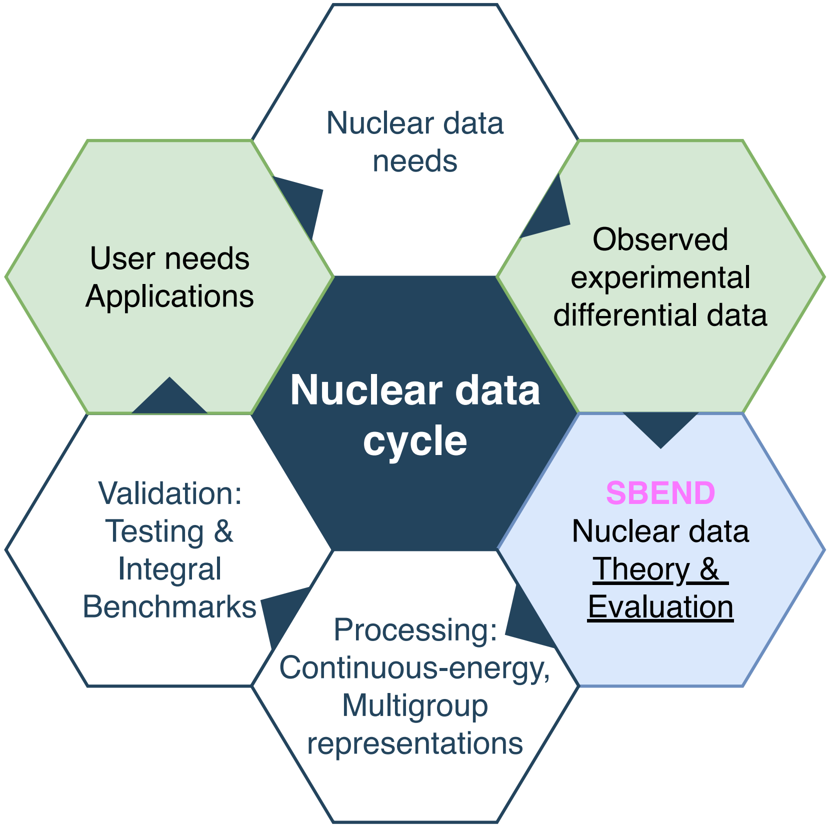
Outline: SBEND project overview

- 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

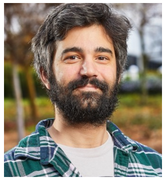
Collaboration

Key personnel

- M. Paris (PI, LANL)
  - Staff scientist Theoretical Divison (T-2)

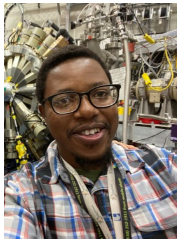
- D. Brown (co-PI, BNL)
  - Staff scientist Nucl. Science & Technology Dept.

- 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}Be system evaluation)
    - Hirokazu Sasaki (LANL/T-2: ^{13}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

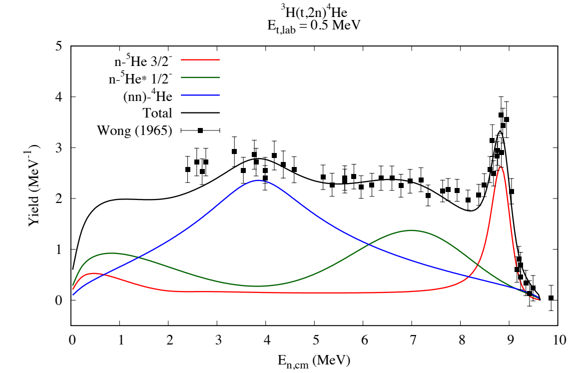
III. Support SC/NP funded research
- Prioritize ND experiments in 2015 LRP for Nuclear Science
  - QCD, Nuclear Astro, Fundamental Symmetries & ν

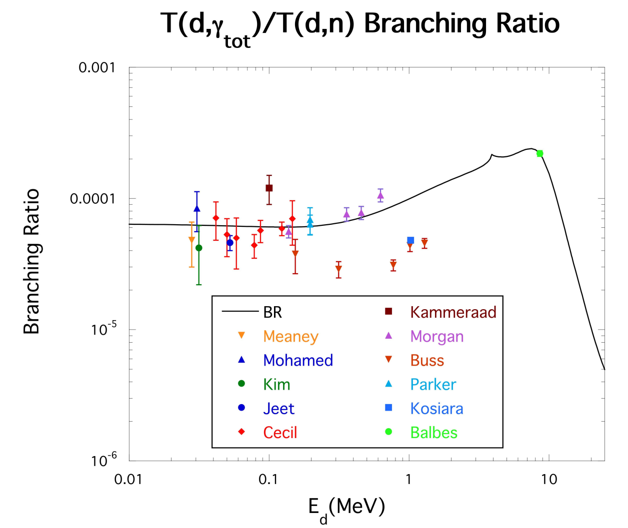
- Elements of interest
  - Material categories: structural, controlled, intervening, detector, source

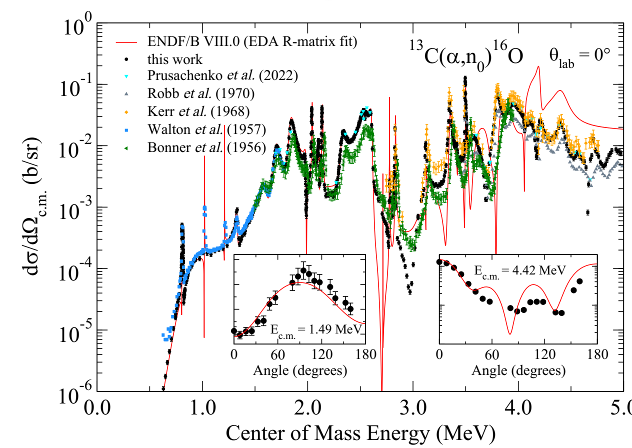
Selected publications

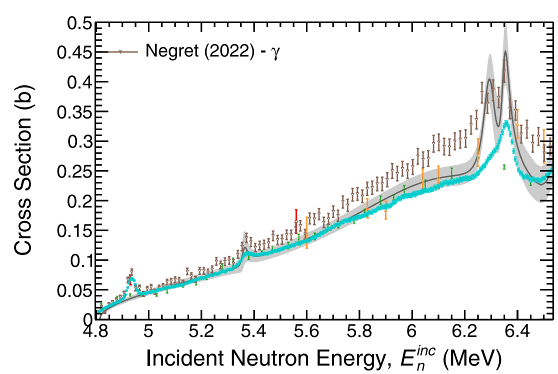
New/recent/upcoming SBEND and related work

- Resonant Faddeev-R-matrix theory for breakup reactions (LANL, Hale & Paris)
  - PHYSICAL REVIEW C (*in preparation*)
- Deuterium-Tritium Fusion γ 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 $^{13}C(\alpha,n_0)^{16}O$ 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 $^{12}C(n,n'\gamma)$ 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}Li, ^{8}Be, ^{10}Be, ^{13}C, ^{15}N, ^{17}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_2O, *n* 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

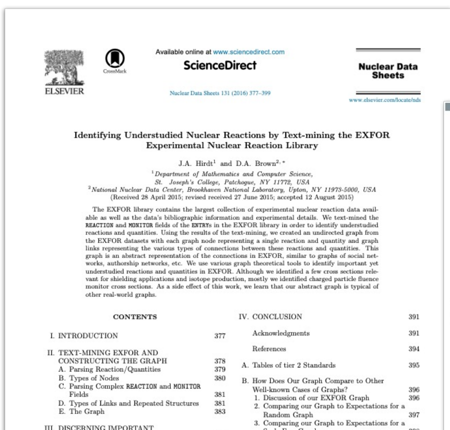
- Elemental processes of interest
  - SBEND initial prioritization
    - subject to need
  - DOE/SC & NNSA motivation

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



Available online at www.sciencedirect.com

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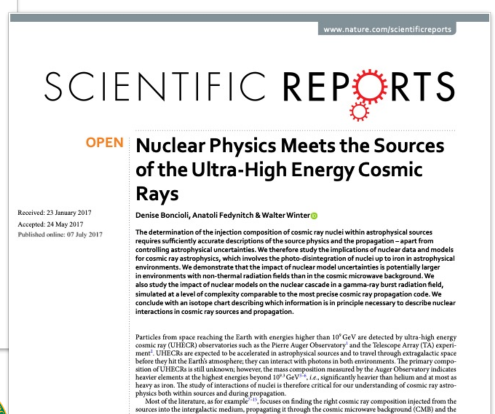
Nuclear Data Sheets

Nuclear Data Sheets 131 (2016) 377–399

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

J.A. Hirdt[1] and D.A. Brown[2,*]



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

Denise Boncioli, Anatoli Fedynitch & Walter Winter

Received: 23 January 2017

Accepted: 24 May 2017

Published online: 07 July 2017

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

Help EXFOR modernization project and NRDC

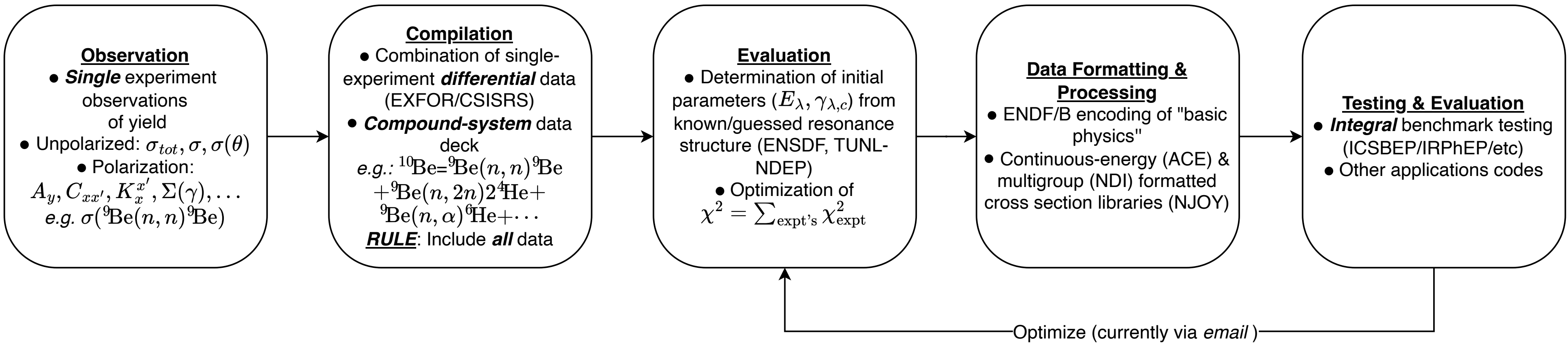
Enable SBEND data extraction

Evaluation pipeline

EDA R-matrix procedure

Nuclear Data Evaluation Pipeline

EDA cross section evaluation

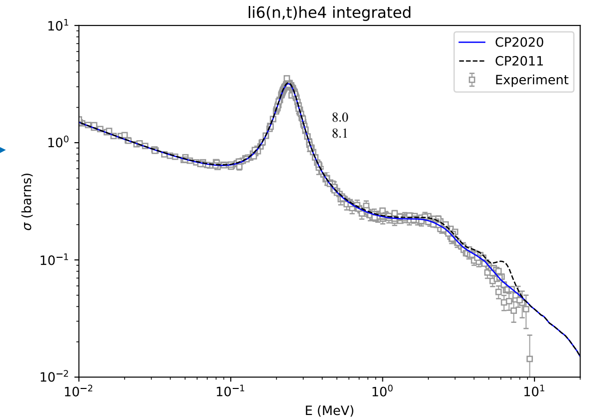


1. **`EDAf90`** code handles all types of data [*EXFOR/CSISRS; publications; priv. comm.*]
   - total, integrated, diff'l, polarized, unpolarized; neutron-, CP-induced, photon: (n,X), (p,X), (d,X), (t,X), (γ,X), ...
2. **`EDAf90`** handles all the compound system (here: ^{10}**Be**) data ***simultaneously***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

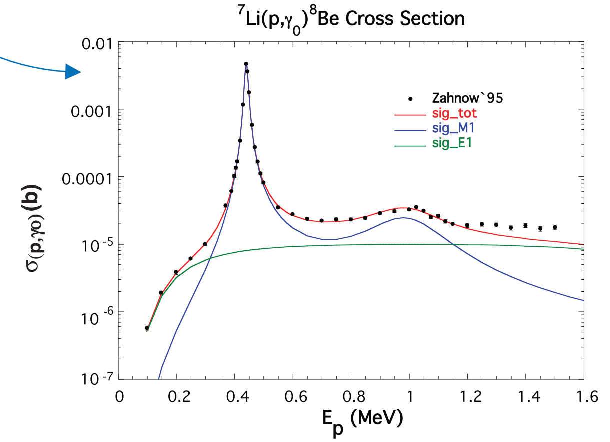
Evaluation updates/publications

**Accepted ENDF/B-VIII.1*

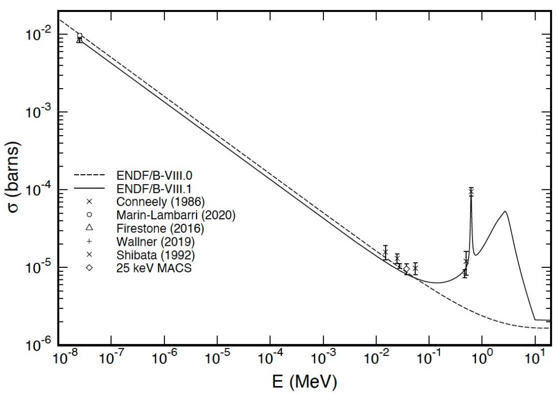
* **^{7}Li system**: n+^{6}Li, t+^{4}He, n_1+^{6}Li*, n_2+^{6}Li**
  - * *To appear* **Nucl. Data Sheets ENDF/B-VIII.1**



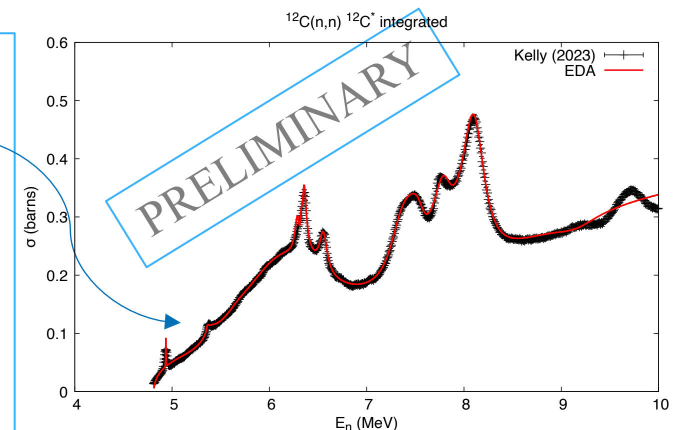
- **^{8}Be system**: α+^{4}He, p+^{7}Li, p_1+^{7}Li*, n+^{7}Be, n_1+^{7}Be*, d+^{6}Li
  - Work with Som Paneru & Hye Young Lee
    - Include inelastic channels
  - Improve ^{8}Be system evaluation
    - Include electromagnetic channels: γ+^{8}Be
  - Follow-up work on "X17" anomaly
    - Hayes, Friar, Hale & Garvey PRC105, 2023



* ^{10}Be system: n+^{9}Be, α+6He, (nn)+^{8}Be*, n_1+^{9}Be*, γ+^{10}Be
  - * *To appear* **Nucl. Data Sheets ENDF/B-VIII.1**



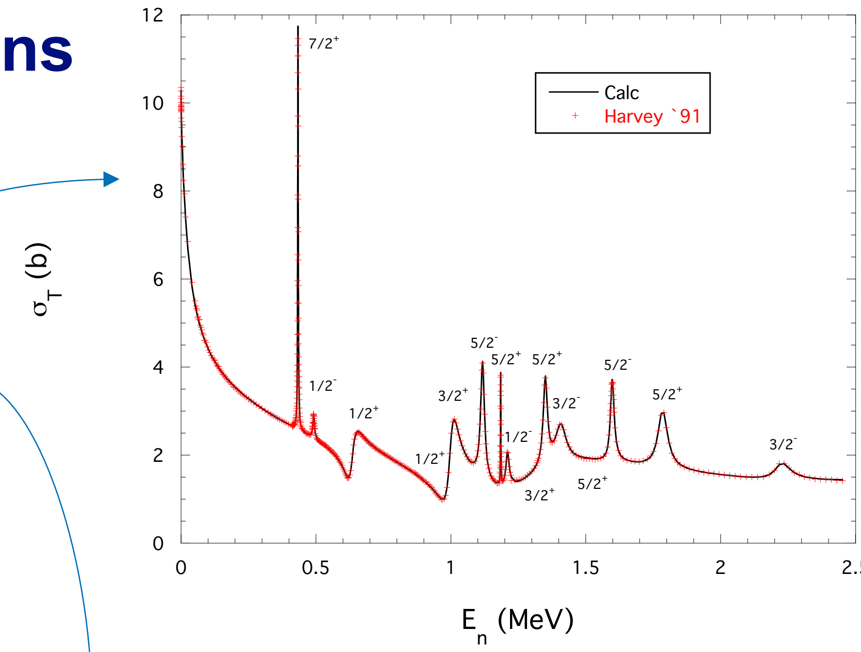
- **^{13}C system**: n+^{12}C, n_1+^{12}C*, α+^{9}Be, γ+^{13}C
  - Work with Hiro Sasaki
  - Goal: increase max E_n from 8 MeV to 20 MeV
  - Good description of new LANL inelastic data
  - **Phys. Rev. C *108*, 014603 (2023)**

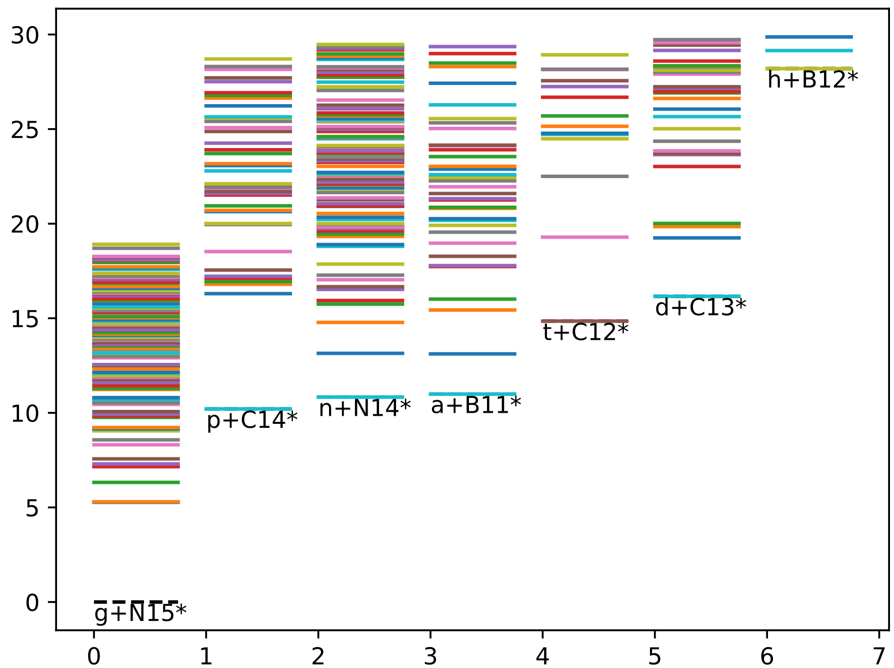


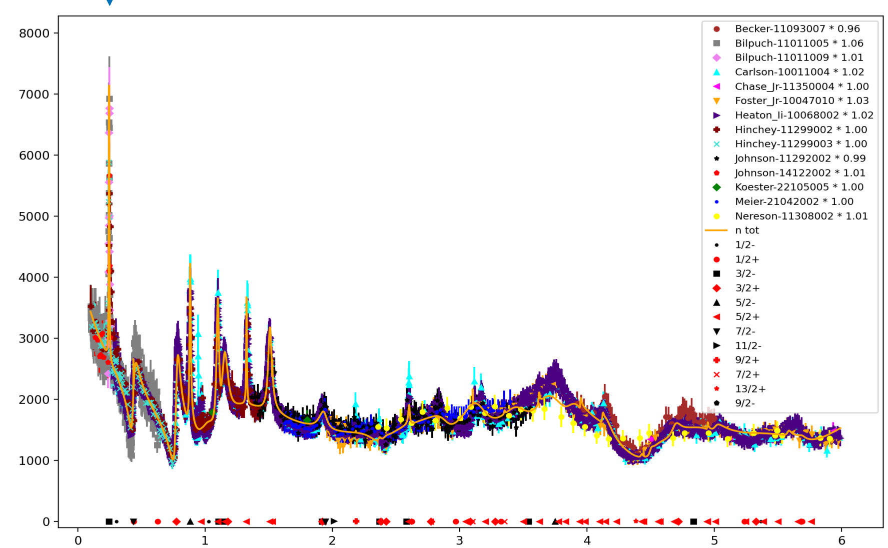
Evaluation updates/publications

LLNL/LANL joint effort;

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





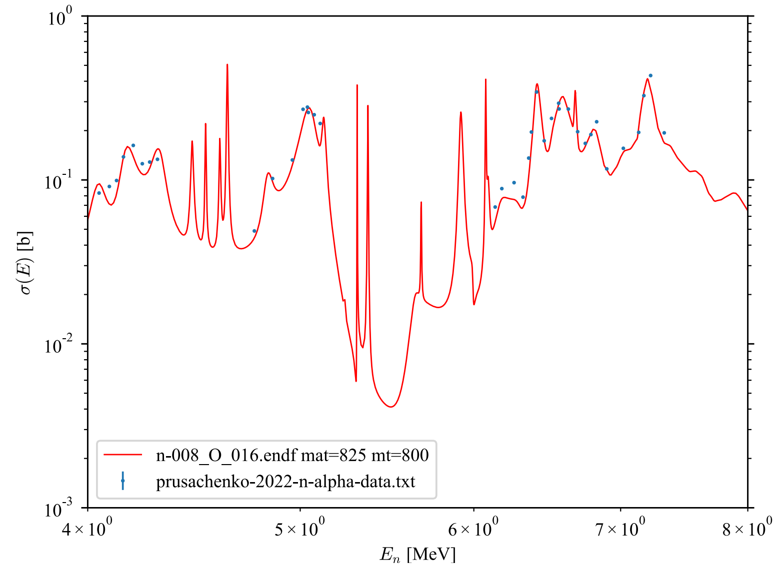


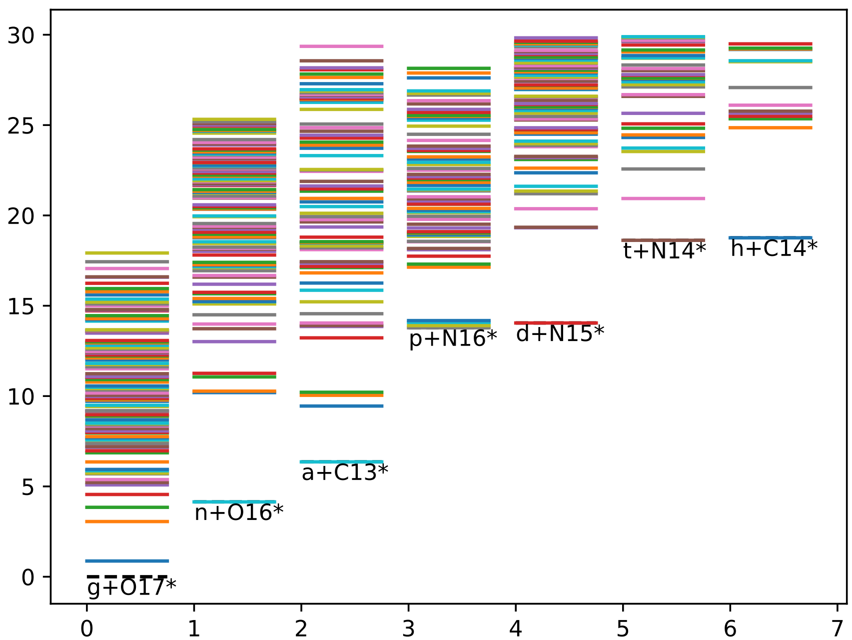
Evaluation updates/publications

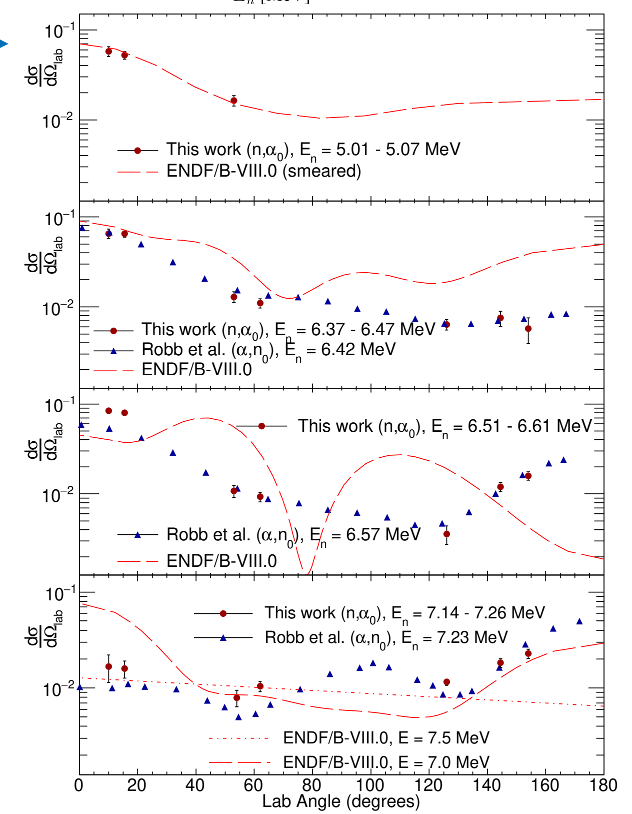
Accepted ENDF/B-VIII.1

* ^{17}O system: n+^{16}O, α+^{13}C, n_1+^{16}O*, n_1+^{16}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

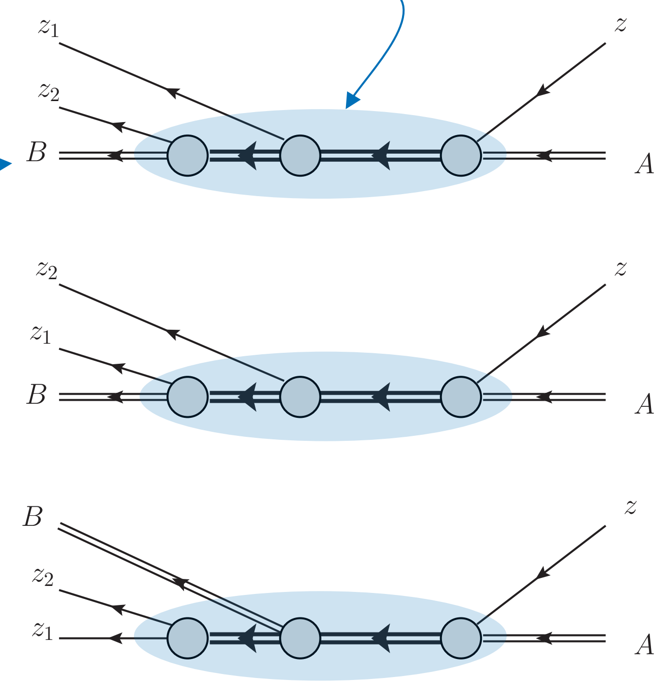
Theoretical modeling

T2: Improved physics modeling and theoretical work

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

Breakup Reactions

$$A(z, z_1 z_2)B$$
$$= A(z,(z_2 B))z_1$$
$$+ A(z,(z_1 B))z_2$$
$$+ A(z,(z_1 z_2))B$$



$$|\psi^+_{\mathbf{k}_0}\rangle = |\chi_{\mathbf{k}_0}\rangle + \mathscr{G}^+_i H'_i |\psi^+_{\mathbf{k}_0}\rangle$$

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

$$|\psi^+_{\mathbf{k}_0}\rangle \doteq -\left(\frac{2\pi\bar{\mu}_i}{\hbar^2}\right)^{1/2}\int_0^\infty dE_{\mathbf{q}_i}\,\frac{e^{ik_i r_i}}{r_i\sqrt{k_i}}|\phi^-_{\mathbf{q}_i}\rangle\langle\phi^-_{\mathbf{q}_i}|H'_i|\psi_{\mathbf{k}_0}\rangle,$$

$$= \int_0^\infty dE_{\mathbf{q}_i}\sqrt{\frac{2\bar{\mu}_i}{\pi\hbar^2 k_i}}\,\frac{e^{ik_i r_i}}{r_i}|\phi^-_{\mathbf{q}_i}\rangle \tilde{T}^{(2)}_{\mathbf{q}_i\mathbf{k}_i,\mathbf{k}_0},$$

Recent work

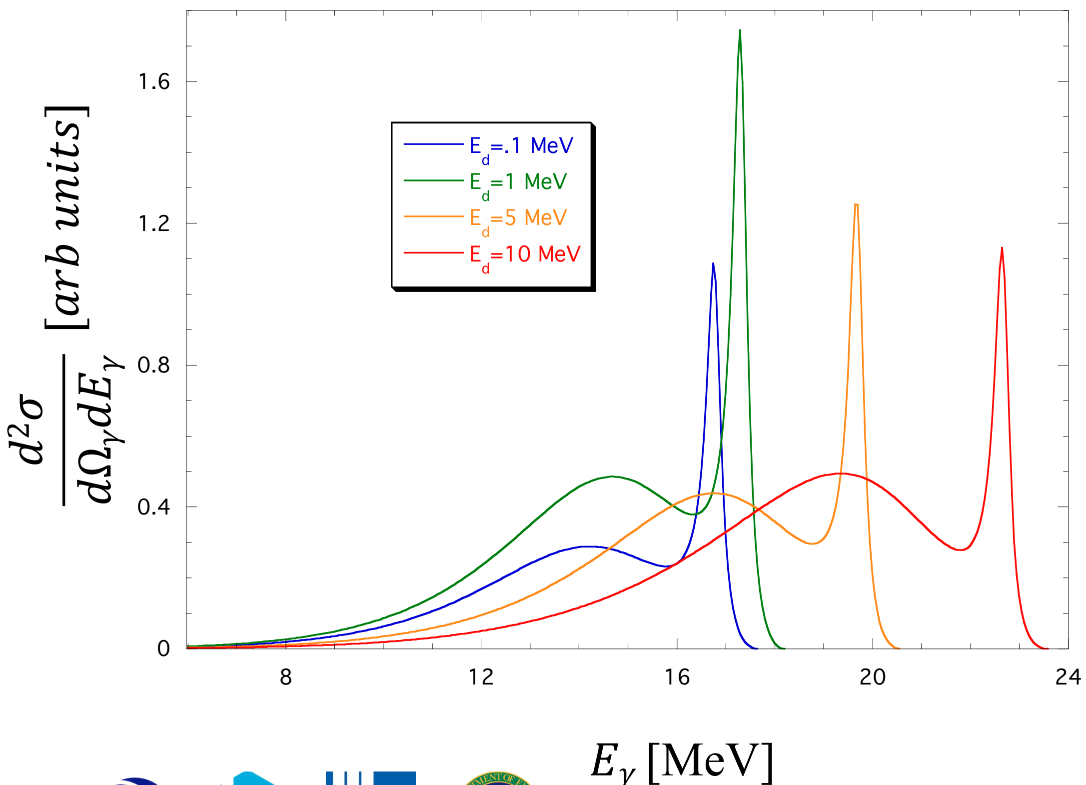
Theoretical modeling & Applications

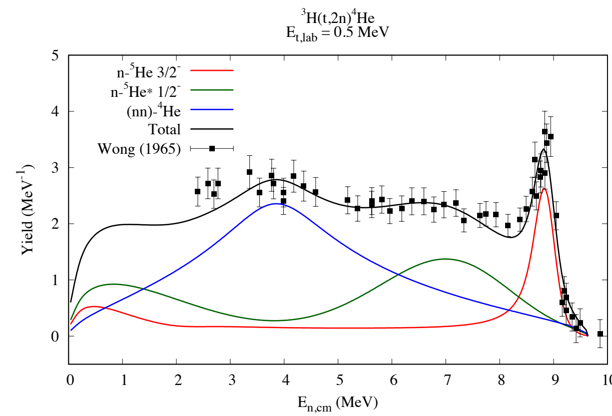
- Applications
  - $^{3}H(d,n\gamma)^{4}He$
  - $^{3}H(t,2n)^{4}He$

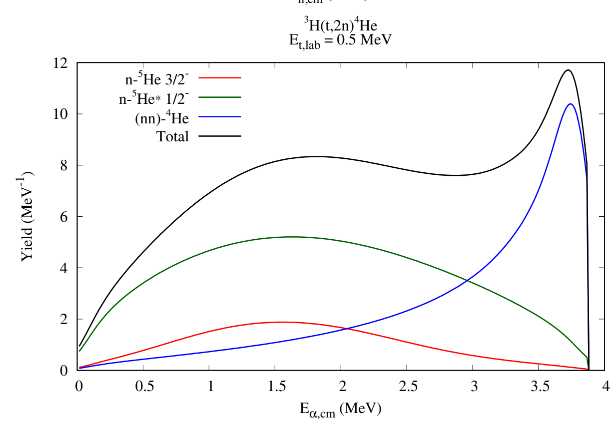
SPECT code calculation

- Employs state-of-the-art Faddeev-like resonance model
- Relativistic kinematics necessary for γ production

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







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 — EDA$_{f90}$
- Coupled-channel approach — XFresco
- Machine learning algos
  - BRR, MDN, QUILTR

R-matrix

Exterior region

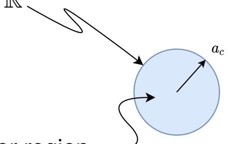
$$|\Psi_c\rangle = |\mathscr{I}_c\rangle - \sum_{c'} |\mathscr{O}_{c'}\rangle S_{c'c}$$

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

$r \to \infty$

Channel surface

$\mathscr{S}_c \in \mathbb{R}^{3A-4}$



Interior region

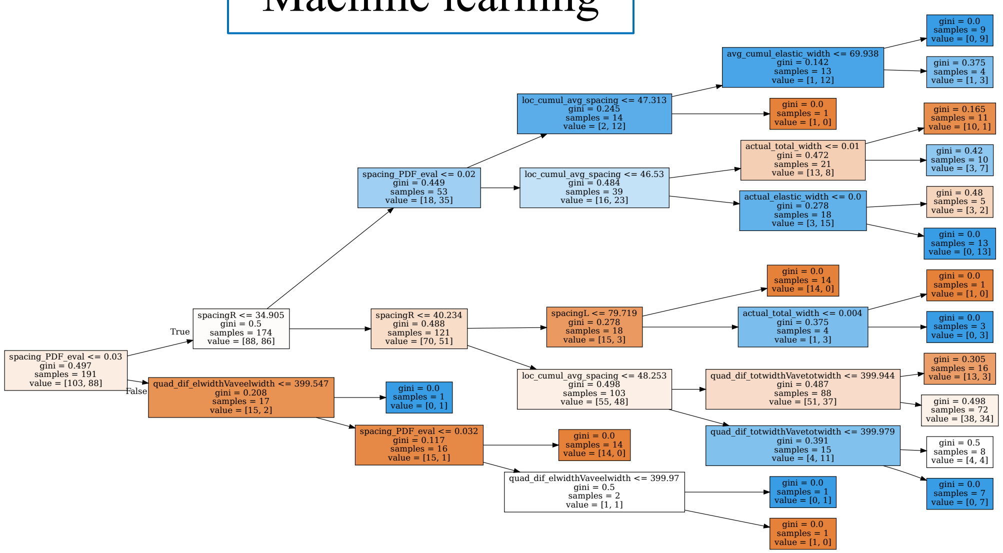
$$[H + \mathscr{L}_B]\,|\lambda\rangle = E_\lambda |\lambda\rangle$$

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

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

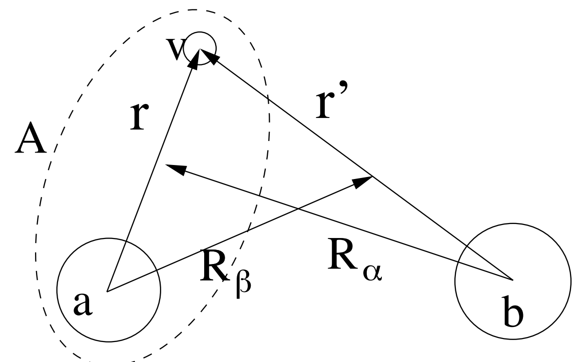
$$R_{B,c'c} = \langle c'|[H + \mathscr{L}_B - E]^{-1}|c\rangle = \sum_\lambda \frac{\langle c'|\lambda\rangle\langle\lambda|c\rangle}{E_\lambda - E}$$

Machine learning



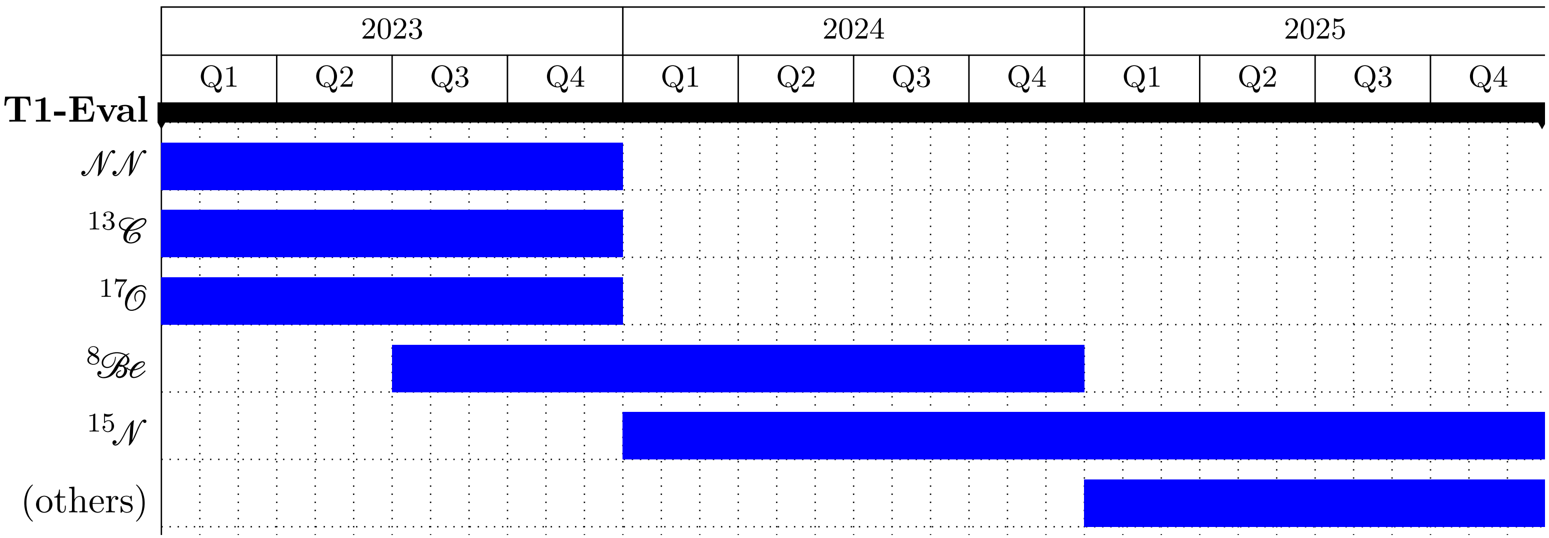
Decision tree @ 5 nodes

Coupled-channel methods



Deliverables: Tasking

- T1: New evaluation work



$$\mathscr{N}\mathscr{N} \sim (\gamma + {}^{2}\mathrm{H}) + (n + p) + (p + p) + (n + n),$$

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

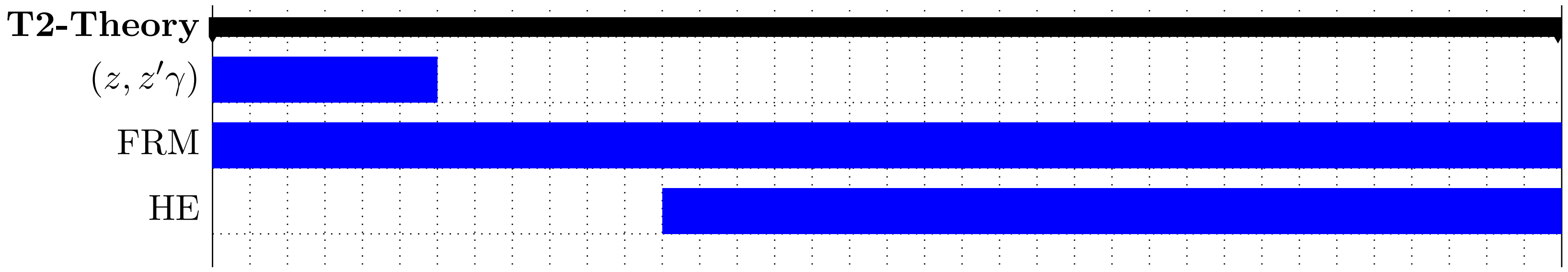
$$^{13}\mathscr{C} \sim (\gamma + {}^{13}\mathrm{C}) + (n + {}^{12}\mathrm{C}) + (n + {}^{12}\mathrm{C}^{*}(E_j) + (\alpha + {}^{9}\mathrm{Be}) + (p + {}^{12}\mathrm{B}) + (d + {}^{11}\mathrm{B}),$$

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

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

Deliverables: Tasking

T2: Improved physics modeling and theoretical work



- $(z, z'\gamma), \quad z, z' = n, p, d, t, \alpha$
  - 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_{f90}	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 σ	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

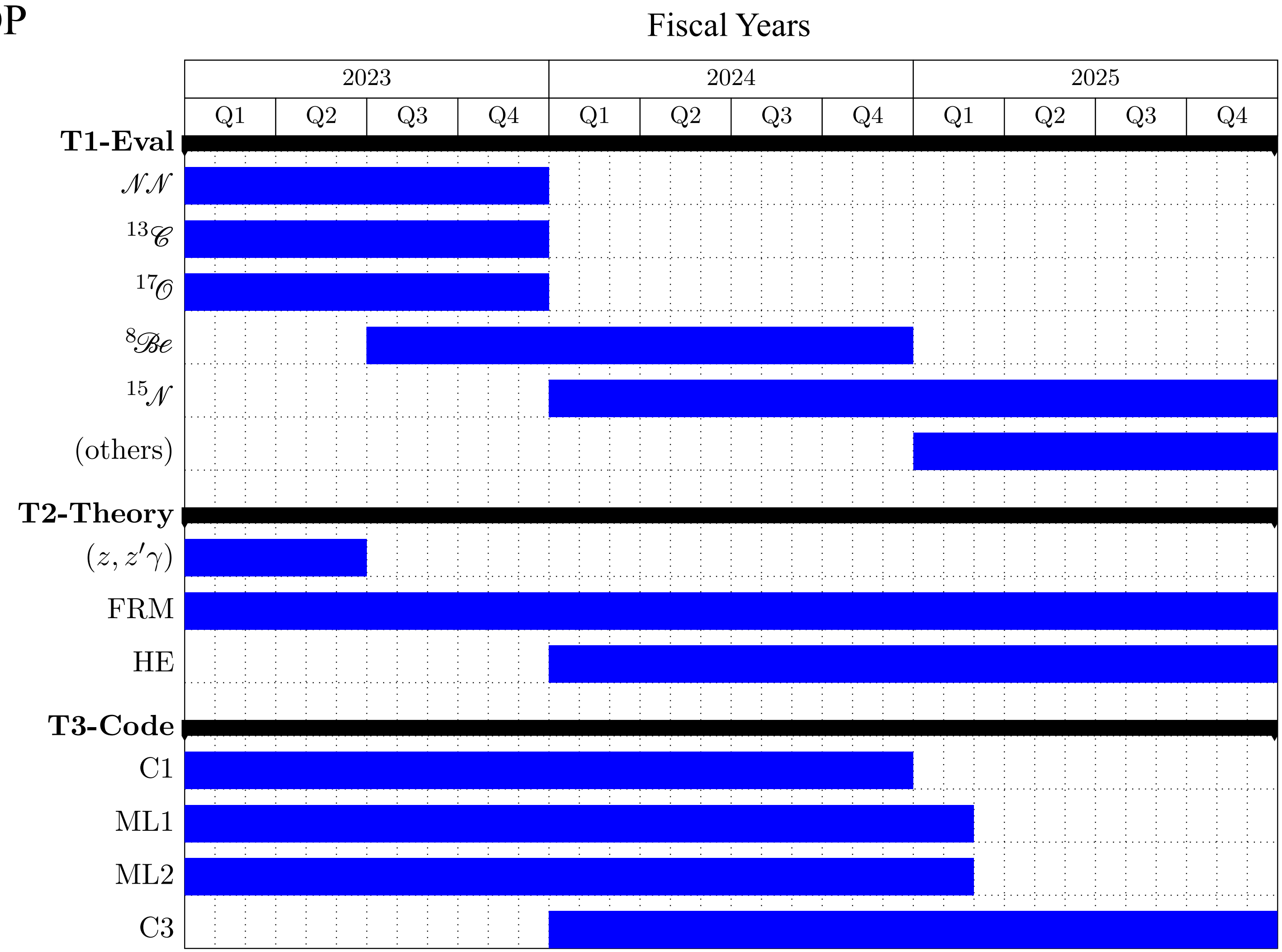
Collaborative work targeting objectives

I. Effectiveness USNDP

II. Multi-user

III. SC/NP support

- T1: Evaluations
- T2: Theory
- T3: Codes
  - analysis
  - development



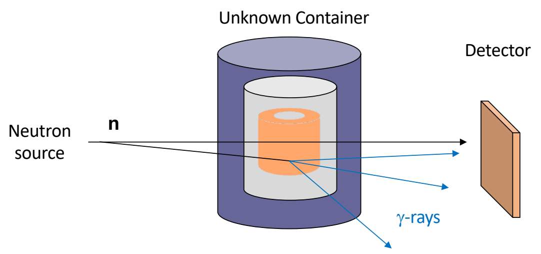
Collaboration work

Recent evaluations

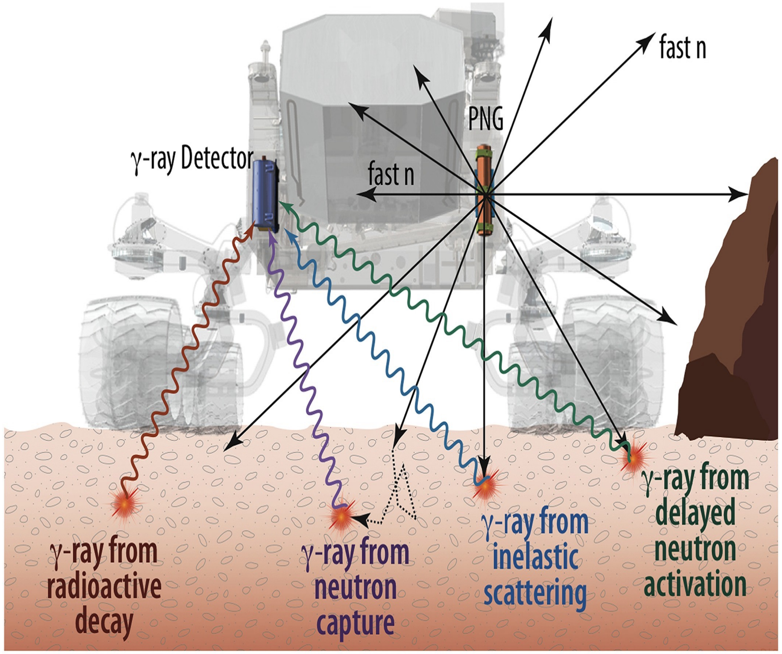
- Neutrino detection: $^{13}C(\alpha,n_x)^{16}O$ $x = 0,\ldots,3$
  - KamLAND detector neutrino spectrum
    - Phys. Rev. Lett. 125, 062501 (2020) [Febbraro *et al.*]
      - agrees well with ENDF/B-VII.1 & ENDF/B-VIII.0 based on LANL R-matrix evaluations
    - "we encourage the KamLAND collaboration to assess the impact of these new results."
- Beyond standard-model (BSM) physics
  - putative BSM candidate *X17*
    - $^{7}Li(p,e^{+}e^{-})\alpha\alpha$
    - require better determinations of isovector & isoscalar *M1* transitions ^{8}Be system
  - Sterile neutrinos and other exotica
    - use Big Bang nucleosynthesis as precision probe [PRD 93, 083522 (2016)]
    - requires ~ 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}Cf(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-γ Coincidence Measurements (PI: Keegan Kelly LANL)
  - Non-destructive active interrogation for non-proliferation
  - M. Paris co-investigator
  - $^{16}O(n,n'\gamma)^{16}O$
- GRIN [next slide]



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

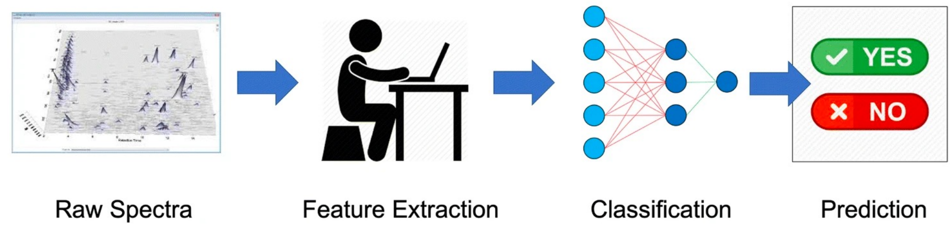


- Outgoing gamma data needed for active interrogation applications in non-proliferation, safeguards, space exploration, soil science, etc.
- Worlds most reliable source of gamma branching ratios, primary gammas is ENSDF
  - This data not reflected in ENDF
  - GRIN project will fix!
  - ENSDF is only 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



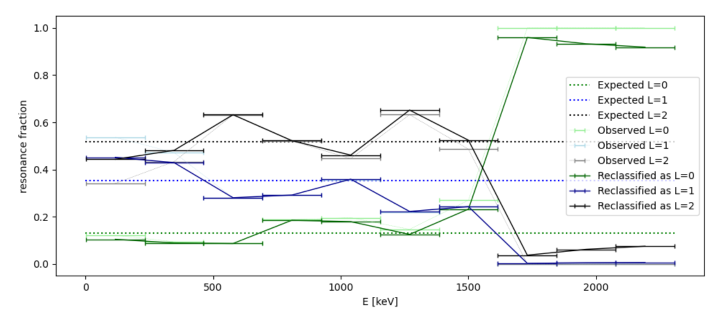
BRR uses a Machine Learning approach

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)**
  - **probabistic 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}Cr resonances



* Fig. taken from K.M. Mendez et al. *Metabolomics* **15,** 142 (2019) https://doi.org/10.1007/s11306-019-1608-0