Neutron Cross Section Standards

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Introduction

Significant improvements have been made in the standard cross section database since the last complete evaluation of the neutron cross section standards, 16 years ago. The emphasis has been on the H(n,n), ^{10}B(n,α), and fission standards. Since 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. 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 Coordinated Research Project (CRP). These groups are working cooperatively to improve the evaluation process.

The new evaluation will include the H(n,n), ^{3}He(n,p), ^{6}Li(n,t), ^{10}B(n,α), ^{10}B(n,$\alpha_1\gamma$), Au(n,γ), ^{235}U(n,f), and ^{238}U(n,f) standard cross sections. The energy region will be extended to ~200 MeV for some of the standards to provide new standards in this important energy region.

Progress on the evaluation

Many of the experiments are not completed that could have an impact on this evaluation. We had hoped to have a cut-off date this year but due to those experiments and the realization that the evaluation process will not be completed until next year, the cut-off date has been extended until spring of 2004. Once the final data are available for these experiments, only a short time is required to add the data to the database and run the evaluation program. It is hoped that most of the experiments will be completed in a timely manner, that are still in the data taking or data analysis stage. We continue to try to get more information/documentation from completed experiments so they can be properly used in the evaluation. For each experiment that has been completed the documentation is investigated for possible corrections that may need to be made and for errors or missing information. The investigative procedure will lead to estimates of the uncertainties and correlations within an experiment and correlations with other experiments. This information will be used to obtain covariance matrices for the measurements that will be used in the evaluation process. Work continues on the encouraging, motivating and coordinating of such measurement activities so they can be used in the evaluation.

The work by Poenitz for the ENDF/B-VI standards evaluation led to many undocumented corrections that he made to various experiments. These corrections had significant effects on the evaluations of the standards for ENDF/B-VI. The documentation for these corrections has not been available until recently. Poenitz has sent to NIST, databooks, correspondence, etc. containing the information he found in his extensive study of the standards database for the ENDF/B-VI standards evaluation. Investigations of this documentation are progressing.

The CRP on the improvement of the standard cross sections has held two Research Coordination Meetings (RCM). The last one was held at NIST October 13-17, 2003. 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 initial efforts of the CRP have led to many results, though much of this work is preliminary and ongoing. The work includes: Improvement to the experimental data in the standards database; R-matrix evaluations of the hydrogen scattering cross section, the ^{6}Li(n,t) cross section and the ^{10}B(n,$\alpha_1\gamma$), and ^{10}B(n,α) cross sections; Work on microscopic calculations leading to independent determinations of R-matrix poles; Generalized least squares evaluations for the ^{6}Li(n,t), ^{10}B(n,α), ^{10}B(n,$\alpha_1\gamma$), Au(n,γ), ^{235}U(n,f), and ^{238}U(n,f) standard cross sections; Combining of R-matrix and generalized least squares evaluations; Studies of the effect of Peelle's Pertinent Puzzle (PPP) and its effect on the standards evaluation; Studies of the small uncertainties resulting from evaluations; Comparisons of R-matrix and model independent least squares codes for values of the cross sections and covariances produced; Methods for handling discrepant data; methods for smoothing evaluated data; Effects of experimental resolution on evaluated results; 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. Many more are expected before the completion of the evaluation.

Hale has evaluated the hydrogen scattering cross section below 30 MeV neutron energy using the R-matrix code EDA. Improvement in the angular distribution was observed compared with recent measurements. Unexpected problems at the 1-2% level appear in the total cross section near 10 MeV neutron energy that require further investigation.

The ^{6}Li(n,t) cross section has been evaluated by Hale using the R-matrix code EDA and by Zhenpeng using the R-matrix code RAC. It is difficult to make detailed comparisons of the two evaluations since the databases used are somewhat different. Also RAC can handle medium range correlations that EDA can not. This tends to produce somewhat larger uncertainties in the RAC output. Zhenpeng has also evaluated the ^{10}B(n,$\alpha_1\gamma$), and ^{10}B(n,α) cross sections; however, the charged particle database he used is not complete.

Theoretical calculations are being made to help describe some of the light element 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 is progressing 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 the R-matrix analysis. 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.

Improvements were made to the generalized least squares program GMA by Pronyaev. An important coding problem was found that resulted in accumulation in the adjustment vector for the 'prior' only for the contribution from the last set of data. This correction does not influence the covariance matrix of the evaluated data. Using the improved program and the database available on September 17, 2003, a run was done to produce an interim evaluation of the standards. Figure 1 shows results for the $^{235}U(n,f)$ cross section compared with those obtained with GMA for the ENDF/B-VI standards evaluation (GMA-1987), the JENDL-3.3 evaluation and an internal LANL evaluation. Figure 2 shows results for the $^{239}Pu(n,f)$ cross section compared with those obtained with GMA-1987 and the JENDL-3.3 evaluation. The results for the $^{235}U(n,f)$ cross section were used in a calculation of the Godiva experiment. MacFarlane used the CSEWG Godiva specifications and the $^{235}U(n,f)$ evaluated cross section in a special ^{235}U evaluation with the elastic scattering modified to preserve the total cross section. The result obtained was 0.99893 which is considerably better than any of the ENDF/B-VI ^{235}U releases. The evaluated cross section will change with the addition of more experimental data and the impact of the R-matrix evaluation through the combining process, however it is expected that the change will be very small.

The R-matrix results for the $^{6}Li(n,t)$ cross section from the RAC code were used as input to the GMA program to provide a combining of R-matrix and generalized least squares outputs. The R-matrix input was cross section, uncertainty and the correlation matrix. The use of the R-matrix results smooths the output considerably. Combining is also being done using EDA output instead of RAC output and comparisons will be made between the two approaches.

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 difference appears to be a result of the PPP problem resulting from the use of discrepant data. A number of methods for removing PPP have been used such as weighting by % uncertainties or the Box-Cox transformation. In the GMA analysis that was done for ENDF/B-VI, Poenitz attempted to remove problems associated with discrepant data by down weighting data greater than three standard deviations away from the output results. 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 is whether PPP is present and if so how can we properly remove it? To understand this better, three different methods for removing PPP effects will be tried on the same data sets, that are limited to the Au and ^{238}U capture database used for GMA.

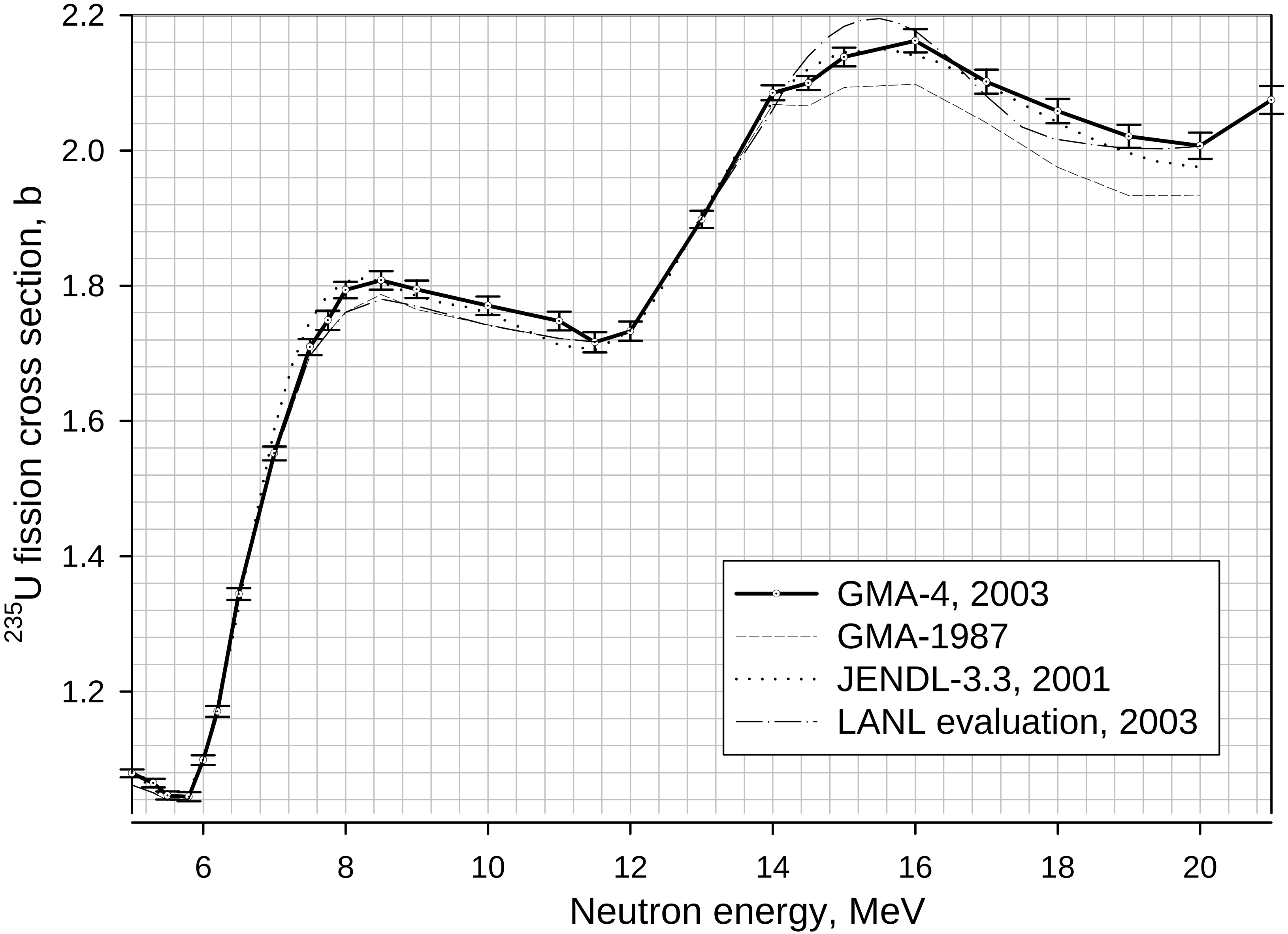
The small uncertainties obtained in the ENDF/B-VI evaluation process are of great concern. An important task for the CRP is to try to understand in detail how standard error propagation in model independent or R-matrix analyses can result in such small uncertainties, and whether there are more reasonable corrections or algorithms to employ. 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. For these comparison tests, five data sets were used: those of Fort, Fort & Marquette, Friesenhahn et al., Lamaze et al. and Poenitz and Meadows. In some cases a thermal point and a total cross section were also 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), a form of KALMAN (Kyushu University) and RAC (Tsinghua University). The generalized least squares codes being used are GLUCS (Obninsk and the University of Vienna), GMA (ANL and JAERI) and KALMAN. For the model independent least-squares work good agreement was obtained for the cross sections for the GMA, GLUCS and SOK codes. Comparisons were in good agreement for the uncertainties and correlations for GMA and GLUCS calculations. The RAC uncertainties are smaller than those of GMA and GLUCS. The EDA, SAMMY and RAC R-matrix analyses that have been done have not used exactly the same databases. Plans have been made to make comparisons using the same databases for each code. The chi-square expressions used in EDA, SAMMY and RAC need to be compared.

It is clear that more work needs to be done to understand the experiments and possible problems with them that may cause discrepancies to exist. During the ENDF/B-VI GMA evaluation process very unusual results were observed with correlated discrepant data. As noted previously, 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 simultaneous evaluation results. 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 large task. There is a more conservative effort underway which involves looking at experiments which have large weights in the evaluation. This will involve extensive investigations of the older data to look for problems with methods, etc. Due to time constraints and the fact that there are thousands of data points, work is being done on analytical procedures for handling discrepant data. In GMA we are now adding a medium energy range correlation component to the experimental data. This results in a much better χ^2 per degree of freedom and larger uncertainty in the evaluated results.

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 could be performed by fitting the output with an R-matrix code. For the heavy element standards, there are some models that may 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 to a maximum neutron energy. Other models should be considered to extend the energy range and allow other reactions (Au(n,γ), ^{238}U(n,γ) and ^{239}Pu(n,f)) to be considered.

For the R-matrix analyses, resolution effects are normally taken into account. For the GMA analysis, they are not. Unfolding of the resolution effects from the various GMA data sets would be difficult and it is not clear that unique solutions are possible. Taking the opposite approach of resolution broadening R-matrix output and also all GMA data sets would also be difficult. Also it would then give resolution broadened cross sections rather than the desired true cross sections. As a simple solution, it was decided to not include poor resolution data in the GMA database.

There is still much work to be done to fully complete this evaluation. There is a need for standards for the new ENDF/B-VII library. The evaluation of the standards depends strongly on the progress of the CRP. It will be necessary to provide an interim library of standards for that library without the detailed uncertainty information, which will be supplied at a later time. It should be emphasized that the activities of the CRP are strongly research orientated so it is difficult to establish a firm schedule for completion of the tasks.



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2.0
1.8
1.6
1.4
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^{235}U fission cross section, b
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8
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12
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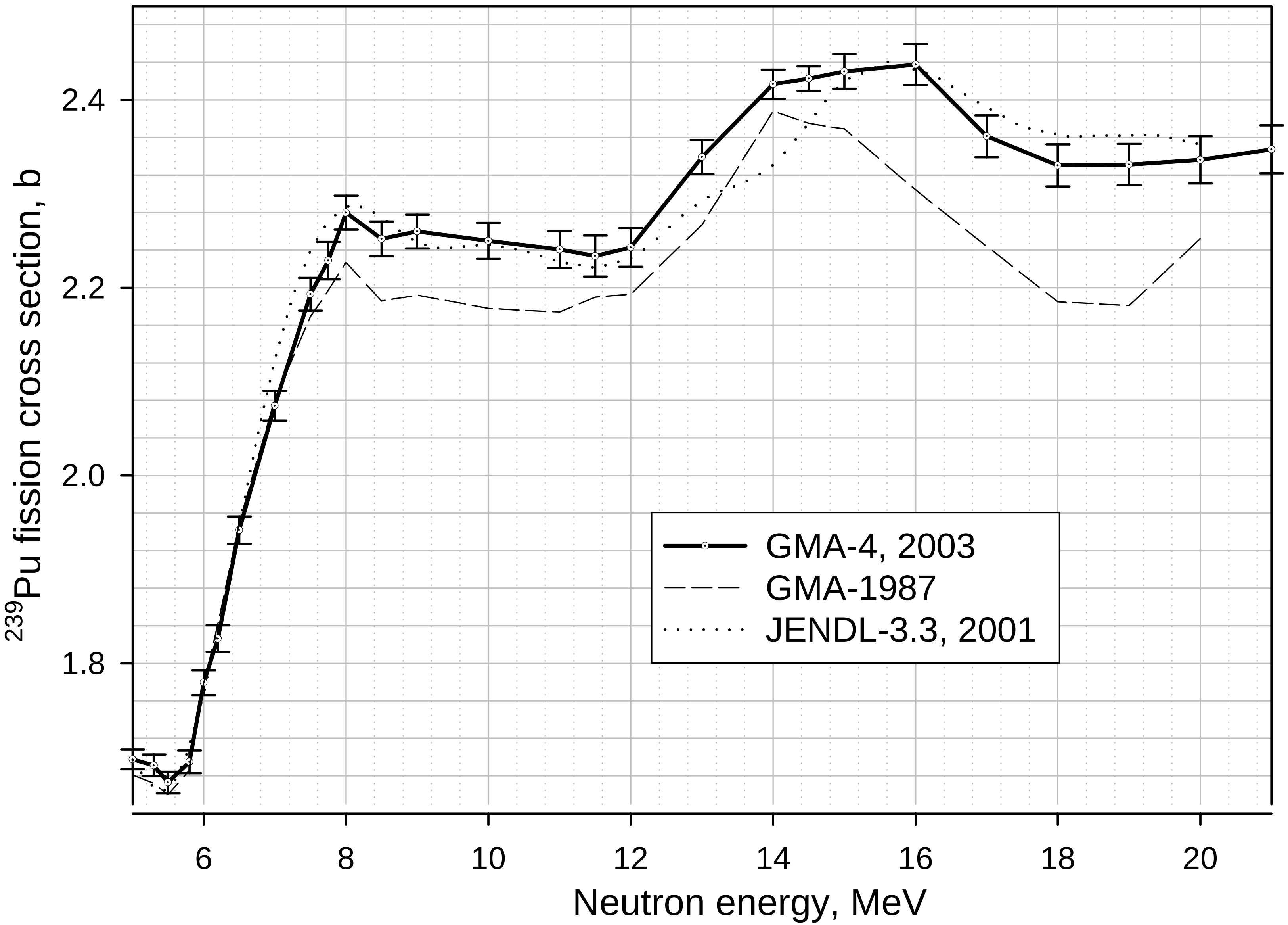
Neutron energy, MeV
GMA-4, 2003
GMA-1987
JENDL-3.3, 2001
LANL evaluation, 2003



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239Pu fission cross section, b
Neutron energy, MeV
GMA-4, 2003
GMA-1987
JENDL-3.3, 2001