Status Report of Subgroup 7 to the NEANSC WPEC
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Nuclear Data Standards
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Introduction

The need for improved neutron cross section standards has led to an international evaluation effort that includes this Subgroup, a CSEWG Task Force and an IAEA Coordinated Research Project (CRP). This strong response was a result of the dated situation for the standards, since the last complete evaluation of the standards was done almost 17 years ago. Also a large amount of experimental work has been done on the standard cross section database since that evaluation, particularly for the H(n,n), $^{10}B(n,\alpha)$, and $^{235}U(n,f)$ reactions. Since improved standards will be the basis for new versions of the neutron reaction cross section libraries, efforts are now underway to update the previous work by including new standards measurements and to improve the evaluation process. In Table 1, the cross section standards are listed and their proposed energy ranges for this evaluation. The C(n,n) cross section will not be evaluated since the database has not changed significantly.

Table 1. The 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

The cut-off date for accepting measurements for the evaluation has been extended until the end of this spring. Once the final data are available for these experiments, it is expected that only a short time will be required to add the data to the database and perform the final evaluation. It is hoped that most of the experiments that are still in the data taking or data analysis stage will be completed in a timely manner. We continue to try to get more information/documentation from completed experiments so they can be properly used in the evaluation. This information will be used to correct the experimental data in some cases or improve uncertainty or covariance data that will be used in the evaluation process.

Work on the experiments considered for the standards database continues. There has been significant support for this work from laboratories involved with the WPEC. 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.

Two Research Coordination Meetings (RCM) of the CRP on the improvement of the standard cross sections have been held. The most recent 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 work of the CRP has led to many results, though much 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; Studies of the small uncertainties resulting from evaluations by comparisons of the results of R-matrix codes and model independent least squares codes; 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; methods for smoothing evaluated data; Effects of experimental resolution on evaluated results. Short summaries of these activities are given below:

More than 30 data sets have been added to the standards database since the formation of the CRP. More are expected before the completion of the evaluation. 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 large task. There is a more conservative effort underway which involves looking at experiments that have large weights in the evaluation. This involves studies of the experiments 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 simplified procedures for handling discrepant data. In GMA we are now adding 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.

Work continues on the problem of obtaining realistic uncertainties for the evaluation. Extremely small uncertainties were obtained for some cases in the ENDF/B-VI evaluation process. The CRP is trying 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 that can be used. The small uncertainty problem has been investigated by comparing the results obtained from several tests of relevant codes. This tests both the cross sections and covariances obtained with different codes. Comparisons have been made of cross sections and their uncertainties using five ^{6}Li(n,t) data sets: 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). For the model independent least-squares work good agreement was obtained for the cross sections and covariances for the GMA (ANL and JAERI), GLUCS (Obninsk and University of Vienna) and SOK (LANL) codes. A similar comparison is underway for the R-matrix codes EDA (LANL), SAMMY (ORNL), and RAC (Tsinghua University). Differences were observed in the results of these R-matrix calculations however these analyses have not used exactly the same databases. Plans have been made to make comparisons starting with the same very small database for each code so that systematic studies can be made to understand possible differences. The uncertainties obtained with the R-matrix codes are smaller than those obtained in the model independent least-squares work.

Evaluating the hydrogen cross section must be one of the first steps in the evaluation process since many standards measurements are made relative to this standard. Hale has completed a preliminary evaluation of the hydrogen scattering cross section below 30 MeV neutron energy that was obtained using the R-matrix code EDA. Improvement in the angular distribution was observed compared with recent measurements. The total cross section is lower than previous evaluations by about 1% near 10 MeV neutron energy and is still being investigated. Improved total cross section data in this energy region would be very helpful. Work is also underway by Hale to extend the energy range to about 150 MeV. Another appropriate evaluation will be merged with the Hale results for the energy region from 150 to 200 MeV. In the 96-200 MeV energy region, problems persist for the cross section at back angles in the CMS. The Indiana University preliminary data do not show the peaking at back angles present in the Uppsala work. The most recent Uppsala measurements extend their angular range so the range is from 74 to 180 degrees in the CMS. This allows that normalization of these shape measurements to the total cross section more accurately.

Preliminary evaluations have also been done for the ^{6}Li(n,t) cross section by both Hale using the R-matrix code EDA and by Zhenpeng using the R-matrix code RAC. There are differences between the two evaluations however it is difficult to make detailed comparisons since the databases used are somewhat different and in some cases data are weighted differently. 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 $^{10}B(n,\alpha)$ cross sections; however, the charged particle database he used is not complete. A special workshop on the R-matrix calculations is scheduled to be held in June at the IAEA headquarters with both Hale and Zhenpeng attending. It is hoped that this workshop will resolve some of the differences obtained with the EDA and RAC codes.

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 in 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 for 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 RRGM 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 can be used by an evaluator to eliminate discrepant experiments from consideration.

Simultaneous evaluations of the $^{6}Li(n,t)$, $^{10}B(n,\alpha)$, $^{10}B(n,\alpha_1\gamma)$, $Au(n,\gamma)$, $^{235}U(n,f)$, and $^{238}U(n,f)$ standard cross sections were successfully obtained using the generalized least squares program GMA. This was done using the version of the program corrected for the coding error found by Pronyaev referred to in the previous report and with an extension in energy range up to 200 MeV for the $^{235}U(n,f)$ and $^{238}U(n,f)$ cross sections.

A procedure for combining R-matrix and generalized least squares outputs was successfully performed by Pronyaev. R-matrix results for evaluation of the $^{6}Li(n,t)$ cross section were used as input to the GMA program. This input was treated in the same manner as an experimental data set. It included cross section, uncertainty and the correlation matrix information. The use of input obtained from an R-matrix code causes output results that are smoothed considerably. R-matrix results obtained with both the RAC and EDA codes were used as input to the GMA program in these tests. Differences were observed between them that were strongly effected by the differences between the RAC and EDA results. These differences will also be a topic of discussion for Pronyaev, Hale and Zhenpeng at the special workshop in June.

It appears that the problems associated with Peelle's Pertinent Puzzle (PPP) may now be under control. Such problems were observed early in the investigations of the CRP. A test run using the least squares code SOK fitting a logarithmic transformation of the data produced higher cross sections than a run fitting the data. There were discrepant data in the test run. The difference was a result of the PPP problem resulting from the use of discrepant data. Pronyaev and Smith implemented a new option that allows the Chiba-Smith method for PPP reduction to be used with the GMA code. This option has been used with the present GMA database and compared with the results obtained using the SOK code with the same database and the logarithmic option. The agreement obtained was generally within a fraction of a percent for both the cross section values and the variances. It has been suggested that the average of the two methods be used when the final analysis is done.

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 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.

A number of meetings will be required in order to make the progress needed to complete this evaluation in a timely manner. In April, a standards workshop was hosted by LANL that led to important work on the standards including: R-matrix analyses; PPP comparisons; Improvement in the understanding of the ^{235}U(n,f) cross section near 1 MeV; Medium energy range correlation components for experimental data that is discrepant; Studies of LANL, JENDL and the present preliminary evaluations of the ^{235}U(n,f) and ^{239}Pu(n,f) cross sections; Consistency of the databases used in these fission evaluations.

The agreement among the LANL, JENDL and present evaluations is about 1-2% for both the ^{235}U(n,f) and ^{239}Pu(n,f) cross sections, except in the 14 MeV energy region for the ^{239}Pu(n,f) cross section where differences as large as 4% exist. At higher energies, the lack of measurements is a major problem for the evaluation effort. For the ^{235}U(n,f) cross section the only recent work is that of Nolte et al. This is an important contribution since these are the only data other than those of Lisowski et al. in the high energy region that have relatively small uncertainties. Except for a data point at 96 MeV, which Nolte et al. suggest may be in error, there is agreement within the uncertainties of these data with the Lisowski et al. data. Since so many cross sections are being measured relative to the ^{235}U(n,f) cross section, additional corroborative measurements of this important standard should be made. Nolte et al. have also made measurements of the ^{238}U(n,f)/ ^{235}U(n,f) cross section ratio, shown in Fig. 1, that are generally in good agreement with the Lisowski et al. measurements, though the uncertainties on the Nolte et al. work are considerably larger. There is a difference between the Shcherbakov et al. and the Lisowski et al. measurements that is a couple of percent at the lowest energies but becomes more than 5% at the highest energies. The most recent measurements of the ^{239}Pu(n,f)/^{235}U(n,f) cross section ratio are those of Lisowski et al., Staples and Morley, and Shcherbakov et al. These data are shown in Fig. 2. The three data sets agree within about 2% up to about 20 MeV neutron energy. Between 20 MeV and 60 MeV neutron energy, the Staples and Morley data are about 4% higher than the Lisowski et al. data. In that same interval the Shcherbakov et al. data increase from 0% to about 3% higher than the Lisowski et al. data. Above 60 MeV neutron energy, the disagreement increases between the

Shcherbakov et al. and Lisowski et al. data sets with the Shcherbakov et al. data being almost 10% higher than the Lisowski et al. data set at 200 MeV.

At the LANL workshop, The lack of high energy measurements for these nuclides led to a discussions with LANL/LANSCE staff concerning the possibility of new measurements being made at that facility. Measurements of the quality required will be a major experimental undertaking. It was suggested that such an effort, independent of where it is done, should be done through an international collaboration. A proposal is being considered to organize a new working group under the WPEC to do this work.

Comparisons were made of spectrum averaged cross sections using the neutron spectra from the GODIVA and JEZEBEL critical assemblies. These average cross sections are a measure of k_{eff} prediction for those assemblies. The present preliminary results for the $^{235}U(n,f)$ cross section were used in a calculation of the Godiva experiment. Mihaila at LANL 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, 0.99971, is in considerably better agreement with the k_{eff} measurement than that obtained with 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. Calculations are underway for the JEZEBEL assembly. The spectrum averaged $^{239}Pu(n,f)$ cross section for the present work suggests that there will be an improved calculation for this critical assembly compared with the ENDF/B-VI cross section.

There is still much work to be done to fully complete this evaluation. A special side meeting is planned at the ND2004 conference that will help the participants to prepare for the next RCM in October. The immediate focus is on producing the standards for the new ENDF/B-VII library. The objective is to provide an interim library of standard cross sections for that library this year. Detailed uncertainty information can be supplied at a later time. Based on the activities that have been focused on this evaluation, it seems reasonable to expect that there will be no remaining technical problems that can not be solved in a timely manner, though a certain level of compromise will be required.

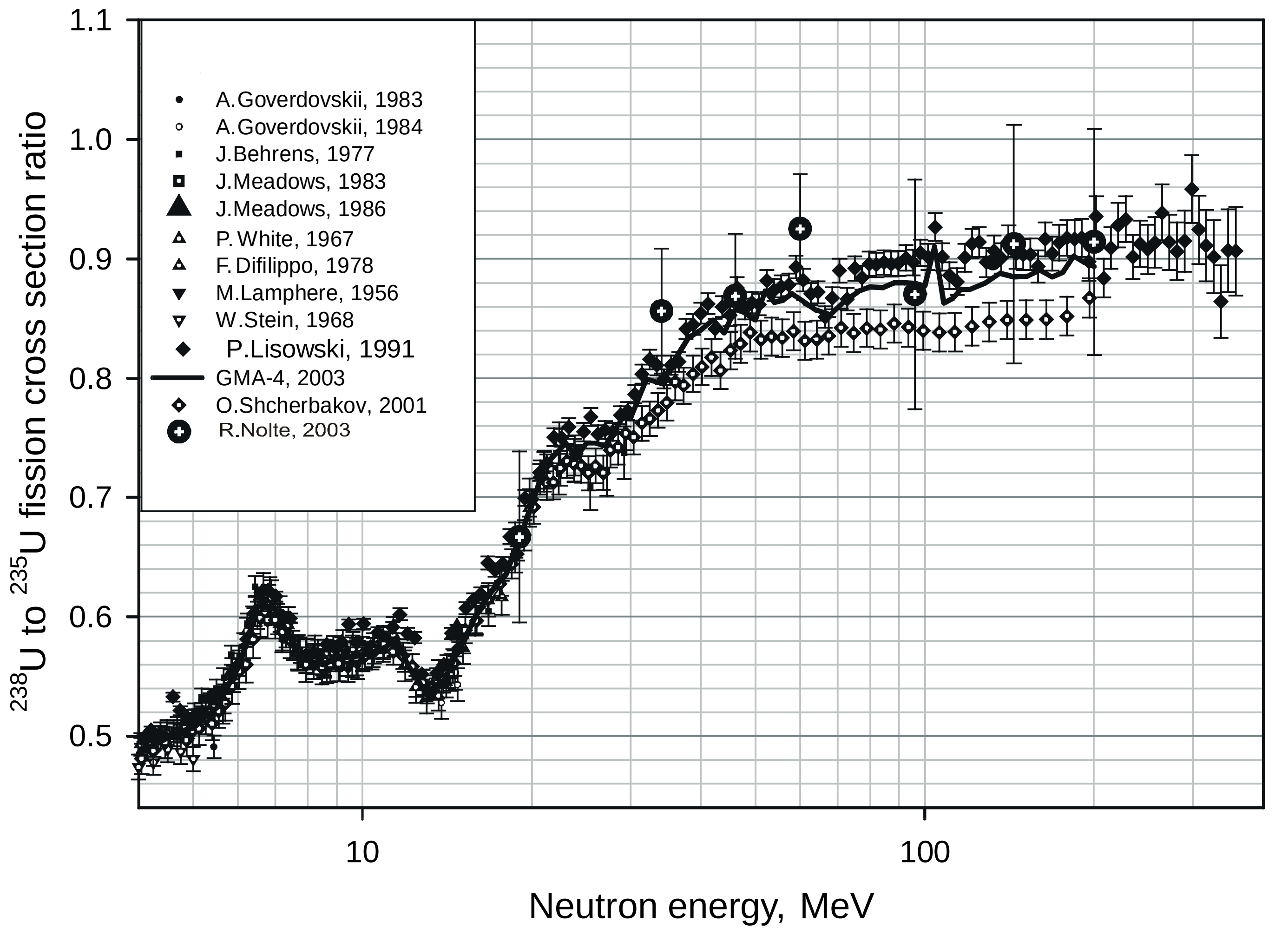

Fig. 1. Measurements of the ^{238}U to ^{235}U fission cross section ratio compared with the present GMA results.

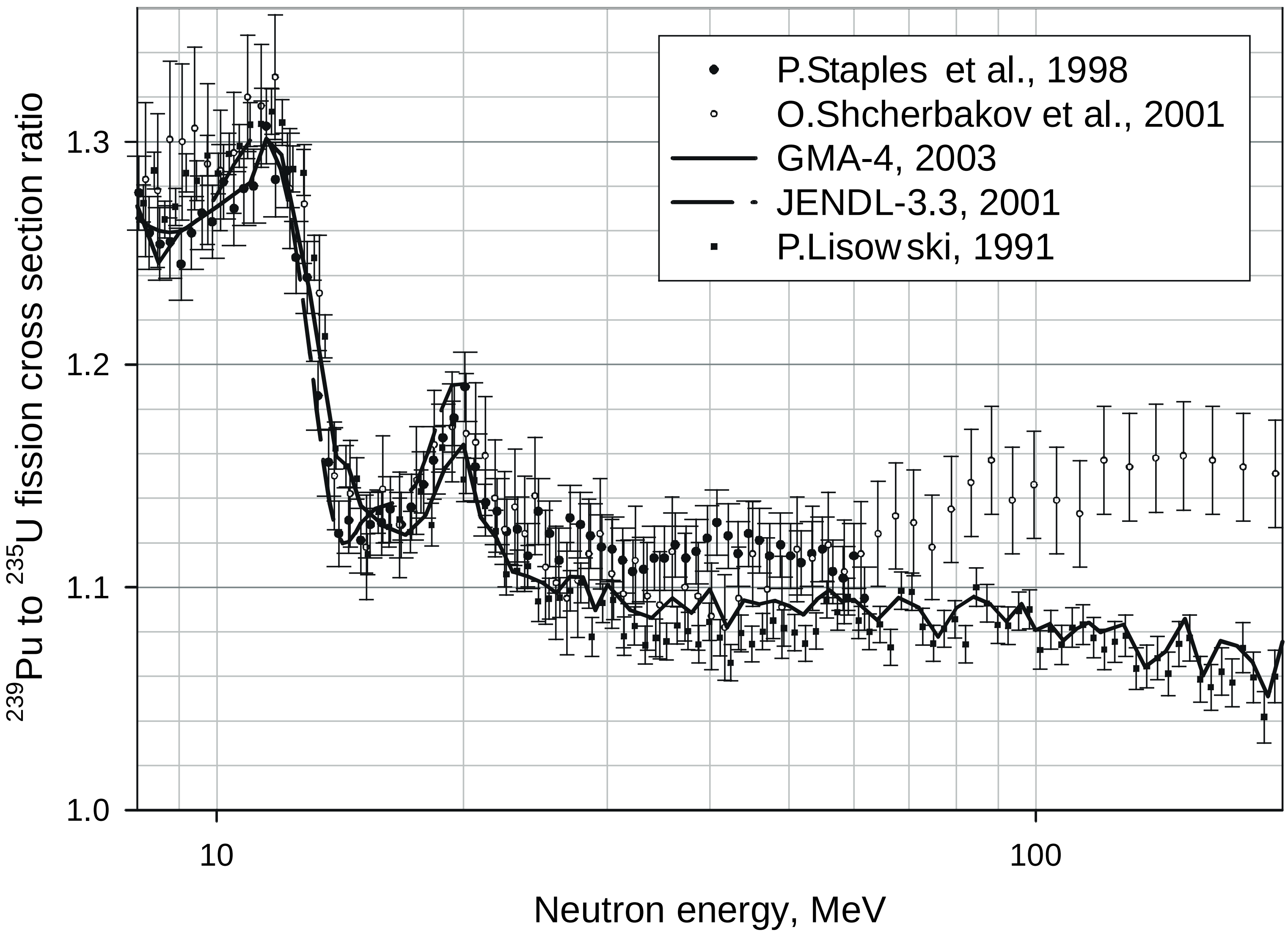

Fig. 2. Measurements of the ^{239}Pu to ^{235}U fission cross section ratio compared with the present GMA results.