Update of GMA Code to Solve the PPP Problem (Technically)

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The GMA code has been updated to introduce the Chiba-Smith option (see report ANL/NDM-121, 1991) to address the problem of PPP. To avoid confusion, we will refer to this code, and results obtained using it, as GMAP. This code revision was accomplished with a minimum of intervention to the original version of GMA in order to avoid introducing coding errors. The Chiba-Smith approach was implemented by means of simple renormalization of the experimental absolute errors (square roots of the variances) after reading them in from the input file. This renormalization was applied to each "experimental" data point and for each class of data, e.g., cross sections, ratios, shape ratios, etc., as $\Delta\sigma'(i)=\Delta\sigma\times(\sigma_p(i)/\sigma)$, where σ represents the experimental data value (whatever it might be) $\Delta\sigma$ is the uncertainty of this experimental data point, $\sigma_p(i)$ is a prior value for this quantity – obtained after i^{th} iteration, and $\Delta\sigma'(i)$ is the renormalized absolute uncertainty of the data after the i^{th} iteration. We use the term "experimental" rather broadly here because it is intended to eventually employ GMAP for merging R-matrix and experimental results, with the R-matrix results introduced as pseudo experimental data. The original GMA code already included an option to iterate the runs with replacement of the prior $\sigma_p(i)$ by the new posterior solution since the prior in GMA is assumed to be ad hoc and non-informative. The convergence to the "true" posterior solution was very fast, usually a few iterations were enough even when first prior was intentionally made discrepant with a bulk of experimental data.

We refer to this option as a "technical" solution to exclude PPP since it is based on the subjective assumption by Chiba and Smith that when experimenters quote absolute total errors these are calculated by multiplying a fractional error (comparable to percent error) by the measured value. Thus, it is supposed that it is the fractional error that actually reflects the accuracy that the experimenter intends to convey to the reader. The PPP problem is a consequence of discrepancies, i.e., the scatter observed for various presumably comparable data obtained by different experimenters that is frequently beyond the quoted errors. Consequently, we believe that the Chiba-Smith approach should be introduced into an evaluation process only after applying the "physical" option, namely, that of identifying the outlying data points (those most discrepant with respect to the main body of evaluated data). Then, where possible, the observed discrepancies should be resolved by applying corrections that were overlooked (or possibly erroneously determined) by the original experimenters, by enhancing quoted errors to compensate for hidden uncertainties not realized by the experimenters, etc. The intent is to reduce the PPP effect as much as possible by objective means before resorting to the above-mentioned "technical" solution. Such an approach is essential to the achievement of a good evaluation since the "corrected" data values are expected to then correspond more closely to the "truth." However, since the PPP phenomenon does not have a threshold and is continuous in nature (see Appendix), we believe that, after exhausting the possibilities for the abovementioned "physical" option, PPP should be excluded by applying a technical approach such as that of Chiba-Smith to correct for residual deficiencies in the database and deficiencies of the least-square procedure, even if the PPP effect is small.

While the example given in the Appendix is illustrative of PPP for a simple hypothetical situation, it is more convincing to explore the phenomenon in the "real world" using a realistic data set. The TEST1 data set, which exhibits a large and clearly seen PPP bias, was adopted by the CRP and used to inter-compare different technical options for PPP exclusion. These data were employed in the various fits without any alterations, i.e., they were original data given by the experimenters. No values were adjusted, no errors were enhanced, etc. Those results indicated in Figs. 1 to 3 as "GMAP" were obtained with three computational steps in the framework of the Chiba-Smith approach to exclude the PPP: the first pass using the assumed prior (ENDF/B-VI), GMAP(1) – the result after one iteration, and GMAP(2) – the result after two iterations. GMA presents results without any technical fixes applied to exclude PPP. Therefore, it exhibits the full extent of the PPP bias. GLUCS03 presents results obtained by S. Tagesen and H. Vonach with inclusion of the Chiba-Smith option in the GLUCS code. GMAJ presents results obtained by Soo-Youl Oh (Table 3, p. 153, report INDC(NDS)-438, 2002) with the GMAJ code. GMAJ is a version of the GMA code completely rewritten by Chiba with inclusion of the Chiba-Smith option to exclude PPP. Oh does not mention whether he iterates the solution obtained using GMAJ, so we will assume for present purposes that there is no iteration. Results showing the use of Box-Cox transformation to exclude the PPP effect are also taken from paper by Soo-Youl Oh (Table 3, p. 153, report INDC(NDS)-438, 2002). The PADE-2 model fit (S. Badikov, Private communication) also was performed without any technical fixes to exclude PPP. Two fits obtained using the RAC R-matrix code – without technical options to exclude the PPP effect – are shown in the Figs. 1 and 2. RAC(2002) presents the "old" fit, where selection of the prior parameters was rather free and problems were known to have existed with regard to ambiguity in the determination of parameters. RAC(2003) presents the "new" fit, where parameters determined from the fit of a large number of data in different reaction channels leading to the formation of ^{7}Li system were taken as the set of non-informative prior R-matrix parameters. It may be the case that the RAC(2003) fit corresponds to a particular local minimum of the chi-square function and perhaps should not be compared to results from the other fitting procedures because of the major differences in the employed approaches.

Results from fits obtained by various means are shown in Fig. 1 as ratios to the GMAP(2) fit. The PPP biases observed in the GMA, RAC(2002) and PADE-2 fits are rather large. The RAC(2003) fit (irrespective of the comment in the preceding paragraph), and all other fits that aim to provide technical exclusion of PPP, give results that are relatively close. It is therefore difficult to judge which approach yields the "best" result since we do not know the true values to which these real data should correspond. Figs. 2a and 2b show in more detail the differences between the GMAP results (one and two iterations, respectively) and the various other approaches used to exclude the PPP effect. It is evident that the Box-Cox approach gives slightly higher values than the other methods. The GMAP and GLUCS03 fits are based on the same technical fix to exclude PPP (Chiba-Smith). Nevertheless, they exhibit some differences that can probably be explained in terms of the precision of the numerical solutions of different equations. Because of such issues related to numerical precision, it is seems unreasonable to claim that one approach is better than another when the observed differences are quite small.

We have found that two distinct effects can lead to the presence of PPP in data evaluated by the least-squares method (see Appendix). One effect can be attributed to the different shapes of distinct strongly correlated data sets. We choose to label the PPP effect that results from these strong correlations as maxi-PPP. The second effect arises when there is a spread of data and absolute uncertainties are assigned. Two data points with the same percent uncertainty (same accuracy), but having different values, will then be weighted differently by the least-squares evaluation process. The lowest point will be assigned the heaviest weight since the weighting factor corresponds to the reciprocal square of the absolute error. We will refer to the PPP effect due to an apparent over-weighting of low values as mini-PPP. The contribution of the mini-PPP effect for the standards data is rather small due to the generally small spread encountered for standard-reaction experimental data values. The contribution of these two components for the TEST1 case can be seen in Fig. 3a and 3b. The thick solid line shows the full PPP bias, based on our assumption that the Chiba-Smith approach, as manifested in GMAP calculations with two iterations, gives the best value. The thin solid line shows the effect of mini-PPP for these five TEST1 data sets. For this particular calculation, all non-diagonal elements of the correlation matrices of all experimental data sets were set to 0, i.e., no correlations (nc). So, in this case the difference between the GMA and GMAP results shows the mini-PPP effect explicitly for the rather discrepant TEST1 database. As we see from Figs. 3a and 3b, this effect is not large. However, we believe it still should be addressed and corrected. Since the thin dashed line in Figs. 3a and 3b shows the ratio of the GMA result with no correlations between data to the comparable GMAP result, it is demonstrated that exclusion only of the correlations is not enough to consider a fit to be effectively free from PPP at levels of accuracy consistent with the requirements for the standard cross sections.

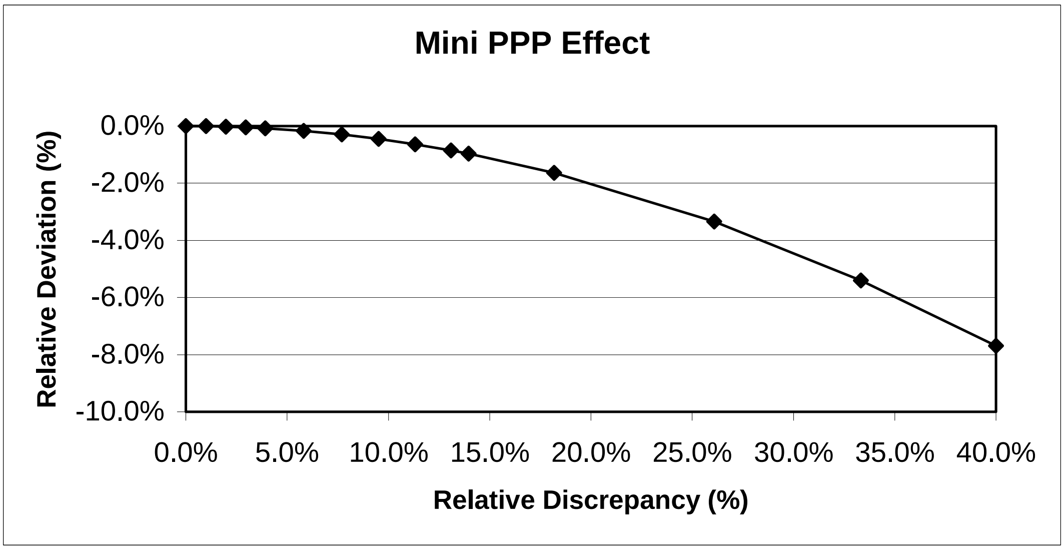
Appendix

Mini- and Maxi- PPP for Peelle's Original Problem

An examination of both simple and complex data evaluation problems by the least squares method shows that the phenomenon known as Peelle's Pertinent Puzzle (PPP) inevitably occurs when data scatter and absolute uncertainties are employed in the evaluation. This appears at a more fundamental level to be attributable to the fact that the least-squares formalism is an approximation to the fundamental Bayesian evaluation approach. Robert Peelle of Oak Ridge National Laboratory first demonstrated the PPP phenomenon, at least to the nuclear data community, in an informal memorandum that he distributed in 1987. Since then, PPP has been the subject of numerous debates within the data evaluation and data adjustment communities. Qualitatively speaking, the PPP phenomenon tends (on average) to lead to evaluated results that are intuitively "too low". Quantitatively, the bias known as PPP resulting from applications of the least-squares methodology can range continuously from zero to values that affect the quality of an evaluation significantly.

A closer examination of the PPP phenomenon shows that it is actually comprised of two components. One component – that for the purpose of convenience will be denoted by mini-PPP – tends to have lesser magnitude. It is observed even when no correlations are present in the uncertainties of data to be evaluated, only scatter. A second aspect of PPP, denoted here by maxi-PPP, is manifested when uncertainty correlations are present. Often this component, which can never be separated from the mini-PPP effect, tends to be the larger effect. In the evaluation of real data with uncertainties, scatter (i.e., discrepancies), and error correlations, one encounters total-PPP, or simply PPP as a composite of the mini-PPP and maxi-PPP components.

In this appendix we demonstrate the effect of both mini-PPP and maxi-PPP by considering Peelle's original problem. Two data are averaged. One has a value 1.5 and the other 1.0. Each has a random uncertainty of 10% and they both have a fully correlated error of 20%. These data are obviously discrepant, and blind application of the least-squares method leads to the non-intuitive result 0.88 ± 0.22 for the evaluated solution! Since both values appear to have the same precision, the intuitive best solution would appear to be 1.25. This is the solution obtained using the method proposed by Chiba and Smith (see report ANL/NDM-121, 1991) to eliminate the PPP effect. Peelle's original problem has been examined using both a spreadsheet routine (EXCEL) and the least squares code LSMOD developed by Smith (see report ANL/NDM-128). The first set of calculations, done with EXCEL, involved switching off the error correlation parameter and varying the discrepancy between these data from zero to 40% (40% corresponds to Peelle's original problem since 0.5/1.25 equals 0.4). The deviation from the Chiba-Smith solution (1.25) varies from zero to about 8% (low) as is seen in the top graph of Fig. A.1. This is the mini-PPP effect. The second set of calculations was performed with LSMOD. The data values 1.5 and 1.0 were retained as originally given, as were the magnitudes of the error components. However, the degree of correlation was varied from zero to 100% (100% corresponds to Peelle's original problem). The results are shown in the bottom graph of Fig. A.1. The correlation strength ranges from 0 to 1.0 (100% correlation). The "mini-PPP effect appears as an 8% reduction for zero correlation strength whereas the full PPP effect at 100% correlation strength is about 30% for this example. The difference is attributed to the maxi-PPP component. Maxi-PPP can be demonstrated only as an observable difference between the reduction seen for total-PPP and that obtained when correlations are neglected (mini-PPP).



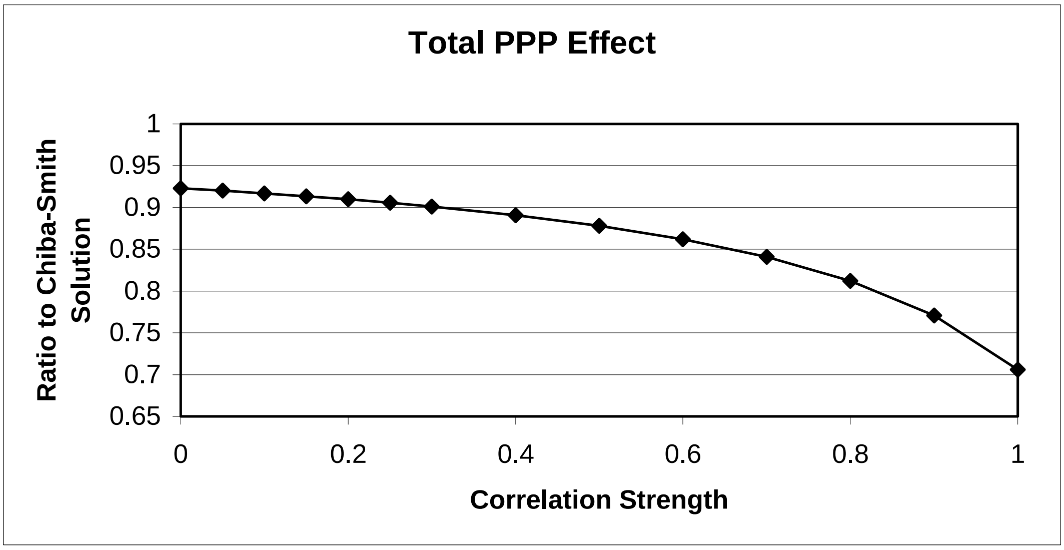


Figure A.1. Demonstration of mini- and maxi-PPP effects

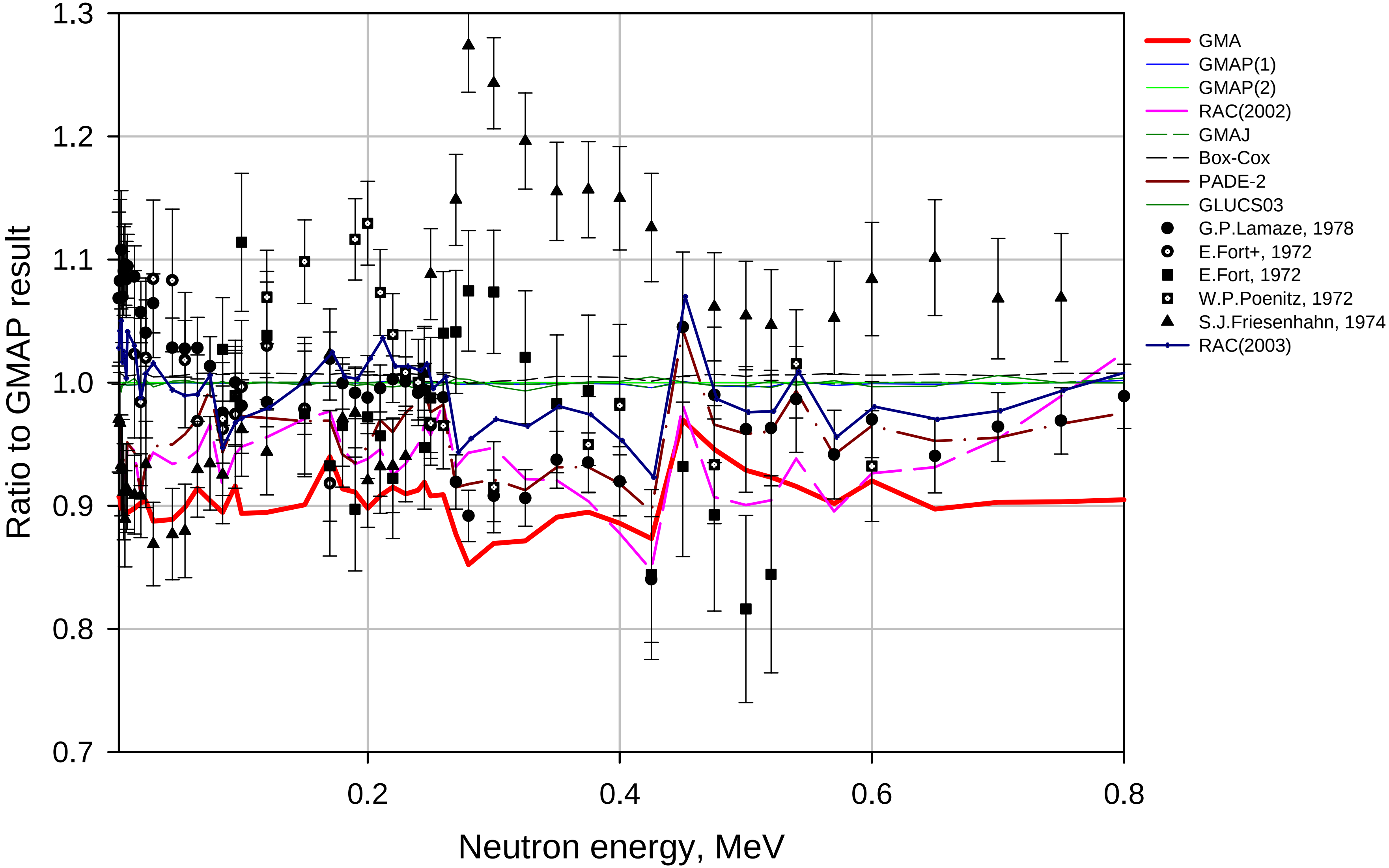


Fig. 1. Ratios of different fits of ^{6}Li(n,t) cross sections to the GMAP(2) iterative fit (Chiba-Smith option).

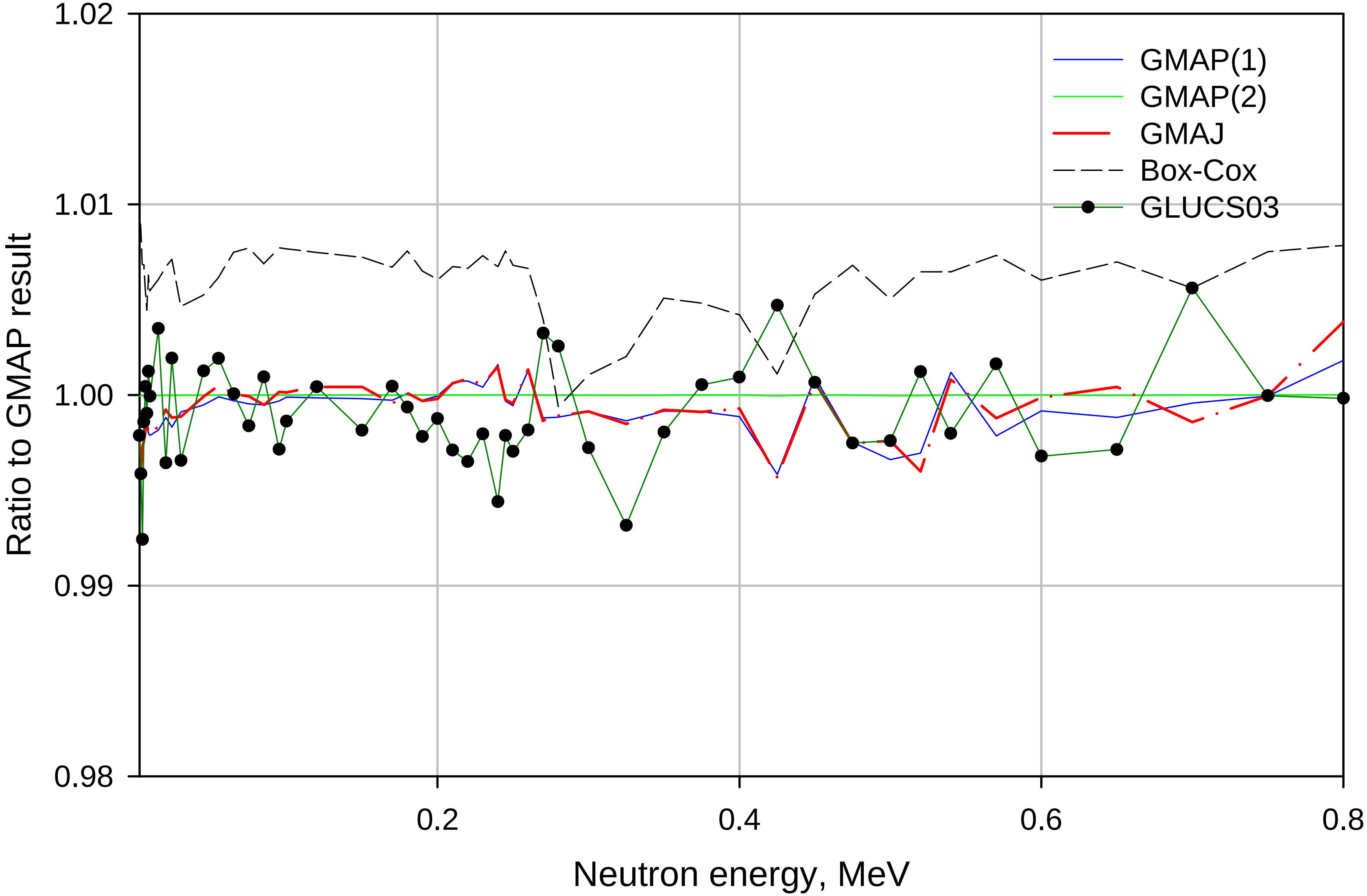


Fig. 2a. Ratios of different fits of ^{6}Li(n,t) cross sections to the GMAP(2) iterative fit (Chiba-Smith option).

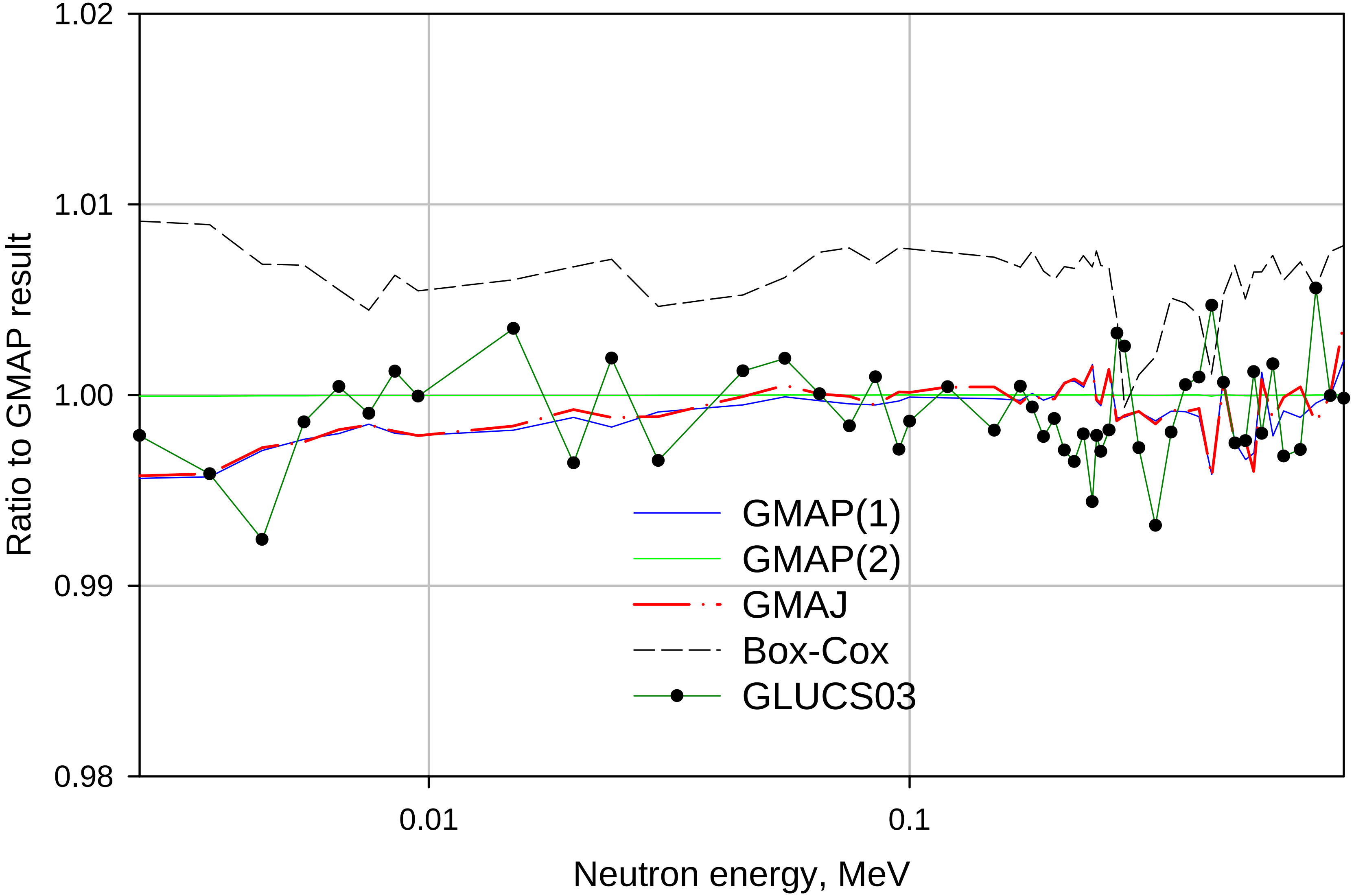


Fig. 2b. Ratios of different fits of ^{6}Li(n,t) cross sections to the GMAP(2) iterative fit (Chiba-Smith option).

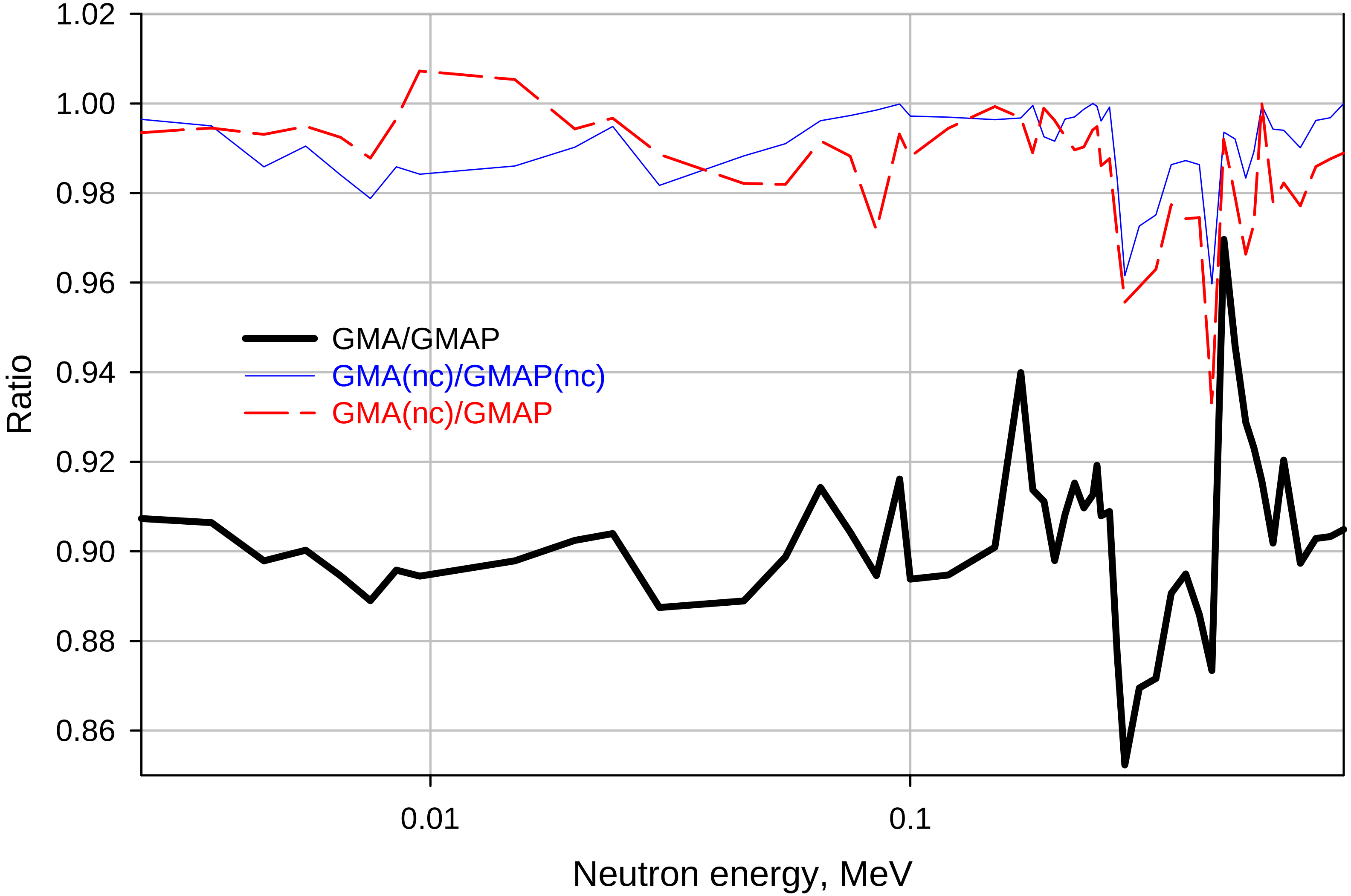


Fig. 3a. Ratios of different fits of ^{6}Li(n,t) cross sections showing the presence of PPP in TEST1 data and the contribution from its components. GMAP result corresponds to two iterations.

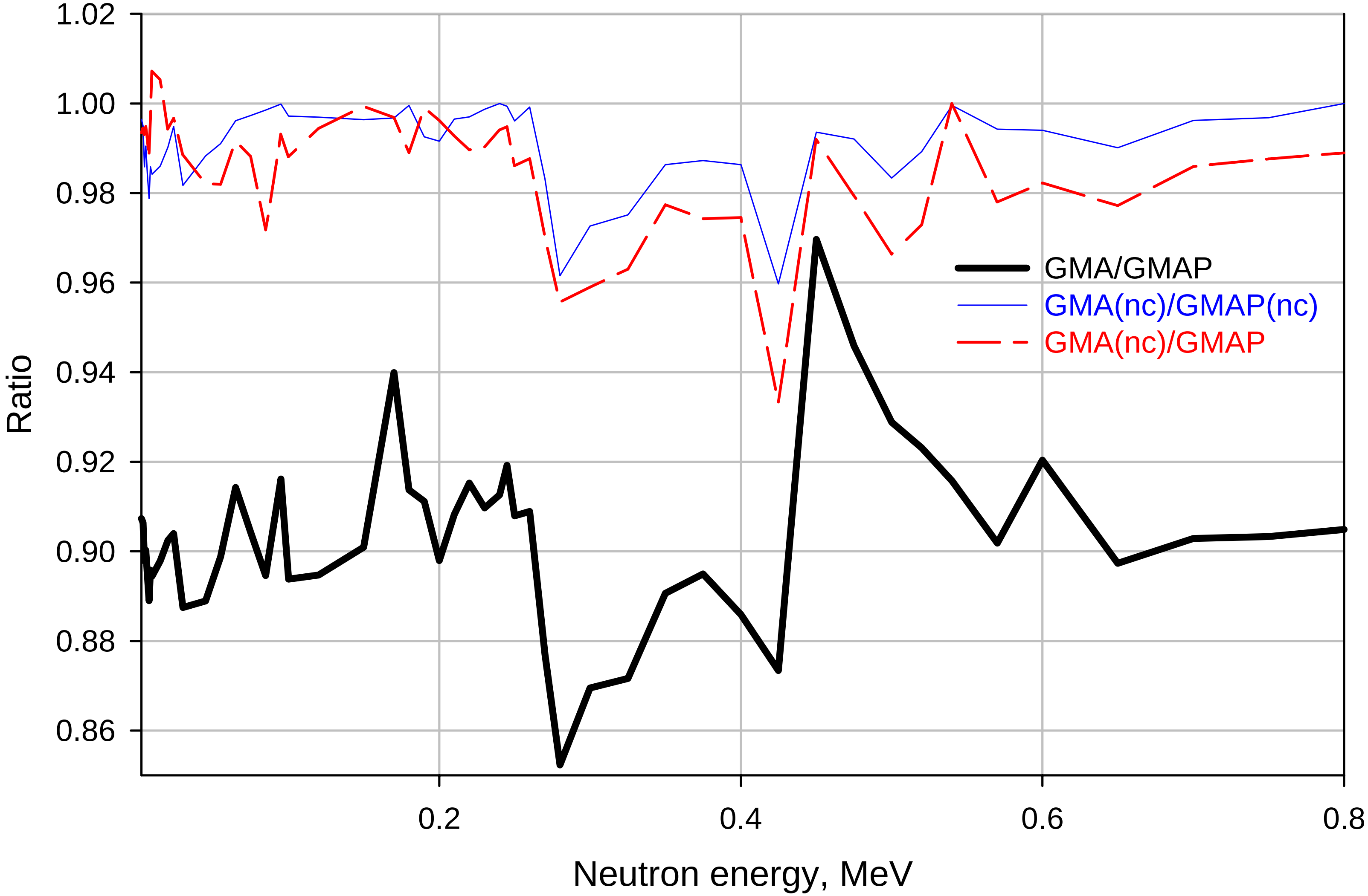


Fig. 3b. Ratios of different fits of ^{6}Li(n,t) cross sections showing the presence of PPP in TEST1 data and the contribution from its components. The GMAP result corresponds to two iterations.