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

"SBEND: Structure-based Evaluation of Nuclear Data"

BNL/LANL/LLNL DOE Collaboration
NSAC Long Range Plan Town Hall Meeting
Nuclear Structure, Reactions & Astrophysics

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

2022-11-15

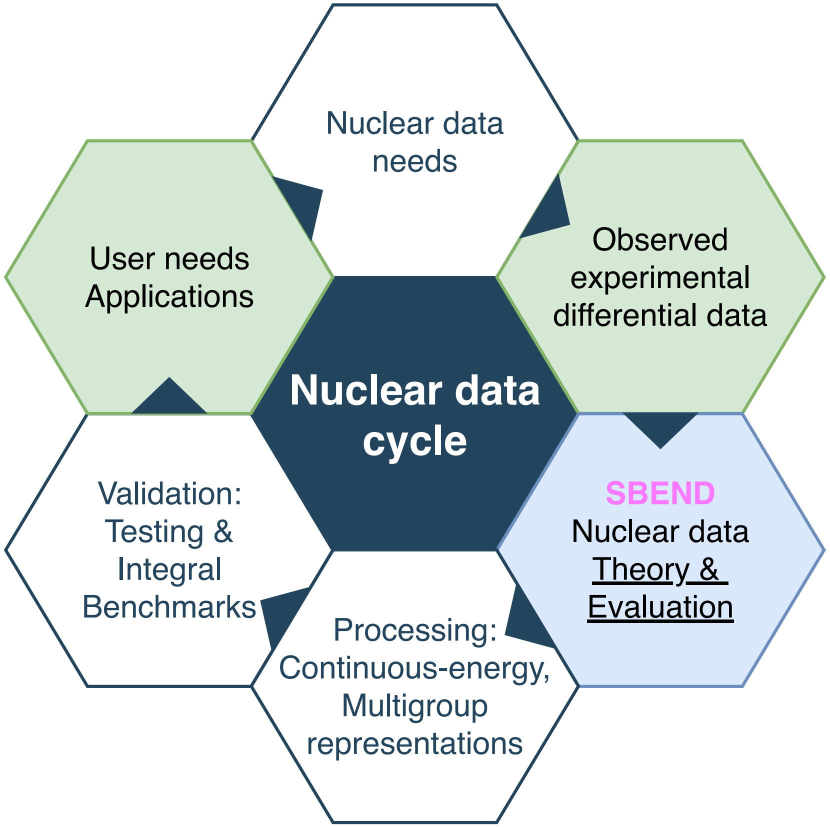
LA-UR-22-31950

Outline

- Collaboration overview
- Collaborative work overview
- Deliverables

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



Collaboration personnel

- M. Paris (PI, LANL)
  - Staff scientist Theoretical Divison (T-2)
  - Consultant to IAEA (standards, R-matrix, Int. Nucl. Data Evaluation Network)
  - NNDC Cross section evaluation working group (CSEWG) member

- 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)

Collaboration work: motivation

- Neutrino detection: $^{13}C(\alpha,n_x)^{16}O \quad x = 0,\dots,3$
  - 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*
    - $^{7}Li(p,e^{+}e^{-})\alpha\alpha$
    - 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

Collaboration work: Objectives & Focus Areas

(FI) Improved physics models and code tools for evaluated nuclear data

- R-matrix
  - $(z, z'\gamma);\ z, z' = n, p, d, t, h(^3He), \alpha$
  - Extend current techniques to compute: $\frac{d\sigma}{d\Omega_{z'} d\Omega_\gamma} = \frac{d\sigma}{d\Omega_{z'}} \frac{W(\Omega_{z'\gamma})}{4\pi}$
- Coupled-channels
  - incorporate statistical γ decays into existing primary (capture) and secondary γ production in CC approach (FRESCO)
- Transitions from low-energy (resolved resonances) → high-energy (unresolved)
  - R-matrix / CC / optical models: unification under Feshbach-Reich-Moore approach

(FII) Machine-learning code modernization

- Resonance identification/classification (decision trees)
- Fitting optimization (supervised learning)
- Uncertainty quantification (Mixture density networks)

(FIII) Data formatting, storage, and transmission

- [See codes table on a subsequent slide]

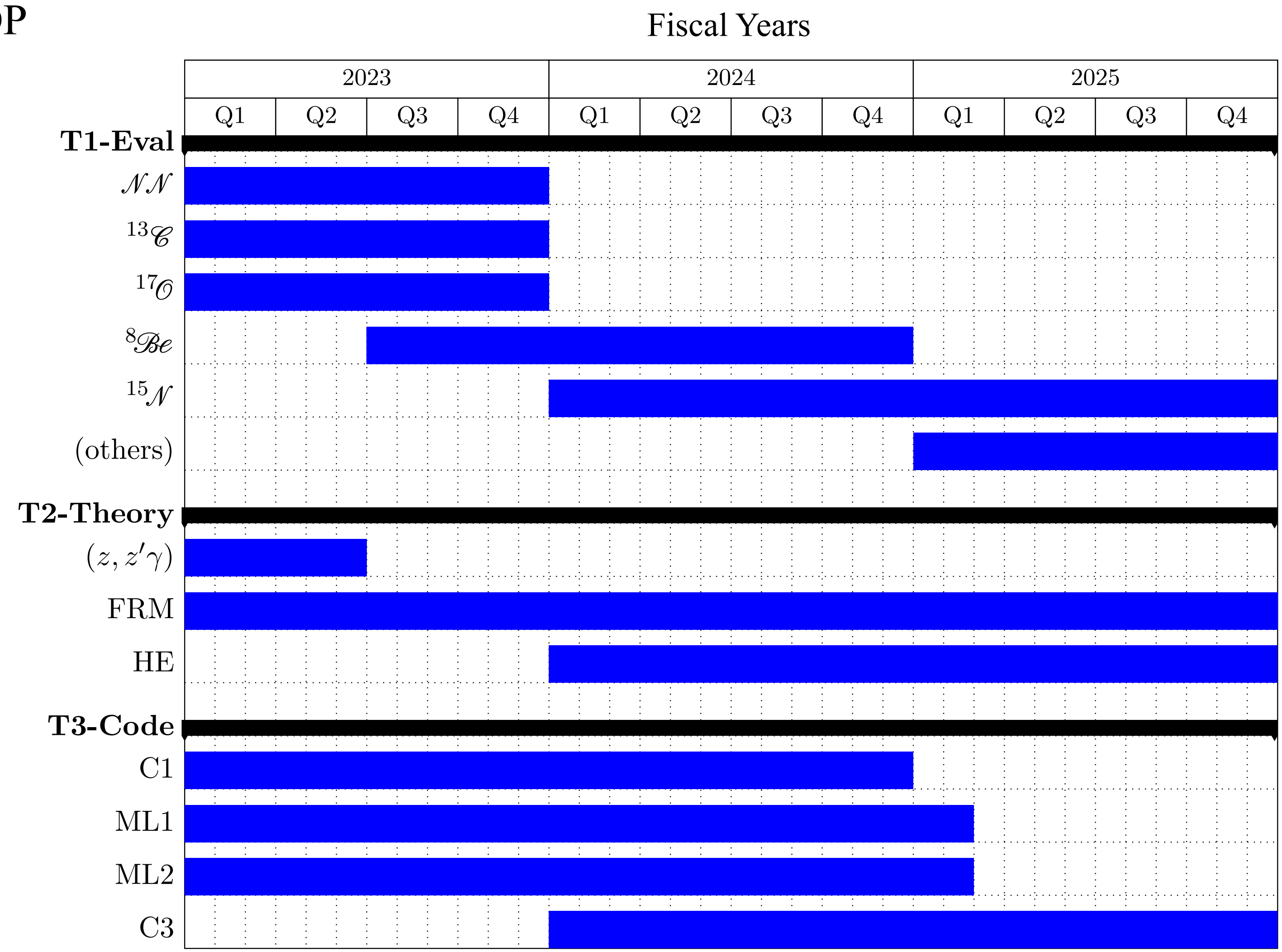
Collaborative work targeting objectives

I. Effectiveness USNDP

II. Multi-user

III. SC/NP support

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



Collaborative work: broad overview

- Materials of interest
  - ***Light elements***
    - methods constraint
  - **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
$^{1}H(n,n)^{1}H$; $^{1}H(n,\gamma)^{2}H$; $^{2}H(\gamma,n)^{1}H$	Reference/monitor cross section; BBN	Reference/monitor for various actinides, *e.g.* $^{235}U(n,f)$; Non-proliferation/interrogation
$^{6}Li(d,\alpha)^{4}He$; $^{7}Li(p,\gamma/\gamma^{*})^{8}Be$	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

Collaboration work: methods & approach

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

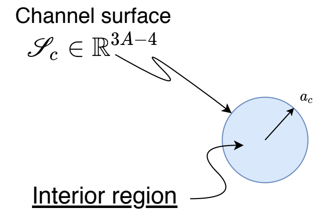
R-matrix

Exterior region

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

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

$r \to \infty$



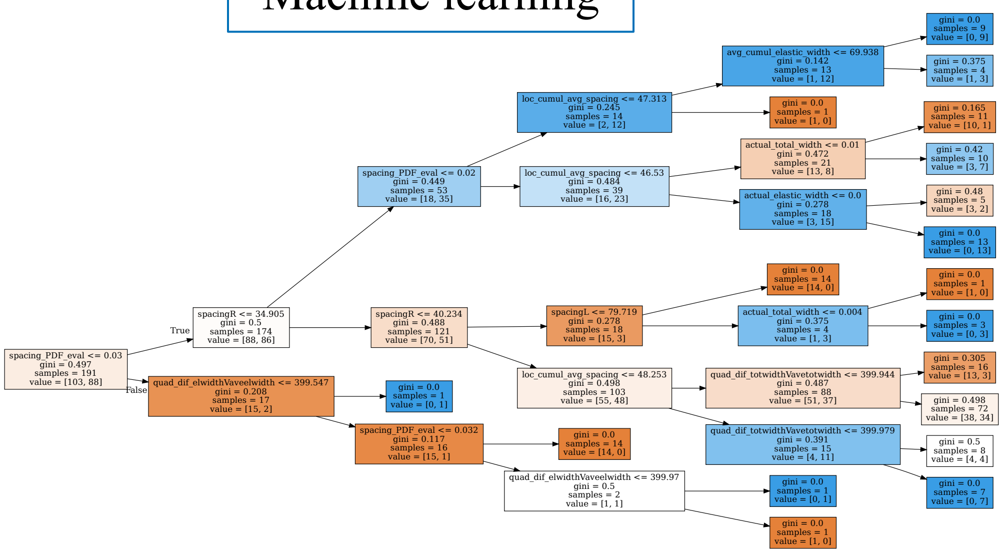
$$[H + \mathscr{L}_B]\,|\lambda\rangle = E_\lambda |\lambda\rangle$$

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

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

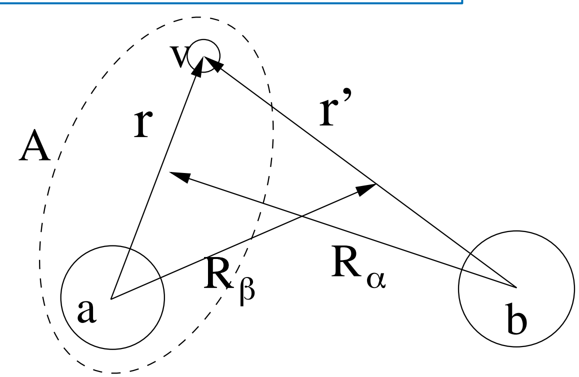
$$R_{B,c'c} = \langle c'|[H + \mathscr{L}_B - E]^{-1}|c\rangle = \sum_\lambda \frac{\langle c'|\lambda\rangle\langle\lambda|c\rangle}{E_\lambda - E}$$

Machine learning



Decision tree @ 5 nodes

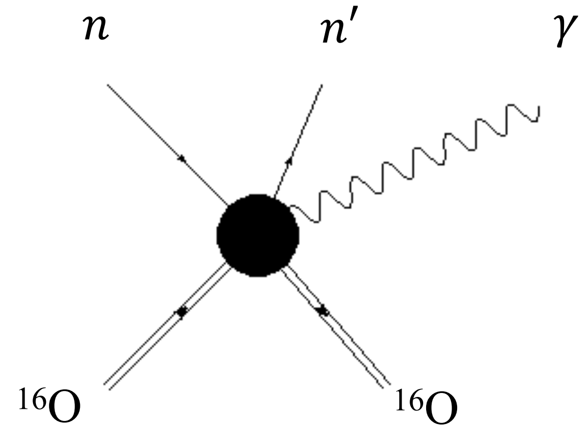
Coupled-channel methods

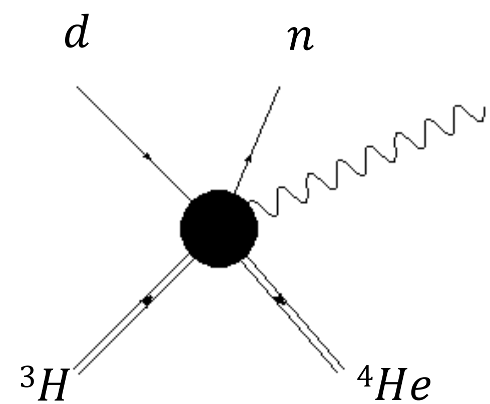


Deliverable example

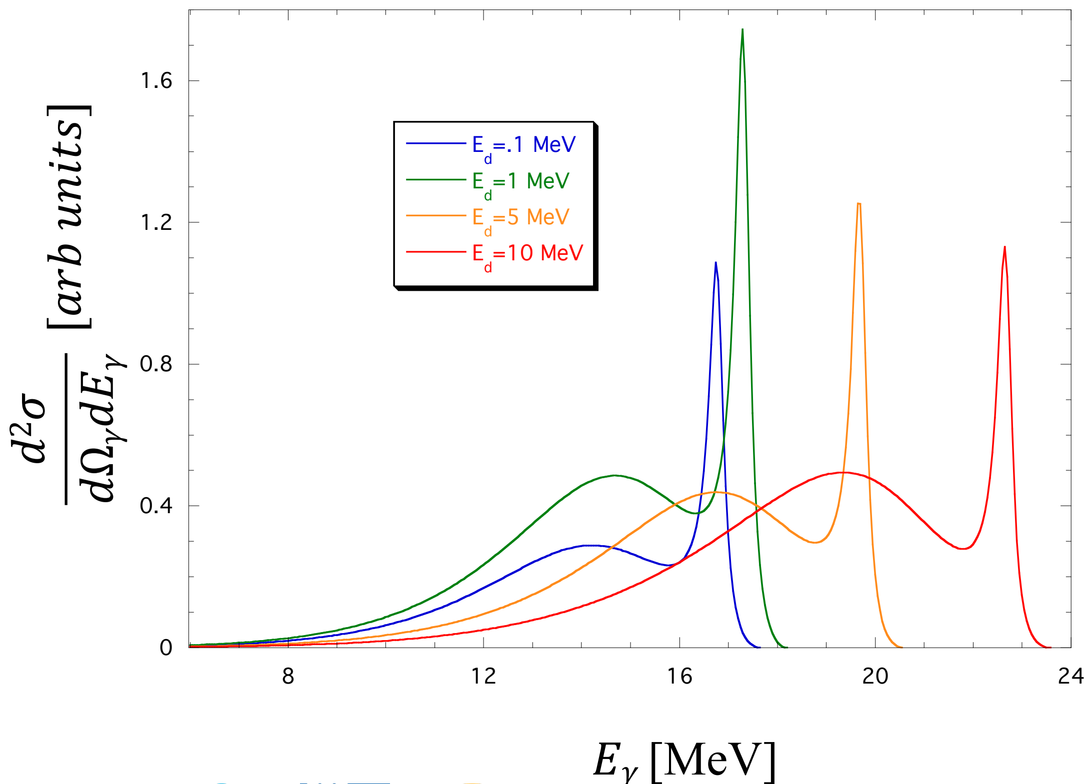
T2: Improved physics modeling and theoretical work

- Central theory effort: develop analytical, numerical tools to calculate, *e.g.* $^{16}\mathrm{O}(n,n'\gamma)^{16}\mathrm{O}$
- **New work** on $^{3}H(d,n\gamma)^{4}He$:





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

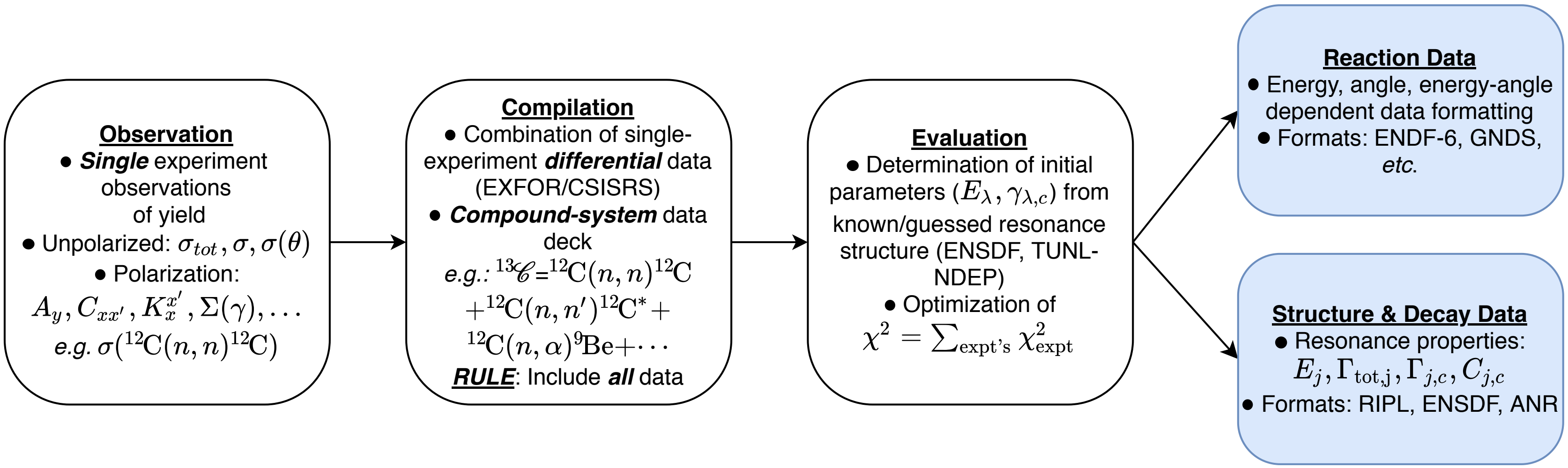


<u>SPECT code calculation</u>

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

Nuclear data evaluation workflow

R-matrix example



- Four phases of Evaluation
  - Assess single experiment observables
  - Compile all process (total, elastic, inelastic, reaction, polarization)
  - Model / parametrization fitting
  - Production of **Reaction Data** and **Structure & Decay Data**

Experimental data desiderata

- General rule
  - the more differential, the better:
  - from Good→Better
    - $\sigma_{tot} \rightarrow \sigma(E) \rightarrow \sigma(E,\theta) \rightarrow \vec{\sigma}(E,\theta)$
  - ***Who is going to measure polarization observables in the future?***
- Better kinematical coverage
  - projectile energy $\mathrm{E_{lab}} \leq$ 20 MeV
  - angular
- Higher precision with higher energies and larger compound systems
  - As A increases, ΔE_R decreases
    - energy resolution needs increase
  - As $\mathrm{E_{lab}}$ projectile increases, higher$-\ell$ contributions
    - angular resolution needs increase

Going forward

- Post-doc search
  - Being run through LANL with online interview talks
- Communication
  - Listserv
  - Regular meetings
    - **Biweekly = "once every two weeks" → these have been occurring since**
- Code & document sharing options
  - BNL-based: NNDC gitlab; listserv

Thanks for your attention

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