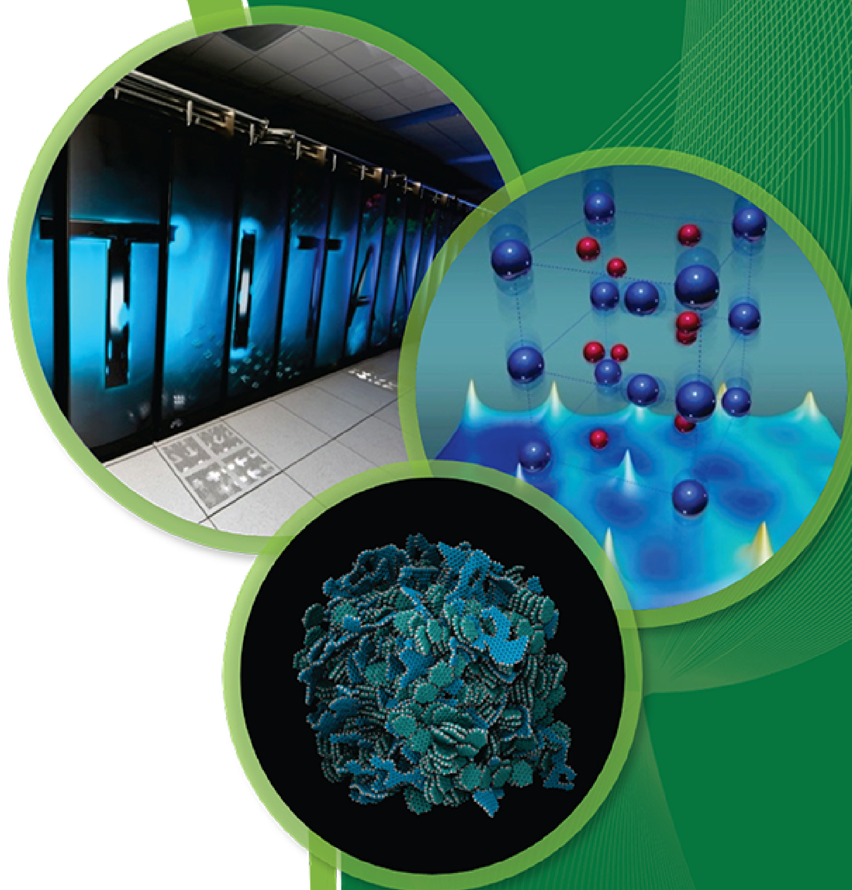
ORNL contribution to ENDF/B-VIII.0 and progress on light nuclei evaluations



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for the US Department of Energy

Outline

- **Neutron evaluation work (Part I)**
  - Resonance evaluation work: $^{182-184,186}$W, ^{40}Ca, ^{235}U, ^{239}Pu
  - On going resonance work: ^{16}O and set of Dy isotopes (FY18)
  - Evaluation work on neutron multiplicities $\bar{\nu}_p$ (see NDAG presentation)

- **Progress on charged-particle evaluations (Part II)**
  - Treatment of the closed-channel effects ($B_c = -l$) in SAMMY
  - R-matrix code project at the International Atomic Energy Agency (IAEA)
  - Test on ^{7}Be compound nucleus
  - Comparison between SAMMY and other R-matrix codes
  - Resonance work on $\alpha+^{17,18}$O evaluations within NA22 program (FY18)

- **Summary and conclusions**

Tungsten RRR evaluations

No.	Nucleus (I^{π})	E_{max} ($E_{max}^{ENDF/B-VII.1}$)	Method	No. Levels	J_0	J_1
1	^{183}W $(1/2^-)$	5 (2.2) keV	RM	387	346	21
2	^{182}W (0^+)	10 (5.0) keV	RM	306	171	135
3	^{184}W (0^+)	10 (4.0) keV	RM	178	94	84
4	^{186}W (0^+)	10 (8.3) keV	RM	169	95	74

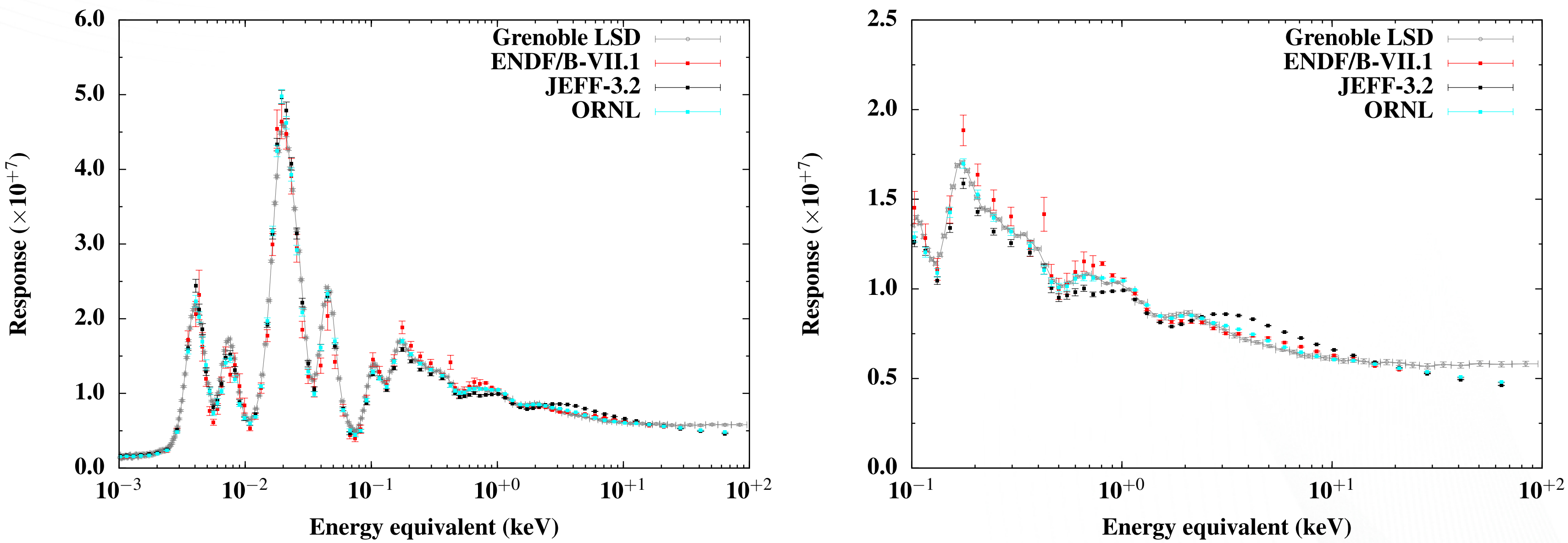


Figure 1: Experimental spectrum of the Grenoble Lead Slowing Down benchmark (gray dots) in the energy range of 1 eV up to 100 keV compared with the spectra obtained with the ENDF/B-VII.1 (red dots), JEFF-3.2 (black dots) and the set of tungsten ORNL evaluations (cyan dots). ND2016 EPJ Web of Conferences **146**, 06010 (2017).

^{235}U RRR evaluation and ^{239}PU

No.	Nucleus (I^{π})	E_{max}	Method	J_{3^-}	J_{4^-}
1	^{235}U $(7/2^-)$	2.25 keV	RM	1433	1731

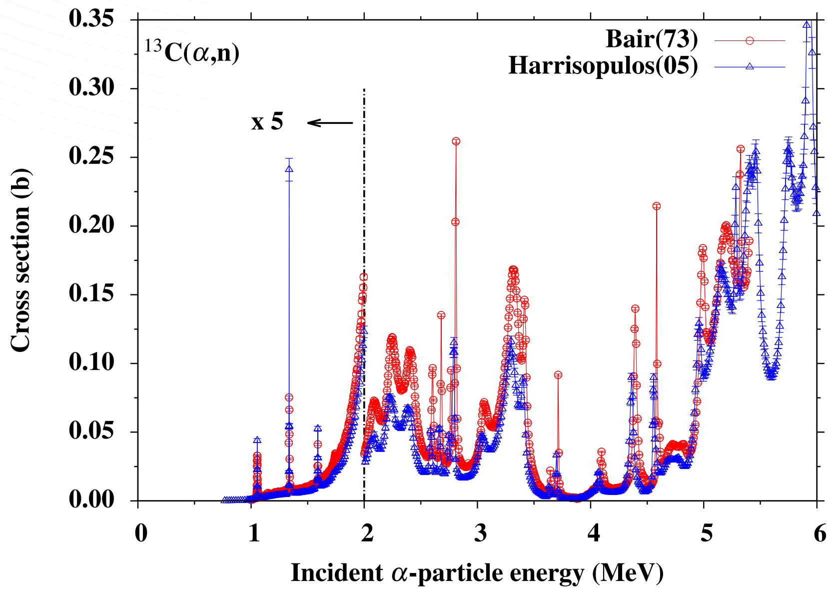
- In the ORNL resonance evaluation in the ENDF/B-VIII.0 library, particular emphasis was devoted to
  - STD-2017 thermal cross sections and the fission integral between 7.8–11 eV
  - Neutron incident energies up to 20 eV for *measurements of* $\alpha = \sigma_\gamma/\sigma_f$ *(or* η*)*
  - New thermal Prompt Fission Neutron Spectra (PFNS) evaluated by the IAEA (Capote/Trkov)
  - Newly evaluated STD-2017 fission average cross sections up 1 keV
- In the covariance analysis, the large number of resonance parameters (about 15,500) led to a related covariance matrix of 1.7 Gb when formatted in an ENDF-compatible file (MT=32 with LCOMP=1)
- Upon request from the IAEA, the resonance covariance file (MT=32) was processed to generate a set of covariance matrices formatted as MT=33
- The covariance file MT=33 is part of the ENDF/B-VIII.0β_5 library but the resonance covariance file (MT=32) should also be stored
- Resonance covariance file (MT=32) for ^{239}Pu was adopted from JEFF-3.2 (SG34) because coupled to the resonance parameter evaluation (MT=2) submitted in September 2012 to the ENDF repository
- Minor corrections were made (last digits) to the resonance parameter in file 32 to match those in file 2

Notes on the ^{16}O(n,α) reaction

The thick-target neutron yield of ^{nat}C can be computed from the thin-target ^{13}C(α,n) cross sections $\sigma(E)$ and (e.g., amorphous) mass stopping power cross sections $L(E)$

$$Y_{\text{nat}}(E) = \eta \cdot \int_0^E \sigma(E')[L(E')]^{-1} dE' , \quad (1)$$

where $\eta = N_A \alpha_{\text{nat}}/(\alpha_{13} A_{\text{nat}})$ is the scaling factor from enriched ^{13}C yield to ^{nat}C yield.



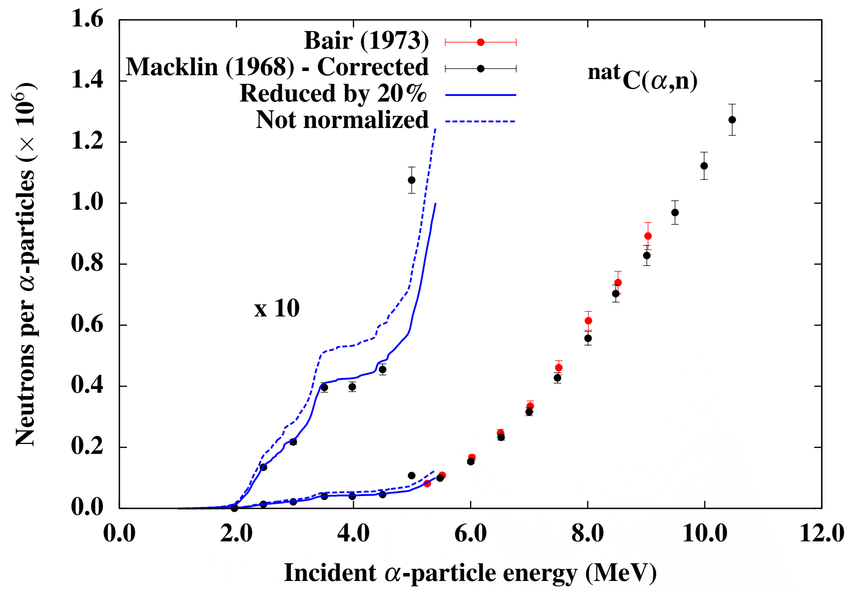


Figure 2: Left : in the plotted ^{13}C(α,n) cross sections, there are differences up to 30%. Right : Total neutron yield vs incident α-particle energy (in blue) calculated from Eq.(1) using Bair's thin-target cross sections. ASTAR mass stopping power cross sections $L(E)$ were used. N_A is the Avogadro number, $\alpha_{13} = 1$ (fraction of ^{13}C in the enriched sample), $\alpha_{\text{nat}} = 0.0107$ (fraction of ^{13}C in a natural sample), the ^{nat}C molar mass A_{nat}=12.0107359 g·mol^{-1}.

- **Newly measured experimental data (Febbruaro et al.) in agreement with Harissopulos' data below 6 MeV**
- **Resonance evaluation, including latest SAMMY updates, i.e., $B_c = -l$ and closed-channels effects, will be completed by FY18**

DY RRR evaluations

- Current status of Dy evaluations in ENDF/B-VII.1 library

Isotope	Abnd. (%)	E_{max} (eV)	ℓ_{max}	Levels	Transmission	(n,γ)
^{156}Dy	0.056	91.0	s	19		
^{158}Dy	0.095	86.2	s	3		
^{160}Dy	2.329	200.8	p	65	✓	
^{161}Dy*	18.889	996.3	s	253	✓	✓
^{162}Dy*	25.475	4845.0	p	75	✓	✓
^{163}Dy*	24.896	99.7	s	114	✓	✓
^{164}Dy*	28.260	699.8	p	69	✓	✓

$(*)$ Relevant to Nuclear Criticality Safety Program

- Experimental data sets (transmission and capture) from RPI and EXFOR library (transmission - H.I. Liou et al.)
- The set evaluations are in progress and are planned to be completed by the end of FY18

Neutron multiplicities $\bar{\nu}_p$ (NDAG)

Formalism

- Based on Fort et al., his formalism can define and compute the fluctuating behavior of prompt neutrons based on the competition of $(n,\gamma f)$ and direct fission (n,f) processes and spin effect,

$$\bar{\nu}_p(E) = \nu^{\text{spin}}(E) - \Delta\nu^{(n,\gamma f)}(E) \quad (2)$$

$$\nu^{\text{spin}}(E) = \left[\sum_J \nu_{c,J} \sum_{k_J} \sigma_{f,k_J}(E)\right] / \sigma_{\text{f}}(E) \quad (3)$$

$$\Delta\nu^{(n,\gamma f)}(E) = \left[\sum_J C_J \sum_{k_J} \sigma_{f,k_J}(E)/\Gamma_{f,k_J}\right] / \sigma_{\text{f}}(E) \quad (4)$$

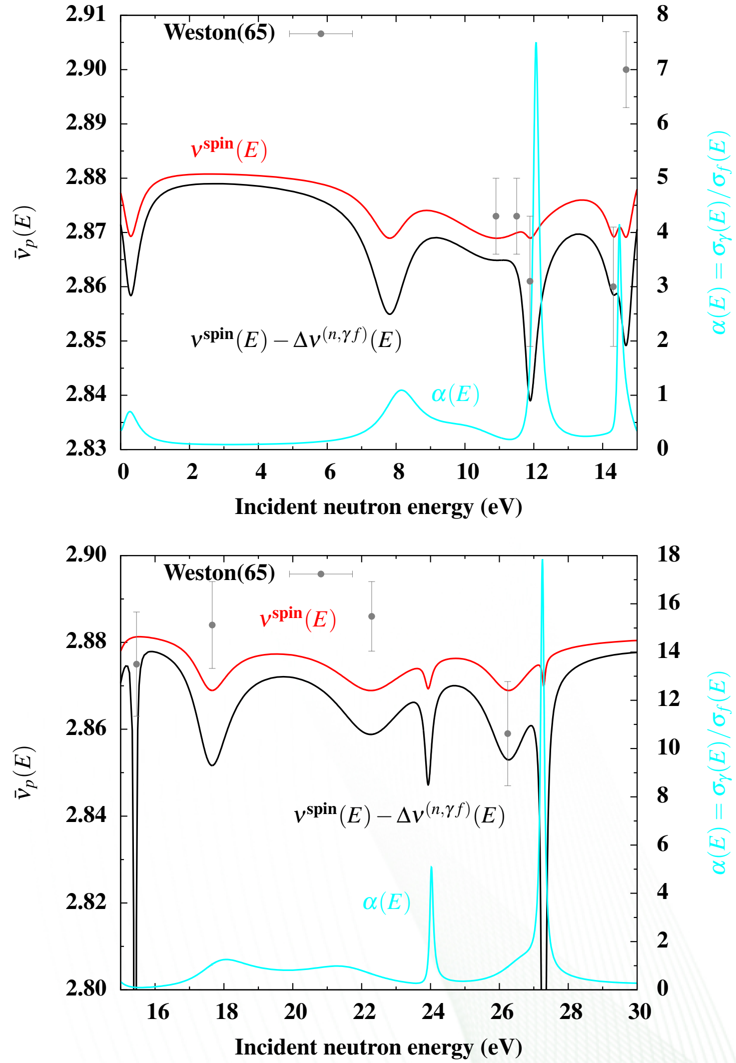
where the quantities $\nu_{c,J}$ and C_J are deduced by the least-squares of the measured data. The resonance fission width Γ_{f,k_J} (taken from ENDF/B-VIII.0) for each resonance is used in SAMMY to calculate the partial energy-dependent fission cross section $\sigma_{f,k_J}(E)$.

  - The coefficients $C_J = (\partial\nu_J/\partial E)\Gamma_{\gamma,f}\cdot E_{\gamma,f}$ are deduced from the linear dependence of $\bar{\nu}_p$ for the direct process assuming, $\Gamma_{\gamma,f}$, $E_{\gamma,f}$ are constant due to the large number of independent channels involved.
  - For ^{239}Pu (having spins $J = 0^+, 1^+$) the parameters used in the calculations are

$$\nu_{c,0^+} = 2.8819 \pm 0.005 \qquad \nu_{c,1^+} = 2.8689 \pm 0.0023$$

$$C_{0^+} = (0.66 \pm 0.091)\cdot 10^{-3}\ \text{eV} \qquad C_{1^+} = (0.629 \pm 0.067)\cdot 10^{-3}\ \text{eV}$$

Spin effect and (n,γf) reaction



The $\bar{\nu}_p$ of ^{239}Pu in the incident neutron energy up 30 eV plotted together with spin effect component. Calculations performed with SAMMY and based on Fort's formalism Eqs.2–4.

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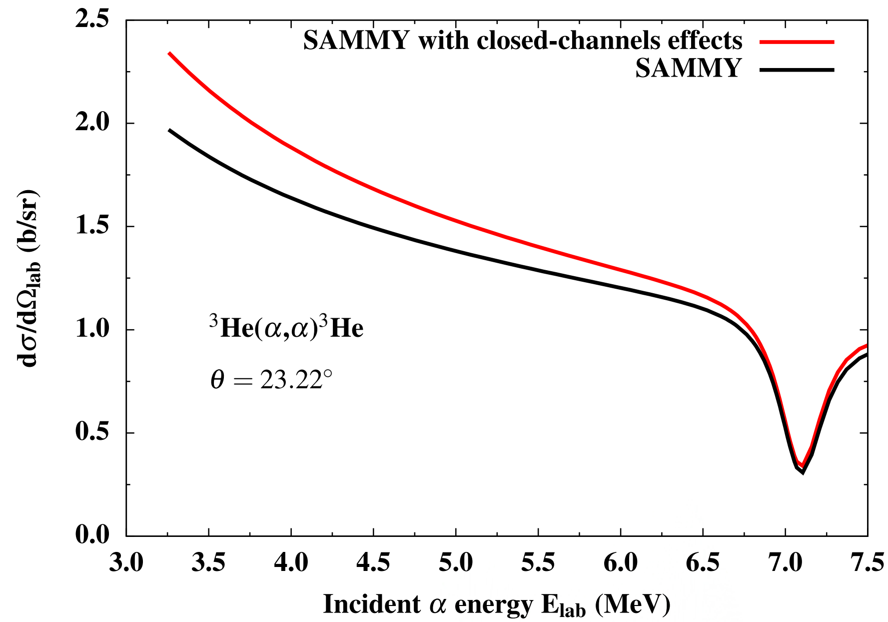
Closed-channel effects

- For heavy nuclei, $\Gamma_c^\ell(E_\lambda)$ s-waves (or at most p-waves) are usually sufficient to describe resolved resonances in the R-matrix formalism; it is also uncommon to have threshold reaction channels opening in the resolved resonance region
- However, for light nuclei, the number of partial waves needed to describe the compound nucleus levels is usually larger, and there may be several excited states opening for reaction channels such as inelastic scattering or charge-particle emissions
- While the elastic channel is by definition always open, reaction channels with Q-value< 0 are measurable only for energies above their corresponding thresholds
- However, R-matrix parameterization (with $B_c = -\ell$) can include closed-channel or sub-threshold effects
  - When $R_{cc'}(E)$ is a function depending on $\Gamma_c^\ell(E_\lambda)$ defined for $E < E_\lambda - E_{thr} < 0$, the shift function $S(E)$ needs to be computed at imaginary $\rho(E)$ and (negative) imaginary $\eta(E)$ being the wave number $k(E)$ imaginary
- Historically, SAMMY was designed for resonance evaluation of heavy nuclei and, so, the boundary condition $B_c = S_c$ was conveniently used as a default option. Within this approximation, the closed-channel effects are suppressed since the shift functions are eliminated

Closed-channel effects

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

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



For ^{3}He(α,α)^{3}He, the threshold for proton emission is about 9.3 MeV. The set of parameters in Tab. 1 has a (bound) energy level with proton widths below the proton channel threshold. This is clearly an example in which closed-channel effects must be included.

R-Matrix Code Project at IAEA

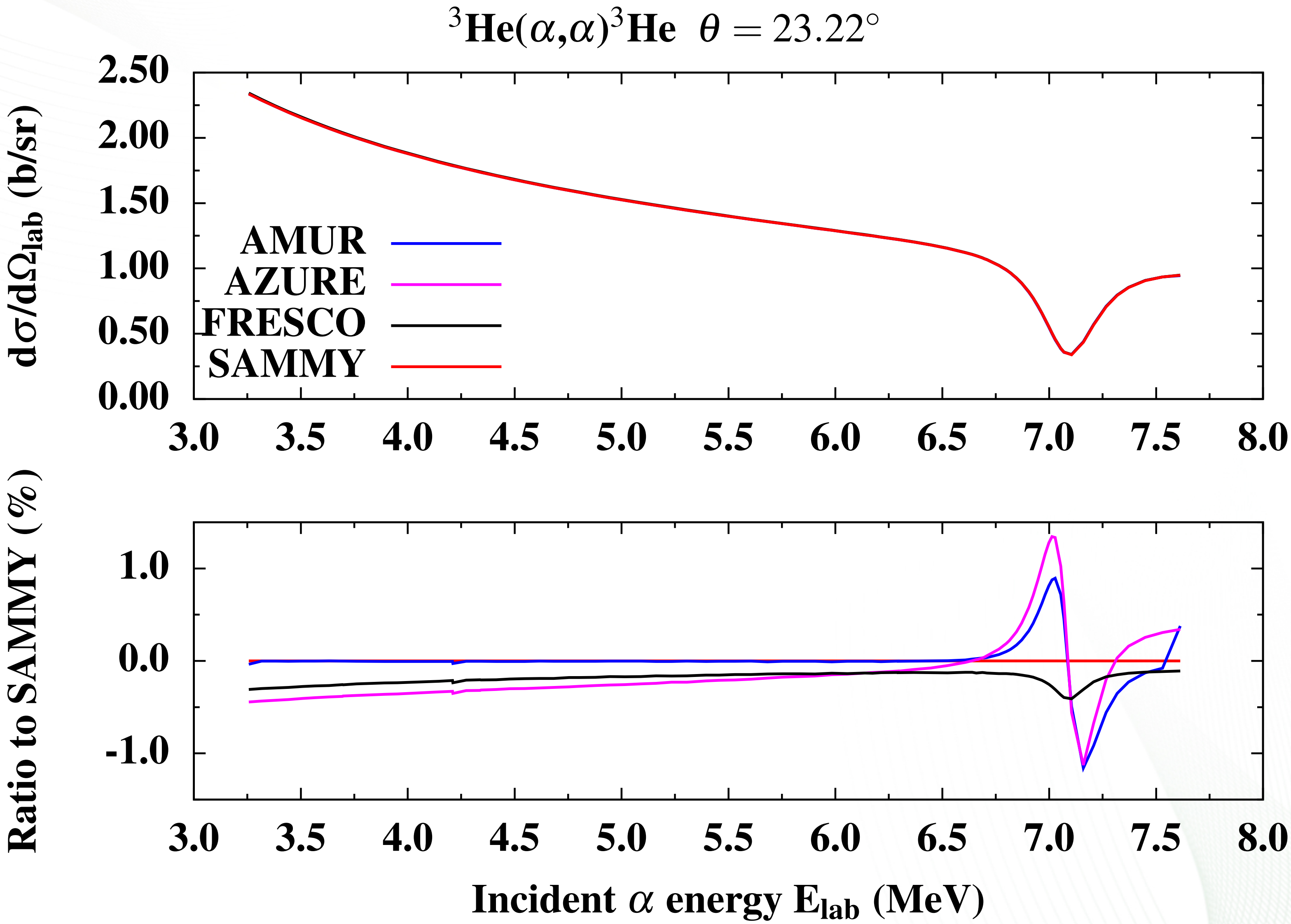
- The Nuclear Data Section (NDS) at the IAEA (Vivian Dimitriou) is leading a series of consultant's meeting on R-matrix codes for charged-particle reactions in the RRR
- The purpose is to gather R-matrix code developers from the various communities of practice (astrophysics, nuclear reactions, neutron data evaluation, etc.) to discuss their R-matrix codes capabilities
- The project goal is as follows:

- To carry out a test exercise to fit the ^{7}Be compound system
- To readily compare the resulting fitted resonance parameters and cross sections and related covariance matrices among five R-matrix codes; AMUR (JAEA), AZURE2 (University of Notre Dame), FRESCO (LLNL), RAC (Tsinghua University), SAMMY (ORNL), and CECC (TUW).

(Project web page and links to NDS reports : www-nds.iaea.org/index-meeting-crp/Rmatrix2017/)

Test on ^{7}Be compound nucleus

(Comparison among SAMMY and other R-matrix codes)



Test on ^{7}Be compound nucleus

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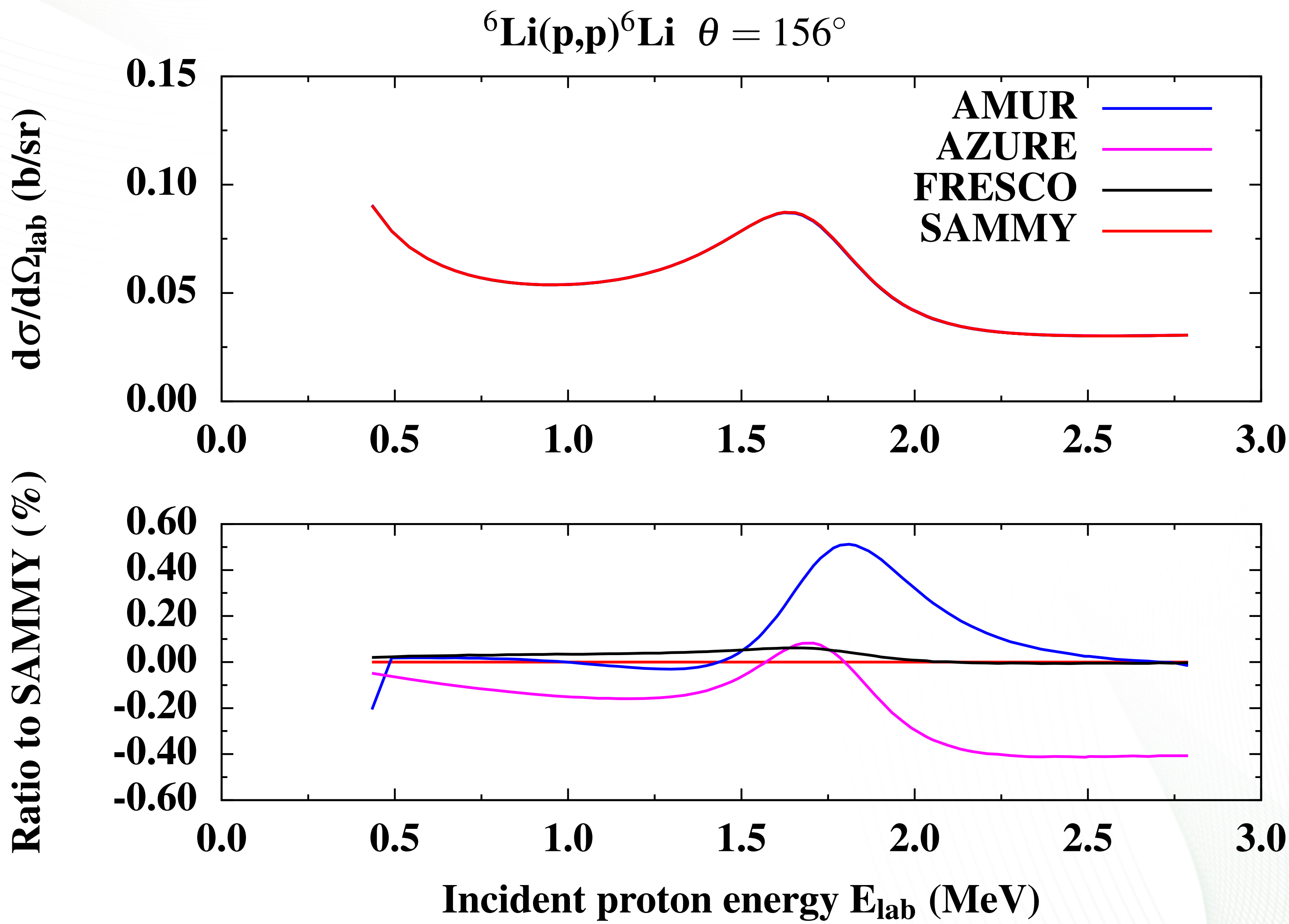

Test on ^{7}Be compound nucleus

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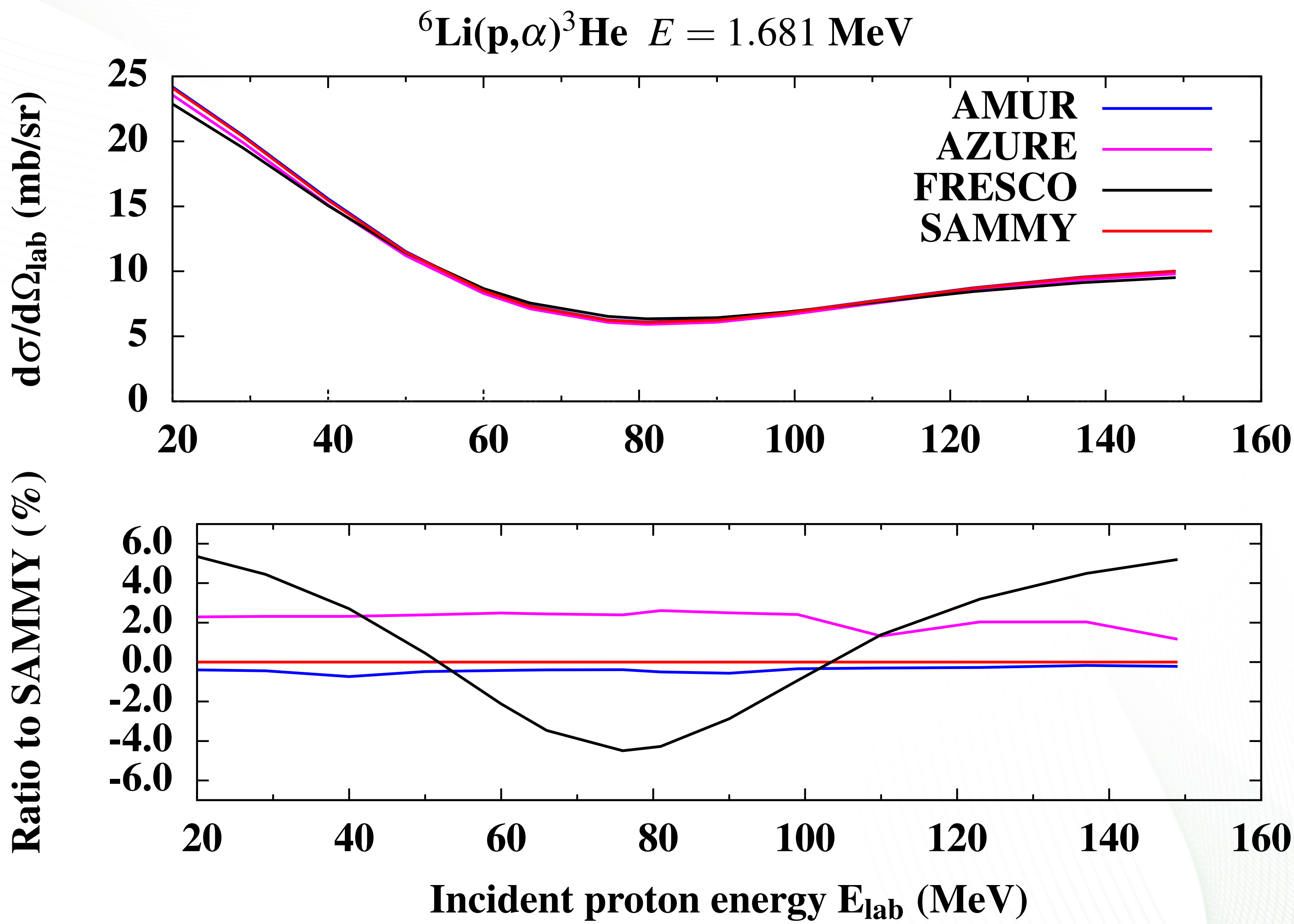
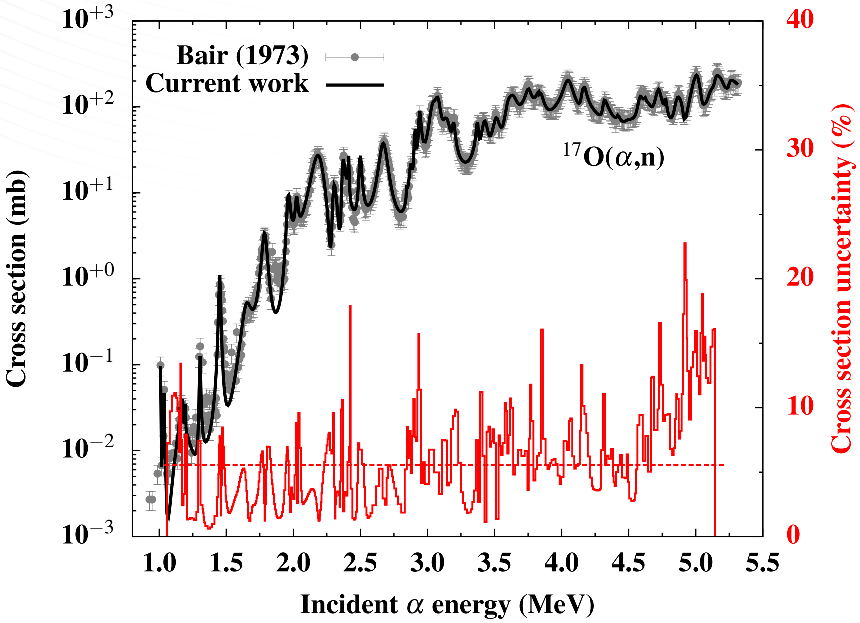


$\alpha+^{17,18}$O evaluations (NA22)

- NA22 program funded two oxygen evaluations for α-particle induced reactions to be completed by FY18
- In the RRR the evaluations will be represented by a set of resonance parameters in a ENDF and GND format



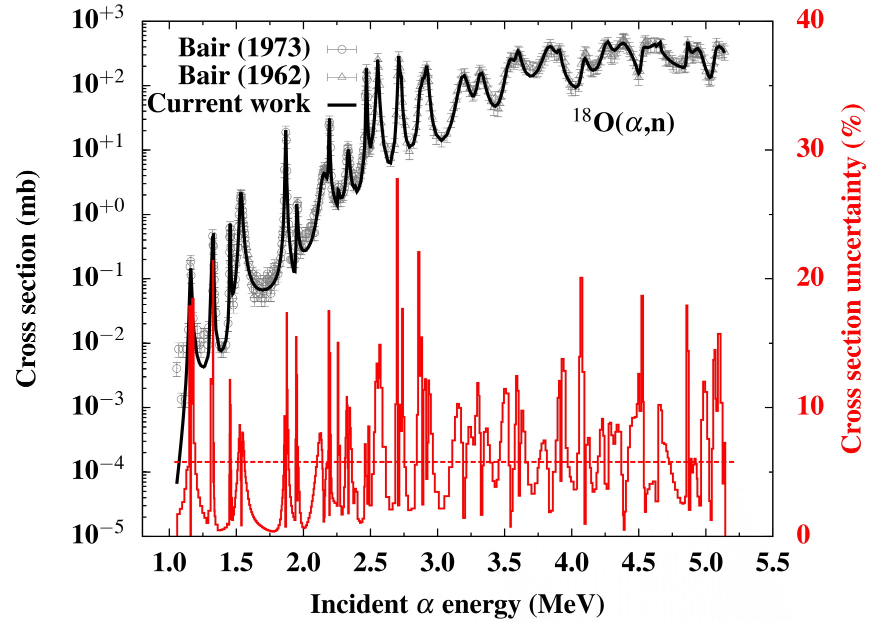


Figure 3: ^{17,18}O(α,n) cross sections reconstructed from the preliminary set of resonance parameters in the energy range of 1–5 MeV compared with Bair's experimental data. Relative cross section uncertainties (in percent) are shown in a continuous red line, along with their average relative uncertainty (≈5%) in a dashed red line. ND2016 EPJ Web of Conferences **146**, 02019 (2017).

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Summary and conclusions

- There have been major contributions to the ENDF/B-VIII.0 library focused on resolved resonance evaluations
- On-going work for future contributions for *neutron*-induced resonance evaluations, set of Dy isotopes, and ^{16}O, is planned to be completed by FY18
- First attempt to couple resonance evaluation to fluctuations in the $\bar{\nu}_p$ is in progress
- For *charged-particle* induced evaluations, resonance work on $\alpha+^{17,18}$O within the NA22 program is planned to be completed by FY18
- The R-matrix code SAMMY was updated to include closed-channel effects that are of fundamental importance for the treatment of thresholds reaction channels
- These updates were tested among other R-matrix codes within R-matrix codes for charged-particle reactions in the RRR and, currently, the agreement among four R-matrix codes is up to a few percents

Acknowledgments

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Thank you!