Verification of R-matrix calculations for charged-particle reactions

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Review

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

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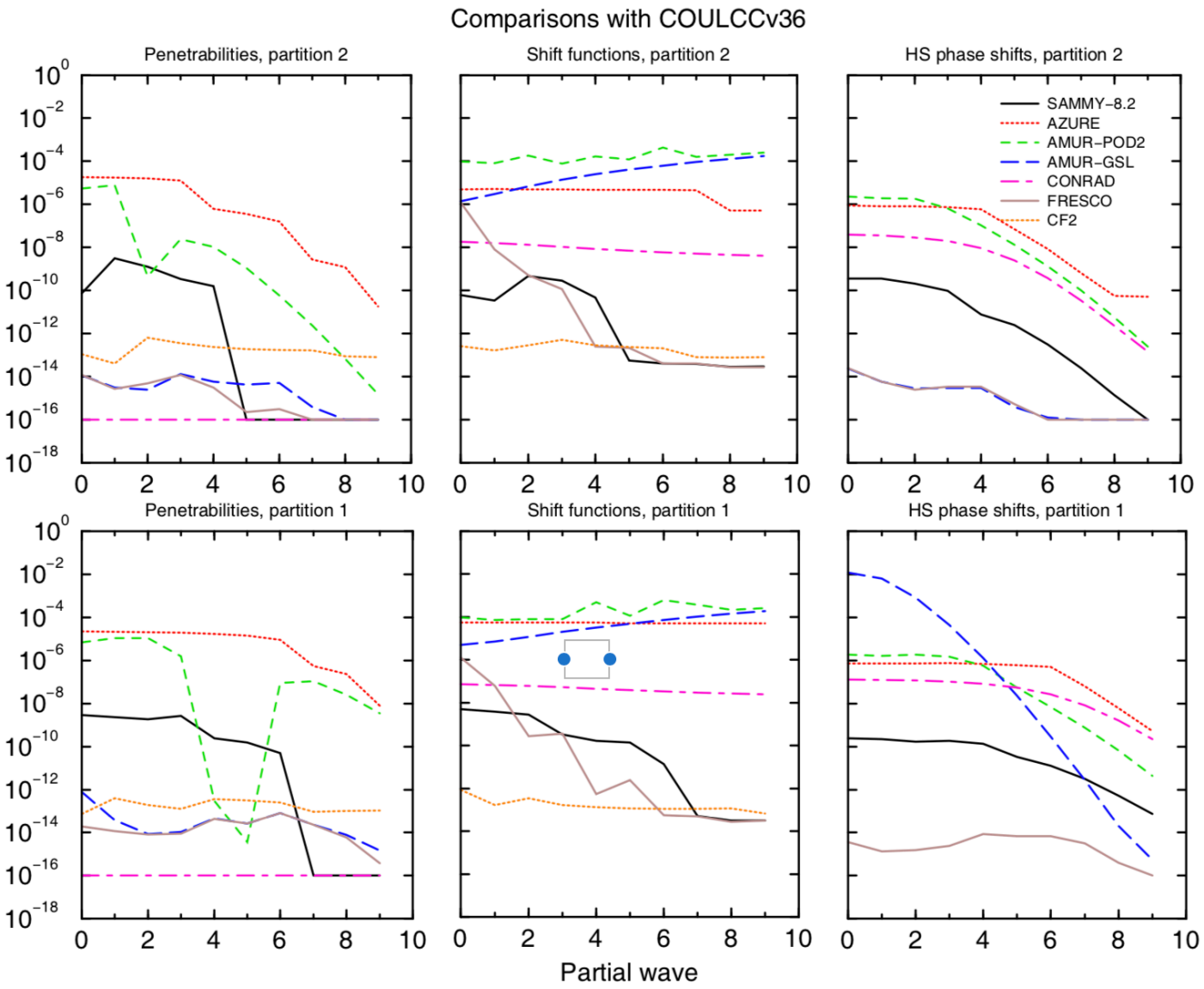
Need to validate R-matrix codes

- AMUR: Japan - S. Kunieda
- AZURE2: Notre Dame – James de Boer
- EDA: LANL – Gerry Hale and Mark Paris
- FRESCOX: LLNL – Ian Thompson
- GECCCOS: TUW – Thomas Srdinko
- SAMMY: ORNL – Marco Pigni and others
- CONRAD: CEA – Tamagno and Archier

Table 1. Summary of R-matrix codes specifications.

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 ($T = 0\,\mathrm{K}$) 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
RRR modification			logarithmic fit	No	Experimental covariances	Marginalization	

Test the Coulomb Functions: S, P, ϕ



Differences of codes with S, P, and ϕ with values from COULCC

Test Case: ^{3}He+^{4}He // p + ^{6}Li.

Energy range

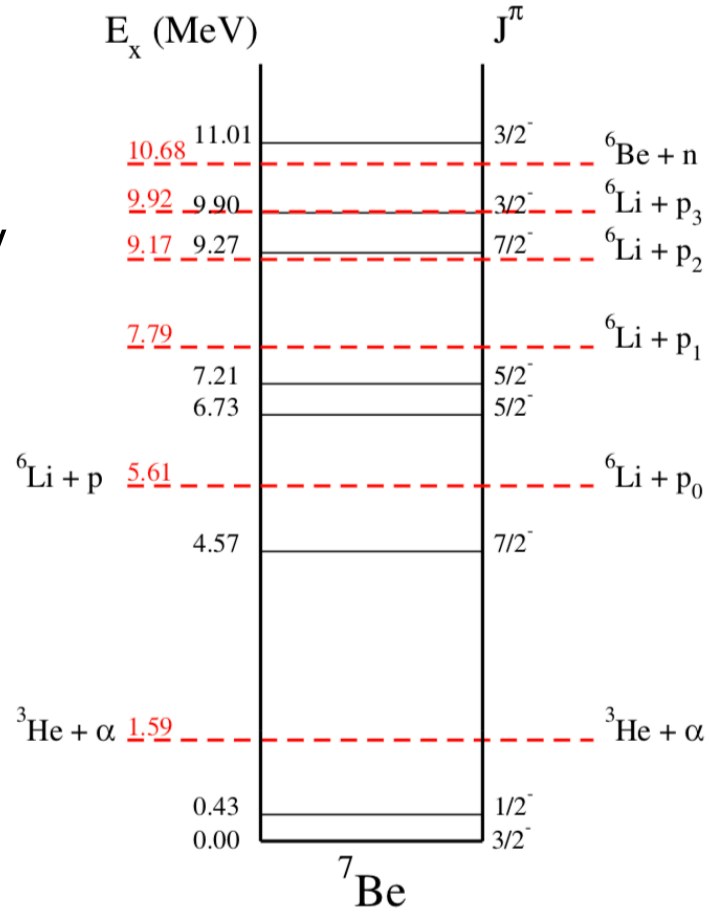


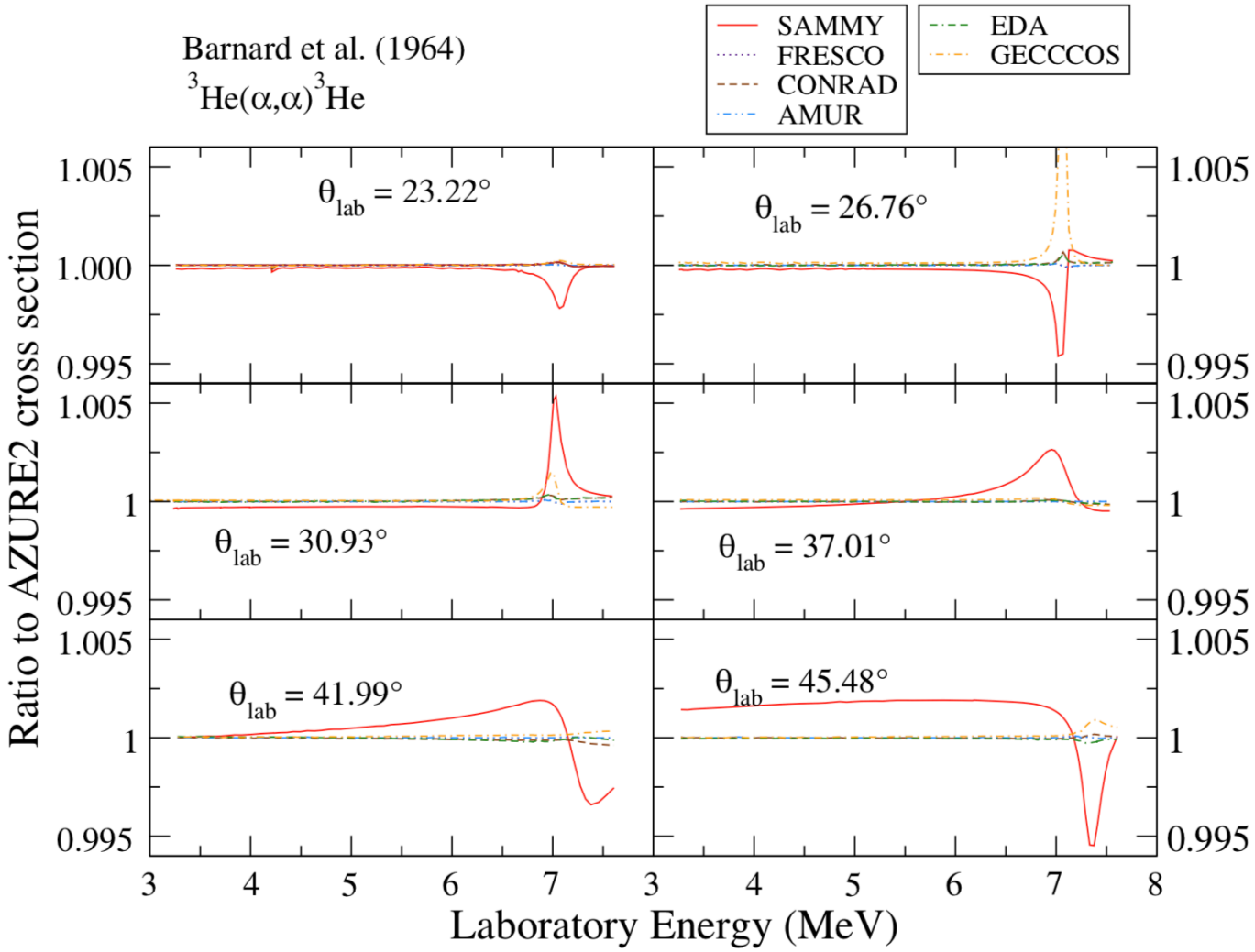
Fig. 1. Level diagram of ^{7}Be. The low mass nucleus has only two bound states, the ground state and the level at E_x = 0.429 MeV.

R-matrix parameters

Table 3. R-matrix parameters in the $B = -\ell$ basis. Pole energies in the center-of-mass frame of the elastic channel. Reduced width amplitudes are given in MeV$^{1/2}$.

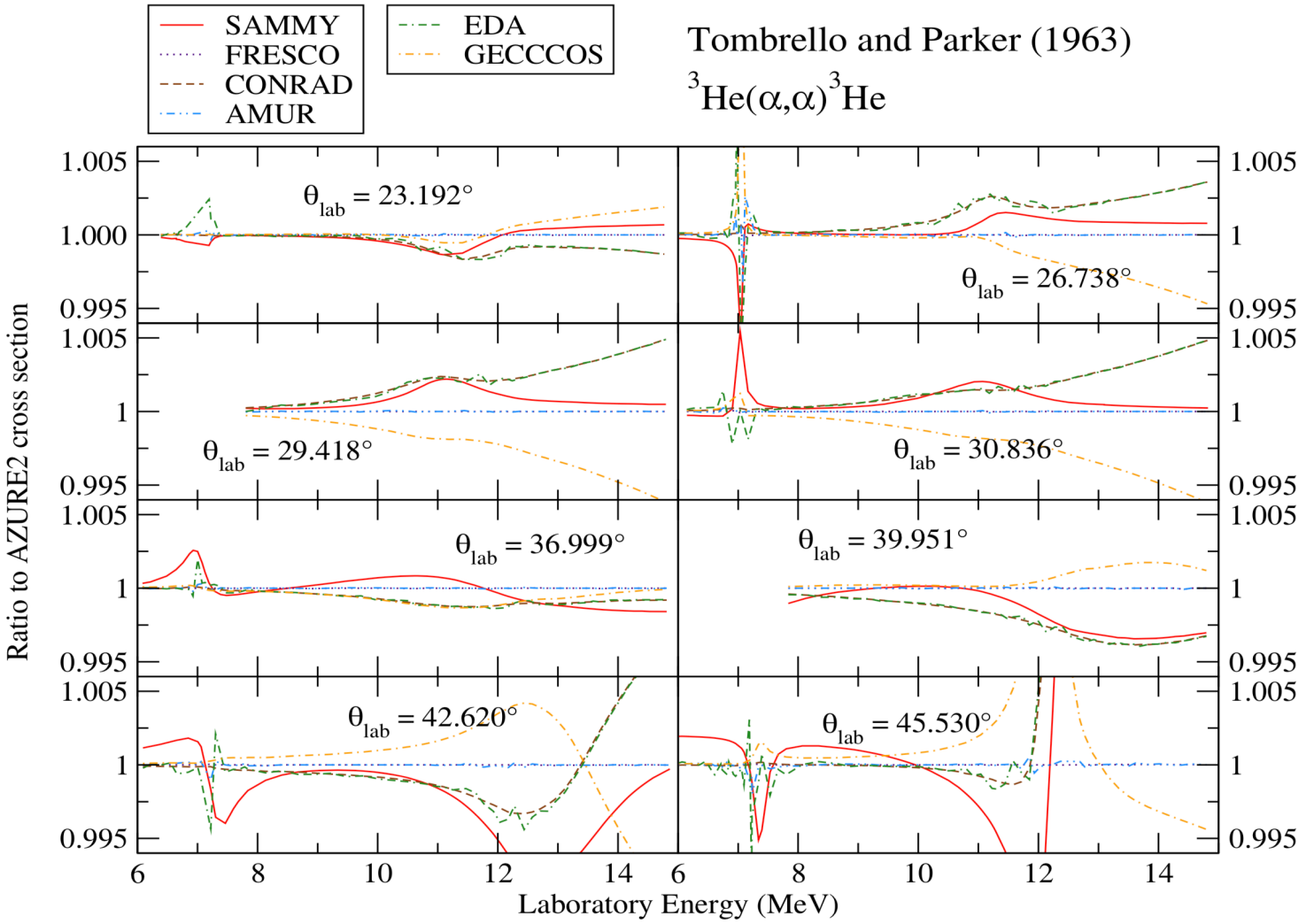
$J^\pi = 1.5^-$				
E	^{1}H+^{6}Li	^{1}H+^{6}Li	^{1}H+^{6}Li	^{4}He+^{3}He
(MeV)	ℓS: 1, 1/2	ℓS: 1, 3/2	ℓS: 3, 3/2	ℓS: 1, 1/2
−1.586097	−1.34077	−0.41816	0.00000	1.05725
$J^\pi = 2.5^-$				
E	^{1}H+^{6}Li	^{1}H+^{6}Li	^{4}He+^{3}He	
(MeV)	ℓS: 1, 3/2	ℓS: 3, 1/2	ℓS: 3, 1/2	
5.746671	0.94880	0.00000	0.18770	
7.088367	−0.34947	0.00000	1.18381	
$J^\pi = 3.5^-$				
E	^{1}H+^{6}Li	^{1}H+^{6}Li	^{1}H+^{6}Li	^{4}He+^{3}He
(MeV)	ℓS: 3, 1/2	ℓS: 3, 3/2	ℓS: 5, 3/2	ℓS: 3, 1/2
3.483949	0.00000	0.00000	0.00000	0.79362

Comparison of calculations to AZURE2 results for the $^{3}He(\alpha,\alpha)^{3}He$



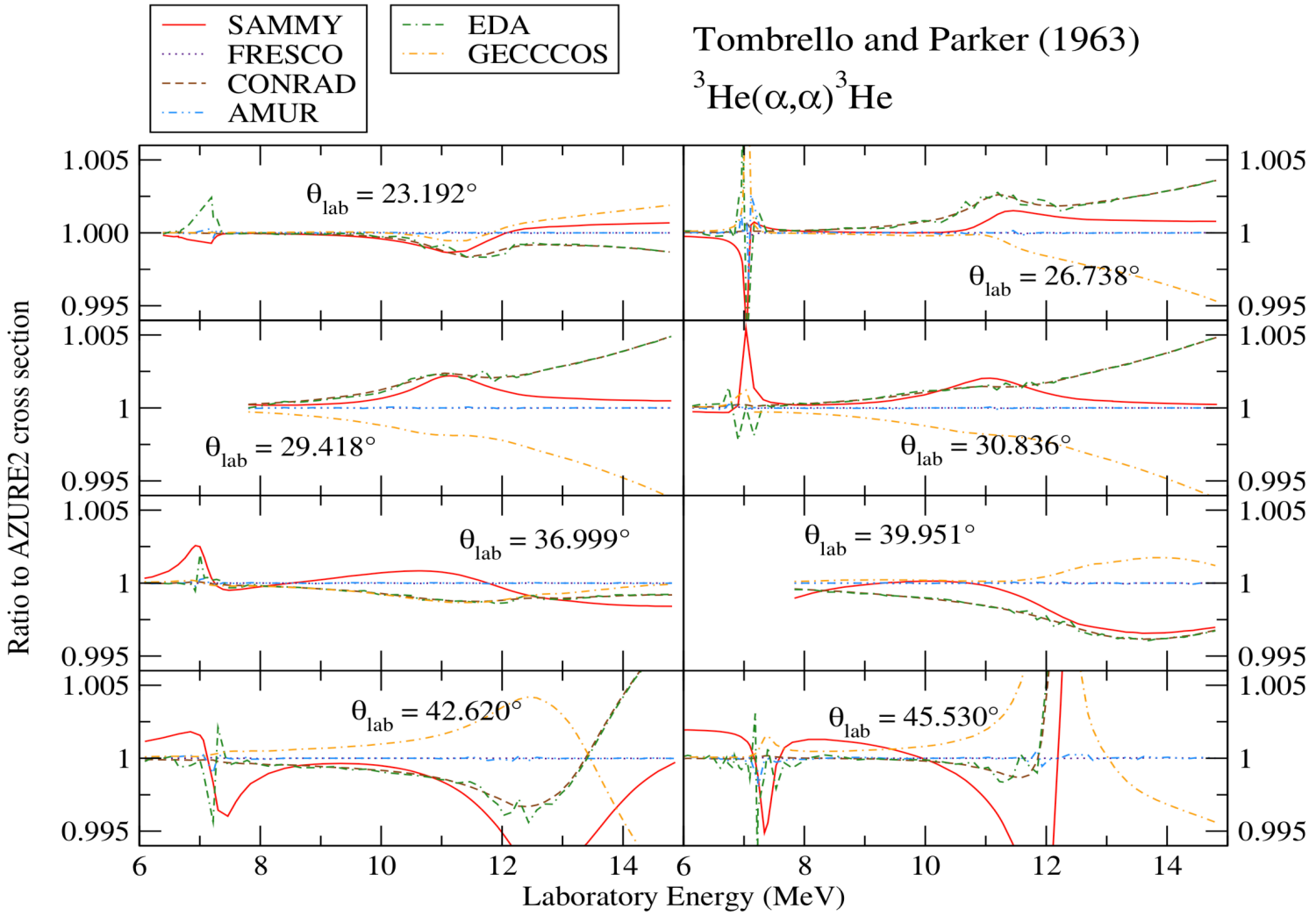
Lower incident energies

Comparison of calculations to AZURE2 for $^{3}He(\alpha,\alpha)^{3}He$



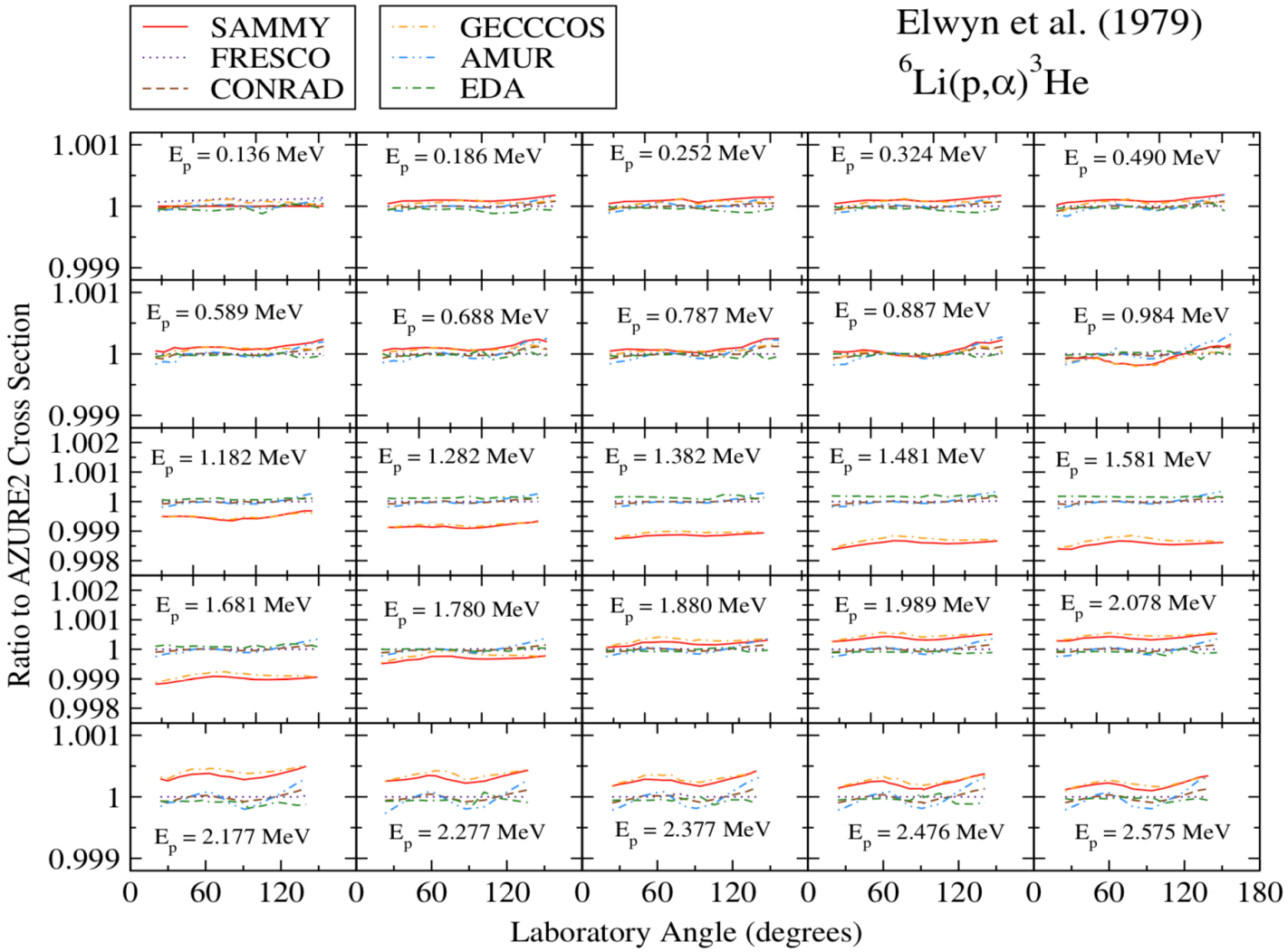
Higher incident energies

Comparison of calculations to AZURE2 for $^{6}Li(p,p)^{6}Li$



Higher incident energies

Comparison of calculations to AZURE2 for $^{6}Li(p, \alpha)^{3}He$



Low incident energies

Conclusions

- A very useful exercise!!
- Used LLNL code FERDINAND.py translate parameter files between all the code inputs.
- We thought this would be all easy, but no -
  - Several bugs were found in several codes.
- On the whole, all the codes agreed to within 0.1–0.3% which is far below the uncertainties of the existing experimental data in this low-energy region.