

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

**"SBEND:** Structure-based Evaluation of Nuclear Data"

**BNL/LANL/LLNL DOE Collaboration** New start; Project duration: CY2023-CY2025

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## **Collaboration personnel**

- M. Paris (PI, LANL)
  - Staff scientist Theoretical Divison (T-2)
  - NNDC Cross section evaluation working group (CSEWG) member
  - Consultant to IAEA (standards, R-matrix, Int. Nucl. Data Evaluation Network)
- D. Brown (co-PI, BNL)
  - Staff scientist Nucl. Science & Technology Dept.
  - Head National Nuclear Data Center (NNDC); CSEWG Chair; ENDF Manager
  - USNDP Chair
  - Chair GNDS Expert Group OECD/NEA-WPEC
- I. Thompson (co-PI, LLNL, Fellow APS/IoP)
  - Staff scientist Nuclear Data & Theory Group
  - USNDP POC
  - Consultant IAEA (R-matrix, INDEN-LE)
- G. Hale (co-Inv, LANL, Fellow APS)
  - Staff scientist T-Division (T-2) [50+ years!]
  - Evaluator for most of the light-element evaluations in ENDF/B
- A. Lovell (co-Inv, LANL)
  - Staff scientist T-Division (T-2)
  - Recent recipient of 2022 FRIB Theory Award (Bayesian analysis & UQ)













## **Collaborative work targeting objectives**





#### Recent activity for work starting CY23

#### • Evaluations

- Nucleon-nucleon evaluation extension to upper energy of 100 MeV (from 50 MeV)
  - data cull via EXFOR, literature search, "archival", etc.
- Other recent, SBEND-relevant evaluation work
  - (by compound system)
  - ${}^{8}\text{Be} \sim d + {}^{6}\text{Li}$  in collaboration with J. DeBoer (U. Notre Dame)
  - <sup>13</sup>C: working with K. Kelly (LANL) CoGNAC experiment
    - Evluation of new (n, n') data
  - <sup>17</sup>O: new evaluation work
    - incorporate <sup>16</sup>O\* excited states for  $(n, n'\gamma)$

## • Theory development

- Faddeev-motivated R-matrix model development for  $(n, n'\gamma) \& (z, z_1 z_2)$ 
  - *Phys. Rev. C* in preparation

## Staff & Postdoc hiring

- New hires this spring/summer
  - L. Hlophe (currently @ LLNL) FRIB-TA Theory Fellow
  - TBA (very soon!) LANL new T-2 group staff position







 $T(d,\gamma)^{5}$ He Spectrum at 90° Lab

# Thanks in advance for your questions & support

## **Planned Code Development**

## **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



Raw Spectra

Feature Extraction Classification

Prediction



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 <sup>52</sup>Cr resonances



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

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