Tools using GNDS for the inter-conversion of inputs and outputs for R-matrix codes

Consultancy Meeting on model code output & application nuclear data form structure.

IAEA.

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R-matrix method used to describe resonances

- All Codes based on Lane and Thomas, RMP (1957)
- Various extensions:
  - Reich-Moore damping for all capture channels
  - Three-body (or more) in final states.
  - Try B=S approximation for resonance energies, or Brune basis
- Many different codes:
  - SAMMY, EDA, AZURE2, CONRAD, SFRESCOX, RFLOW, AMUR, etc.
  - Fitting data by varying parameters to minimize χ^2/dof.
  - All with different input and output formats.
- ENDF and GNDS evaluation formats can describe (most) parameter sets and the cross-section fits.

Feature	EDA	AZURE2	AMUR	FRESCOX	SAMMY	CONRAD	GECCCOS
R-matrix	Full	Full	Limited (for γ's)	Full	SLBW, MLBW, RM, Full[a]	SLBW, MLBW, RM, Full[a]	Full
Derivatives	Analytic	Numerical	Numerical	Numerical	Analytical ($T = 0$ K) Numerical[b]	Analytic	Numerical
Reference frame	Lab/CM	In Lab, Out CM	Lab/CM	Lab/CM	Lab/CM	Lab/CM	Lab/CM
(Non)Relativistic kinematics	R + NR	NR	NR	R, NR	N-R	R, NR	NR
Channel Radii	Varied	Varied	Fitted (option)	Fixed	Varied	Varied	Fixed/Varied
Photons	In/Out	Out	Out	In/Out	Out	Out	
Observables: E, θ cross sections	All	All	All	All	All	All	All
Observables: polarization T_{kq}	All	No	Yes	All	No[c]	No	No (planned)
Inverse reactions	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Decay gammas	Post-processing	No	No	Post-processing	No	No	No
Isobaric reactions simultaneously	Yes	No	No	No	No	No	No
Doppler broadening	No	No	Yes	No	Yes	Yes	No
Resolution broadening	Yes	Yes	Yes	No	Yes	Yes	No
Normalization	Yes	Yes	Yes	yes	Yes	Yes	Yes
Background subtraction	No	No	Yes	No	Yes	Yes	No
Background R-matrix terms	E-dependent	Distant poles	Distant poles	Distant poles	Yes	No (planned)	Yes
Sample-size corrections	No	Yes	No	No	Yes	Yes	No
Close-geometry Q-corrections	No	Yes	No	No	Yes	No	No
Fitting procedure	LSQ	MINUIT2	KALMAN	MINUIT1	Bayesian (GLS)	Bayesian (GLS)	DAKOTA [41]
Multiple data sets S: Simultaneously	S	S	S	S	S	S	S
Uses data covariances	No	No	Yes	No	Yes	Yes	No[d]
Prior parameter covariances	Yes	No	Yes	No	Yes	Yes	No[d]
Data covariances (MF 32)	No	No	No	No	Yes	Yes	No
Brune parameter output	No (planned)	Yes	No	No	No (planned)	No (planned)	No (planned)
ENDF-6 format output	Yes	No	Yes	No	Yes	Yes	No[d]
ENDF-6 input	No	No	No	No	Yes	Yes	No
Code language	F77	C++	C++	F90	F77[e]	C++	F03
Export controlled	Yes	No	Yes	No	RSICC[f]	Yes	No
Documentation	No	Yes	No	Yes	Online	No	No[g]
Parallelized	No	Yes	Yes	No	No	Yes	Yes
Interactive fitting	Yes	No	No	Yes	Yes	Yes	No
PPP modification			logarithmic fit	No	Experimental covariances	Marginalization	

[a] Full R-matrix in SAMMY and CONRAD is achieved by treating γ-channels as reaction channels.

[b] Analytic derivatives of cross sections at $T = 0$ K, numerical derivatives of Doppler-broadened and resolution-broadened cross sections.

[c] SAMINT links to IBE.

[d] provides the input for a separate Bayesian evaluation code, which delivers all the mean values and covariances of considered observables.

[e] SAMMY modernization in progress: the SAMRML code has been modernized into C++.

[f] SAMMY may have its export-controlled classification removed.

[g] Source code documentation available, manual in preparation.

Need to Verify the various R-matrix codes

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Review

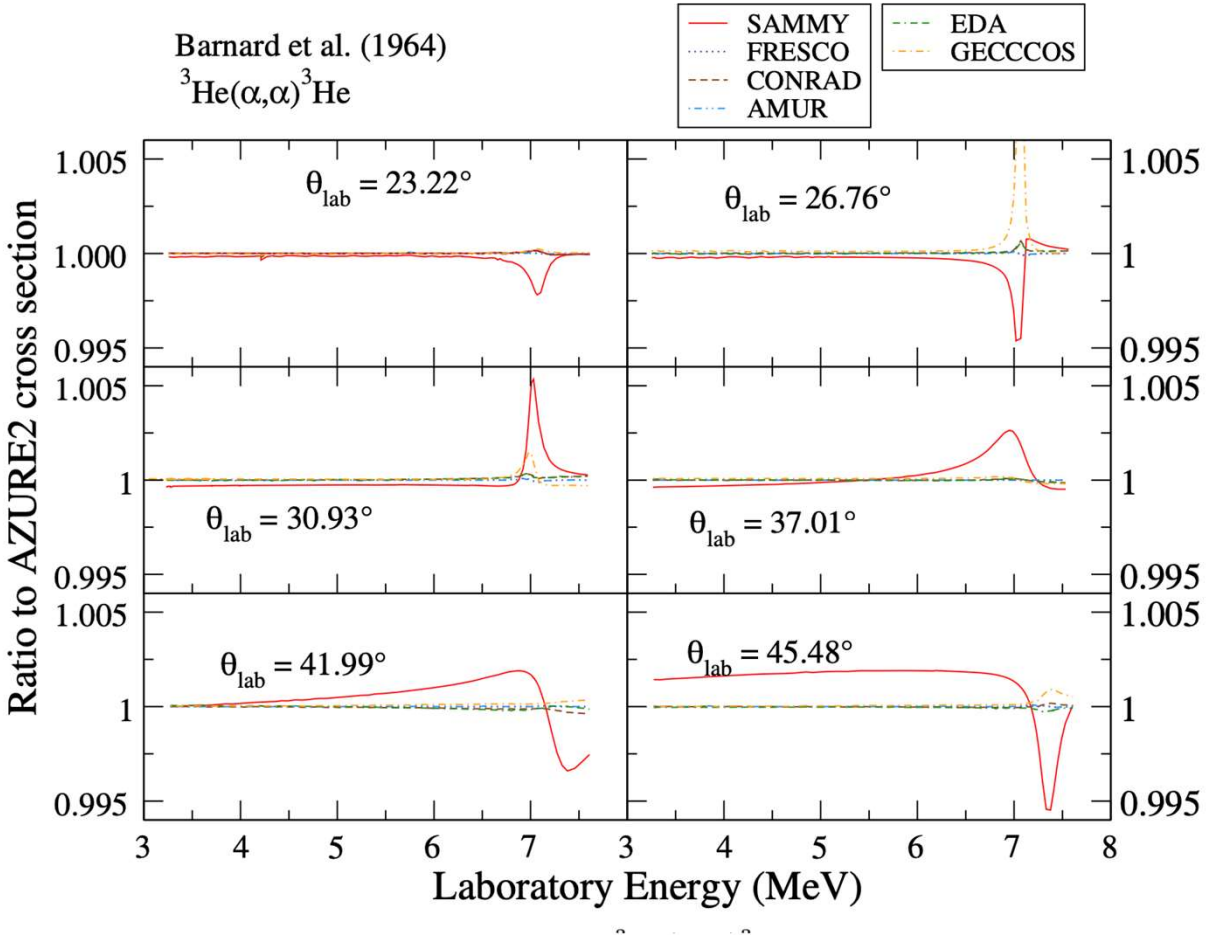
Verification of R-matrix calculations for charged-particle reactions in the resolved resonance region for the ^{7}Be system

Ian J. Thompson[1], R.J. deBoer[2,3], P. Dimitriou[4,a], S. Kunieda[5], M.T. Pigni[6], G. Arbanas[6], H. Leeb[7], Th. Srdinko[7], G. Hale[8], P. Tamagno[9], and P. Archier[9]

The results of a comprehensive effort to verify the most widely used R-matrix codes in the various fields of nuclear science and applications:
AMUR, AZURE2, CONRAD, EDA, FRESCO, GECCCOS, and SAMMY.

Emphases on Accuracy and Replication

Comparisons of Codes



Comparison of calculations to AZURE2 results for the 3He(α,α)3He reaction

Ferdinand.py : translation of all code inputs & outputs

- To compare codes, we need to be able to translate input R-matrix parameters, even if not converged.
  - All codes need to have a common format for these parameters, usable for inputs as well as outputs converged-so-far.

- I use GNDS as common interchange format
  - Read & write ENDF, GNDS standard formats for MF=2 and <RMatrix>
  - Read AMUR, AZURE, EDA, FRESCO and RAC formats
  - Write AZURE, EDA, FRESCO, HYRMA and latex formats.
  - Convert
    - standard ↔ Brune basis (a GNDS extension)
    - rwa ↔ formal widths,
    - different boundary condition numbers B
    - add/remove a Reich-Moore damping channel
    - re-normalization factors for experimental data sets (a GNDS extension)
    - covariance matrices for parameters to GNDS/ENDF (a few codes only)

Current and Future Work

- Include excited residual states in R-matrix fits: p1, p2, etc.
- Predict angular particle distributions giving the excited states
- Predict secondary gamma distributions from residual-state decays. Method: Brune & deBoer, PRC 102, 024628 (2020).
- Extend to higher energies into smooth-cross-section region
  - Transition properly to optical-model scattering and Hauser-Feshbach methods using optical potentials.
  - Even for lighter nuclei if excitation energies high enough.

Related codes

1. Rflow: GPU R-matrix code using Tensorflow.
2. validateWithX4plotlibc.py : compare GNDS with EXFOR data
3. data4rflows.py get EXFOR data for Rflow, making spreadsheet of meta-data for checking and other imports.
4. Pointwise-reconstruction using FRESCO or Tensorflow.

Improvements

- More uniform treatment of covariance matrices
  - Order of parameters
  - Parameter transformations ⇒ covariance transformation
  - Include fitted data normalizations?

- EXFOR, clearly specifying:
  - systematic vs statistical uncertainties
  - final levels in residual nuclei
  - averaging intervals and resolution - for angles and energies in and out.

- Organized cross-over to Hauser-Feshbach statistical models at higher beam energies when cross-sections smooth

- RECENT (in PREPRO) needs updates for pointwise reconstructions:
  a) charged projectiles (giving Coulomb+Nuclear elastic scattering)
  b) angular distributions, not just total and angle-integrated data.
  c) different boundary conditions B (or Brune basis)
  d) general LRF=7 R-matrix specifications including excited states.