Status Report of WPEC Subgroup 7
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Nuclear Data Standards
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Introduction

The standards are the basis for the neutron reaction cross section libraries. It is important to reevaluate them taking into account new experimental data and improved evaluation techniques. Significant improvements have been made in the standard cross section database since the last complete evaluation of the neutron cross section standards, almost 20 years ago. In response to requests for improvements in the standards the CSEWG formed a Task Force, the WPEC formed a subgroup and the IAEA formed a CRP. These groups have worked cooperatively to improve the evaluation process. The emphasis has been on the H(n,n), $^{10}B(n,\alpha)$, and fission standards. Table 1 shows the standards and the expected energy ranges that should result from the new evaluation. The $^{238}U(n,f)$ cross section, which is an NEANDC/INDC standard, was accepted as an ENDF standard at the Fall 2004 CSEWG meeting. However 2 Mev was recommended as the lower bound for use of this cross section as a standard. The use of this cross section from threshold to 2 MrV is discouraged due to the very rapid change of this cross section in that energy range and the very small cross section in the threshold energy region. Extended energy ranges compared with the ENDF/B-VI results are expected for H(n,n) from 20 MeV to ~200 MeV; for $^{10}B(n,\alpha)$ and $^{10}B(n,\alpha_1\gamma)$ from 250 keV to 1 MeV; and for $^{235}U(n,f)$ and $^{238}U(n,f)$ from 20 MeV to 200 MeV. Changes in the energy ranges of the other standards may occur depending on the results of the evaluation process.

Table 1. Neutron Cross Section Standards

Reaction	Proposed energy range
H(n,n)	1 keV to 200 MeV
$^{3}He(n,p)$	0.0253 eV to 50 keV
$^{6}Li(n,t)$	0.0253 eV to 1 MeV
$^{10}B(n,\alpha)$	0.0253 eV to 1 MeV
$^{10}B(n,\alpha_1\gamma)$	0.0253 eV to 1 MeV
C(n,n)	0.0253 eV to 1.8 MeV
$Au(n,\gamma)$	0.0253 eV, 0.2 to 2.5 MeV
$^{235}U(n,f)$	0.0253 eV, 0.15 to 200 MeV
$^{238}U(n,f)$	Threshold to 200 MeV

Progress on the evaluation

A number of meetings have been held since the last WPEC meeting in order to make the progress needed for the completion of this evaluation in a timely manner. In addition to the CRP RCM in October, a side meeting was held at the ND2004 conference to discuss the status of the database; progress on the individual evaluations; problems and possible solutions concerning the ^{6}Li(n,t) analyses; establishing the ^{235}U(n,f) cross section required for the ENDF/B-VII library and thermal data concerns.

The cut-off date for including experiments in the database for the evaluation was extended until the spring of last year. For each experiment in the database, the documentation was investigated for possible corrections that may need to be made and for errors or missing information. This investigative procedure in many cases led to estimates of the uncertainties and correlations within an experiment and correlations with other experiments. This information was used to obtain covariance matrices for the measurements that were used in the evaluation process. Work continues on the encouraging, motivating and coordinating of new measurements that can be used in the next evaluation of the standards. The database also includes data involving the ^{238}U(n,γ) and ^{239}Pu(n,f) cross sections. There are many very accurate measurements of these cross sections. The use of these additional data improves the database as a result of ratio measurements of those cross sections to the traditional standards. Also scattering and total cross section data have been included for ^{6}Li and ^{10}B since they provide information on the standard cross sections. No evaluation of the C(n,n) cross section is planned since very little new data have been obtained since the last evaluation and what was obtained is in good agreement with that evaluation.

The CRP on the improvement of the standard cross sections has held three RCMs. The second one was held at NIST October 13-17, 2003. The other two were held at IAEA headquarters in Vienna, Austria in 2002 and 2004. The CRP has included membership from Austria, Belgium, China, Germany, Japan, the Republic of Korea, Russia and the USA. The main objectives of the CRP are the following: Improve the methodology for determination of the covariance matrix used in cross section evaluations; Upgrade the computer codes using this methodology; Study the reasons for uncertainty reduction in R-matrix and model independent fits; Evaluate cross sections and covariance matrices for the light elements, H(n,n), ^{3}He(n,p), ^{6}Li(n,t), ^{10}B(n,$\alpha_1\gamma$), and ^{10}B(n,α); Establish the methodology and computer codes for combining the light element with the heavy element evaluations leading to a final evaluation of the neutron cross section standards. The efforts of the CRP have led to many results, though some of this work is preliminary and ongoing. The work includes: improvements to the experimental data in the standards database and methods for handling discrepant data; R-matrix evaluation of the hydrogen scattering cross section and conversion of measurements relative to the hydrogen cross section to the new standard; studies of the effect of Peelle's Pertinent Puzzle (PPP) and its effect on the standards; evaluation work on microscopic calculations leading to independent determinations of R-matrix poles; studies of the small uncertainties resulting from evaluations; results provided for the ENDF/B-VII standards; smoothing procedures; and work on the thermal constants; Short summaries of some activities follow.

In addition to the data sets introduced after the ENDF/B-VI evaluation and before the formation of the CRP, more than 30 data sets have been added to the standards database. Work has been done to understand the experiments and possible problems with them that may cause discrepancies to exist. During the ENDF/B-VI GMA evaluation process unusual results were observed with correlated discrepant data. To remove problems associated with these discrepancies, data greater than three standard deviations away from the output results were down weighted in the ENDF/B-VI GMA evaluation. This had the effect of making χ^2 per degree of freedom essentially one. It would clearly be better to find the sources of the discrepancies. Then the evaluation could be done with consistent data sets. This is a very difficult task. Due to time constraints and the fact that there are thousands of data points, a simplified procedure for handling discrepant data was established. In GMA we have added a medium energy range correlation component to the experimental data that is discrepant. This component is added if the difference from the evaluation is more than two sigma for a single point or more than one sigma for two or more consecutive energy points. This results in a much better χ^2 per degree of freedom and larger uncertainty in the evaluated results. Results obtained for the ^{235}U(n,f) cross section using this method are shown in Fig. 1. Note that the change in the cross section from this procedure is small.

Hale has evaluated the hydrogen scattering cross section below 30 MeV neutron energy using the R-matrix code EDA. Calculations of the angular distribution using these R-matrix parameters are in much better agreement with recent measurements than the ENDF/B-VII evaluation. Comparisons of the ENDF/B-VII evaluation with other evaluations are shown in Fig. 2. With the availability of the new hydrogen standard, all data in the database relative to hydrogen cross sections were converted so they are relative to the ENDF/B-VII standard. The database contained measurements relative to several different versions of total cross sections. Also a number of experiments were in the database which used different laboratory angles, and different versions of the differential cross section. In Fig. 3, results obtained for the ^{235}U(n,f) cross section with the present database using the ENDF/B-VI hydrogen standard are compared with those obtained using the ENDF/B-VII hydrogen standard. An intermediate result is also shown. Effects as large as about 0.5% are present. Hale is extending the hydrogen evaluation to 200 MeV neutron energy. When that work has been completed, the data in the database at those higher energies that are relative to the hydrogen cross section will be converted to the new standard.

Problems associated with PPP were observed early in the investigations of the CRP. A test run using a model independent least squares code fitting the logarithm of the cross section produced higher cross sections than a run fitting the cross section. There were discrepant data in the test run. The problem appears to be largely a result of using discrepant data. A number of methods for removing PPP have been used such as using percent uncertainties, using a logarithmic transformation or the Box-Cox transformation. The EDA R-matrix analysis that uses only random and normalization uncertainties does not appear to suffer the PPP problem; but the RAC R-matrix analysis that includes medium range correlations does. The question that was addressed was whether PPP is present and if so how can it be properly removed or minimized? After the second RCM, Donald Smith, as an IAEA consultant for the standards work, and Vladimir Pronyaev updated the GMA code (called GMAP) by adding the Chiba-Smith option to handle PPP problems. This option renormalizes the experimental absolute errors on the assumption that it is the fractional error that actually reflects the accuracy the experimenter has provided. This approach appears to have reduced the effect of PPP significantly. In Fig

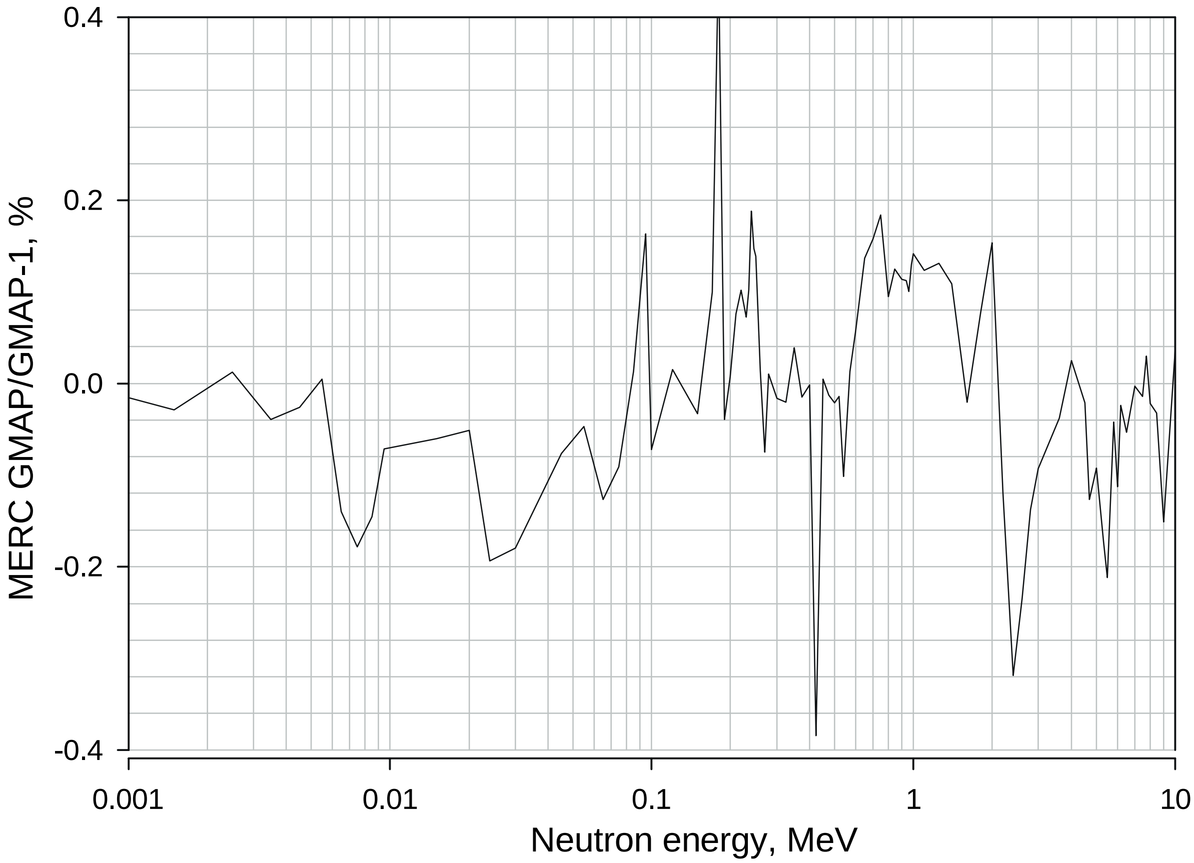

Fig. 1. Effect of adding a medium energy range correlation component for the $^{235}U(n,f)$ experimental data. This is the ratio of the corrected to uncorrected data.

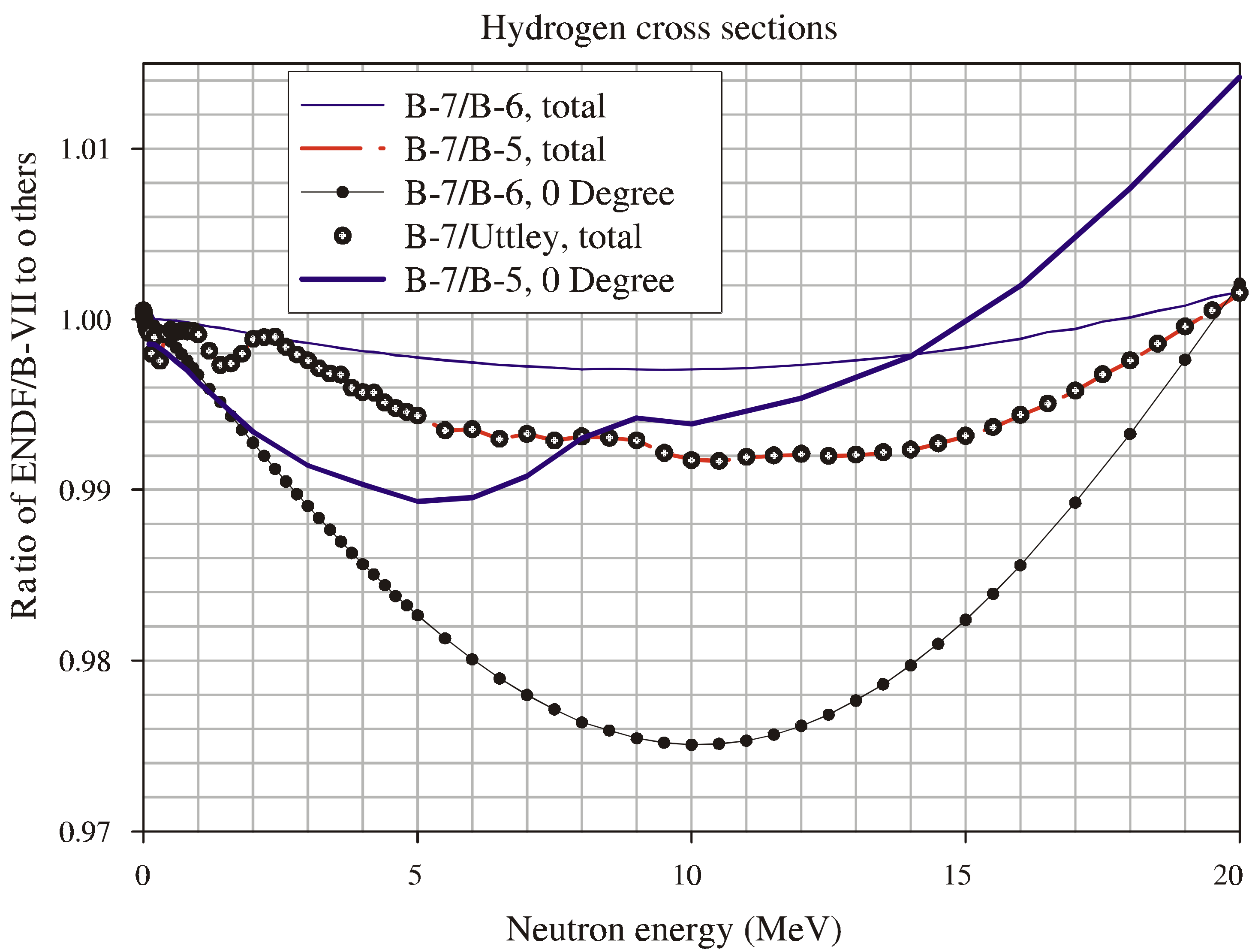

Fig. 2. Comparison of the ENDF/B-VII hydrogen evaluation to other evaluations.

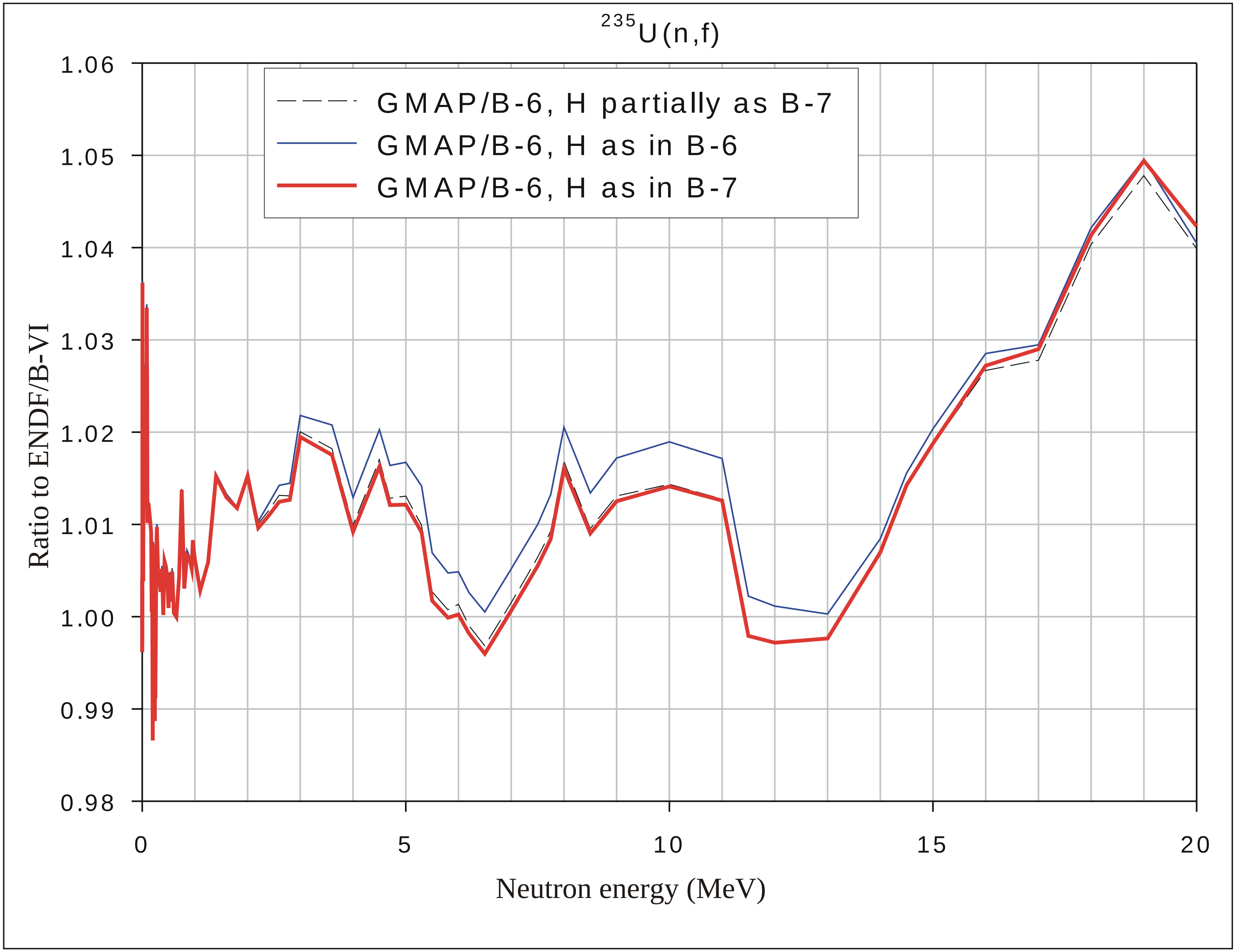

Fig. 3. Changes in the U-235 fission cross section as a result of converting the standards database from the ENDF/B-VI to the ENDF/B-VII hydrogen standard.

4-6, the effect of using the GMAP correction for three of the cross sections is shown. Comparisons with a method using a logarithmic transformation indicate good agreement for a number of test cases.

Theoretical calculations are being made to help describe some of the light-nuclei standard cross sections. Since there are a relatively small number of nucleons involved for the ^{4}He compound nucleus, it is possible to use the Refined Resonating Group Model (RRGM), to obtain information about the ^{3}He(n,p) cross section. This model allows realistic nuclear interactions to be used however it requires very large computer resources. Using effective NN potentials allows heavier nuclei to be studied such as the A=7 case which leads to the ^{6}Li(n,t) standard. Using effective potentials allows the calculations to be done with a standard personal computer. The work on these two standards has progressed well. The calculations produce results that are rather close to those given by R-matrix analyses. Transforming the RGM results to R-matrix poles should allow them to be used in R-matrix analyses. This work should lead to improved values of the parameters and more realistic uncertainties in the cross sections. In some cases the information on the poles allows an evaluator to eliminate experiments from consideration.

The small uncertainties obtained in the ENDF/B-VI evaluation process are of great concern. An important task for the CRP is to try to understand in detail how standard error propagation in model independent or R-matrix analyses can result in such small uncertainties, and whether there are more reasonable corrections or algorithms to employ. An important result of the studies by the CRP is that it is essential to consider the covariances not just the variances in applications of cross sections to practical systems. Work has been done on the small uncertainty problem through comparisons of several tests of codes. Comparisons are underway of cross sections and their uncertainties obtained for several R-matrix codes that fit data from a common database. It is necessary to select a database containing measurements that can be properly used in the comparison. For example some of the codes can not handle certain types of input data correlations. A similar comparison is underway for model independent least-squares codes. Again the database must be carefully selected so that the types of data and correlations present in the measurements are consistent with the codes being investigated. Initial work was done with five ^{6}Li(n,t) experimental data sets. The EDA, SAMMY and RAC R-matrix analyses that have been done with these data sets have not used exactly the same databases. New comparisons are now being made using exactly the same databases for each code and an improved database selection. For the new comparison tests, cross sections from one ^{6}Li(n,n), one ^{6}Li total and four ^{6}Li(n,t) measurements were used. Also one "created" ^{6}Li total cross section was used. For the comparison tests, it was assumed that no correlations exist between these data sets. The only correlations within the data sets are assumed to be short energy range (statistical) and long energy range (normalization). The R-matrix codes being used in this study are EDA (LANL), SAMMY (ORNL), and RAC (Tsinghua University). The generalized least squares codes being used are GLUCS (Obninsk), GMA (IAEA and Obninsk) and SOK (LANL). Additional code comparisons are being considered. The chi-square expressions used in EDA, SAMMY and RAC are also being investigated.

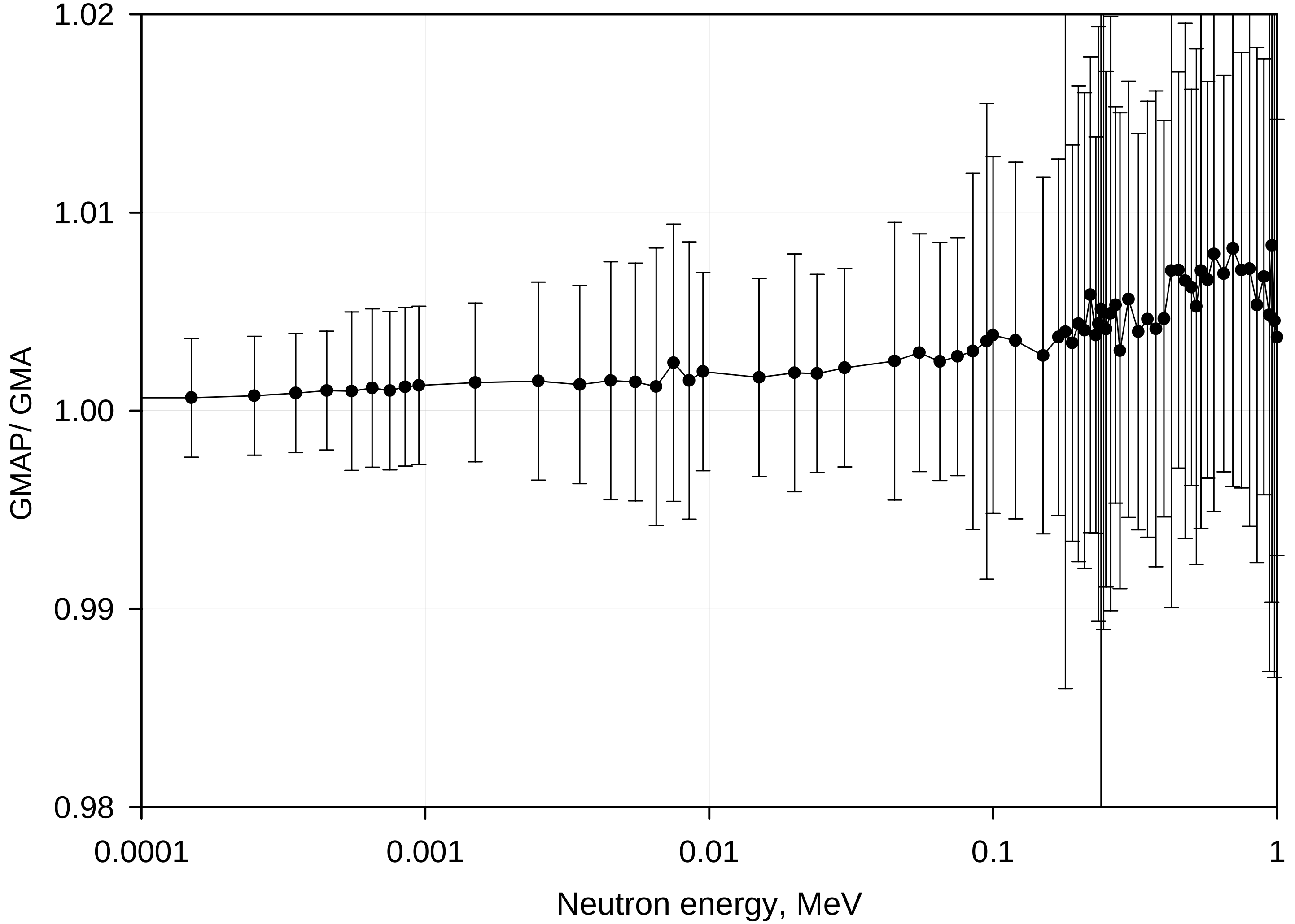

Fig. 4. Ratio of GMAP fit to minimize PPP to the standard GMA fit for the $^{10}B(n,a1)$ reaction. Note MERC was used so these are lower bounds to the PPP effect.

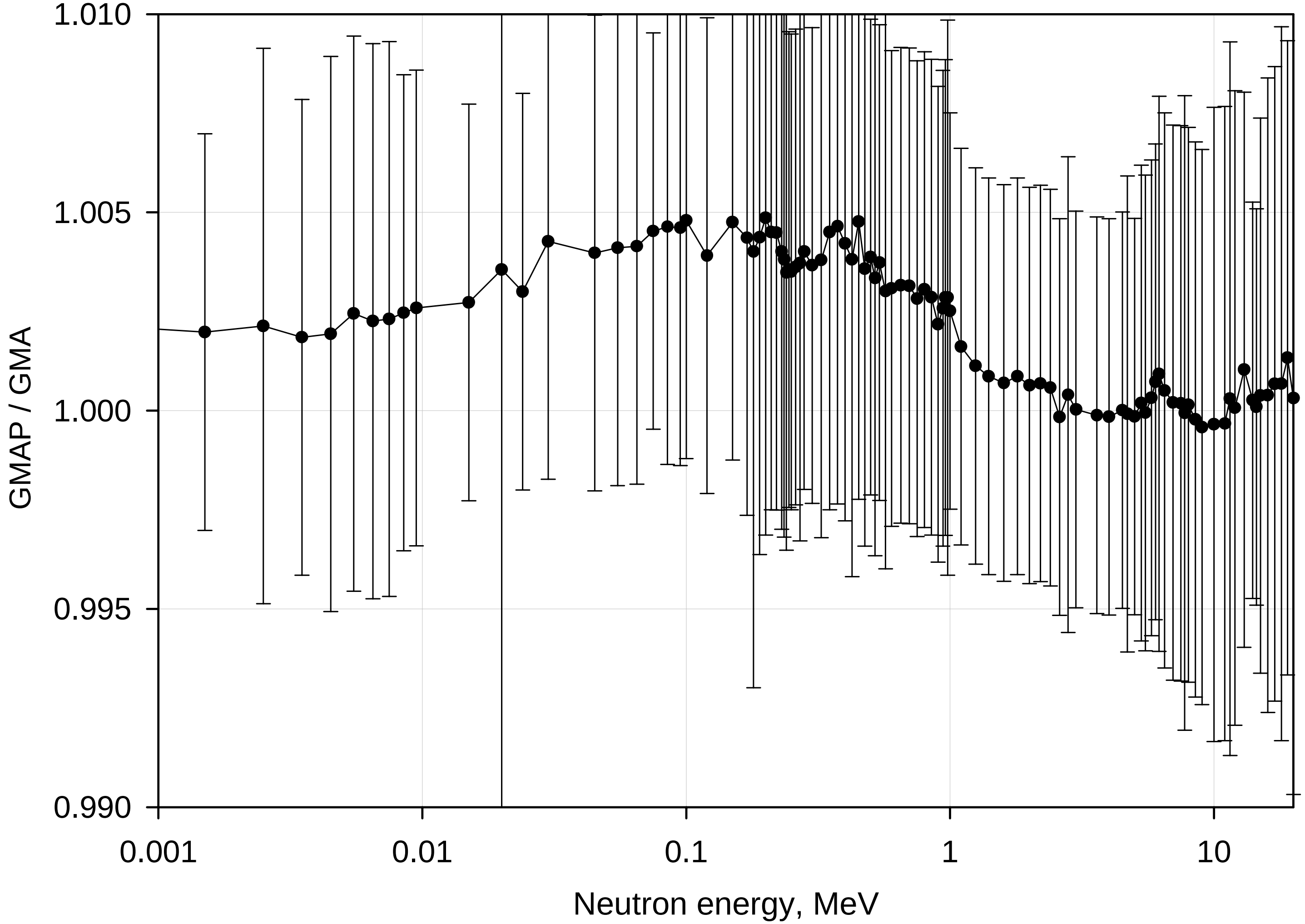

Fig. 5. Ratio of GMAP fit to minimize PPP to the standard GMA fit for the ^{235}U(n,f) reaction. Note MERC was used so these are lower limits to the PPP effect.

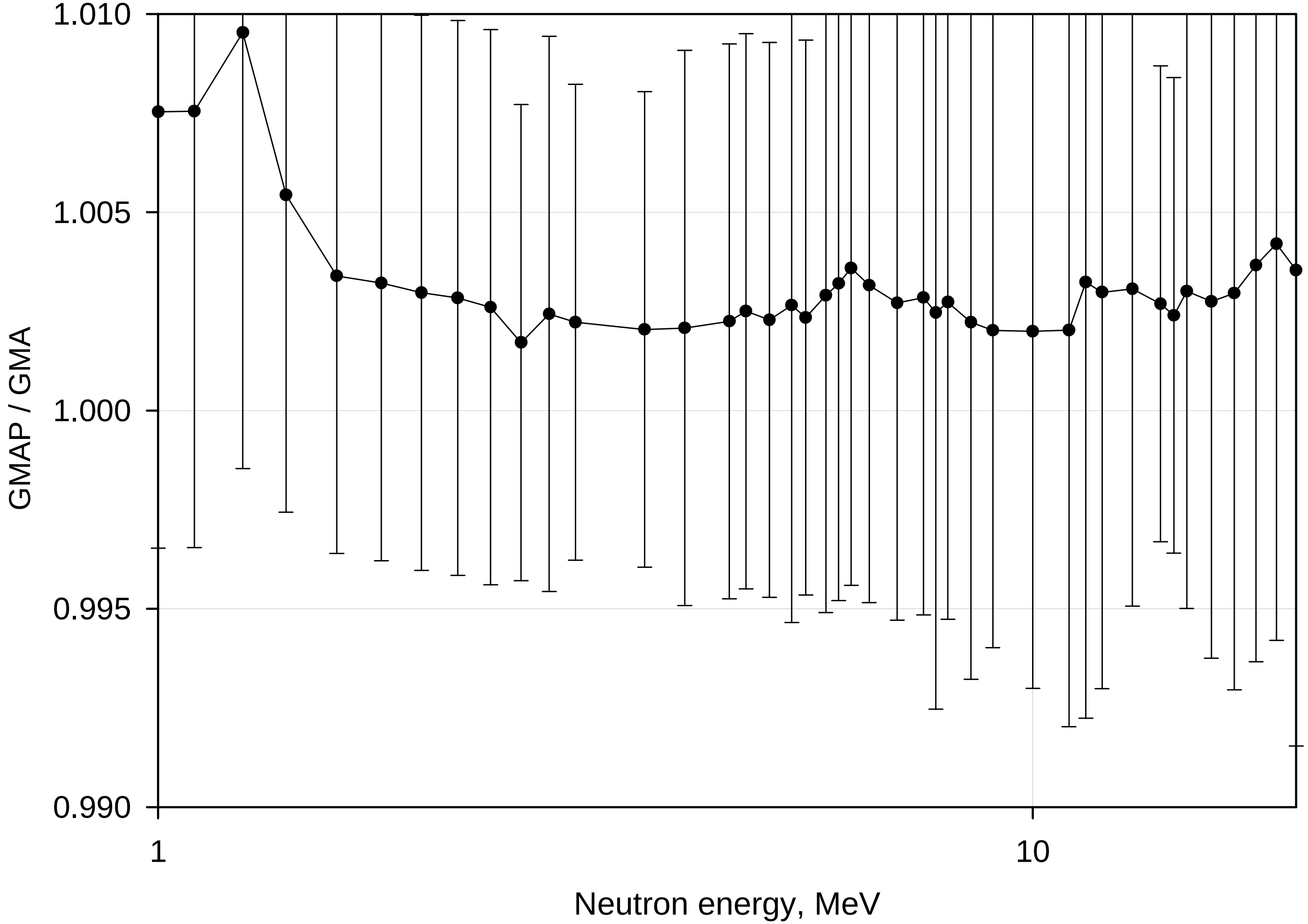

Fig. 6. Ratio of GMAP fit to minimize PPP to the standard GMA fit for the ^{238}U(n,f) reaction. Note MERC was used so these are lower limits to the PPP effect.

For the results to be provided for the ENDF/B-VII evaluation it was decided that both the EDA and RAC analyses should be used. The R-matrix analyses will be using charged-particle data and the entire lithium and boron neutron databases. The only lithium and boron data for use in the GMA program will be the ratio measurements. Thus the R-matrix and GMA data sets have no common or correlated data sets. For the ^{6}Li(n,t) R-matrix work, the central values (cross sections) obtained for the RAC and EDA analyses were not identical. In an effort to provide the most important standards for the ENDF/B-VII library, a compromise evaluation procedure was adopted. For this procedure the RAC and EDA central values were averaged (unweighted) and used as the R-matrix input to GMA. The covariance matrix used with these central values was that from RAC since its results appeared more physically reasonable. The R-matrix input was treated like the addition of another data set to the GMA program. The basic procedure used is outlined in Fig. 7. At each energy point, half the difference between the RAC and GMA results was treated as a model uncertainty that was added to the RAC covariance of uncertainties. This then takes into account the small differences obtained between the RAC and EDA analyses. Unfortunately only the RAC analysis for boron was available in time for the release of the standards for the ENDF/B-VII library; so the boron cross sections will not be released at this time. The RAC boron results alone were used as input to GMA to provide data for the impact on the other cross sections from the R-matrix boron analysis. The effect was found to be small. Fig. 8 shows that the effect for the ^{235}U(n,f) cross section. In the region where it is a standard the effect is very small. The cross sections obtained from this combination process for the ^{6}Li(n,t), Au(n,γ), ^{235}U(n,f), and ^{238}U(n,f) standard cross sections as well as the ^{238}U(n,γ) and ^{239}Pu(n,f) cross sections are shown in Fig. 9-14. These cross sections and the H(n,n) results up to 20 MeV were given to the CSEWG in November as the proposed standards for the ENDF/B-VII library. It is anticipated that the additional work being done on the hydrogen cross section to extend it to 200 MeV will have only a very small effect on the hydrogen cross section below 20 MeV. Only the cross sections were released for use in the ENDF/B-VII library. The covariances are still under investigation. When both boron R-matrix results are available, the boron input will be obtained in a manner similar to that used for the lithium case described above. The boron cross sections will then be obtained from the GMA program using both the lithium and boron R-matrix input. The ^{3}He(n,p) cross section is being evaluated independently by Hale. It is anticipated that the boron cross sections, the ^{3}He(n,p) cross section, and the extension of the H(n,n), ^{235}U(n,f), ^{238}U(n,f) and ^{239}Pu(n,f) cross sections to 200 MeV will be released later this year.

The results of the combination procedure will not be smooth. For the ^{6}Li(n,t), ^{10}B(n,$\alpha_1\gamma$), and ^{10}B(n,α) cross sections smoothing will not be required since the highest weight will go to the cross sections used in the R-matrix analyses. For the heavy element standards, there are some models that provide insight on how to define the curves. One model for the ^{235}U(n,f) cross section was discussed by Hambsch at the second RCM. This model is now limited as to its maximum neutron energy. Evaluations by Maslov extend to higher neutron energies. The CRP felt that a simple smoothing algorithm would be satisfactory for most cases. It was used sparingly for the heavy element cross sections. A patch using the shape of the Maslov evaluated curve was applied in the 50-60 MeV region for the

NEW STANDARDS EVALUATION PROCEDURE

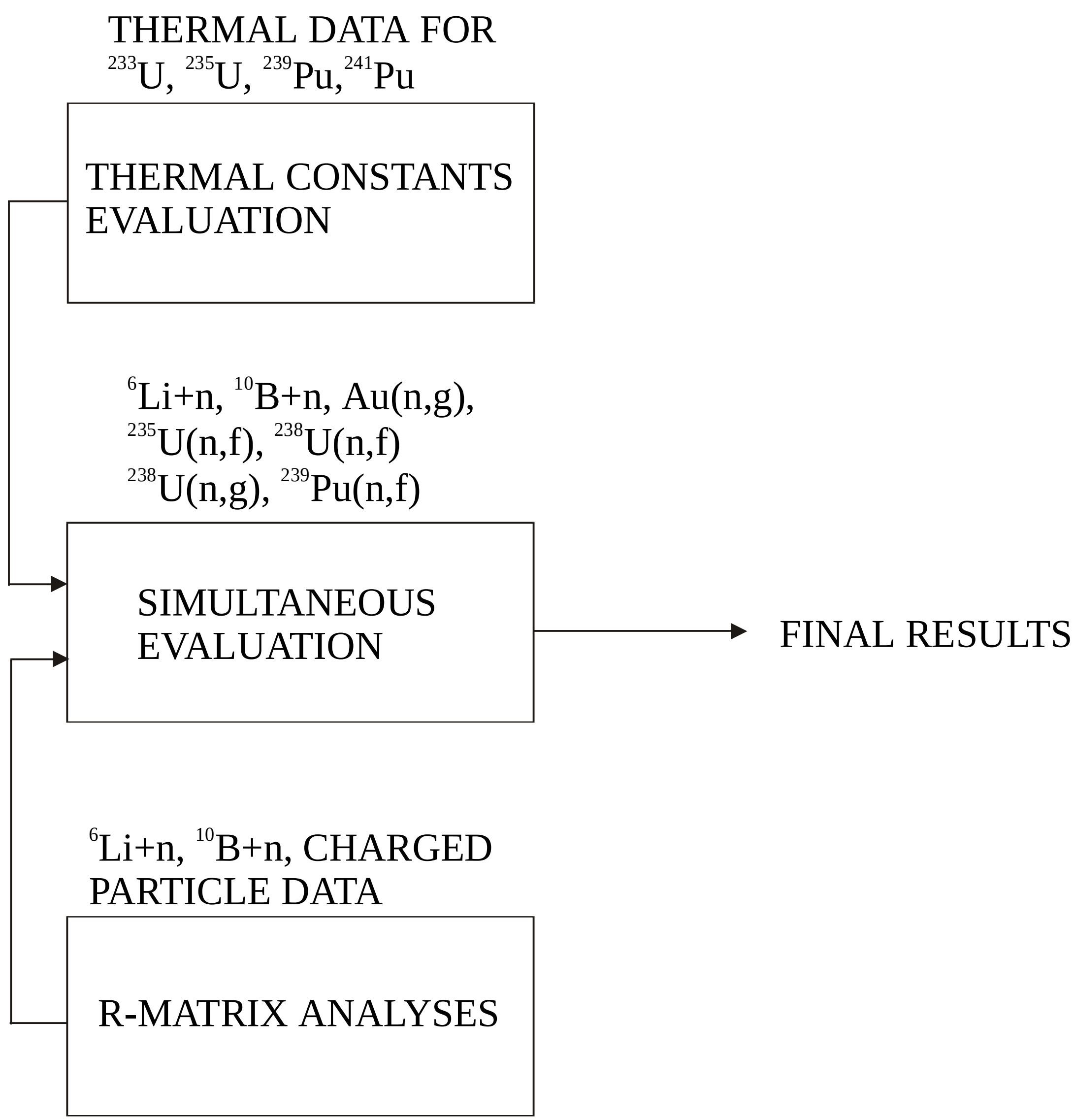

Fig. 7. New evaluation procedure for the standards evaluation

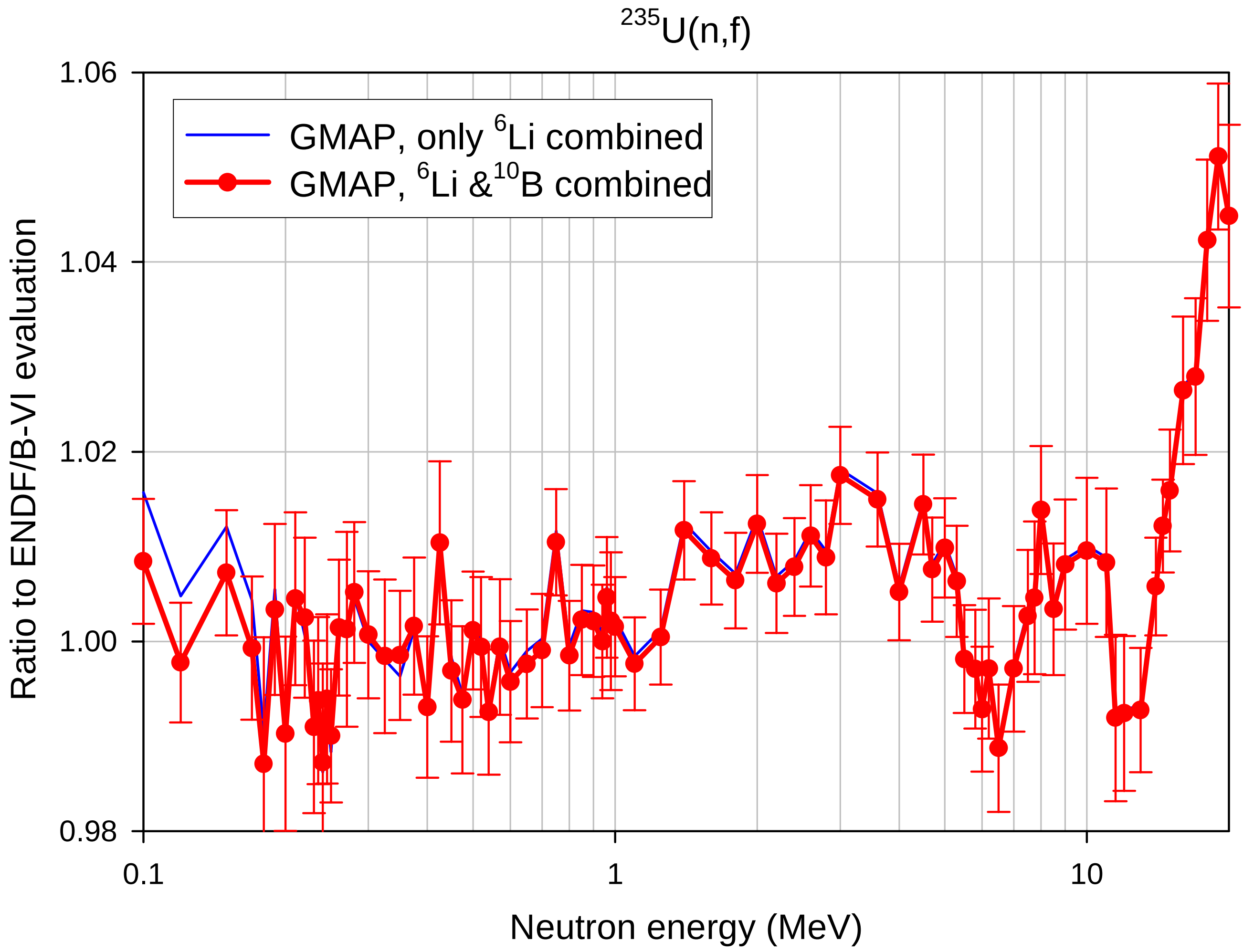

Fig. 8. The effect of the R-matrix boron results on the evaluation of the $^{235}U(n,f)$ cross section.

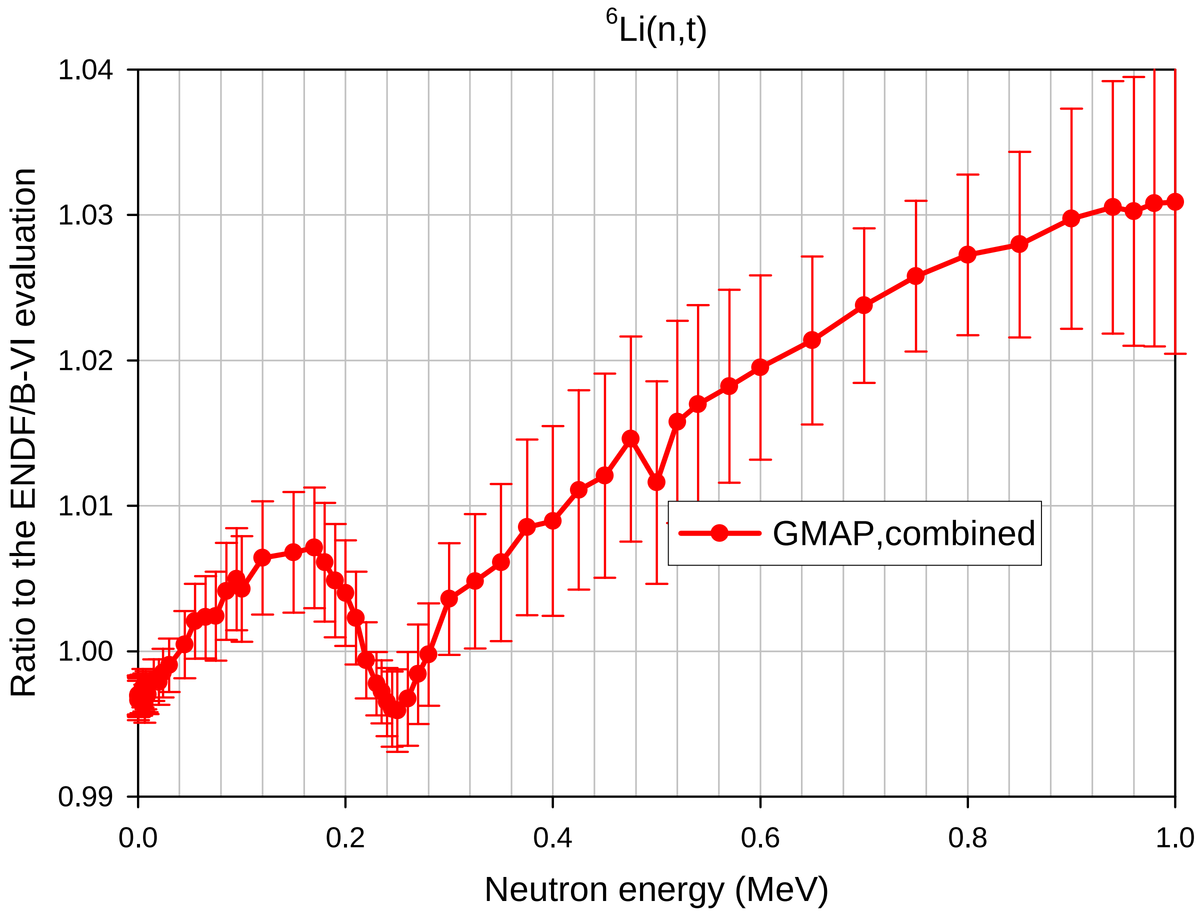

Fig. 9. The GMAP +R-matrix (combined) evaluation for the ^{6}Li(n,t) cross section.
This is the ENDF/B-VII evaluation.

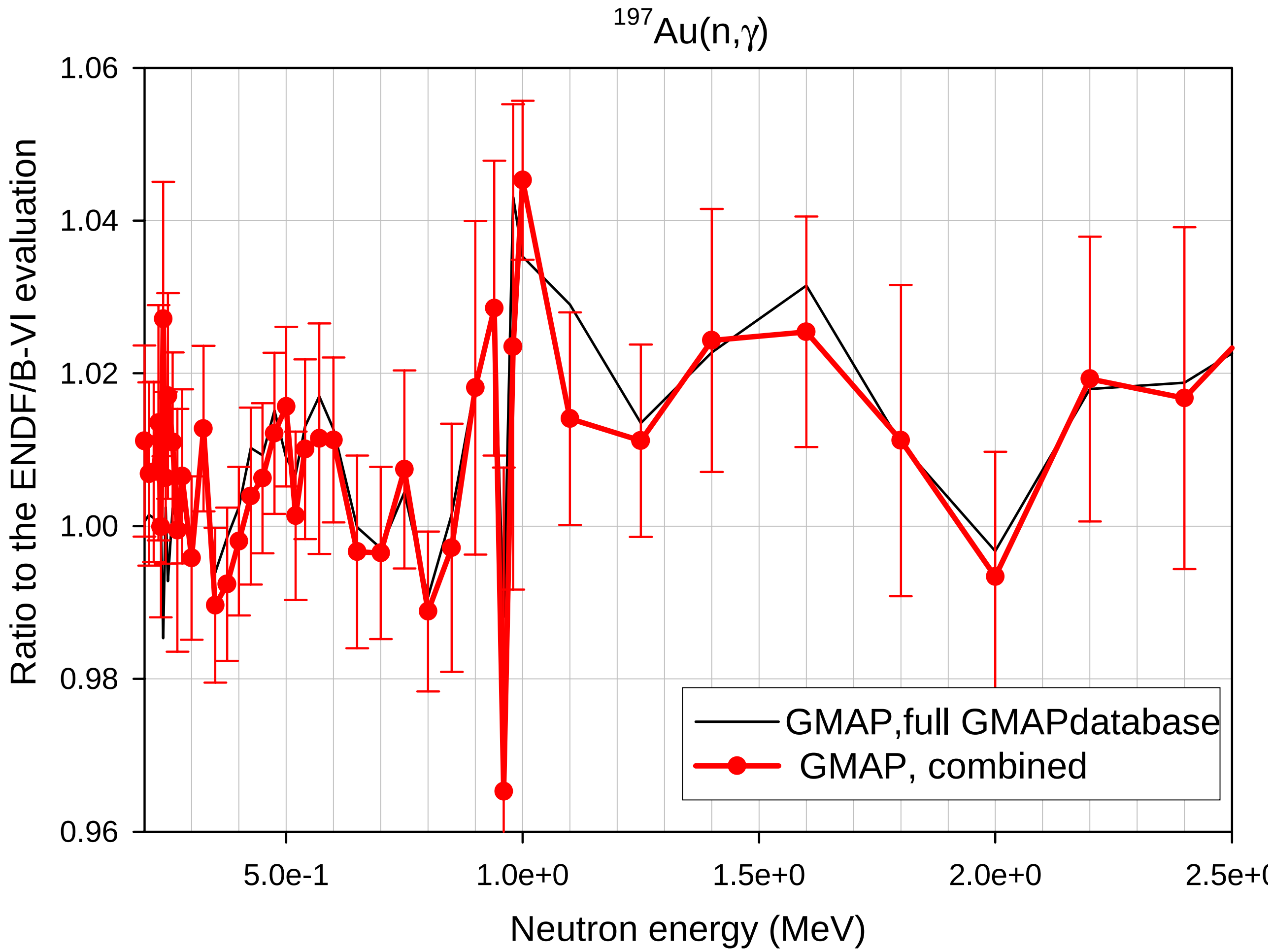

Fig. 10. Comparison of the GMAP alone and the GMAP+R-matrix (combined) evaluations for the Au(n,γ) cross section. The ENDF/B-VII evaluation is the combined result.

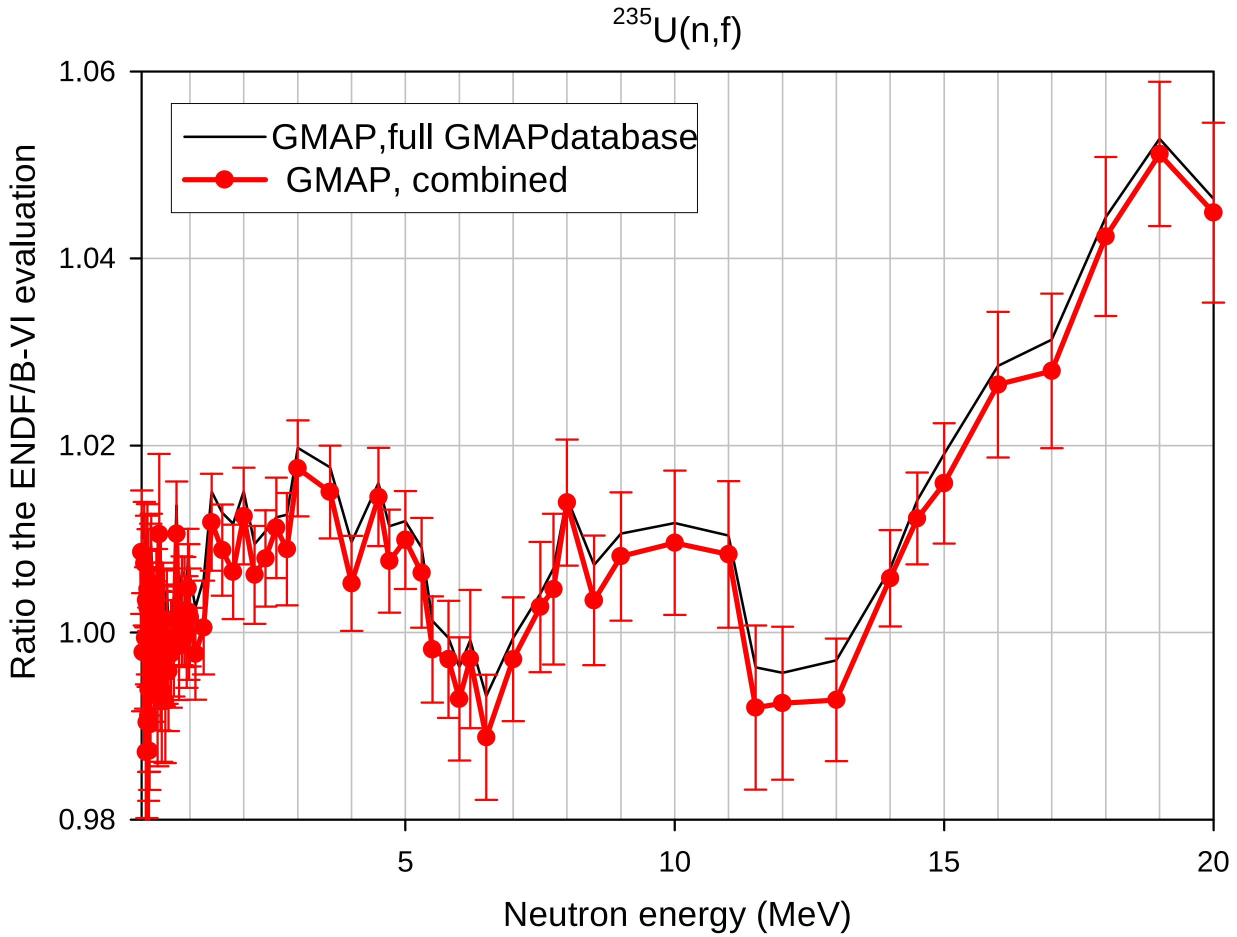

Fig. 11. Comparison of the GMAP alone and GMAP+R-matrix (combined) evaluations for the ^{235}U(n,f) cross section. The ENDF/B-VII evaluation is the combined result.

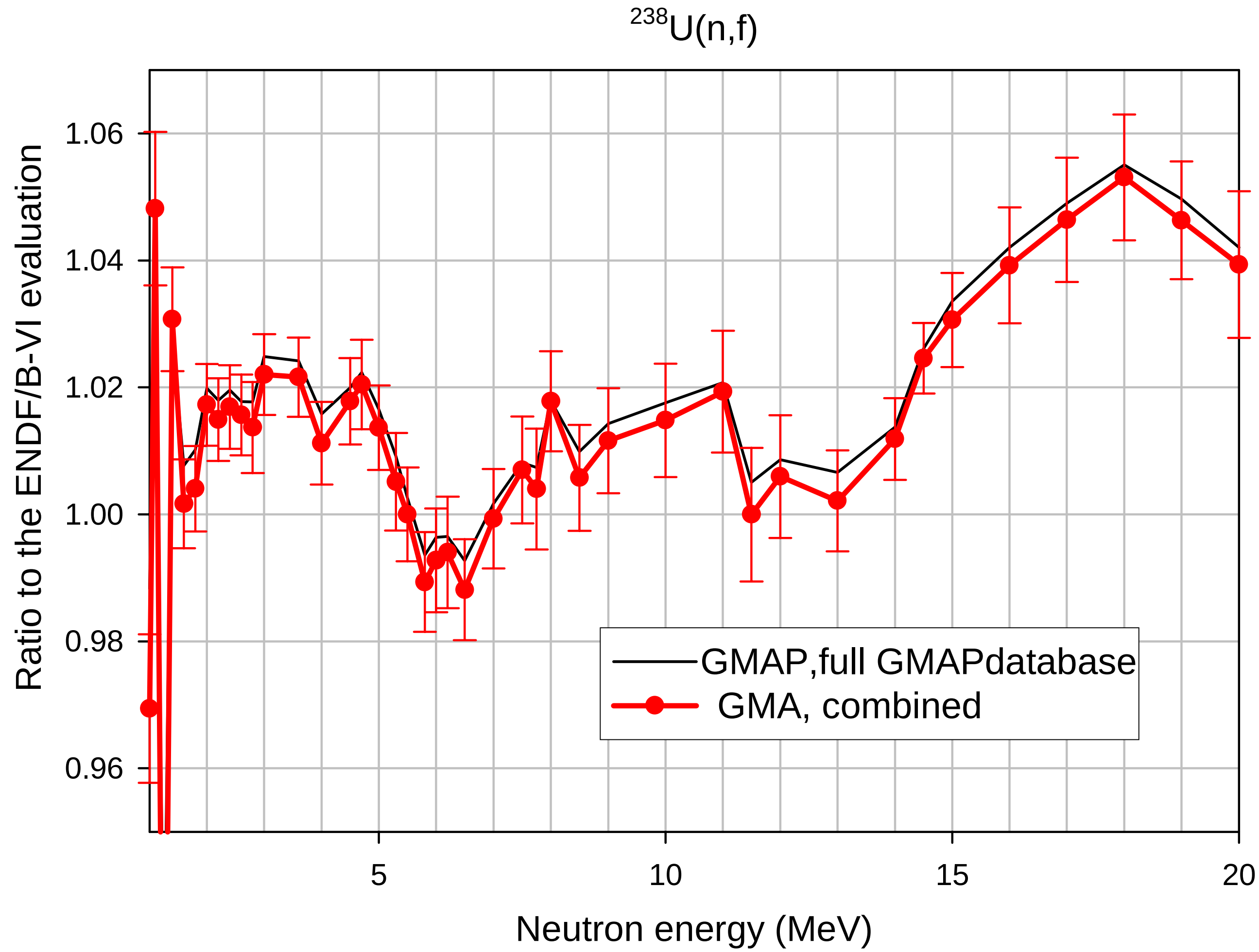

Fig. 12. Comparison of the GMAP alone and the GMAP+R-matrix (combined) evaluations for the ^{238}U(n,f) cross section. The ENDF/B-VII evaluation is the combined result.

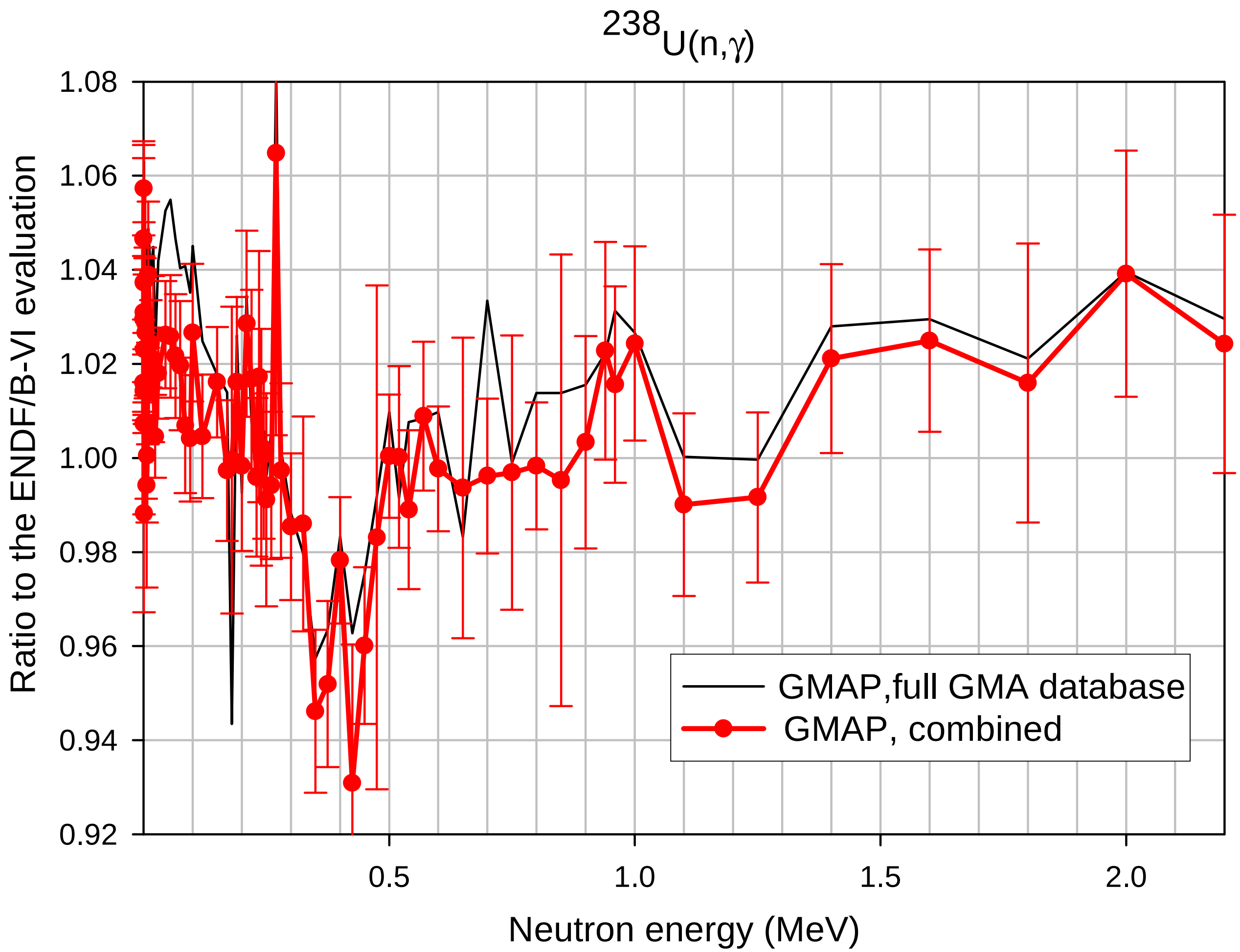

Fig. 13. Comparison of the GMAP alone and the GMAP+R-matrix (combined) evaluations for the $^{238}U(n,\gamma)$ cross section. The ENDF/B-VII evaluation is the combined result.

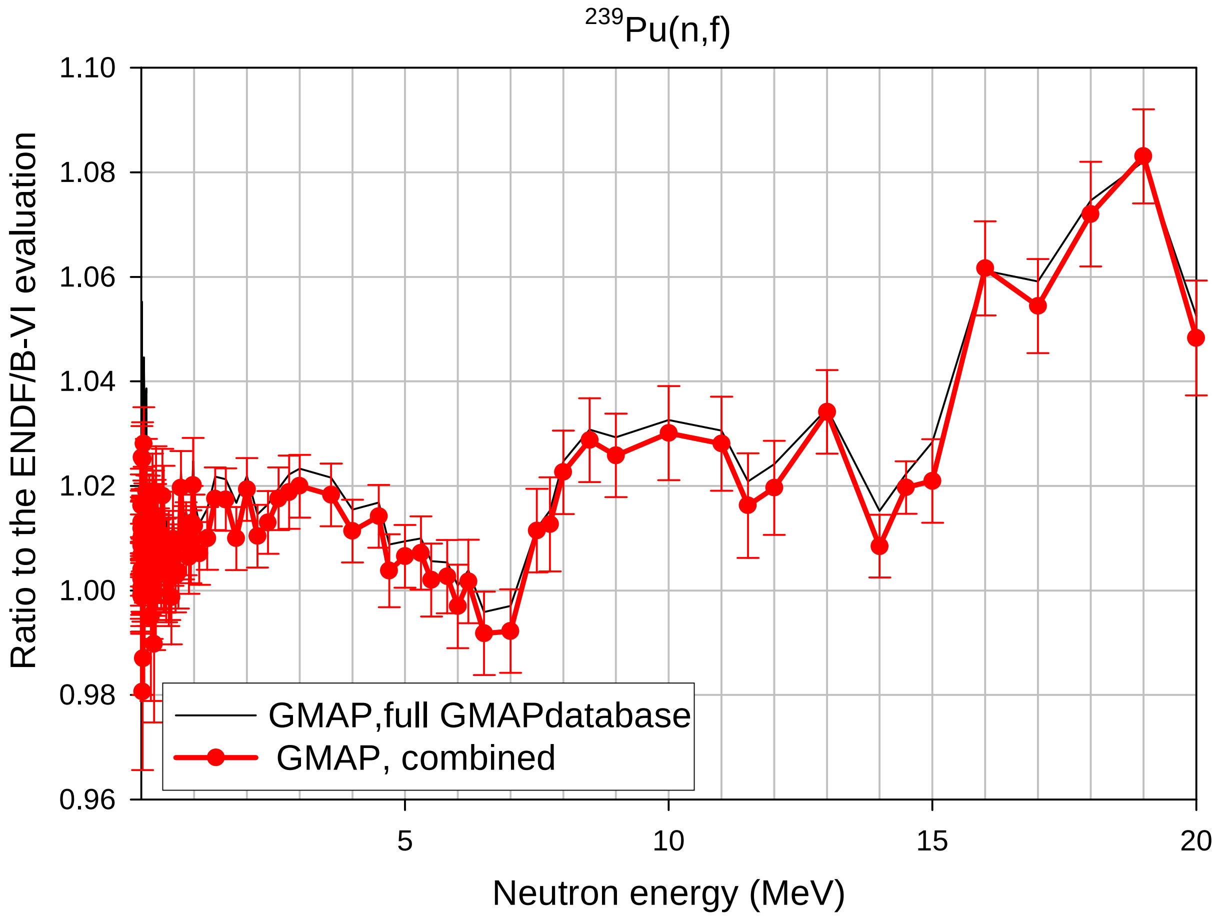

Fig. 14. Comparison of the GMAP alone and GMAP+R-matrix (combined) evaluations for the ^{239}Pu(n,f) cross section. The ENDF/B-VII evaluation is the combined result.

^{235}U(n,f) cross section where a rather large fluctuation, assumed to be statistical, occurred.

Significant improvements were obtained for the thermal constants obtained from the evaluation. This was largely due to the very accurate coherent scattering measurements for ^{235}U obtained by Arif and an improved analysis of the Gwin ν bar uncertainties. K1 calculated from the evaluation is 721.6 b. This should be compared with the "preferred" value of 722.7 b determined by Hardy. The agreement is quite good when one considers that the uncertainty in the Hardy value is 3.9 b. The evaluated cross sections are now being used in calculations of criticality experiments. The preliminary results are generally in better agreement than those obtained with the ENDF/B-VI standards. These results may change since other data involved in the calculations may be changing.

Conclusions

Significant progress has been made on the evaluation of the neutron cross section standards. Completion of this effort will require considerably more work. The most pressing concern for last year was satisfied since the most important standards were supplied for the new ENDF/B-VII library. However the remaining standards and the detailed uncertainty information must be provided. The CRP is continuing its work to provide that information. Also a new IAEA Data Development Project has been approved that is focused on the maintenance of the neutron cross section standards. This project could provide a method for obtaining standards evaluations that will be up-to-date as they are needed by the various nuclear data evaluation projects.