Reproducibility in light-element evalautions

NEA/WPEC/Subgroup 49

Reproducibility in Nuclear Data Evaluation

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Outline

- **EDA** evaluation pipeline
  - Overview/reminder
- *High-fidelity, unitary* **R-matrix** approach
  - Simultaneous evaluation of ***all*** data
- Evaluation reproduction
  - Challenges in push-button/script-driven reproducibility for our approach

NB: our evaluation approach is currently heavily hand-spun

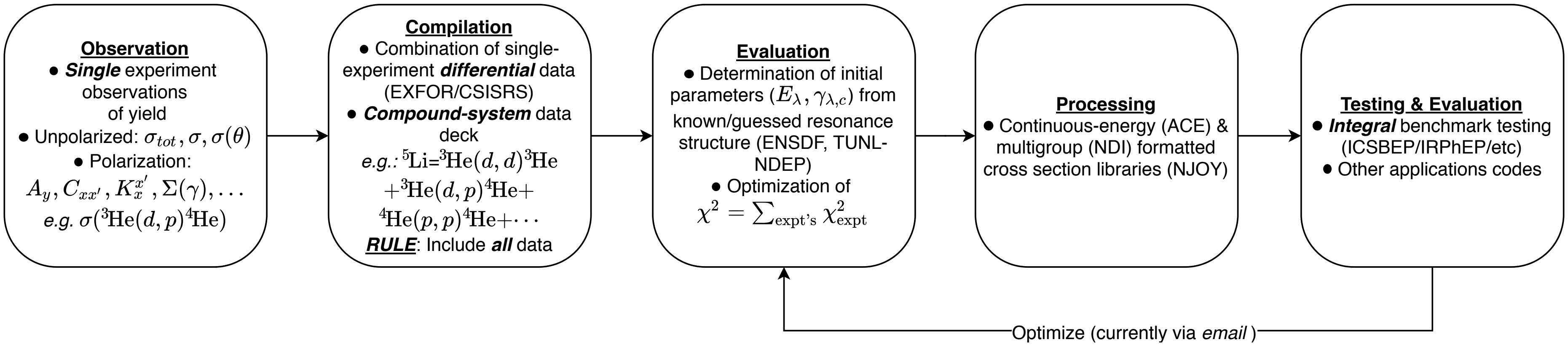
- Automation *limited* but *under development*

Overview/reminder

Light-element evaluation

Nuclear Data Pipeline

EDA **cross section evaluation**

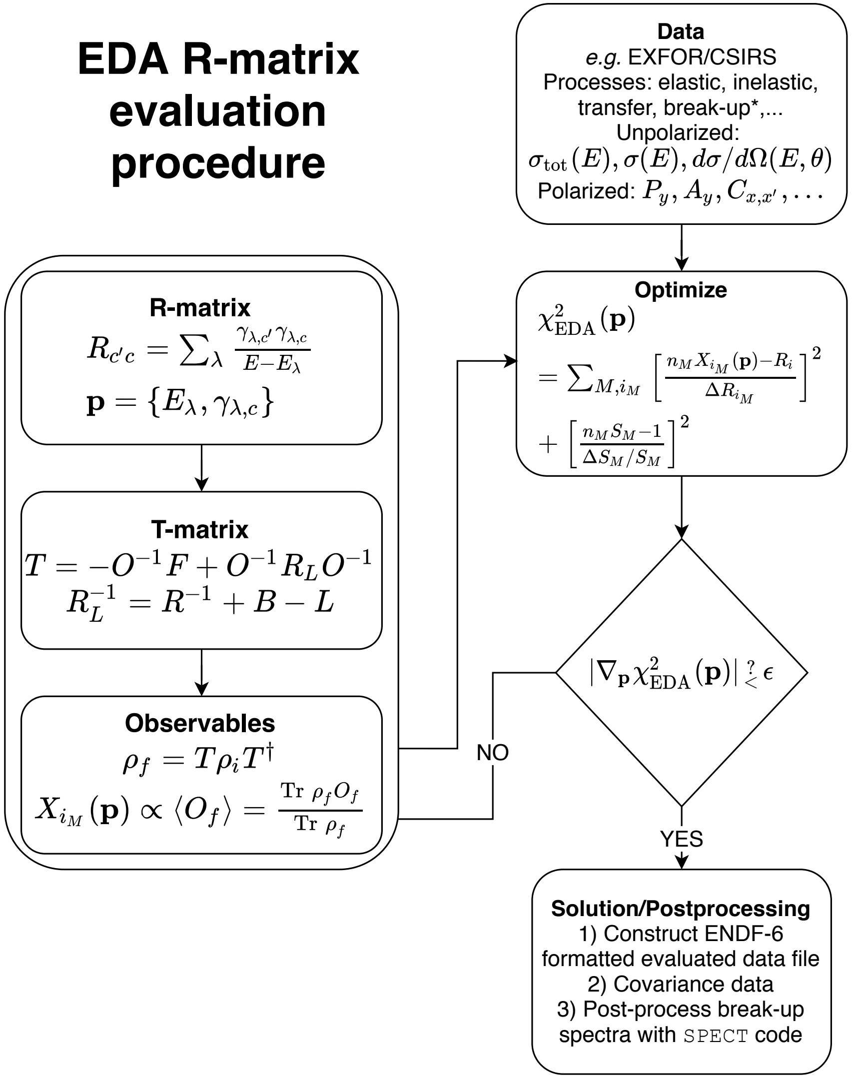


- Data-cull: observables from single experiments are compiled
- Evaluation: one set of variational parameters for all data
  - Unitary parametrization: highly constraining between different processes
    - Elastic & reaction cross sections are coupled in complex ways
  - Not simply drawing smooth curves
- Processing

R-matrix evaluation

^{5}Li system

EDA R-matrix evaluation procedure



Channel	a_c (fm)	l_{max}
$d + {}^3\text{He}(\frac{1}{2}^+)$	4.8	4
$p + {}^4\text{He}(0^+)$	2.9	4
$p + {}^4\text{He}^*(0^+; 20.2\text{ MeV})$	3.4	2
$d_0 + {}^3\text{He}(\frac{1}{2}^+)$	5.1	0

Reaction	Energy Range (MeV)	# Data Points	Observables
${}^3\text{He}(d,d){}^3\text{He}$	$E_d = 0.32 - 10.0$	2,229	$\sigma(\theta), A_i, A_{ii}, C_{i,j}, C_{ij,k}, K_{i,j'k'}, K_{ij,k'l'}$
${}^3\text{He}(d,p){}^4\text{He}$	$E_d = 0.13 - 10.0$	3,839	$\sigma(E), \sigma(\theta), A_i, A_{ii}, C_{i,j}, K_{ij,k'}$
${}^3\text{He}(d,p){}^4\text{He}^*$	$E_d = 3.70 - 6.70$	28	$\sigma(\theta)$
${}^4\text{He}(p,p){}^4\text{He}$	$E_p = 0.92 - 34.3$	867	$\sigma(E), \sigma(\theta), A_y, P_y$
	Total:	6963	

Table 1: Channel configuration (top) and data summary (bottom) for the ^{5}Li system analysis. The column labeled "Observables" indicates the following data types: $\sigma(E)$, integrated cross section; $\sigma(\theta)$, unpolarized angular distributions (energy-dependence suppressed); A initial-state analyzing power; P final-state polarization; C spin correlation coefficients; K polarization transfer coefficients. (We have suppressed the indices $i, j, \ldots$ which take on values x, y, z for spins/polarization directions in configuration space.) All polarization and spin distributions are angular distributions, which depend on the angle of the outgoing particle. Chi-squared per degree of freedom for the analysis is $\chi^2/\text{dof} \simeq 2.7$ over 7,178 data points, 215 of which were discarded by eliminating individual data points which contribute to $\chi^2 > 40$.

Evaluation reproduction

Ideal Script Scenario

Provide compound system to script: *NN, ^{3}H, ^{3}He, ^{4}He, ^{5}He, ^{5}Li, etc.*

➡ `python edaEvaluate --cs 5Li`

- **Data**
  - Retrieve all available data from SG50's (future) relational database URL
    - ^{5}Li: ^{4}He(p,p)^{4}He, ^{4}He(p,d)^{3}He, ^{3}He(d,d)^{3}He, ^{3}He(d,p)^{4}He, ^{3}He(d,np)^{3}He, ...
    - $\sigma(\theta), A_i, P_j, A_{ii}, C_{i,k}, C_{ij,k}, K_{i,j'k'}, K_{ij,k'l'}, \ldots$
  - Construct internal/native code (EDA) representation (frames for Lab/CM, spectra, etc.)
  - [Construct data covariance for GLS]
  - [Import sets of detector instrument response functions]
- **Evaluation configuration**
  - Load partition (p+4He, d+3He, n+p+3He, etc.) and channel information from input deck
  - Load R-matrix parameters
  - Load code-run parameters (search method, convergence criteria, etc.)
- **Execute evaluation**

Evaluation reproduction
Realistic Scenario

- **Data**
  - Using “all” data in database is generally not feasible
  - ‘Data-cull’ is complex, human-intensive endeavor
    - Consult original literature for meaning, interpretation, accuracy, etc.
    - Cull-out data beyond range of applicability of theory/fit
  - Solution: specifiy details of evaluation data-selection
    - VERY COMPLEX
- **Evaluation configuration**
  - Generally straightforward
  - Can get complex as code versions change
    - Improved physics models
    - Error/bug corrections, etc.
  - Solution: detailed versioning required
- **Evaluation execution & testing**

Thank you.

Follow-on material

NN evaluation: configuration & data

- Neutron energies $E_n \leqq 50$ MeV
- Charge-independent analysis

$$R(E) = \sum_{\lambda,T} \frac{\gamma_\lambda^{(T)} \tilde{\gamma}_\lambda^{(T)}}{E_\lambda^{(T)} - E},$$

  - T=1 (pp, np-isovector)
  - T=0 (np-isoscalar)
  - Coulomb energy-level shift

$$E_\lambda^{(T=1)} = E^{(T=0)} + \Delta_Z$$

    - Fit to $a_{nn} = -18.5$ fm
  - Predict nn scattering
- High-fidelity description

$$\chi^2/\text{dof} = 0.9$$

- Planned evaluation
  - $E_n \lesssim 250$ MeV

TABLE II. Channel configuration (top) and data summary (bottom) for the charge-independent $N-N$ analysis up to 50 MeV. Since the number of free parameters is 43 resonance parameters + 83 normalizations, the chi-squared per degree of freedom for the analysis is 0.90.

Channel	a_c (fm)	$l_{\max}$
$p+p$	3.26	3
$n+p$	3.26	3
$\gamma+d$	84.6	1
$n+n$	3.26	3

Reaction	# Pts.	χ^2	Observable Types
$p(p,p)p$	675	951	$\sigma(\theta), A_y(p), C_{x,x'}, C_{y,y'}, K_x^{x'}, K_y^{y'}, K_z^{x'}$
$p(n,n)p$	4815	3764	$\sigma_T, \sigma(\theta), A_y(n), C_{y,y'}, K_y^{y'}$
$p(n,\gamma)d$	86	179	$\sigma_{\text{int}}, \sigma(\theta), A_y(n)$
$d(\gamma,n)p$	88	77	$\sigma_{\text{int}}, \sigma(\theta), \Sigma(\gamma), P_y(n)$
$n(n,n)n$	1	0	a_0
Norms.	80	86	
Total:	5745	5057	20