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Summary Report of the First Research Co-ordination Meeting on Improvement of the Standard Cross Sections for Light Elements

IAEA Headquarters
Vienna, Austria

23 - 27 September 2002

Prepared by
A. D. Carlson, G.M. Hale and V.G. Pronyaev

January 2003

IAEA NUCLEAR DATA SECTION, WAGRAMER STRASSE 5, A-1400 VIENNA

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Abstract

Results obtained during the first six months of the Coordinated Research Project (CRP) on Improvement of the Standard Cross Sections for Light Elements were presented. Attention focused on studies of the reduction in uncertainty for the model and non-model least squares fits, intercomparison and testing of different computer codes based on the nuclear model, non-model general least square and Bayesian approaches to the evaluation of standard reaction cross sections and covariance matrix of their uncertainties. The reasons leading to the underestimation of uncertainties and bias in the evaluated values were discussed and solutions to these problems were outlined. A coordinated working plan was prepared which will result in the preparation of new reaction cross section standards for light and heavy elements by 2004.

January 2003

CONTENTS

1. Meeting summary

V. Pronyaev, the Scientific Secretary, opened the meeting and presented a welcome address by A. Nichols, Head of the Section, who was unable to attend the meeting. After brief self-introductions by the participants, A. Carlson was elected as a Chairman and G. Hale as Rapporteur of the meeting. The Agenda was adopted with a few corrections and changes (see Appendix 1).

The objectives of the Coordinated Research Project (CRP) as formulated at the Consultants' Meeting on Improvement of the Standard Cross Sections for Light Elements (2-4 April 2001, Report INDC(NDS)-425 (2001), available on http://www-nds.iaea.org/indc_sel.html) were converted into an Action Plan and presented by V. Pronyaev. Primary aims will be to improve the evaluation methodology for the covariance matrices of the uncertainty in the R-matrix model fits, R-matrix evaluation of standards cross sections for light elements, and combining the light and heavy elements standards evaluations. At their May 2002 meeting, the Working Party on Evaluation Cooperation (WPEC) urged the RCM to accelerate the preparation of new standards evaluations, because work has already begun on new versions of national evaluated data libraries with their expected releases as early as 2005. These general purpose and specialized evaluations will require knowledge of the updated standards. Therefore, substantial changes should be introduced in the CRP working plan with extension of the objectives on evaluation of both light and heavy element standard reactions, and aiming the issue of the first version of the Standards evaluation in 2004. A. Carlson, as Chairman of Subgroup 7 of the WPEC (Nuclear Data Standards), which coordinates the measurements and updating of the data base for the standards, informed participants about the recommendations from the last WPEC meeting. He also summarized the evaluation process used for the ENDF/B-VI standards and provided recommendations for improvements to the new international evaluation process. RCM participants have agreed with the requested changes in the working plans. A problem is that some participants are heavily involved in laboratory tasks not related directly with standards, and cannot devote much time to the desired evaluations.

Session 1 was devoted to presentations by participants and follow-up discussions.

The capabilities of the microscopic resonating group model (RGM) with realistic two- and three-nucleon forces for prediction of the ^{3}He(n,p) reaction cross section (states in ^{4}He system) were demonstrated by H. Hofmann. This method requires very large amounts of computer time. Using three-body force calculations, the practical limit is approximately A=5. With two-body force calculations, it may be possible to calculate A=7, thus contributing to the ^{6}Li(n,t) cross section evaluation. The RGM results show more poles effecting the energy region where the cross section can be used as a standard, although some poles are very broad. The transformation to the R-matrix type of pole is needed in order to use them in the R-matrix analysis.

The results of R-Matrix fits of 5 sets (numbered from 0 to 4, see Attachment 1) of ^{6}Li(n,t) reaction cross section data treated as absolute for the TEST1 intercomparison were shown by G. Hale. The thermal value of the reaction cross section and one experimental data set for the total cross section were added to avoid an ambiguous determination of 10 free parameters. The normalization for Set 4 (Friesenhahn), which was discrepant compared with

all the others, was eventually released (constrained by error), but made only a small improvement in the fit. In fact, the EDA fit was not influenced very much by the Friesenhahn data, perhaps due to inconsistencies with the other data sets. The cross sections as well as covariance matrix for 13 energy points were calculated from the evaluated parameters and their covariance matrices. It was shown that the uncertainty of the evaluated curve increases from 0.5% at low energy (2.5 keV), where the influence of the additional thermal point value is extremely high, up to 1.5% at high energy (0.8 MeV). The correlation matrix shows clearly some strong medium energy range correlations, which are intrinsic features of the model fits, and small anticorrelations between some energies. Hale noted that all three R-matrix codes (EDA, RAC, and SAMMY) gave the same results when calculating cross sections from the same R-matrix parameters, using non-relativistic kinematics. Unfortunately, the additional data sets used for the EDA parameter search did not permit direct intercomparison with the results of the TEST1 exercise for other model and non-model fits. The participants discussed later in the meeting how the test data might be expanded and modified to allow such direct comparisons to be made (see the item about R-matrix intercomparison below).

Detailed studies of error propagation in the R-matrix model fitting were presented by Chen Zhenpeng. The simulated data set for each type of data (channel) was prepared from realistic R-matrix parameters for standard reactions passing though ^{7}Li, ^{11}B or ^{16}O composite systems in the energy region of interest. Realistic uncertainties were assigned to the simulated cross sections in different channels. The covariance matrix of the simulated data was constructed from 3 components: Long Energy Range Correlation (LERC), Medium Energy Range Correlation (MERC) and Short Energy Range Correlation (SERC) components. The relative contributions of components can be varied, keeping the total variance unchanged and the Error Propagation Coefficient (EPC) was defined as the ratio of the average relative uncertainty of the model evaluated data to the same quantity for the experimental data of a given type. Thus EPC shows which role is played by different components of the uncertainty for a given type of data (channel). The result for the ^{6}Li(n,t) reaction shows that consideration and inclusion of MERC can substantially increase the EPC. Hence treatment of all non-statistical components of error only as a LERC will lead to the underestimation of the uncertainty. An empirical formula for evaluation of the EPC was proposed.

The intercomparison of capabilities of different R-matrix fitting codes EDA, RAC and SAMMY was given by N. Larson. Because the codes were initially oriented for solution of different tasks, each of them has its own specific features. The SAMMY code presented by N. Larson can (and should, where it is possible) work with raw data. This means that counts per channel in time-of-flight measurements can be introduced as primary data. Cross sections and their covariance matrices will be obtained through data reduction based on the use of the error propagation law and detailed information about the experiment (spectrometer resolution function, background, etc.) and corrections, which should be applied. There are built-in options for possible adjustment of the data considered as discrepant due to possible errors in energy calibration, background separation, etc. These features of data reduction in the SAMMY code can be used for the preparation of cross sections and covariance matrices used by other R-matrix codes for evaluation of standard cross sections. It was pointed out that the raw data (counts) could be fitted with a covariance matrix that is diagonal (purely statistical, non-correlated). However, it is not likely that many experimentalists would provide necessary information to do this.

Carlson presented studies of the database for the standard reaction cross sections and new experimental data, obtained after the last standards evaluation, that should be incorporated in the database. Although many experiments have been completed, a large number are still in the data processing and analysis stage. The list of experiments for which data have been obtained or measurements are underway was given. Contributions, which can lead to significant changes in the evaluated values, are expected in the H(n,n), ^{10}B(n,α), ^{235}U(n,f) and ^{238}U(n,f) cross sections. As a result some important discrepancies in the experimental database for the H(n,n) and ^{10}B(n,α) reactions are expected to be resolved. A new evaluation of the ^{235}U(n,f) cross section completed by T. Kawano et al. for the JENDL library with inclusion of all the latest data is several percent higher than the present ^{235}U(n,f) standard in the energy region from about 1 to 5 MeV. It is unclear to which extent this discrepancy is due to inclusion of new data or because data from EXFOR were used without their renormalization to new standards and additional corrections (as was done by W. Poentz for the standards database).

The problem of the underestimation of evaluated cross-section uncertainties is addressed in paper presented by S.Badikov and E.Gai. Two basic sources of the underestimation of evaluated cross-section uncertainties - a) inconsistency between declared and observable experimental uncertainties and b) inadequacy between applied statistical models and processed experimental data - are considered. Both the sources of the underestimation are mainly a consequence of existence of the uncertainties unrecognized by experimenters. A model of a “constant shift” is proposed for taking unrecognised experimental uncertainties into account. The model predicts for each data set the renormalization coefficient, systematic and statistical uncertainties. The model is applied for statistical analysis of the ^{238}U(n,f)/^{235}U(n,f) reaction cross-section ratio measurements. The authors demonstrate that multiplication by sqrt(χ^2) as instrument for correction of underestimated evaluated cross-section uncertainties fails in case of correlated measurements. It is also shown that arbitrary assignment of uncertainties and correlation in a simple least squares fit of two correlated measurements of unknown mean (like in case of Peelle’s Puzzle) leads to physically incorrect evaluated results.

The problem of obtaining reliable (in the sense of statistical significance) evaluated covariance matrices in the least squares model and non-model fits with implementation of full error propagation law were discussed by Soo-Youl Oh. The simple model of three non-correlated sets presenting data at four points was taken to avoid unneeded complexity. Model fits with splines of different orders and non-model GMA fits were done. As expected, the model fit with a spline of third order gives the same evaluated central value and covariance matrix as non-model GMA fit. Fits with second order, linear and inverse linear splines give different evaluation of central values and covariance matrices. Because of near-linear dependence of the fitted data, the difference in central values is small. The general tendency is the increasing the diagonal and decreasing off-diagonal covariances, with the growth of the order used for the spline. This is how such an intrinsic property of the model function as shape propagates into the covariance matrix of evaluated data. A peculiar feature observed is that with good accuracy all fits give the same univariate (one-group) collapsed variance, namely the sum of all elements of a covariance matrix does not depend on the order of the spline or type of model/non-model fit (type of sum rule for uncertainty). The presence of the Peelle’s Pertinent Puzzle (PPP) in the fitting of discrepant data, which can lead to an unphysical decrease of evaluated values and use of Box-Cox transformation to overcome this problem, was demonstrated. In many cases it requires just a logarithmic transformation of the

data and uncertainties, a least squares fit and back transformation of evaluated data and uncertainties. Although the expert's solution for removing discrepancies is preferable, the inclusion of this procedure in the least squares fitting codes is desirable.

The use of the KALMAN system for error analysis was presented by T. Kawano. The system includes the SOK code, which provides preparation of data and their least square fitting based on the Bayesian approach. Runs with TEST1 data was undertaken for a spline function with a variable number of nodes (parameters): 10, 18 and 35. Unfortunately, direct intercomparison with the fits using non-model GMA, GLUCS and R-matrix model RAC code for TEST1 case was impossible, because these codes evaluate data for 51 points (nodes). The general tendency observed is that with increasing number of nodes (that gives larger freedom to the shape of the model function) all elements of the covariance matrix of uncertainty of the data evaluated in these nodes decreases with a larger decrease of the non-diagonal elements in comparison with the diagonal ones. The uncertainties of data evaluated at 35 nodes for a very complex model function were still well above that of non-model least square fitting. If the fitting could be done with a spline of 51 nodes, evaluated data and covariance matrix uncertainty would be identical to the non-model fitting for 51 points (as was shown by Soo-Youl Oh above for case of four nodes). Another model function selected for test, was a Lorentzian resonance with 1/v addition, which (as could be expected) with only four parameters might describe the shape of fitted data. The fitting with this model function was carried out at 35 points to make possible a comparison with 35 knots spline fitting. Chi-square of fitting was rather large due to a clear inability of the model to describe the energy dependence on the right side of the resonance at 247 keV. Adding the constant term as a fifth parameter will substantially improve the chi-square of fitting.

V. Pronyaev presented the results of TEST1 data fitting with the generalized least square code GMA versus the Bayesian code GLUCS. A simple correction was introduced in the version of the GMA code transferred to the IAEA in November 1999. Without this correction, GMA accumulated in the adjustment vector of the evaluated cross section the contribution only from the last block (correlated set) of the data. This correction does not influence the covariance matrix of uncertainty of the evaluated data. The results of fitting of TEST1 discrepant data with GMA and GLUCS codes based on different numerical algorithms, had shown a difference of stochastic nature in the limits not exceeding 0.5%. A check was made to ensure that the order of data input does not influence the final GMA and GLUCS results. TEST2 was prepared, to check the numerical convergence of the results of calculations with GLUCS and GMA when large numbers of data are treated by the codes. Thus, TEST2 was designed in such a way, that the result of evaluation of the cross section in the limit of a large number of data sets should asymptotically converge to the values known prior to the process of evaluation. For 501 data sets fitted with GMA, the difference from the known asymptotic value was to be less than 0.1%. The conclusion about good performance of GMA code should be still reviewed independently in other conditions of GMA fitting. The effect of PPP was clearly observed in the fitting of TEST1 data sets over the resonance in the ^{6}Li(n,t) reaction. Fitting the logarithms of the data points and revising the uncertainties of discrepant data sets might exclude the PPP effect.

The next session was devoted to the discussions of open (unsolved) problems in the standards evaluation, which are summarized below. An Action List based on these discussions was prepared after the meeting and agreed upon by the participants.

Problems with least-squares fits: Kawano stated that he uses log(sigma) in data fitting. Although GLUCS and GMA appear to agree very well, Kawano will do his calculations with SOK. This comparison will involve using the same starting values. Kawano and Talou have done comparison work at Los Alamos with GLUCS, which appears (visually) to give the same results. Pronyaev will send information to Kawano to make direct comparisons using the same starting values. Badikov pointed out that GMA handles more different types of input data than GLUCS. However, overall, there were no real problems seen with least-squares fitting. Pronyaev pointed out that large variation in cross sections may cause numerical instabilities in GMA/GLUCS fittings if correlations are large. It could be worthwhile incorporating Chiba's modifications to GMA into a new GMAR, and PPP problem might be overcome. Perhaps we should also make a new GMA version (GMAR4) incorporating the logarithmic transformation discussed by Oh. Badikov suggested further discussion on PPP. Vonach pointed out that RAC calculations shown in the Pronyaev presentation "Test and Intercomparisons…" is systematically lower than the experimental data in the low-energy range. Chen replied that he has a newer solution that is better.

Oh noted the interesting result that the correlation matrix for his fitting of an approximately linear function was the same for any function having the same number of fitting parameters.

Kawano showed SOK results with and without the logarithmic transformation. When there are cross-energy correlations in the data sets, the results with the log(sigma) transformation are different (and better) than those without; without cross-energy correlations, the results are the same. Also, he confirmed that the log transformation gives a reasonable result for combining the correlated points in the classic PPP example. SOK results without the log transformation agree within a few tenths of a percent with those of GMA/GLUCS. Differences may be explained by rounded-off values of covariances used for input in SOK.

Oh pointed out that the log transformation is a special case of the Box-Cox transformation, and may work in PPP because this transformation linearizes the dependence on normalization factors.

Non-diagonal elements of covariance matrices: Chen talked about the effect of long- and medium-range correlations on output covariances in R-matrix fitting. For only statistical (uncorrelated) error, the error reduction is about 1/20. For non-zero amounts of Y (long-range correlations) and M (medium-range correlations), the error-reduction factors rise rapidly. He showed contour plots of the correlation coefficients for the ^{6}Li(n,t) cross section with features that correspond to local and non-local effects of the resonance parameters. He also showed results for ^{16}O(n,n) reaction that has more resonances. He showed results of ^{6}Li(n,t) to illustrate effect of input covariances on the output values. Input correlations tend to increase output correlations. This work is important and needs further study, elucidation and documentation.

Chen also showed various RAC fits which included the five ^{6}Li(n,t) cross sections, supplemented by various other measurements, including a thermal value, total cross sections, and charged-particle data. The results using only the five reaction cross section sets were similar to those from GMA/GLUCS. Removing the discrepant Friesenhahn data changed the RAC fit considerably. This result is different from that obtained by Hale in his EDA analysis.

Badikov commented on "ill-posed" mathematical problems for the case where there is no unique solution. For a positive definite covariance matrix of the parameters, the propagated covariance matrix is also positive definite if the rank of the sensitivity matrix is equal to the number of parameters. If the rank exceeds the number of parameters, the result is semipositive-definite (zero eigenvalues), and the predicted uncertainties are only lower limits. Hofmann pointed out that numerical round off could even cause such matrices to have negative eigenvalues that are meaningless.

Pronyaev discussed uncertainty for correlated data, starting from the standpoint of information entropy. For the case of a simple univariate Gaussian, this becomes proportional to the log of the variance. In the multivariate case, it is proportional to the log of the determinant of the covariance matrix. Further, he discussed a means of collapsing (grouping) the multivariate case to produce a single quantity. He showed how Chen's RAC fit for the first data set (Lamaze) changes the uncertainties on the input experimental data. The variances changed, but the covariances exhibited little changes. Also he showed the behavior of GMA, GLUCS, and RAC when all five data sets were fitted. There was again a reduction of the variances, but very little difference in the output off-diagonal covariances of the three different codes.

R-matrix intercomparison: Hale proposed that a common set of initial data and covariances be used to compare the behavior of the three R-matrix codes. He volunteered to put together a set of neutron total cross sections and a thermal reaction value to supplement the existing 5 sets of reaction data. Pronyaev suggested gradually reduce the influence of these additional data to see the effect on the R-matrix fits. In the limit that the additional data became noninformative, his expectation was that the R-matrix results would approach those of the model-independent fits. However, the physical constraints on the energy dependence of the R-matrix calculations would not allow this sort of equivalence to be realized fully, even in that limit.

Improvements in R-matrix codes were discussed briefly. One item that might eventually be required is the addition of medium-range initial correlations to EDA, but that would be difficult to achieve because of the structure of the code. Another was checking for positive-definiteness of the parameter covariance matrix at a solution in RAC and SAMMY, as does EDA.

Proposed format for resonance data and their uncertainties was presented by Larson. The Reich-Moore format is too restrictive for many cases of interest. The proposed format is more general, but not all the necessary conventions have been considered. She also proposed a compact format for storing the parameter covariances from a resonance analysis that involved truncating them to two significant digits. Hofmann again pointed out the problem with this truncation introducing spurious negative eigenvalues, and suggested tabulating the most significant eigenvalues and their associated eigenvectors.

Kawano raised concerns about how Poenitz had renormalized the cross sections that were used in the ENDF/B-VI. Carlson emphasized that the larger effects from Poenitz were corrections to experiments he deduced by studying the documentation, etc. The renormalization to the new hydrogen cross section was a rather small correction in most cases. Poenitz is attemping to obtain from long-term storage his data books containing the information he used to make the various corrections. These books could then be used to

verify the corrections that were made, before being properly archived.

Pronyaev showed measurements from EXFOR and CINDA that were made after, or had not been included in, Poenitz's data base. Several data sets appeared to have been missed, and Carlson said he would check on them. There were many new data sets for ^{235}U(n,f), including a large high-resolution measurement with much structure at energies between 0.1 and 2 keV. Carlson was unsure how much effort would be necessary in dealing with such data (energy averaging), but would consider the possibility later in the meeting. The same question arose with a similar measurement for ^{239}Pu(n,f). Pronyaev volunteered to help obtain experimental papers and possibly data, especially from Russian reports which are more easily obtained from the IAEA, to ensure that the data listed in EXFOR reflect the latest, revised values. Pronyaev's suggestion that the hydrogen cross section be included in the GMA data base initiated a long discussion about whether the ratios or cross sections had been included in the ENDF/B-VI GMA data base. It appears that cross sections were used, but Kawano pointed out that it was not always obvious what (earlier) hydrogen standard had been used to obtain the ratio data that were then converted to cross sections using the Version VI hydrogen cross section. Carlson pointed out that it was usually easy to determine what hydrogen standard was used in a given experiment from the documentation. When direct information was not given in the documentation, it was assumed that the standard used was that of the ENDF/B version available at the time of the experiment. This assumption is quite likely to be correct since so few evaluations of the hydrogen cross section have been made.

Hale gave a brief update on the status of the n-p analysis, which continues to give a very good fit to the n-p total cross section and differential scattering cross sections at energies up to 30 MeV.

Kawano described work on ^{235}U(n,f) and other standards using SOK. He saw differences with ENDF/B-VI presumably starting from the same experimental data base. The differences may come from the logarithmic transformation of the cross sections in SOK, and from the treatment of normalizations and experimental corrections by Poenitz. Czirr shape data have a very strong effect on the outcome, and therefore it is very sensitive to the corrections made by Poenitz (and others) for this data set.

Pronyaev showed recent results from Mannhart's evaluation of the ^{235}U thermal neutron induced fission neutron spectrum averaged ^{235}U(n,f) cross section. The new value (1219 ± 14 mb) had increased somewhat (1.6%) from his 1985 value. The same tendency is seen for ^{252}Cf spectrum averaged cross sections. Result of NIST (I.G. Schroder et al., 1985) measurements of ^{252}Cf spectrum averaged ^{235}U(n,f) cross section (1234 ± 17 mb) is also about 2% above the 1987 Mannhart evaluation (1210 ± 15 mb). There is a strong need to re-evaluate the ^{252}Cf spontaneous fission neutron spectrum averaged cross sections, as well as thermal neutron spectrum averaged cross sections.

A definite schedule for the work plan was discussed. The R-matrix codes will be compared starting from the same data set, as constructed by Hale. This data set will include the five ^{6}Li(n,t) cross-section sets given by Pronyaev, a thermal value, and total cross sections from thermal up to about 1 MeV. The construction of this data set is will take less than two months, while further comparison of the R-matrix results (solutions, output covariances) will take another two months. The next step is to investigate the effects of medium-range correlations in RAC and SAMMY on the output covariances (estimated to take two months).

During the same six-month period, Hofmann and Hale will investigate how to extract R-matrix parameters from microscopic resonating group calculations. They will first try the procedure on the ^{4}He system, in the hope of improving the ^{3}He(n,p) cross section, and then extend to resonances in the ^{7}Li system, in order to obtain information about background levels and possibly unknown broad states in the region of interest. The work on ^{7}Li system is expected to improve the ^{6}Li(n,t) cross-section standard.

The group returned to matters related to the generalized least-squares codes. There was a long discussion about the use of the logarithmic transformation (or its generalization) in these codes to take care of PPP-type effects. An alternative is to adjust the errors on discrepant data (or neglect them), so that the PPP effects may not appear. Oh will investigate the 5-set test data using GMA with and without the logarithmic transformation (estimated to take three months).

New experimental data for the analyses should be available before August of 2003.

Discussion followed on the combination process. The most likely path is to use the output from the R-matrix and least-squares codes to undertake the combination, probably using GMA. Other possibilities would be to use Muir's code ZOTT, or to modify SAMMY to treat the results from the GMA analysis. Kawano pointed out that SOK can also be used, and has the advantage that the experimental data do not have to be placed on a fixed grid. GLUCS is no longer needed now that favorable comparisons have been established. Further CRP work with GLUCS would require significant additional coding effort.

Preparation of the experimental data base will be handled by Carlson and Pronyaev (EXFOR), with help from Vonach and possibly others. Techniques developed by Badikov and Gai will be useful for identifying data that require special attention. Also the procedure suggested by Vonach using auto-correlation studies should be considered. A similar procedure was used in an iron total cross-section evaluation.

Kawano will produce simulated data with known means in order to investigate what happens with the different codes in the case when the data are forced to be discrepant, and with strong correlations. By fitting these data with R-matrix parameters, as for ^{56}Fe, Kawano may gain insight into how the PPP may enter R-matrix fits. Badikov also has a simple procedure for producing such data sets. Vonach suggested looking at these effects in just some (say two) of the data sets. Kawano did this for sets 0 (Lamaze) and 3 (Poenitz) using SOK, and saw no difference using the log transformation. Pronyaev could use GMA to investigate the effect of increasing the off-diagonal correlations for this test case. The covariance matrices of experimental data should be prepared for this test as the sum of covariance matrices for long-range (LER) and short-range (SER) correlation components, but not through artificially assigning the same correlation coefficient to all the off-diagonal elements of the correlation matrix.

Based on work done by Zhou, the consistent view of the group was that PPP relates to an idealization that should not occur in practice. It was felt that a more physical construction of covariances would eliminate this problem in GMA. This feeling was reinforced by the GMA test of the Lamaze/Poenitz data (they are rather consistent) performed by Pronyaev, in

which the output cross sections were much lower than the measurements for 99% long-ranged correlations. Vonach pointed out that such a large correlation is not physically possible, but a similar effect was also evident for 50% correlation. This raised concerns about whether this effect actually occurred in ENDF/B-VI, and could occur in the new GMA evaluation. Again, the possibility was raised that the logarithmic transformation could mitigate this effect. Carlson reminded the CRP that Poenitz increased the uncertainties of data which were greater than three standard deviations away from the output results in an effort to remove problems with discrepancies.

Carlson suggested that a trial combination of the ^{6}Li and ^{10}B data along the lines of the ENDF/B-VI combination be done with GMA about six months into the next year. Hale will provide preliminary output from the ^{7}Li and ^{11}B system analyses at that time for this trial.

Larson said she would investigate putting a GMA-type algorithm in SAMMY to evaluate the physical reasonableness of covariance matrices. She described how experimental covariances are constructed with SAMMY. Vonach suggested an iterative procedure for correcting his estimates of the medium-range correlations.

Kawano commented that the log transformation has the effect of weighting all data with the same percentage uncertainty the same way, independent of the size of the cross section; whereas using the cross section tends to weight smaller values with the same percentage uncertainty more heavily. He also asked about the role of normalization parameters and their covariances in GMA analyses.

Oh asked about energy uncertainties in GMA. There is a “slot” to give this type of information in the input to the code, and all agreed that this feature should be used. However, Carlson was not sure how these uncertainties were actually used (if at all) in the fitting process, and suggested this behavior be checked.

Pronyaev commented on the types of publications that could be produced in connection with the project. He advised us that, while not required, electronic publications of any length dealing with any part of the research can be put on the IAEA website. The proceedings of this meeting are planned to be published within about two months. He will produce, with help from Carlson and Hale, an initial draft of recommendations (primarily the work plan) and conclusions from the meeting, and then circulate them for comment to all participants.

The next meeting was tentatively scheduled for 13-17 October of 2003 near Washington DC (NIST at Gaithersburg, MD).

2. Action list

1. Input from Resonating Group Microscopic Nuclear Model (RGM) predictions to the R-Matrix (RM) Phenomenological Model Fit

No.	Action	Participant(s)	Terms
1.1.	To prepare specification for conversion of the RGM parameters in the parameters of the R-Matrix model.	H. Hofmann, G. Hale	October 2002
1.2.	To prepare the subroutines for this conversion.	H. Hofmann	February 2003
1.3	To make RGM calculations which account for all channels contributing in the energy range of the interest of standards for system with A=4 and A=7 trough poles located in this energy range or through distant poles. To prepare the information on R-Matrix poles.	H. Hofmann	July 2003

2. R-Matrix codes inter-comparison and data evaluation: testing of different approaches to the implementation of the error propagation law in codes EDA, SAMMY and RAC, testing of the convergence in the parameters search, testing in the cases when strong non-linearity in parameters/cross section exists; comparison of the results of the R-matrix model with non-model fit based on the same sets of the experimental data

No.	Action	Participant(s)	Terms
2.1.	To prepare specification for R-Matrix codes search and covariance matrix inter-comparison, which should include 5 data sets for ^{6}Li(n,t) reaction specified for TEST1 (all treated as absolute cross-section measurements), thermal cross section and one data set for each ^{6}Li(n,total) and ^{6}Li(n,elastic). Data for additional cross sections/channels can be used for unambiguous determination of R-Matrix parameters which will be used as starting values in fittings with gradual conversion of additional cross sections/channels in the non-informative ones. To distribute data for this test to all participants.	G.Hale	October 2002
2.2.	To test to what extent the linear approximation for presentation of sensitivity coefficients is good for case of R-Matrix fit of ^{6}Li(n,t) reaction. To test the accuracies of numerical versus analytical determination of sensitivity coefficients applied in different R-matrix codes.	G.Hale, Chen Zhenpeng, N.Larson	November 2002
2.3.	To run PADE-2 model fit for TEST1 case (5 data sets) and send results to the NDS for intercomparison.	S.Badikov	November 2002
2.4.	To intercompare the results of least-squares fits with R-Matrix codes EDA, RAC and SAMMY and R-Matrix codes versus non-model codes GLUCS, GMA and SOK. To demonstrate the factors leading to the reducing of the variances in the R-Matrix model fits: unitarity following from relations between total and partial channels and intrinsic medium and long energy range correlations induced by model through predetermined functional shape.	G.Hale, Chen Zhenpeng, N.Larson, S.Tagesen, V.Pronyaev, Soo-Youl Oh, T.Kawano	December 2002

2.5.	To finalize the studies of error propagation in the model fits and send the paper to the NDS/IAEA for publication as INDC report.	Chen Zhenpeng	January 2003
2.6.	To review and prepare data for neutron induced channels in ^{3}He+n, ^{10}B+n and ^{6}Li+n reactions, which will be processed by R-matrix codes and exclude these data from the non-model fits.	G.Hale, N.Larson, A.Carlson, H.Vonach, V.Pronyaev	January 2003
2.7.	To review and prepare data for all other channels which are needed for R-matrix fitting of ^{3}He+n, ^{10}B+n and ^{6}Li+n reactions.	G.Hale, N.Larson, A.Carlson, H.Vonach, V.Pronyaev	February 2003
2.8.	To extend SAMMY code with inclusion of the option for simultaneous fits of direct and inverse channels.	N.Larson	May 2003
2.9.	To evaluate ^{3}He(n,t), ^{10}B(n,α) and ^{6}Li(n,t) reactions in R-Matrix model fits with EDA, RAC and SAMMY codes.	G.Hale, Chen Zhenpeng, N.Larson	September 2003

3. GMA database of experimental cross sections for standards evaluation and evaluation of data with GMA.

No.	Action	Participant(s)	Terms
3.1.	To prepare the list of experimental data which are not included in the Poenitz database (as September 1997) for standards and compile them in EXFOR (or EXFOR-like shortened format).	A.Carlson, V.Pronyaev	December 2002
3.2.	To explore the possibility of re-evaluation of thermal cross sections and resonance integrals needed for standards evaluations (revision of Axton evaluation, paying attention to the solution of the "puzzles" in the least squares fit and benchmark experiments).	A. Carlson	December 2002
3.3.	To analyze new data and prepare input for generation of covariance matrices of these data with RCL.F and DAT.F codes (data preparatory codes for GMA). Test these new data for consistency with other data in the database.	A.Carlson, H.Vonach, V.Pronyaev	February 2003

3.4.	To analyze all of the database for data consistency and local discrepancy and to improve discrepant data by correcting (including cutting of the data at the edges) or revision of their covariance matrices using method of introducing of medium energy correlations for data discrepant with a posterior evaluated data (by H. Vonach and S. Tagesen) or method of treatment of unrecognized systematical error proposed by S.Badikov.	A.Carlson, H.Vonach, S.Badikov, S.Tagesen, V.Pronyaev	July 2003
3.5.	To run GMA with a full database and to estimate quality of the fitting, paying special attention to the energy regions where cross sections has no smooth behavior ((n,f) and (n,γ) cross sections at heavy elements for energy below 10 keV).	Soo-Youl Oh, V.Pronyaev	September 2003
3.6.	To prepare database of cross sections for high energy standard cross sections (En > 20 MeV) and input for GMA	A.Carlson, V.Pronyaev	September 2003
3.7.	To make decision about possible exclusion of data for this region, if data reduction introduces large uncertainty in data.	A.Carlson, Soo-Youl Oh, V.Pronyaev	September 2003
3.8.	To run GMA with updated GMA database with exclusion of data, which where used in R-Matrix fit.	Soo-Youl Oh, V.Pronyaev	October 2003
3.9.	To run GMA with inclusion of high energy standard cross sections	Soo-Youl Oh, V.Pronyaev	November 2003

4. Study of Peelle's Pertinent Puzzle (PPP) and improvement of the GMA and other general least-squares codes to exclude bias of evaluated data caused by the PPP.

No.	Action	Participant(s)	Terms
4.1.	To prepare the MC numerically simulated data for testing at the PPP presence, e.g.: ^{6}Li(n,t) reaction with 51 data points as in TEST1 grid (cross sections are calculated from resonance parameters) with an equal Long Energy Range Correlation (LERC, 20%) and average Short Energy Range Correlation (SERC, 20%) components. Few tens (statistically significant number) of such uncorrelated data sets should be prepared, where each (central values) biased randomly (as MC numerically simulated) relative to the basic unbiased curve calculated from resonance parameters. The average value (half-width) of normally distributed bias could be taken as sqrt(20**2+20**2)=28.3%.	T.Kawano	November 2002

4.2.	To introduce Box-Cox transformation (logarithm transformation of data and covariance matrices of data if parameter λ=1) in the GMA code, which reduces PPP.	Soo-Youl Oh	November 2002
4.3.	To run GMA and SOK with and without logarithm transformation for test data prepared under 4.1. for study of presence of PPP.	T.Kawano, Soo-Youl Oh	November 2002
4.4.	To study the possibility of implementing S.Chiba&D.Smith ansatz in the GMA and SOK for exclusion of the PPP. Run test case prepared under 4.1., to demonstrate exclusion of PPP and comparison with logarithm transformation ansatz.	Soo-Youl Oh, T.Kawano	February 2003

5. Combining of the results of R-Matrix model fits for ^{10}B(n,α) and 6Li(n,t) reaction cross sections with general least-squares non-model evaluations of light and heavy element standards evaluations.

No.	Action	Participant(s)	Terms
5.1.	To study an option when light-element standard cross sections evaluated in R-Matrix model are introduced as data sets with their evaluated covariance matrix in the final combined GMA fit of light and heavy elements.	Soo-Youl Oh, T.Kawano, V.Pronyaev	November 2003
5.2.	To study an option in which R-matrix parameters, their covariance matrices and sensitivity coefficients are used and combined with the results of non-model general least square fits (ZOTT, KALMAN).	T.Kawano	November 2003
5.3.	To study an option when cross sections and their full covariance matrix evaluated in the non-model least-squares fit are used as input data set for R-matrix fitting.	N.Larson	November 2003

6. Other different important topics.

No.	Action	Participant(s)	Terms
6.1	To prepare CRP Web-site and make available to participants for downloading and uploading	V. Pronyaev	February 2003
6.2.	To make best evaluation of the numerical uncertainties introduced by the method of solution and numerical procedures (GLUCS versus GMA).	S.Tagesen, V.Pronyaev	February 2003
6.3.	To undertake best evaluation of the components of the uncertainty related with the underestimation of cross-energy, cross-reaction or cross-material correlations in the GMA database, which could be added to the final evaluated result.	H.Vonach	July 2003
6.4.	To study the data reduction and preparation of the covariance matrices of experimental data selected for R-Matrix model fit based on implementation of law of error propagation for separate components of the uncertainties.	N.Larson	May 2003

3. Annexes

Annex 1. Agenda and time schedule

International Atomic Energy Agency
First Research Co-ordination Meeting on
Improvement of the Standard Cross Sections for Light Elements
IAEA Headquarters, Vienna, Austria
23–27 September 2002
Meeting Room A-1972 (phone extension 21381)

Monday, 23 September

08:30 - 09:30 **Registration** (at Gate 1, IAEA Headquarters)

09:30 - 10:45 **Opening Session:**

- Welcome
- Round table self-introductions by participants
- Election of Chairman and Rapporteur
- Adoption of Agenda (Chairman)
- Objectives of CRP (V.G. Pronyaev and A.D. Carlson)

10:45 – 11:00 Coffee break

11:00 - 12:20 **Session 1: Presentations by Participants, and Discussions**

(max. 40 minutes for each presentation and discussion):

1. *Microscopic Calculations in the ^{4}He Systems using realistic two- and three-nucleon forces,* ***Hartmut M. Hofmann***, Universität Erlangen-Nürnberg, Erlangen, Germany.
2. *R-matrix Results from n+^{6}Li Test Data Using EDA,* ***Gerry M. Hale***, Los Alamos National Laboratory, USA.

12:20 - 14:00 **Lunch and Administrative/Financial Matters (Ms. Monica Wirtz)**

14:00 - 17:15 **Session 1: Presentations by Participants, and Discussions (cont.)**
[Coffee break when appropriate]

3. *Covariance Propagation in R-matrix Model Fitting,* ***Chen Zhenpeng,*** Tsinghua University, Beijing, China.
4. *A Different Perspective on Resonance Fitting,* ***Ms. Nancy M. Larson***, Oak Ridge National Laboratory, USA.
5. *Status of Experimental Database for Standard Reactions,* ***Allan D. Carlson***, National Institute of Standards and Technology, Gaithersburg, USA.

17:15 **Reception**, NDS: floor A-23 (adjacent to room A-2340)

Tuesday, 24 September

9:00 - 12:30 **Session 1: Presentations by Participants, and Discussions (contd.)**

[Coffee break when appropriate]

6. *Some Sources of Underestimation of Evaluated Cross Section Uncertainties*, ***Sergei A. Badikov, Evgenij V. Gai***, Institute of Physics and Power Engineering, Obninsk, Russia.
7. *Arbitrariness of Evaluated Covariance in Least-Squares Method,* ***Soo Youl Oh***, KAERI, Republic of Korea.
8. *Error Analysis with the KALMAN Code,* ***Toshihiko Kawano***, Kyushu University, Kasuga, Japan.
9. *Tests and Intercomparisons of Data Fitting with General Least Squares Code GMA Versus Bayesian Code GLUCS,* ***Vladimir G. Pronyaev***, IAEA Nuclear Data Section, Austria.

Session 2: Discussions and Presentations (everyone) - Objectives of CRP Revisited – Work to be Performed

- problems in least squares fits;
- non-diagonal elements of covariance matrix in R-matrix fit (*Chen Zhenpeng*);
- positive definiteness of covariance matrices (*S.A. Badikov*);
- measure of uncertainty for correlated data (*V.G. Pronyaev*);
- test to compare uncertainty reduction in model and non-model least squares fit;
- R-matrix codes intercomparison (*G.M. Hale, Chen Zhenpeng and Ms. N.M. Larson*);
- improvements in R-matrix codes;
- new ENDF format for resonance data and their uncertainties (*Ms. N.M. Larson*);
- reductions in uncertainty (under accounting for data correlations; discrepant data);
- GMA code and experimental database;
- evaluation of basic scattering standards [H(n, n) and C(n, n)];
- ^{235}U and ^{239}Pu (n,f) evaluation for JENDL-3.3 (*T. Kawano*);
- combining R-matrix and basic scattering standards with general GMA least squares fit
- etc.

12:30 - 14:00 **Lunch**

14:00 - 17:00 **Session 2: Discussions and Presentations - Objectives of CRP Revisited - Work to be Performed (cont.)**
[Coffee break when appropriate]
- see above.

Wednesday, 25 September

09:00 - 12:30 **Session 2: Discussions (cont.)**

[Coffee break when appropriate]
- see above.

12:30 - 14:00 **Lunch**

14:00 - 17:00 **Session 2: Discussions (cont.)**
[Coffee break when appropriate]
- see above.

19:30 **Dinner at restaurant**

Thursday 26 September

09:00 - 12:30 **Session 3: Distribution of Workloads**

[Coffee break when appropriate]

Assignment of tasks, including name and contents of the package,

List of actions,

TECDOC: structure and individual writing assignments?

12:30 - 14:00 **Lunch**

14:00 - 15:00 **Session 3: Distribution of Workloads (cont.)**
[Coffee break when appropriate]

Friday, 27 September

09:00 - 12:30 **Session 4: Drafting of the Meeting Report, and Conclusions**

[Coffee break when appropriate]
- prepare meeting report (in Working Groups),
- recommendations,
- review of actions.

Any other business
- next RCM.

12:30 **Lunch**

Annex 2. List of participants

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Annex 3. List of working papers presented at session 2 or submitted after the meeting

1. *"Evaluation of Covariance Matrices for Resolved and Unresolved Resonance Regions"* by T.Kawano, K.Shibata.

1. "^{235}U and ^{239}Pu (n,f) evaluation for JENDL-3.3" by T.Kawano.

2. *"Standard Error Propagation in R-matrix Model Fitting for Light Elements"* by Chen Zhenpeng, Zhang Rui, Sun Yeying and Liu Tingjin.

3. *"New Function for Deal with Covariance Matrix in RAC"* by Chen Zhenpeng and Sun Yeying.

4. *"Progress Report on Calculation of ^{6}Li(n,t) with RAC"* by Chen Zhenpeng and Sun Yeying.

5. *"Does Model Fit Decrease the Uncertainty of the Data in Comparison with a General Non-model Least Squares Fit?"* by V.G.Pronyaev.

6. *"Peelle's Pertinent Puzzle: Way of Solution"* by V.G.Pronyaev.

7. *"Standards Database Extension: New Results Since 1997 (data not included in ANL/NDM-139, 1997)"* by V.G.Pronyaev.

8. *"Proof that Bayes and Least Squares Give Exactly Equivalent Results for Arbitrary Number of Data Sets (assuming linearity)"* by N.M.Larson.

8. *"Box-Cox Transformation for Resolving Peelle's Pertinent Puzzlein Curve Fitting"* by Soo-Youl Oh.

Annex 4. Input data for TEST1 intercomparison

Five pseudo-experimental (but realistic) data sets (cross section and covariance matrices for ^{6}Li(n,α) reaction) have been prepared for testing GMA, GLUCS and RAC codes and study of the uncertainty reduction in the least-squares fits.

Data set #0 which covers all energy nodes and can be used as a prior for Bayesian fit.

```
CROSS SECTION      6Li(n,a)

 YEAR 1978 TAG  1 AUTHOR:  G.P.LAMAZE ET AL.   NSE68,183(1978)

SYSTEMATICAL (LONG ENERGY RANGE CORRELATION - LERC) UNCERTAINTY 1.6%

NO MEDIUM ENERGY RANGE CORRELATION (MERC) UNCERTAINTY

  ENERGY/MEV   VALUE   TOT. ABS.UNCERT. TOT. UNCERT./%

  0.2500E-02  0.3042E+01  0.2125E+00      7.0
  0.3500E-02  0.2570E+01  0.1695E+00      6.6
  0.4500E-02  0.2302E+01  0.1099E+00      4.8
  0.5500E-02  0.2078E+01  0.7621E-01      3.7
  0.6500E-02  0.1934E+01  0.6919E-01      3.6
  0.7500E-02  0.1821E+01  0.6031E-01      3.3
  0.8500E-02  0.1720E+01  0.5398E-01      3.1
  0.9500E-02  0.1585E+01  0.4060E-01      2.6
  0.1500E-01  0.1275E+01  0.3167E-01      2.5
  0.2000E-01  0.1130E+01  0.2807E-01      2.5
  0.2400E-01  0.1003E+01  0.2728E-01      2.7
  0.3000E-01  0.9217E+00  0.2220E-01      2.4
  0.4500E-01  0.7724E+00  0.1860E-01      2.4
  0.5500E-01  0.7240E+00  0.1690E-01      2.3
  0.6500E-01  0.6908E+00  0.1716E-01      2.5
  0.7500E-01  0.6516E+00  0.1569E-01      2.4
  0.8500E-01  0.6578E+00  0.1443E-01      2.2
  0.9500E-01  0.6619E+00  0.1594E-01      2.4
  0.1000E+00  0.6514E+00  0.1385E-01      2.1
  0.1200E+00  0.6984E+00  0.1397E-01      2.0
  0.1500E+00  0.8613E+00  0.1723E-01      2.0
  0.1700E+00  0.1140E+01  0.2500E-01      2.2
  0.1800E+00  0.1341E+01  0.2851E-01      2.1
  0.1900E+00  0.1597E+01  0.3395E-01      2.1
  0.2000E+00  0.1897E+01  0.4033E-01      2.1
  0.2100E+00  0.2275E+01  0.4292E-01      1.9
  0.2200E+00  0.2770E+01  0.5226E-01      1.9
  0.2300E+00  0.3107E+01  0.6214E-01      2.0
  0.2400E+00  0.3222E+01  0.7066E-01      2.2
  0.2450E+00  0.3181E+01  0.6976E-01      2.2
  0.2500E+00  0.3062E+01  0.6715E-01      2.2
  0.2600E+00  0.2797E+01  0.5594E-01      2.0
  0.2700E+00  0.2398E+01  0.5259E-01      2.2
  0.2800E+00  0.1956E+01  0.4159E-01      2.1
  0.3000E+00  0.1425E+01  0.3030E-01      2.1
  0.3250E+00  0.1022E+01  0.2386E-01      2.3
  0.3500E+00  0.8002E+00  0.1868E-01      2.3
  0.3750E+00  0.6561E+00  0.1580E-01      2.4
  0.4000E+00  0.5624E+00  0.1576E-01      2.8
  0.4250E+00  0.4666E+00  0.2361E-01      5.1
  0.4500E+00  0.4512E+00  0.2758E-01      6.1
  0.4750E+00  0.4248E+00  0.2352E-01      5.5
  0.5000E+00  0.3877E+00  0.1962E-01      5.1
  0.5200E+00  0.3684E+00  0.1725E-01      4.7
  0.5400E+00  0.3489E+00  0.1503E-01      4.3
  0.5700E+00  0.3309E+00  0.1184E-01      3.6
  0.6000E+00  0.3153E+00  0.9896E-02      3.1
  0.6500E+00  0.2867E+00  0.8510E-02      3.0
  0.7000E+00  0.2742E+00  0.7682E-02      2.8
  0.7500E+00  0.2568E+00  0.6986E-02      2.7
  0.8000E+00  0.2463E+00  0.6308E-02      2.6

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  0.55 0.62 0.62 0.58 0.53 0.53 0.53 0.58 1.00
  0.17 0.18 0.25 0.33 0.34 0.36 0.38 0.47 0.48 0.48 0.44 0.50 0.50 0.52 0.48 0.50 0.55 0.50 0.57 0.60 0.60 0.55 0.57 0.57
  0.57 0.64 0.64 0.60 0.55 0.55 0.55 0.60 0.55 1.00
  0.17 0.18 0.25 0.33 0.34 0.36 0.38 0.47 0.48 0.48 0.44 0.50 0.50 0.52 0.48 0.50 0.55 0.50 0.57 0.60 0.60 0.55 0.57 0.57
  0.57 0.64 0.64 0.60 0.55 0.55 0.55 0.60 0.55 0.57 1.00
  0.16 0.17 0.23 0.30 0.31 0.33 0.35 0.43 0.44 0.44 0.40 0.46 0.46 0.47 0.44 0.46 0.50 0.46 0.52 0.55 0.55 0.50 0.52 0.52
  0.52 0.58 0.58 0.55 0.50 0.50 0.50 0.55 0.50 0.52 0.52 1.00
  0.16 0.17 0.23 0.30 0.31 0.33 0.35 0.43 0.44 0.44 0.40 0.46 0.46 0.47 0.44 0.46 0.50 0.46 0.52 0.55 0.55 0.50 0.52 0.52
  0.52 0.58 0.58 0.55 0.50 0.50 0.50 0.55 0.50 0.52 0.52 0.47 1.00
  0.15 0.16 0.22 0.29 0.30 0.32 0.34 0.42 0.43 0.43 0.39 0.44 0.44 0.46 0.43 0.44 0.48 0.44 0.50 0.53 0.53 0.48 0.50 0.50
  0.50 0.56 0.56 0.53 0.48 0.48 0.48 0.53 0.48 0.50 0.50 0.46 0.46 1.00
  0.13 0.14 0.19 0.25 0.26 0.28 0.29 0.36 0.37 0.37 0.34 0.38 0.38 0.39 0.37 0.38 0.42 0.38 0.43 0.46 0.46 0.42 0.43 0.43
  0.43 0.48 0.48 0.46 0.42 0.42 0.42 0.46 0.42 0.43 0.43 0.39 0.39 0.38 1.00
  0.07 0.08 0.11 0.14 0.14 0.15 0.16 0.20 0.20 0.20 0.19 0.21 0.21 0.22 0.20 0.21 0.23 0.21 0.24 0.25 0.25 0.23 0.24 0.24
  0.24 0.27 0.27 0.25 0.23 0.23 0.23 0.25 0.23 0.24 0.24 0.22 0.22 0.21 0.18 1.00
  0.06 0.06 0.09 0.11 0.12 0.13 0.13 0.16 0.17 0.17 0.15 0.17 0.17 0.18 0.17 0.17 0.19 0.17 0.20 0.21 0.21 0.19 0.20 0.20
  0.20 0.22 0.22 0.21 0.19 0.19 0.19 0.21 0.19 0.20 0.20 0.18 0.18 0.17 0.15 0.08 1.00
  0.07 0.07 0.10 0.13 0.13 0.14 0.15 0.18 0.19 0.19 0.17 0.19 0.19 0.20 0.19 0.19 0.21 0.19 0.22 0.23 0.23 0.21 0.22 0.22
  0.22 0.25 0.25 0.23 0.21 0.21 0.21 0.23 0.21 0.22 0.22 0.20 0.20 0.19 0.17 0.09 0.08 1.00
  0.07 0.08 0.11 0.14 0.14 0.15 0.16 0.20 0.20 0.20 0.19 0.21 0.21 0.22 0.20 0.21 0.23 0.21 0.24 0.25 0.25 0.23 0.24 0.24
  0.24 0.27 0.27 0.25 0.23 0.23 0.23 0.25 0.23 0.24 0.24 0.22 0.22 0.21 0.18 0.10 0.08 0.09 1.00
  0.08 0.08 0.11 0.15 0.15 0.17 0.17 0.21 0.22 0.22 0.20 0.23 0.23 0.23 0.22 0.23 0.25 0.23 0.26 0.27 0.27 0.25 0.26 0.26
  0.26 0.29 0.29 0.27 0.25 0.25 0.25 0.27 0.25 0.26 0.26 0.23 0.23 0.23 0.20 0.11 0.09 0.10 0.11 1.00
  0.09 0.09 0.12 0.16 0.17 0.18 0.19 0.23 0.24 0.24 0.22 0.25 0.25 0.25 0.24 0.25 0.27 0.25 0.28 0.30 0.30 0.27 0.28 0.28
  0.28 0.31 0.31 0.30 0.27 0.27 0.27 0.30 0.27 0.28 0.28 0.25 0.25 0.25 0.21 0.12 0.10 0.11 0.12 0.13 1.00
  0.10 0.11 0.15 0.20 0.20 0.22 0.23 0.28 0.29 0.29 0.26 0.30 0.30 0.31 0.29 0.30 0.33 0.30 0.34 0.36 0.36 0.33 0.34 0.34
  0.34 0.38 0.38 0.36 0.33 0.33 0.33 0.36 0.33 0.34 0.34 0.31 0.31 0.30 0.26 0.14 0.12 0.13 0.14 0.15 0.17 1.00
  0.12 0.12 0.17 0.22 0.23 0.25 0.26 0.32 0.33 0.33 0.30 0.34 0.34 0.35 0.33 0.34 0.37 0.34 0.38 0.41 0.41 0.37 0.38 0.38
  0.38 0.43 0.43 0.41 0.37 0.37 0.37 0.41 0.37 0.38 0.38 0.35 0.35 0.34 0.29 0.16 0.13 0.15 0.16 0.17 0.19 0.23 1.00
  0.12 0.13 0.18 0.24 0.24 0.26 0.27 0.34 0.35 0.35 0.32 0.36 0.36 0.37 0.35 0.36 0.39 0.36 0.41 0.43 0.43 0.39 0.41 0.41
  0.41 0.46 0.46 0.43 0.39 0.39 0.39 0.43 0.39 0.41 0.41 0.37 0.37 0.36 0.31 0.17 0.14 0.16 0.17 0.18 0.20 0.24 0.27 1.00
  0.13 0.14 0.19 0.25 0.26 0.28 0.29 0.36 0.37 0.37 0.34 0.38 0.38 0.39 0.37 0.38 0.42 0.38 0.43 0.46 0.46 0.42 0.43 0.43
  0.43 0.48 0.48 0.46 0.42 0.42 0.42 0.46 0.42 0.43 0.43 0.39 0.39 0.38 0.33 0.18 0.15 0.17 0.18 0.20 0.21 0.26 0.29 0.31
  1.00
  0.13 0.14 0.20 0.26 0.26 0.28 0.30 0.37 0.38 0.38 0.35 0.39 0.39 0.40 0.38 0.39 0.43 0.39 0.44 0.47 0.47 0.43 0.44 0.44
  0.44 0.50 0.50 0.47 0.43 0.43 0.43 0.47 0.43 0.44 0.44 0.40 0.40 0.39 0.34 0.19 0.15 0.17 0.19 0.20 0.22 0.26 0.30 0.32
  0.34 1.00
  0.14 0.15 0.21 0.27 0.28 0.30 0.32 0.39 0.40 0.40 0.37 0.42 0.42 0.43 0.40 0.42 0.46 0.42 0.47 0.50 0.50 0.46 0.47 0.47
  0.47 0.53 0.53 0.50 0.46 0.46 0.46 0.50 0.46 0.47 0.47 0.43 0.43 0.42 0.36 0.20 0.16 0.18 0.20 0.21 0.23 0.28 0.32 0.34
  0.36 0.37 1.00
```

Data set #1.

```
YEAR 1972 TAG  1 AUTHOR:  E.FORT+J.P.MARQUETTE  EANDC(E)148"U"

SYSTEMATICAL (LONG ENERGY RANGE CORRELATION - LERC) UNCERTAINTY 4.4%

NO MEDIUM ENERGY RANGE CORRELATION (MERC) UNCERTAINTY

  ENERGY/MEV    VALUE  TOT. ABS. UNCERT. TOT. UNCERT./%

  0.1500E-01  0.1201E+01  0.8181E-01      6.8
  0.2000E-01  0.1052E+01  0.7166E-01      6.8
  0.2400E-01  0.9835E+00  0.6404E-01      6.5
  0.3000E-01  0.9390E+00  0.5977E-01      6.4
  0.4500E-01  0.8134E+00  0.4729E-01      5.8
  0.5500E-01  0.7176E+00  0.3947E-01      5.5
  0.6500E-01  0.6509E+00  0.3503E-01      5.4
  0.8500E-01  0.6490E+00  0.3493E-01      5.4
  0.9500E-01  0.6449E+00  0.3879E-01      6.0
  0.1000E+00  0.6617E+00  0.3562E-01      5.4
  0.1200E+00  0.7309E+00  0.3812E-01      5.2
  0.1500E+00  0.8620E+00  0.4591E-01      5.3
  0.1700E+00  0.1027E+01  0.6038E-01      5.9

   CORRELATION MATRIX OF DATA BLOCK

  1.00
  0.42 1.00
  0.44 0.44 1.00
  0.45 0.45 0.47 1.00
  0.49 0.49 0.51 0.52 1.00
  0.52 0.52 0.54 0.55 0.61 1.00
  0.53 0.53 0.55 0.57 0.62 0.65 1.00
  0.53 0.53 0.55 0.57 0.62 0.65 0.67 1.00
  0.47 0.47 0.49 0.51 0.55 0.59 0.60 0.60 1.00
  0.53 0.53 0.55 0.57 0.62 0.65 0.67 0.67 0.60 1.00
  0.54 0.54 0.57 0.58 0.64 0.67 0.69 0.69 0.62 0.69 1.00
  0.53 0.53 0.56 0.57 0.63 0.66 0.68 0.68 0.60 0.68 0.70 1.00
  0.48 0.48 0.51 0.52 0.57 0.60 0.61 0.61 0.55 0.61 0.63 0.62 1.00
```

Data set #2.

```
YEAR 1970 TAG  1 AUTHOR:  E.FORT  70HELSINKI,CN26/72

SYSTEMATICAL (LONG ENERGY RANGE CORRELATION - LERC) UNCERTAINTY 4.0%

NO MEDIUM ENERGY RANGE CORRELATION (MERC) UNCERTAINTY
```

ENERGY/MEV	VALUE	TOT. ABS. UNCERT.	TOT. UNCERT./%
0.8500E-01	0.6926E+00	0.2913E-01	4.2
0.1000E+00	0.7396E+00	0.4132E-01	5.6
0.1200E+00	0.7369E+00	0.3821E-01	5.2
0.1500E+00	0.8583E+00	0.4397E-01	5.1
0.1700E+00	0.1043E+01	0.4712E-01	4.5
0.1800E+00	0.1295E+01	0.6475E-01	5.0
0.1900E+00	0.1445E+01	0.7225E-01	5.0
0.2000E+00	0.1867E+01	0.9335E-01	5.0
0.2100E+00	0.2187E+01	0.1068E+00	4.9
0.2200E+00	0.2548E+01	0.1244E+00	4.9
0.2450E+00	0.3032E+01	0.1516E+00	5.0
0.2500E+00	0.3133E+01	0.1530E+00	4.9
0.2600E+00	0.2945E+01	0.1472E+00	5.0
0.2700E+00	0.2716E+01	0.1358E+00	5.0
0.2800E+00	0.2357E+01	0.1151E+00	4.9
0.3000E+00	0.1685E+01	0.8425E-01	5.0
0.3250E+00	0.1151E+01	0.6194E-01	5.4
0.3500E+00	0.8390E+00	0.4687E-01	5.6
0.3750E+00	0.6973E+00	0.4251E-01	6.1
0.4000E+00	0.6012E+00	0.3850E-01	6.4
0.4250E+00	0.4688E+00	0.3226E-01	6.9
0.4500E+00	0.4023E+00	0.2935E-01	7.3
0.4750E+00	0.3830E+00	0.2989E-01	7.8
0.5000E+00	0.3289E+00	0.2510E-01	7.6
0.5200E+00	0.3230E+00	0.2576E-01	8.0

CORRELATION MATRIX OF DATA BLOCK

```
1.00
0.68 1.00
0.73 0.55 1.00
0.74 0.56 0.60 1.00
0.84 0.63 0.68 0.69 1.00
0.76 0.57 0.62 0.62 0.71 1.00
0.76 0.57 0.62 0.62 0.71 0.64 1.00
0.76 0.57 0.62 0.62 0.71 0.64 0.64 1.00
0.78 0.59 0.63 0.64 0.73 0.66 0.66 0.66 1.00
0.78 0.59 0.63 0.64 0.73 0.66 0.66 0.66 0.67 1.00
0.76 0.57 0.62 0.62 0.71 0.64 0.64 0.64 0.66 0.66 1.00
0.78 0.59 0.63 0.64 0.73 0.66 0.66 0.66 0.67 0.67 0.66 1.00
0.76 0.57 0.62 0.62 0.71 0.64 0.64 0.64 0.66 0.66 0.64 0.66 1.00
0.76 0.57 0.62 0.62 0.71 0.64 0.64 0.64 0.66 0.66 0.64 0.66 0.64 1.00
0.78 0.59 0.63 0.64 0.73 0.66 0.66 0.66 0.67 0.67 0.66 0.67 0.66 0.66 1.00
0.76 0.57 0.62 0.62 0.71 0.64 0.64 0.64 0.66 0.66 0.64 0.66 0.64 0.64 0.66 1.00
0.71 0.53 0.57 0.58 0.66 0.59 0.59 0.59 0.61 0.61 0.59 0.61 0.59 0.59 0.61 0.59 1.00
0.68 0.51 0.55 0.56 0.63 0.57 0.57 0.57 0.59 0.59 0.57 0.59 0.57 0.57 0.59 0.57 0.53 1.00
0.62 0.47 0.51 0.51 0.58 0.52 0.52 0.52 0.54 0.54 0.52 0.54 0.52 0.52 0.54 0.52 0.49 0.47 1.00
0.59 0.45 0.48 0.49 0.55 0.50 0.50 0.50 0.51 0.51 0.50 0.51 0.50 0.50 0.51 0.50 0.46 0.45 0.41 1.00
0.55 0.42 0.45 0.45 0.51 0.46 0.46 0.46 0.48 0.48 0.46 0.48 0.46 0.46 0.48 0.46 0.43 0.42 0.38 0.36 1.00
0.52 0.39 0.42 0.43 0.49 0.44 0.44 0.44 0.45 0.45 0.44 0.45 0.44 0.44 0.45 0.44 0.41 0.39 0.36 0.34 0.32 1.00
0.49 0.37 0.40 0.40 0.45 0.41 0.41 0.41 0.42 0.42 0.41 0.42 0.41 0.41 0.42 0.41 0.38 0.37 0.34 0.32 0.30 0.28 1.00
0.50 0.38 0.40 0.41 0.46 0.42 0.42 0.42 0.43 0.43 0.42 0.43 0.42 0.42 0.43 0.42 0.39 0.38 0.34 0.33 0.30 0.29 0.27 1.00
0.48 0.36 0.39 0.39 0.44 0.40 0.40 0.40 0.41 0.41 0.40 0.41 0.40 0.40 0.41 0.40 0.37 0.36 0.33 0.31 0.29 0.28 0.26 0.26
1.00
```

Data set #3.

```
YEAR 1972 TAG  1 AUTHOR:  W.P.POENITZ+J.W.MEADOWS  72VIENNA,95(1972)

SYSTEMATICAL (LONG ENERGY RANGE CORRELATION - LERC) UNCERTAINTY 1.4%

NO MEDIUM ENERGY RANGE CORRELATION (MERC) UNCERTAINTY
```

ENERGY/MEV	VALUE	TOT. ABS. UNCERT.	TOT. UNCERT./%
0.8500E-01	0.6546E+00	0.2347E-01	3.6
0.9500E-01	0.6550E+00	0.2591E-01	4.0
0.1200E+00	0.7590E+00	0.2861E-01	3.8
0.1500E+00	0.9672E+00	0.3290E-01	3.4
0.1900E+00	0.1798E+01	0.5952E-01	3.3
0.2000E+00	0.2169E+01	0.7378E-01	3.4
0.2100E+00	0.2453E+01	0.8568E-01	3.5
0.2200E+00	0.2871E+01	0.9505E-01	3.3
0.2300E+00	0.3130E+01	0.1065E+00	3.4
0.2400E+00	0.3250E+01	0.1135E+00	3.5
0.2450E+00	0.3238E+01	0.1101E+00	3.4
0.2500E+00	0.3068E+01	0.1044E+00	3.4
0.2600E+00	0.2732E+01	0.9542E-01	3.5
0.3000E+00	0.1436E+01	0.5280E-01	3.7
0.3750E+00	0.6663E+00	0.2574E-01	3.9
0.4000E+00	0.6001E+00	0.2374E-01	4.0
0.4750E+00	0.4005E+00	0.1926E-01	4.8
0.5400E+00	0.3591E+00	0.1590E-01	4.4
0.6000E+00	0.3030E+00	0.1370E-01	4.5

CORRELATION MATRIX OF DATA BLOCK

```
1.00
0.14 1.00
0.15 0.13 1.00
0.16 0.15 0.15 1.00
0.17 0.15 0.16 0.17 1.00
0.16 0.15 0.15 0.17 0.17 1.00
0.16 0.14 0.15 0.16 0.17 0.16 1.00
0.17 0.15 0.16 0.17 0.18 0.17 0.17 1.00
0.16 0.15 0.15 0.17 0.17 0.17 0.16 0.17 1.00
0.16 0.14 0.15 0.16 0.17 0.16 0.16 0.17 0.16 1.00
0.16 0.15 0.15 0.17 0.17 0.17 0.16 0.17 0.17 0.16 1.00
0.16 0.15 0.15 0.17 0.17 0.17 0.16 0.17 0.17 0.16 0.17 1.00
0.16 0.14 0.15 0.16 0.17 0.16 0.16 0.17 0.16 0.16 0.16 0.16 1.00
0.15 0.13 0.14 0.16 0.16 0.16 0.15 0.16 0.16 0.15 0.16 0.16 0.15 1.00
0.14 0.13 0.13 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.14 1.00
0.14 0.13 0.13 0.15 0.15 0.15 0.14 0.15 0.15 0.14 0.15 0.15 0.14 0.13 0.13 1.00
```

```
  0.11 0.10 0.11 0.12 0.12 0.12 0.12 0.12 0.12 0.12 0.12 0.12 0.12 0.11 0.11 0.10 1.00
  0.12 0.11 0.12 0.13 0.13 0.13 0.13 0.13 0.13 0.13 0.13 0.13 0.13 0.12 0.11 0.11 0.09 1.00
  0.12 0.11 0.11 0.13 0.13 0.13 0.12 0.13 0.13 0.12 0.13 0.13 0.12 0.12 0.11 0.11 0.09 0.10 1.00
```

Data set #4.

```
YEAR 1974 TAG  1 AUTHOR:  S.J.FRIESENHAHN ET AL. INTEL-RT7011-001(197

SYSTEMATICAL (LONG ENERGY RANGE CORRELATION - LERC) UNCERTAINTY 2.7%

NO MEDIUM ENERGY RANGE CORRELATION (MERC) UNCERTAINTY

  ENERGY/MEV    VALUE  TOT. ABS. UNCERT. TOT. UNCERT./%

  0.2500E-02  0.2763E+01  0.1178E+00      4.3
  0.3500E-02  0.2296E+01  0.9439E-01      4.1
  0.4500E-02  0.1938E+01  0.7967E-01      4.1
  0.5500E-02  0.1809E+01  0.7037E-01      3.9
  0.6500E-02  0.1616E+01  0.6286E-01      3.9
  0.7500E-02  0.1478E+01  0.5749E-01      3.9
  0.8500E-02  0.1451E+01  0.5242E-01      3.6
  0.9500E-02  0.1322E+01  0.4218E-01      3.2
  0.1500E-01  0.1067E+01  0.3404E-01      3.2
  0.2000E-01  0.9708E+00  0.3321E-01      3.4
  0.2400E-01  0.9001E+00  0.3135E-01      3.5
  0.3000E-01  0.7525E+00  0.2574E-01      3.4
  0.4500E-01  0.6587E+00  0.2424E-01      3.7
  0.5500E-01  0.6198E+00  0.2367E-01      3.8
  0.6500E-01  0.6247E+00  0.2430E-01      3.9
  0.7500E-01  0.6009E+00  0.2294E-01      3.8
  0.8500E-01  0.6240E+00  0.2519E-01      4.0
  0.9500E-01  0.6535E+00  0.2542E-01      3.9
  0.1000E+00  0.6387E+00  0.2439E-01      3.8
  0.1200E+00  0.6698E+00  0.2333E-01      3.5
  0.1500E+00  0.8824E+00  0.3073E-01      3.5
  0.1700E+00  0.1144E+01  0.4210E-01      3.7
  0.1800E+00  0.1303E+01  0.5068E-01      3.9
  0.1900E+00  0.1571E+01  0.5675E-01      3.6
  0.2000E+00  0.1768E+01  0.6751E-01      3.8
  0.2100E+00  0.2130E+01  0.8133E-01      3.8
  0.2200E+00  0.2576E+01  0.9836E-01      3.8
  0.2300E+00  0.2919E+01  0.1074E+00      3.7
  0.2450E+00  0.3224E+01  0.1186E+00      3.7
  0.2500E+00  0.3452E+01  0.1270E+00      3.7
  0.2700E+00  0.2996E+01  0.1102E+00      3.7
  0.2800E+00  0.2794E+01  0.1067E+00      3.8
  0.3000E+00  0.1951E+01  0.7179E-01      3.7
  0.3250E+00  0.1349E+01  0.5247E-01      3.9
  0.3500E+00  0.9862E+00  0.3980E-01      4.0
  0.3750E+00  0.8116E+00  0.3157E-01      3.9
  0.4000E+00  0.7030E+00  0.2943E-01      4.2
  0.4250E+00  0.6254E+00  0.2765E-01      4.4
  0.4750E+00  0.4555E+00  0.2013E-01      4.4
  0.5000E+00  0.4249E+00  0.1878E-01      4.4
  0.5200E+00  0.4004E+00  0.1802E-01      4.5
  0.5700E+00  0.3699E+00  0.1694E-01      4.6
  0.6000E+00  0.3524E+00  0.1614E-01      4.6
  0.6500E+00  0.3358E+00  0.1565E-01      4.7
  0.7000E+00  0.3038E+00  0.1491E-01      4.9
  0.7500E+00  0.2833E+00  0.1462E-01      5.2

   CORRELATION MATRIX OF DATA BLOCK

  1.00
  0.42 1.00
  0.42 0.43 1.00
  0.44 0.46 0.46 1.00
  0.44 0.46 0.46 0.48 1.00
  0.44 0.46 0.46 0.48 0.48 1.00
  0.47 0.49 0.49 0.52 0.52 0.52 1.00
  0.54 0.56 0.56 0.59 0.59 0.59 0.63 1.00
  0.54 0.56 0.56 0.59 0.59 0.59 0.63 0.72 1.00
  0.50 0.52 0.52 0.55 0.55 0.55 0.59 0.67 0.67 1.00
  0.49 0.51 0.51 0.54 0.54 0.54 0.58 0.66 0.66 0.61 1.00
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Annex 5. Participants' presentations and working papers submitted for inclusion in the report

Microscopic calculations in the $^4\mathrm{He}$ System using realistic two- and three-nucleon forces

Hartmut M. Hofmann
Institut für Theoretische Physik III
Universität Erlangen-Nürnberg

September 22 2002

Motivation
Model and Potentials
Model spaces, binding energies, ...

Results

phase shifts

Cross sections

Triton-proton elastic
Standard neutron
$^3\mathrm{H}(\mathrm{p},\mathrm{n})^3\mathrm{He}$
$^2\mathrm{H}(\mathrm{d},\mathrm{p})^3\mathrm{H}$
Deuteron-deuteron elastic

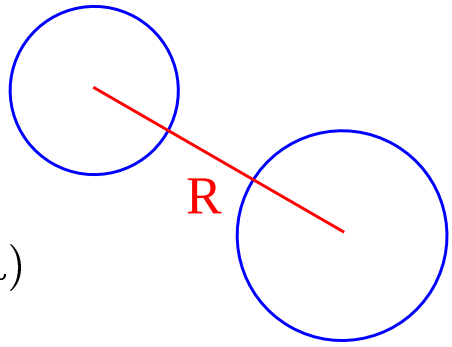
Motivation

The $^4\mathrm{He}$ nucleus is the lightest, stable nucleus with

- many two-body reaction-channels
- different fragmentations
- well developed resonances
- deeply bound ground state
- standard cross-sections
- huge amount of data
- well studied theoretically
- benchmark for models
- still open questions

Resonating Group Model Ideas

Composite system



RGM Ansatz $\Psi_l = \sum_{k=1}^{chan} \psi_{chan}^k \cdot \chi_{rel}^{lk}(\mathbf{R})$

Variation $\langle \delta\Psi_l \mathcal{A} | \mathrm{H} - \mathrm{E} |\ \Psi_l \rangle = 0$

Channel function $\psi_{chan} = [Y_L(\hat{\mathbf{R}}) \otimes [\phi_1^{j1} \otimes \phi_2^{j2}]^{S_c}]^J$

Ansatz $\psi = \psi_{chan}(\sum_i b_i \cdot \mathrm{Gaussian})$ (bound state)

or $\chi_{rel}^{lk}(R) = \delta_{lk} \cdot F_k(R) + a_{lk} \cdot \tilde{G}_k(R) + \sum_i b_{lki} \cdot$ Gaussian (scattering state)

Variational parameters a_{lk} and $b_{(lk)i}$

Decompose Hamiltonian

$H - E = H_1 - E_1 + H_2 - E_2 +$
$\sum_{\substack{i\in 1\\ j\in 2}} V_{ij} - V_{Coul} +$
$T_R + V_{Coul} - (E - E_1 - E_2) =$
$H_1 - E_1 + H_2 - E_2 + V_{short} + H_R - \tilde{E}$

with $\mathcal{A} \cdot (H_i - E_i)\phi_i = 0$ and $(H_R - \tilde{E})F/G = 0$

$\Rightarrow$ All integrals shortranged
Note: Relative thresholds fixed by $\tilde{E}$

Resonating Group Model Technicalities

$\Rightarrow$ Expand all functions including F and G

- in terms of Gaussians
- times solid spherical harmonics

$\Rightarrow$ All individual integrals analytically calculable,
provided potential is of Gaussian form including differential operators
All operators allowed which occur in Argonne and Bonn (r-space) potentials and in Urbana IX NNN-force

- Correct center of mass motion
- No limit on number of channels
- NNN-forces limit number of nucleons to 4

$\Rightarrow$ Allow for distortion of fragments via different ϕ

Three- and more-body channels approximately treated via two-body channels (unitary pole approximation)

Fragment wave functions ϕ_1 and ϕ_2 must be strongest bound in given model-space
$\Rightarrow$ Relative thresholds can only be changed by increasing dimension of model-space or using other potentials

Model spaces, binding energies

Deuteron: E_b = -2.224 MeV $J^\pi = 1^+ \Rightarrow$ S=1, L=0,2

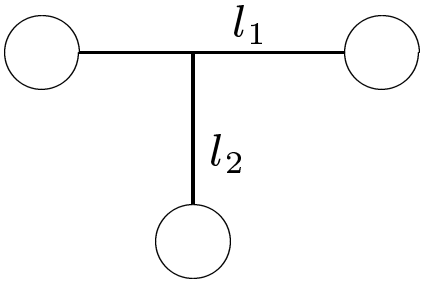
$\Rightarrow$ model space ${}^3S_1, {}^3D_1$

dimension (3,1) E_b = -0.929 MeV

dimension (3,2) E_b = -1.921 MeV

dimension (5,2) E_b = -2.095 MeV

dimension (5,3) E_b =- 2.213 MeV



E_b determined via genetic algorithm

Triton / ${}^3\mathrm{He}$: $\mathrm{E_b}$ = -8.481 MeV $J^\pi = \frac{1}{2}^+$, isospin $= \frac{1}{2}$

$\Rightarrow S = \frac{1}{2}, \frac{3}{2}; (l_1, l_2)^L$ all combinations $(L, S)^J$ with $l_1 + l_2$ even

additional $T_{12} = 0$, 1 possible

Model spaces

dimension 29 : $(l_1, l_2)^L$ = (0,0), (2,0), (0,2), $(2, 2)^{1,2}$

AV18 E_b = -7.068 MeV, AV18 + UIX E_b = -7.586 MeV

dimension 35 : $(l_1, l_2)^L$ = (0,0), (2,0), (0,2), $(2, 2)^{0,1,2}, (1, 1)^1$

AV18 E_b = -7.413 MeV, AV18 + UIX E_b = -8.241 MeV

dimension 70 : $(l_1, l_2)^L$ = (0,0), (2,0), (0,2), $(2, 2)^{0,1,2}, (1, 1)^{1,2}$

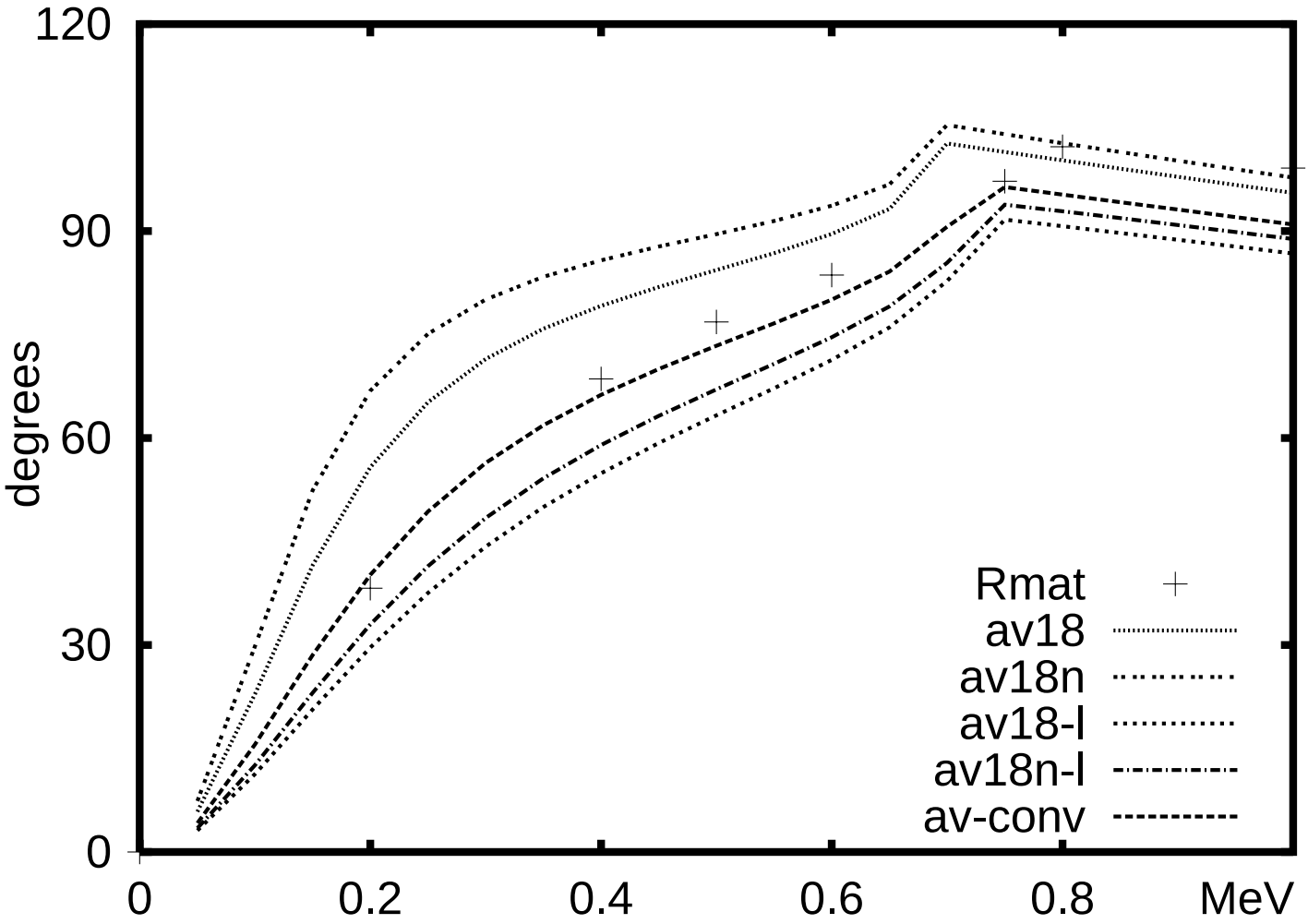
AV18 E_b = -7.572 MeV, AV18 + UIX E_b = -8.460 MeV

Thresholds relative to ^{3}H - p

model space	AV18		AV18 + UIX	
	${}^3\mathrm{He} - p$	$d - d$	${}^3\mathrm{He} - p$	$d - d$
	0.698	3.227	0.710	3.745
large	0.725	3.572	0.748	4.400
converged	0.715	3.145	0.747	4.033
exp.	0.763	4.033	0.763	4.033

Triton – proton 0^+ phase shift

Various model spaces, NN–interaction only

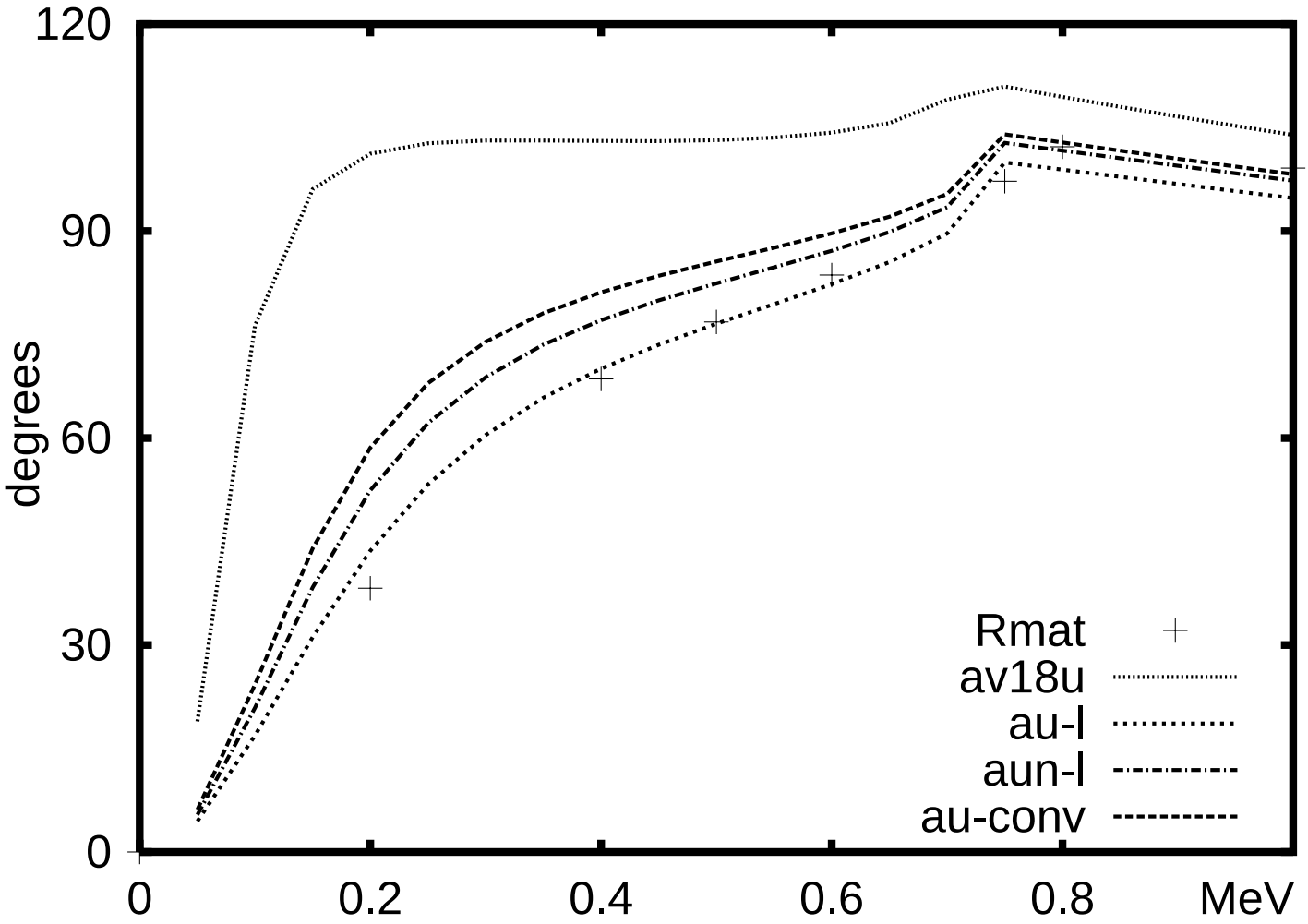


Converged results close to R-matrix analysis
^{4}He binding energy -23.597 $\cdots$ -24.112 MeV

S-matrix pole position $E_0 = E_r - i\Gamma/2$
E_0 = 0.093 - i 0.174 MeV, Γ_{tot} = 0.265 MeV
Pole position far from 90-degrees crossing

Triton – proton 0^+ phase shift

Various model spaces, NN–interaction + NNN–Urbana IX

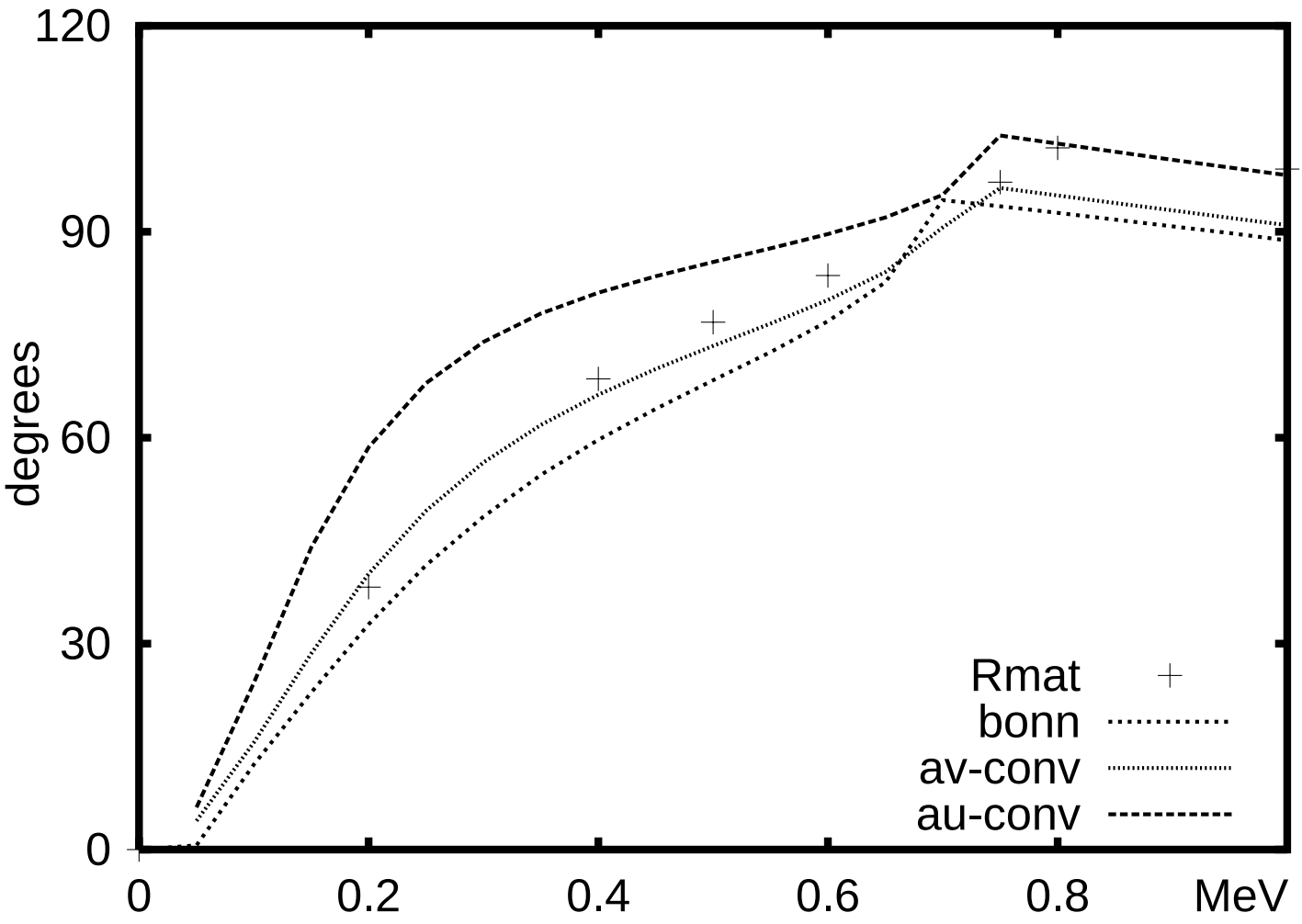


Results for large model space close to R-matrix ones
Converged results too attractive
^{4}He binding energy -27.106 $\cdots$ -28.328 MeV

S-matrix pole position
$E_0 = 0.096$ - i 0.114 MeV, $\Gamma_{tot} = 0.173$ MeV
Pole position far from 90-degrees crossing

Triton – proton 0^+ phase shift

Various potentials, largest model space

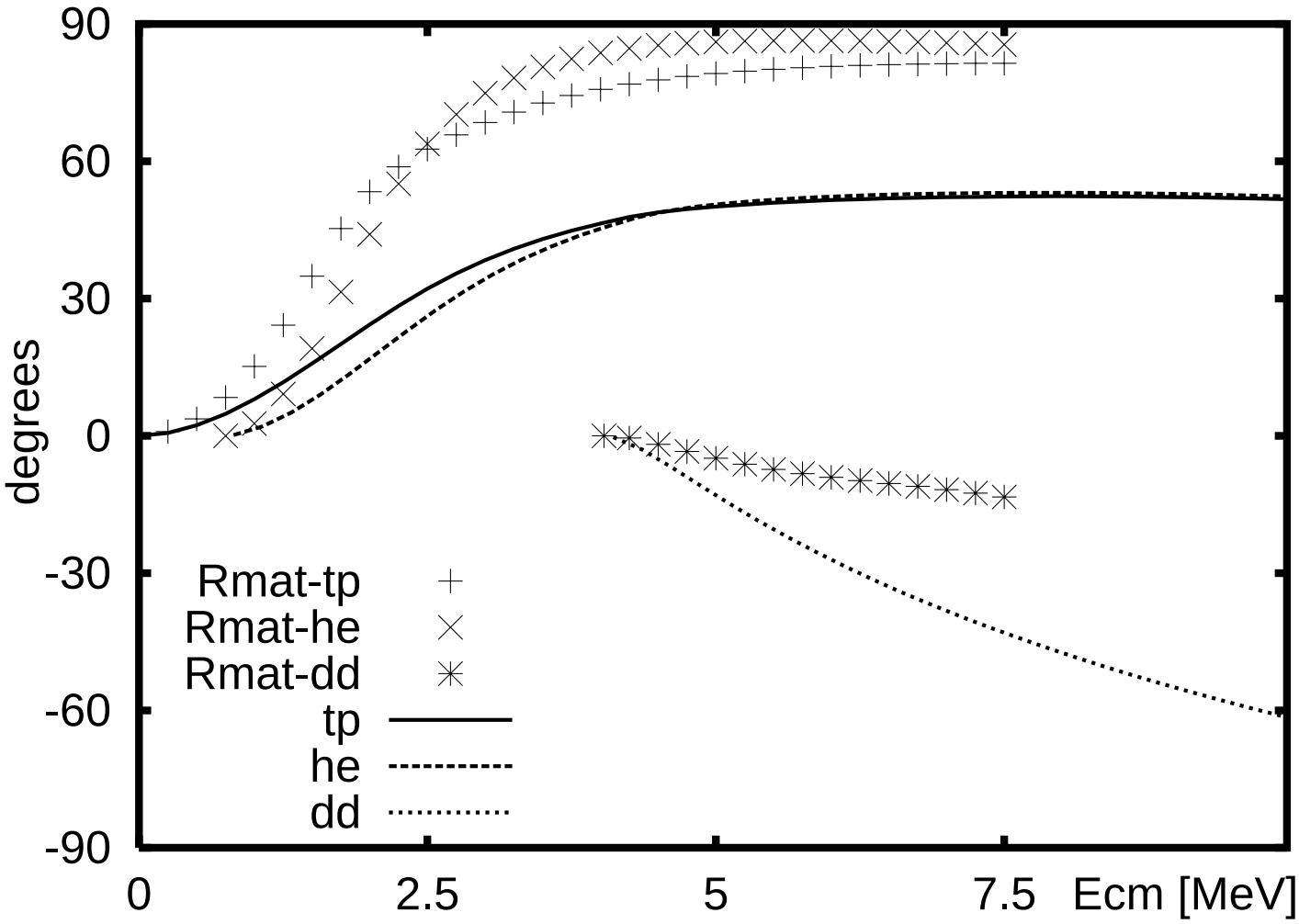


Argonne v18 + Urbana IX too attractive

Operator structure of UIX ?

2^- phase shifts

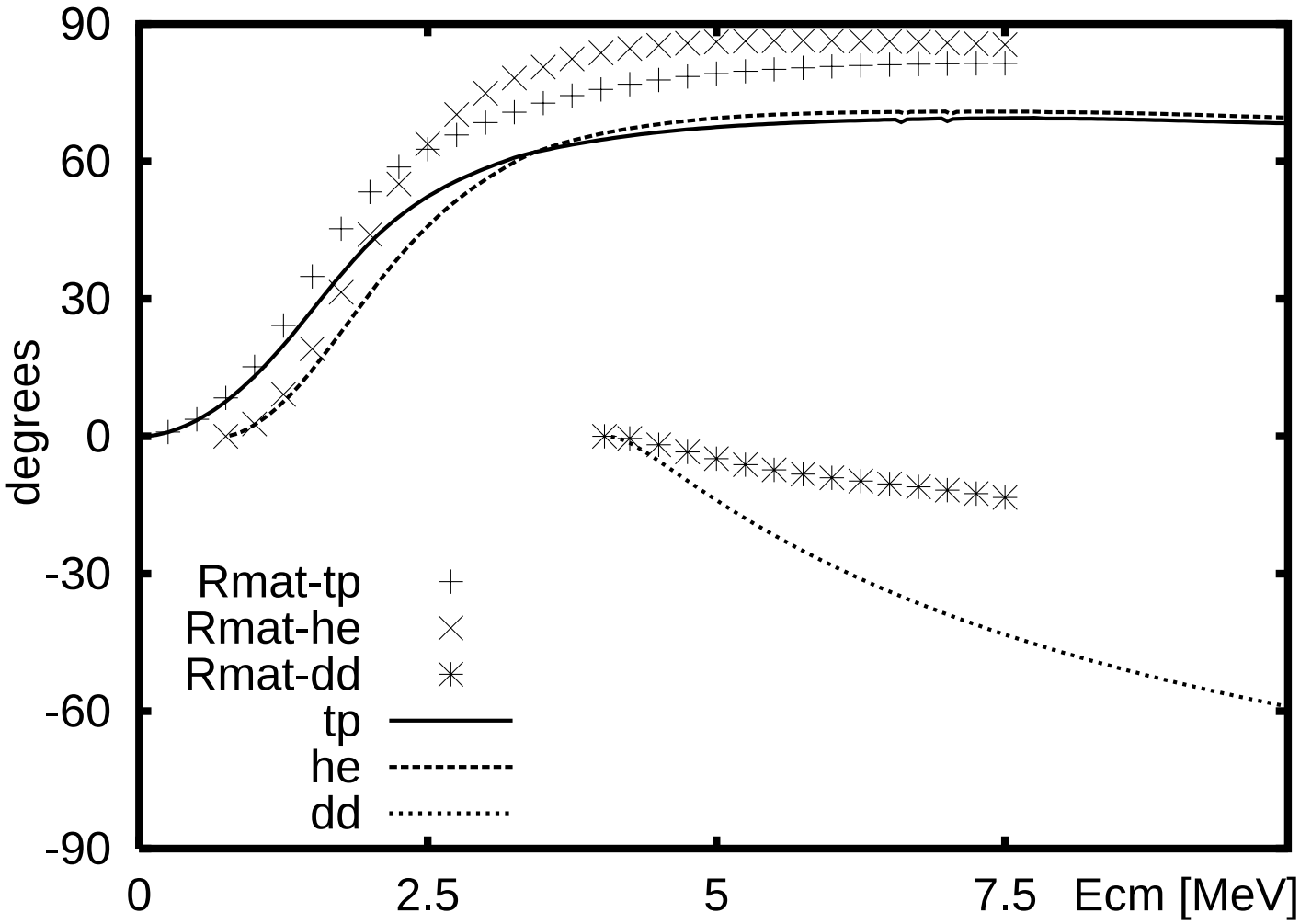
Bonn potential



Too small t–p phase shift reason for missing the polarization data

2^- phase shifts

Argonne v18 potential

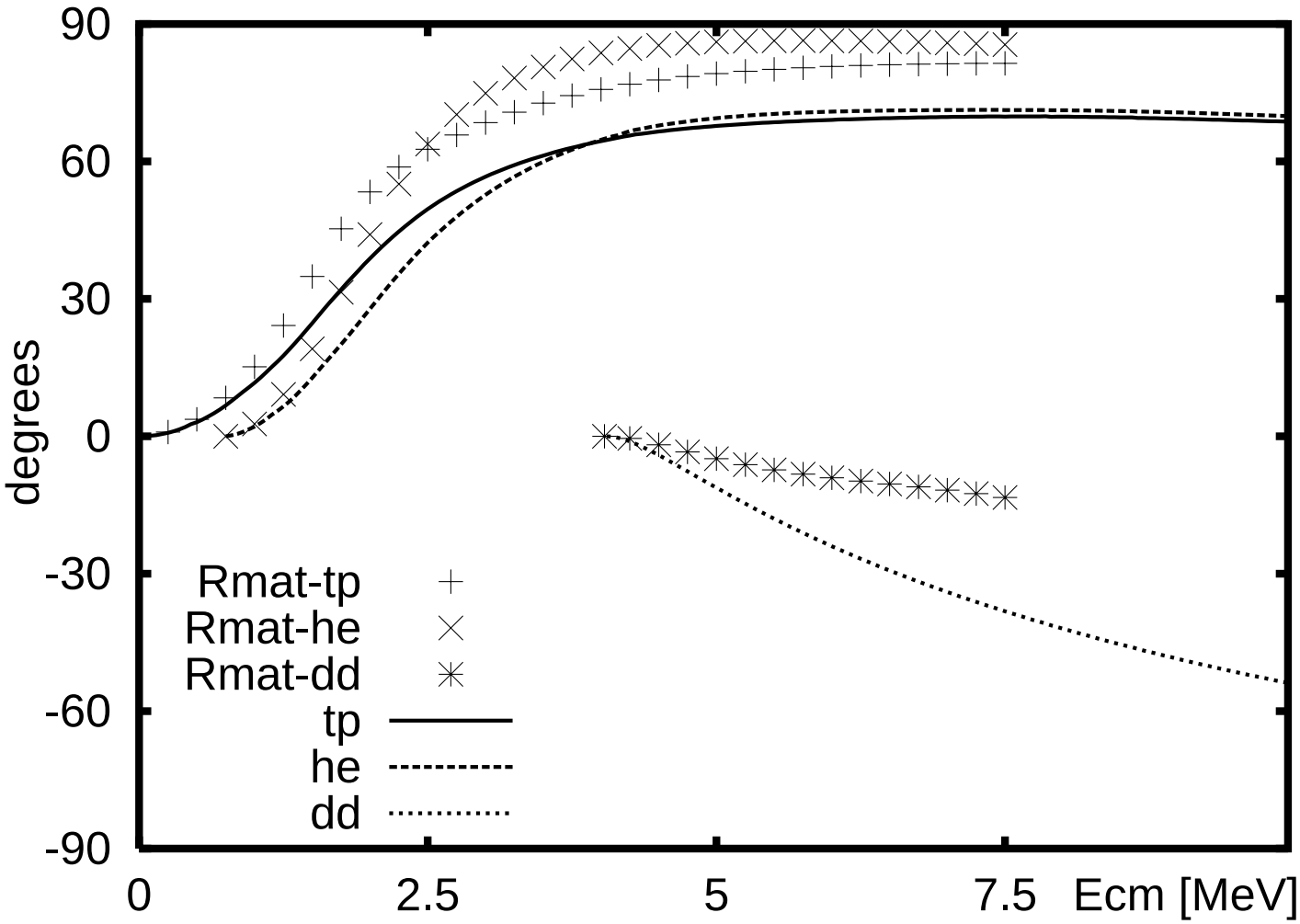


Triton - proton channel gains attraction

Stronger coupling to $^3\mathrm{He}$ - n channel

2^- phase shifts

Argonne v18 + Urbana IX potentials



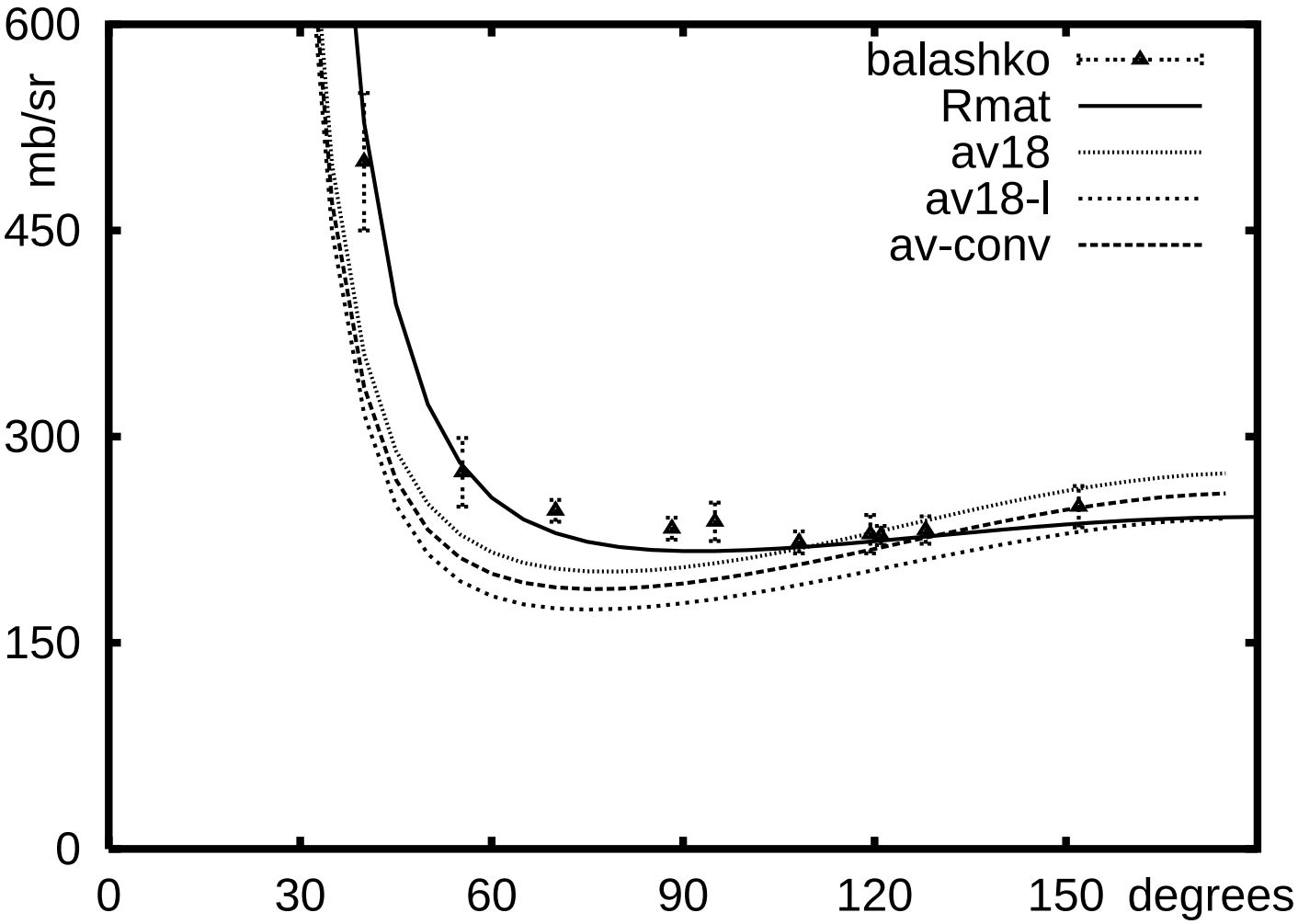
Compared to NN-force alone

Small modifications

Slightly less attractive

Coupling matrix element reduced by 5 percent

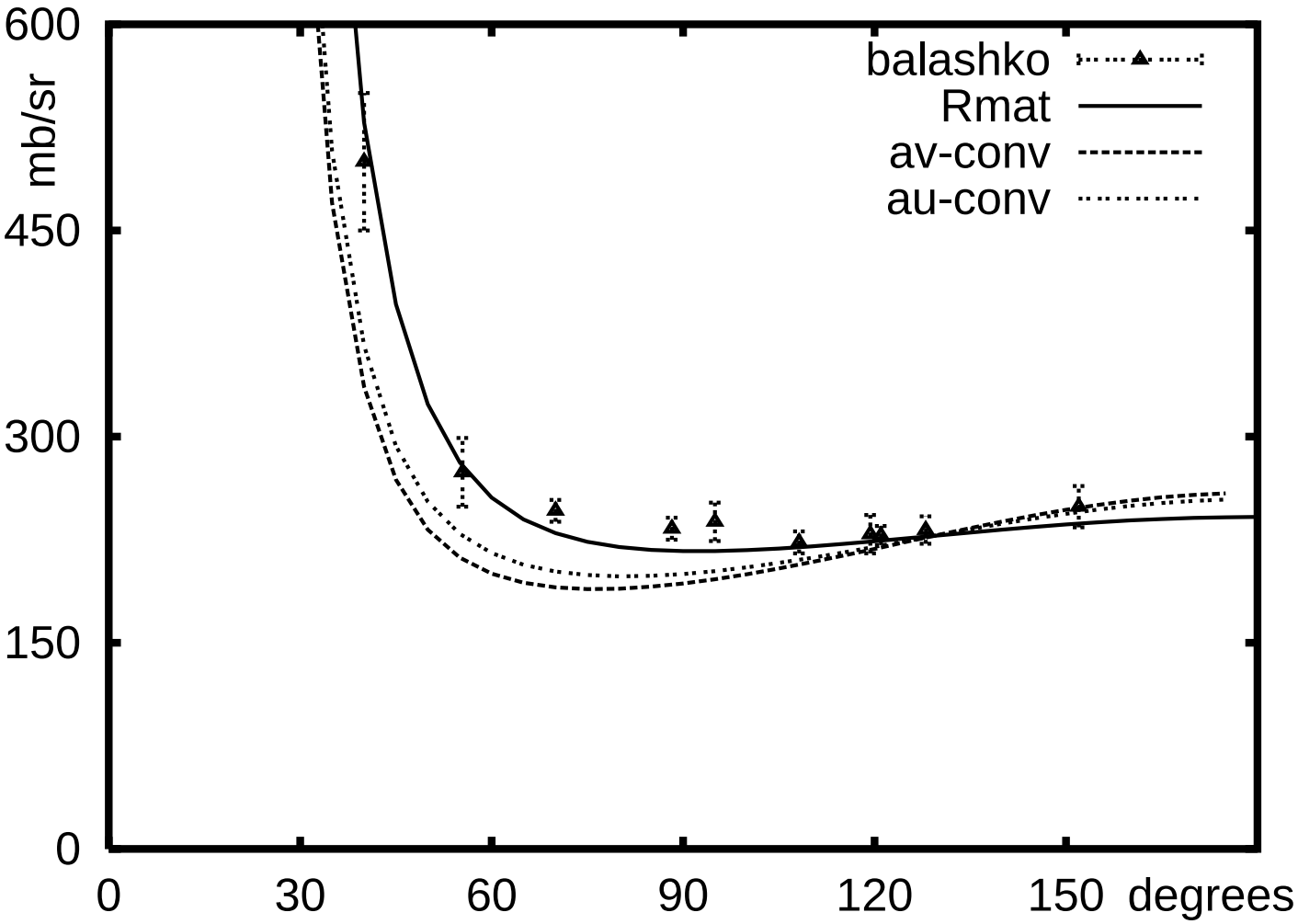
Triton – proton elastic scattering



Differential cross section at $E_{cm} = 600$ keV

Coulomb – nuclear interference?
Data?

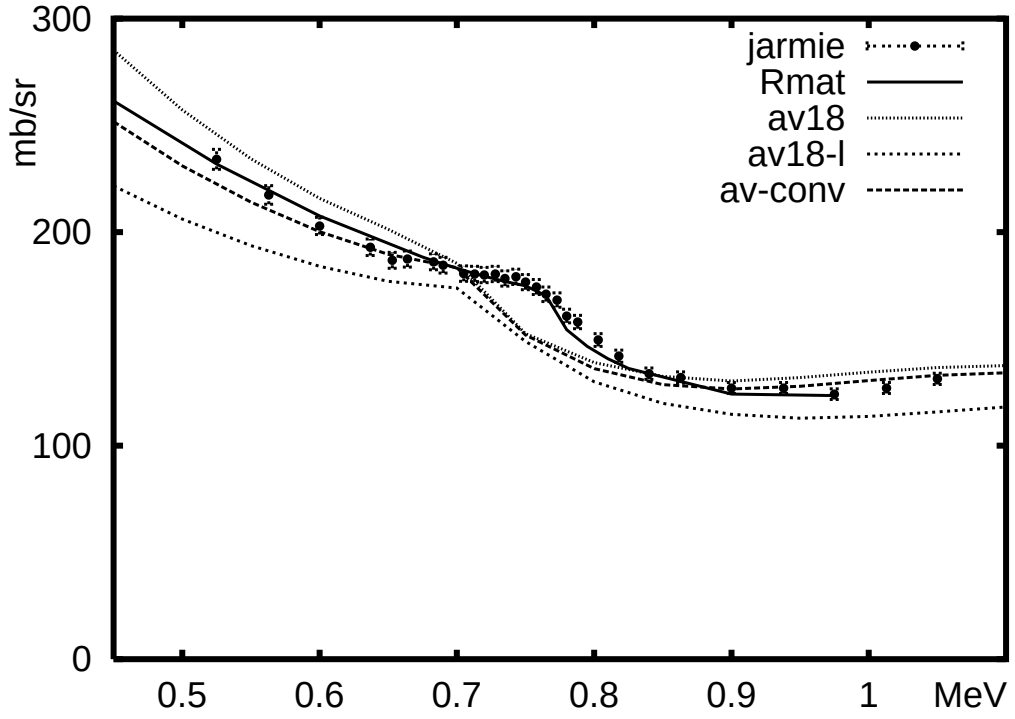
Triton – proton elastic scattering



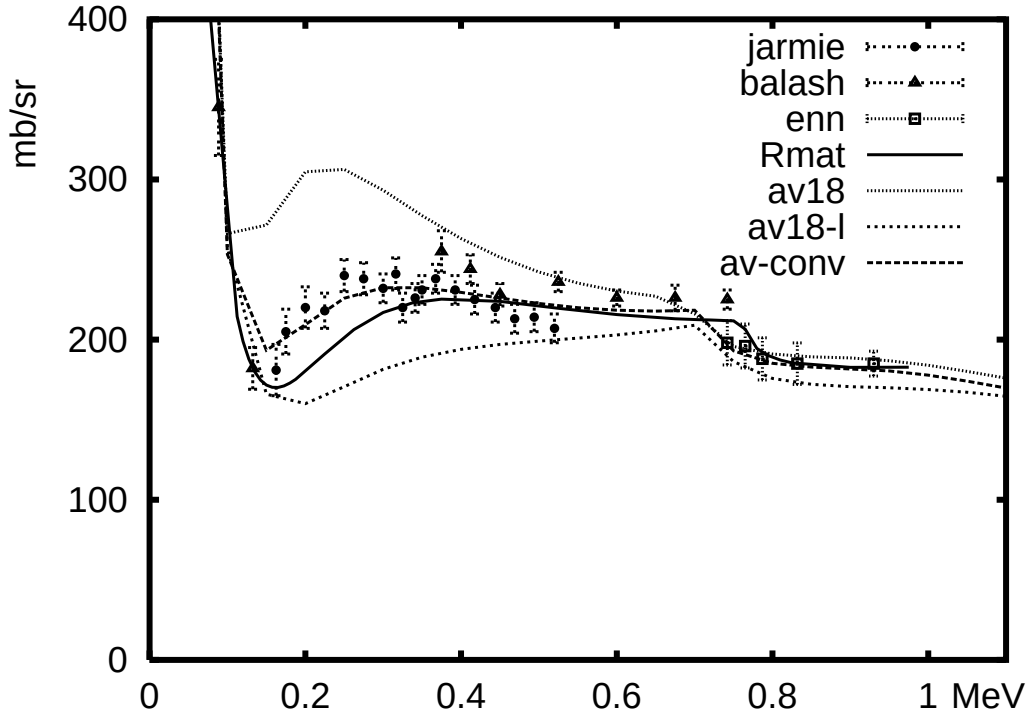
Differential cross section at $E_{cm} = 600$ keV

NNN – force effects tiny

Triton – proton elastic scattering



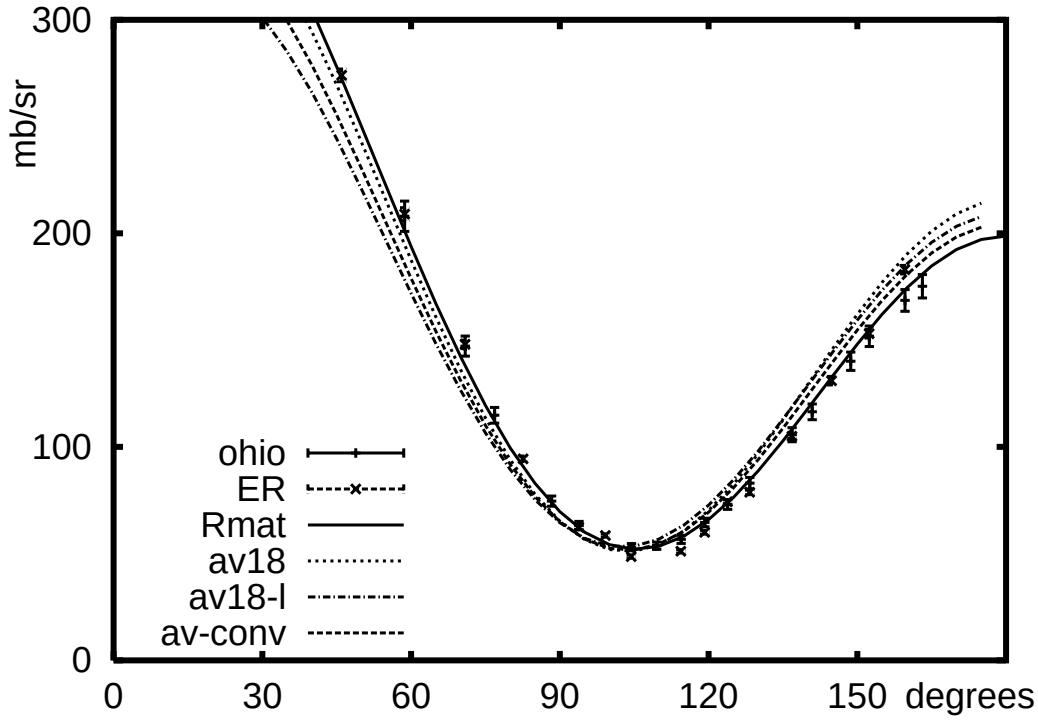
Excitation function at $\Theta = 58^\circ$ as function of center-of-mass energy



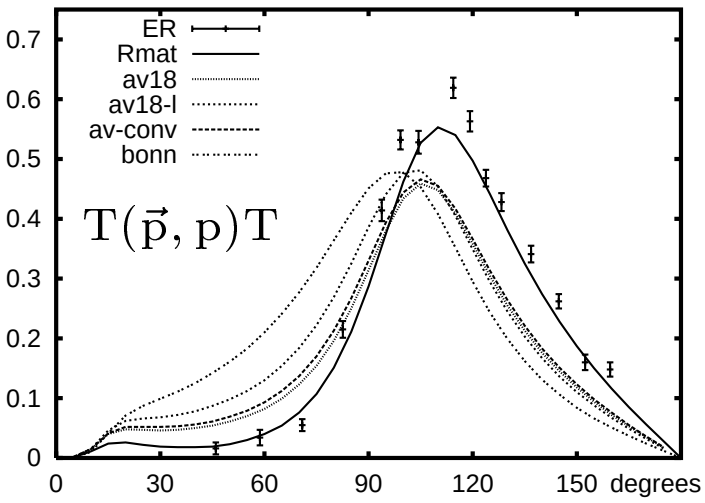
Excitation function at $\Theta = 120^\circ$ as function of center-of-mass energy
Converged results through data

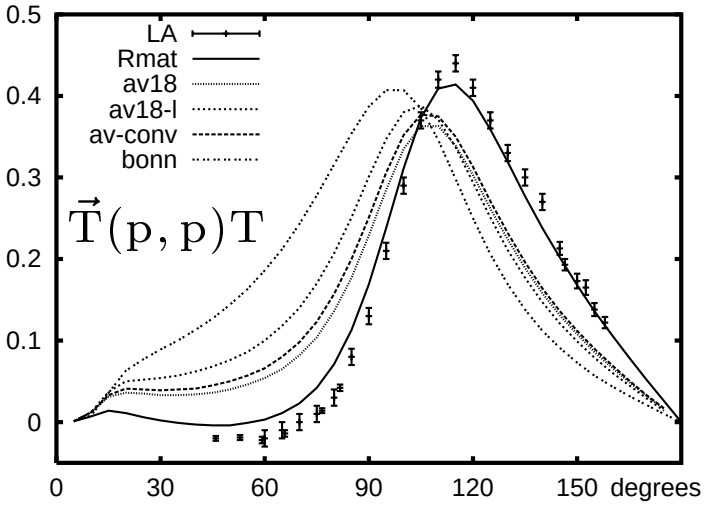
Triton – proton elastic scattering

The data are for 4.15 MeV protons



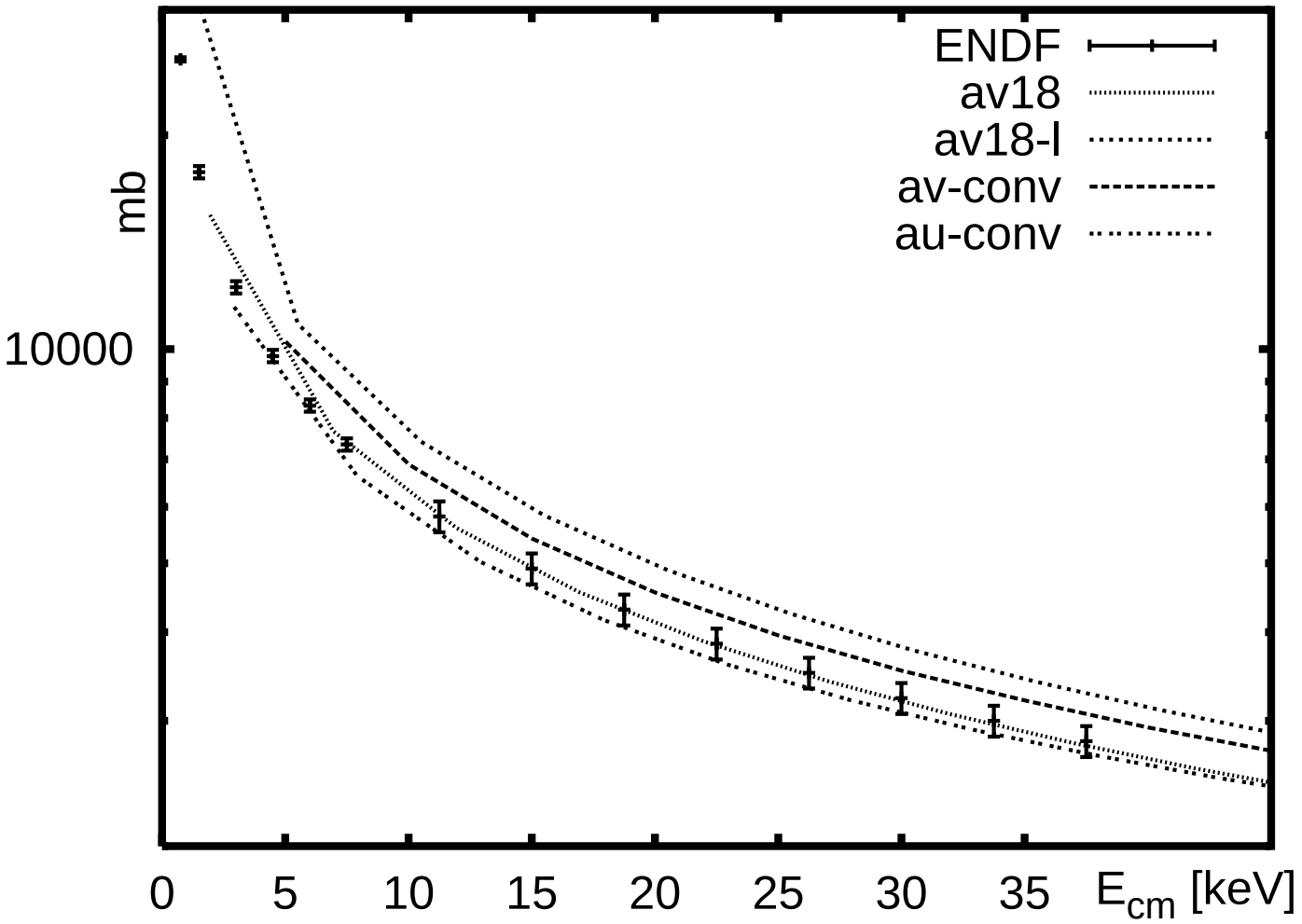
Cross section reasonably well reproduced





Some improvement, but still large discrepancies

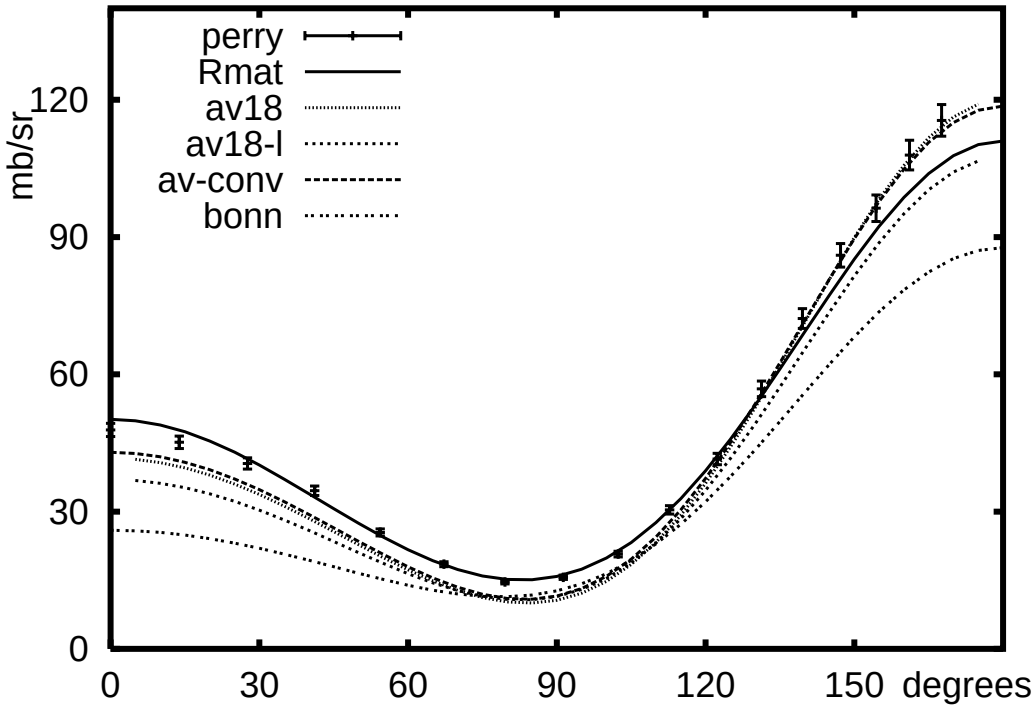
Standard cross section $^3\mathrm{He}$(n,p)



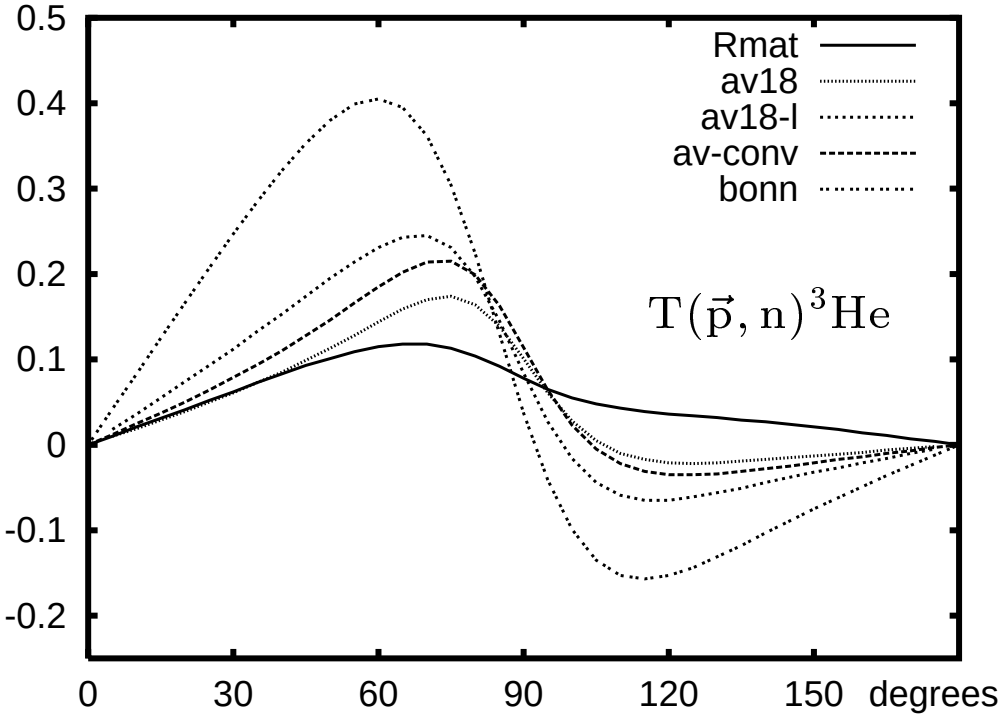
Converged results close to data

Dominant contribution $^1S_0$
P-wave 0.2 $\cdots$ 7 percent
$^3S_1$ 0.7 $\cdots$ 0.5 percent
D-wave negligible

^{3}H(p,n)^{3}He Reaction

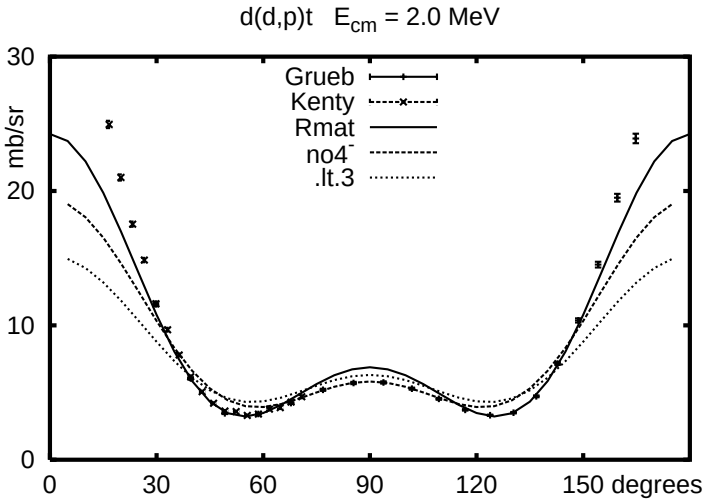


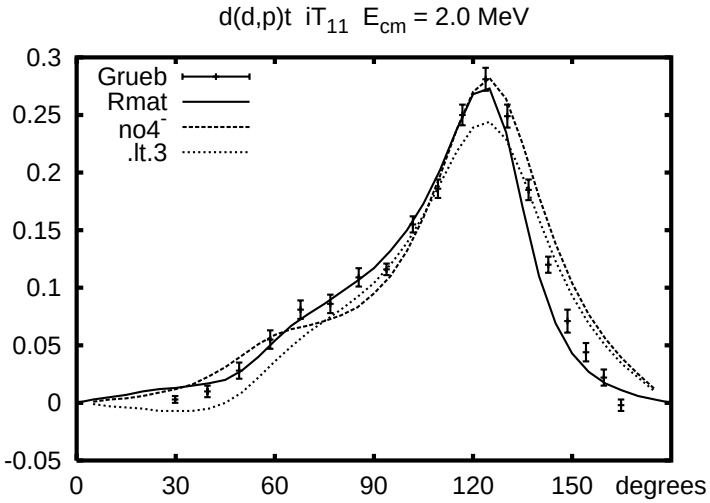
Converged calculation reproduces cross section reasonably well

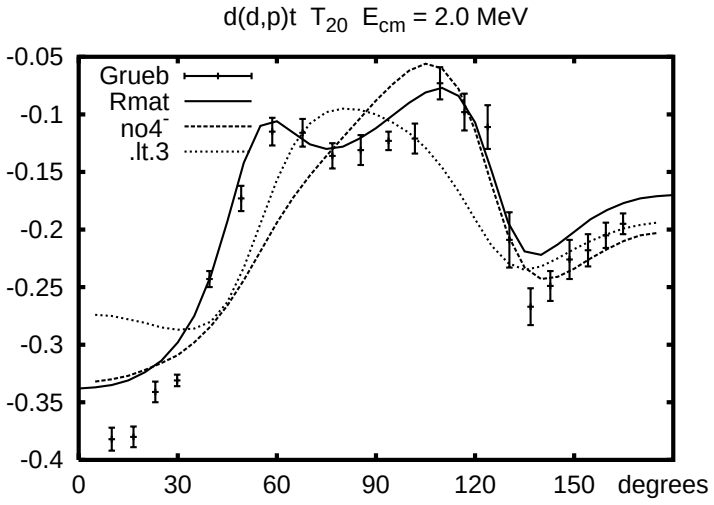


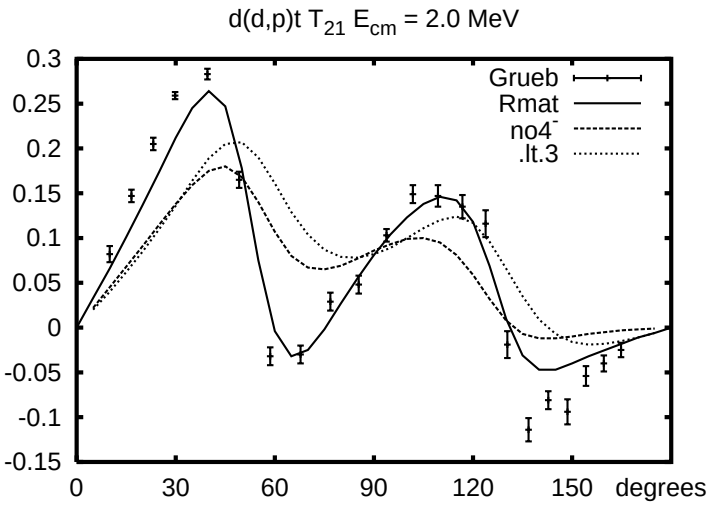
Large differencies

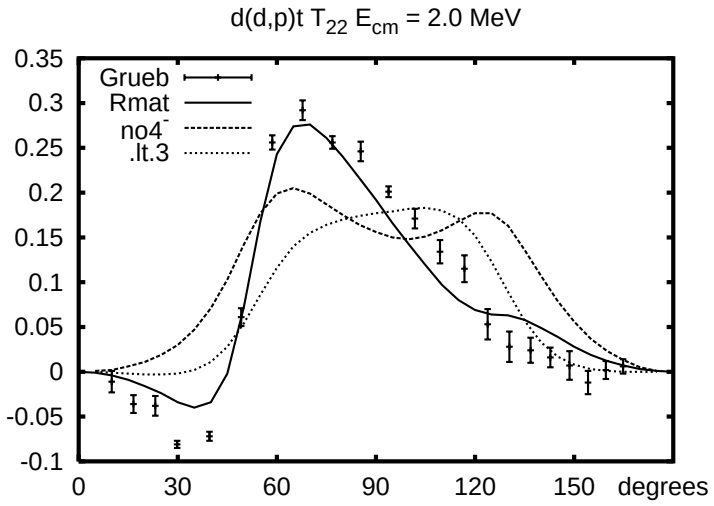
Deuteron – Deuteron fusion
R – matrix analysis





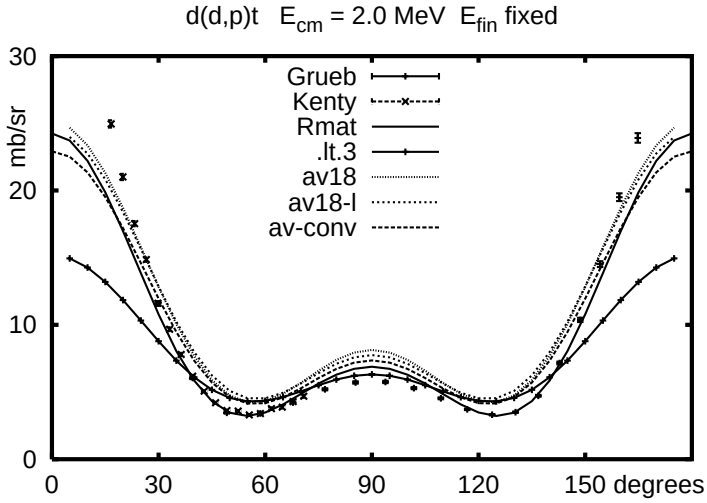


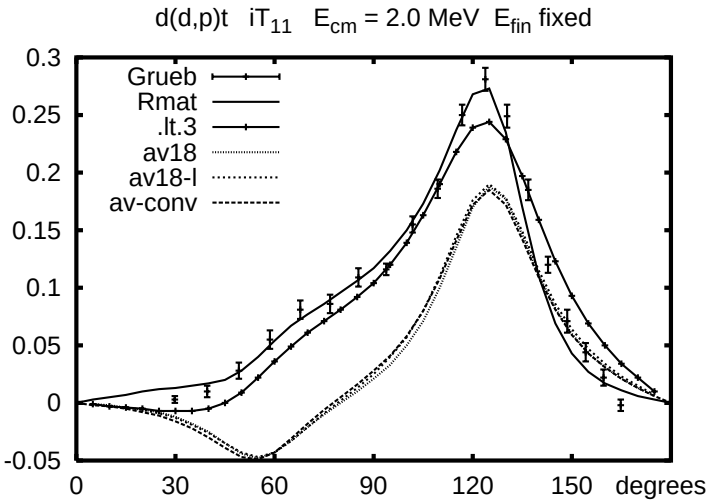


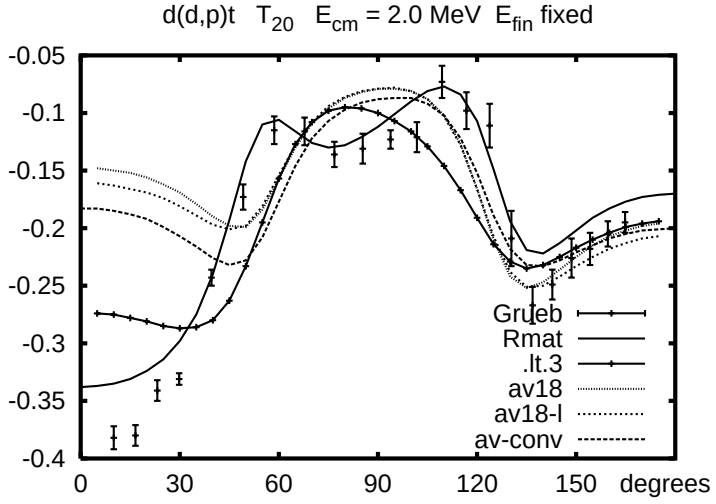


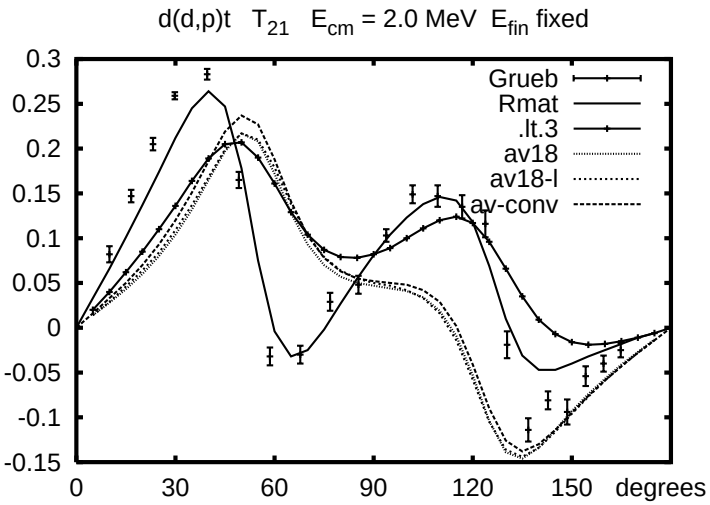
4^- causes big effects, 3^- still large, other missing channels negligible

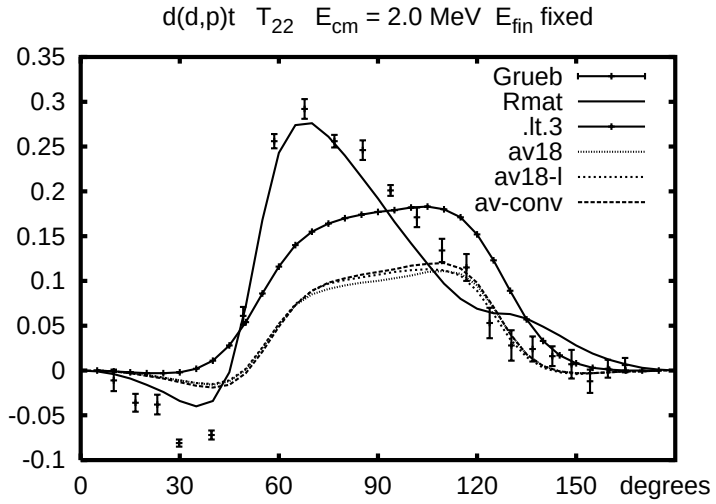
Deuteron – Deuteron fusion RGM calculation







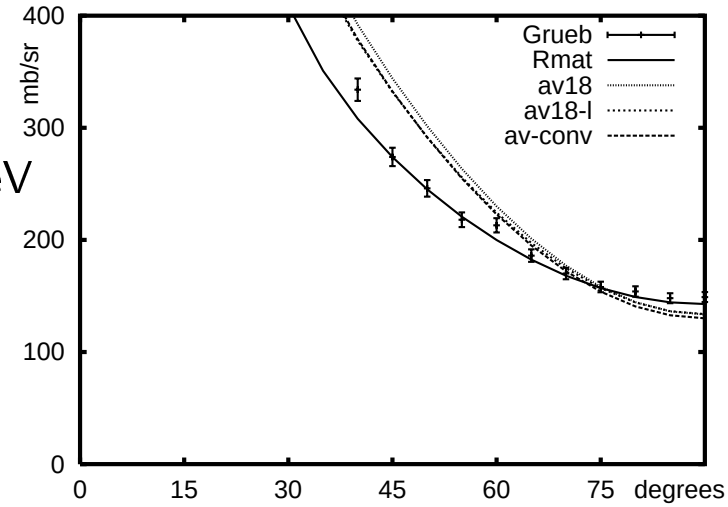


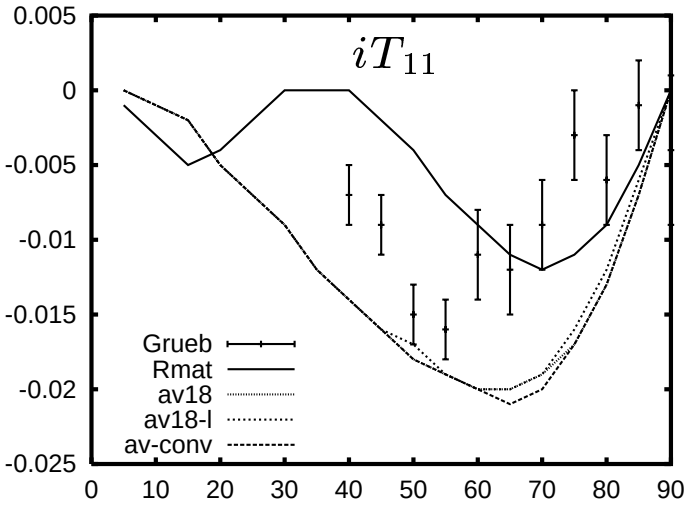


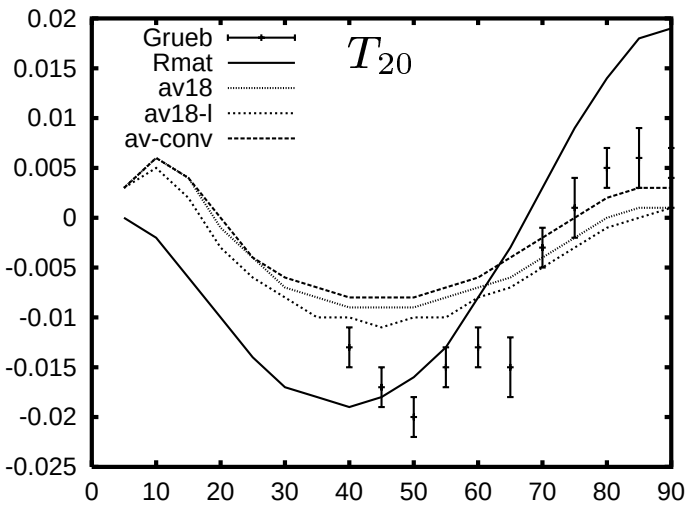
In restricted modelspace R-matrix and RGM results similar

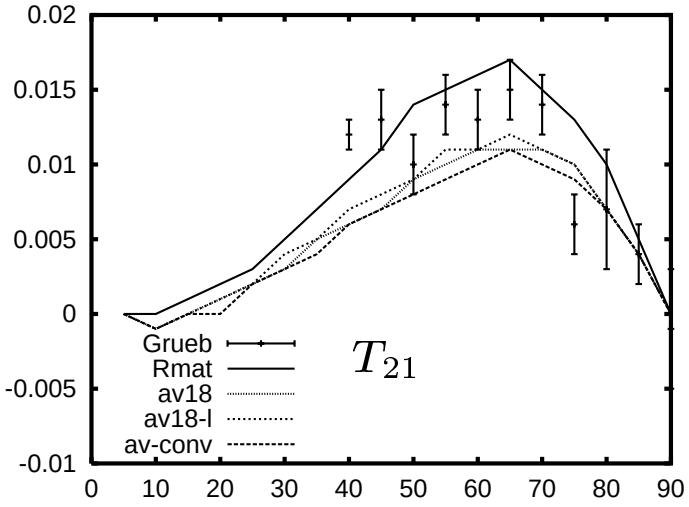
Deuteron – Deuteron elastic RGM calculation

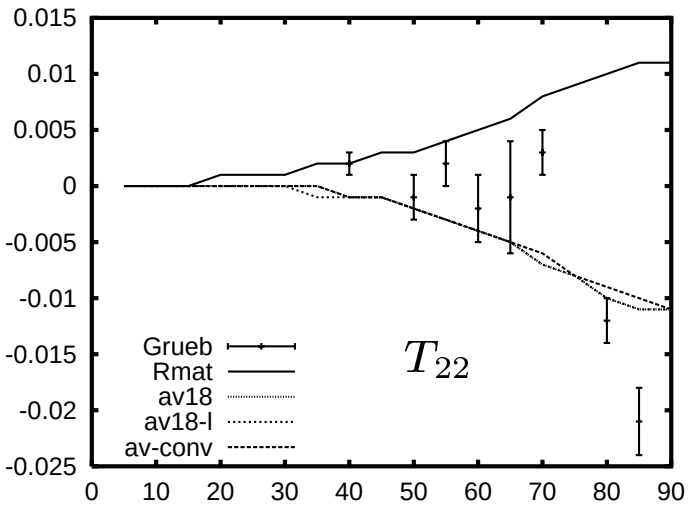
$E_{cm} = 3.11$ MeV











Polarisation data reasonably well reproduced

Resonating Group Model
S – matrix approach

RGM Ansatz $\Psi_l = \sum_{k=1}^{chan} \psi_{chan}^k \cdot \chi_{rel}^{lk}(\mathbf{R})$

Variation $\langle \delta\Psi_l \mathcal{A} | \mathrm{H} - \mathrm{E} |\ \Psi_l \rangle = 0$

Channel function $\psi_{chan} = [Y_L(\hat{\mathbf{R}}) \otimes [\phi_1^{j_1} \otimes \phi_2^{j_2}]^{S_c}]^J$

Ansatz $\psi = \psi_{chan}(\sum_i b_i \cdot \mathrm{Gaussian})$ (bound state)

or $\chi_{rel}^{lk}(R) = -\delta_{lk} \cdot \tilde{H}_k^-(R) + S_{lk} \cdot \tilde{H}_k^+(R) + \sum_i d_{lki} \cdot$ Gaussian (scattering state)

With $H^{\pm}(R) = G(R) \pm iF(R)$; $\lim_{R\to\infty} H^{\pm}(R) = e^{\pm ikR}$

Variational parameters S_{lk} and d_{lki}

Note: $\chi_{rel}^{lk}(R)$ regular at origin $\Rightarrow$ regularize $H^{\pm}(R)$ around origin

For complex k huge cancelations neccessary

Solution

$$S = i\left[\left(\tilde{H}^-|\tilde{\mathrm{H}} - \mathrm{E}|\tilde{\mathrm{H}}^-\right) - \left(\tilde{H}^+|\tilde{\mathrm{H}} - \mathrm{E}|\tilde{\mathrm{H}}^-\right)^T \left(\tilde{H}^+|\tilde{\mathrm{H}} - \mathrm{E}|\tilde{\mathrm{H}}^+\right)^{-1} \left(\tilde{H}^+|\tilde{\mathrm{H}} - \mathrm{E}|\tilde{\mathrm{H}}^-\right)\right]$$

Numerically more stable than standard approach
But no guarantee for unitary S

S – matrix pole positions

		R-matrix		RGM AV18 + UIX conv		
J^π	T	E_r	$-i\Gamma/2$	E_r	$-i\Gamma/2$	Γ_{tot}
0^+	0	0.114	0.196	0.096	0.114	0.173
	0	7.680	3.565	4.344	2.288	0.280
				12.230	2.186	0.840
1^+	0	8.416	3.008	6.288	3.104	0.419
				9.699	1.766	0.369
				12.619	1.851	0.738
2^+	0	4.840	3.159	3.156	2.914	0.393
	0	8.535	1.600	16.942	2.001	1.205
0^-	0	1.031	0.301	0.911	0.224	0.417
	1	4.550	11.79	1.657	3.064	0.963
				9.858	4.140	0.220
				12.611	0.268	0.514
1^-	0	2.804	2.336	0.750	1.887	0.704
	1	7.404	10.91	1.528	2.339	1.868
	0	8.051	1.801	2.028	2.556	1.567
				7.902	2.229	0.047
				9.936	3.336	0.326
				17.500	1.500	0.577
2^-	0	1.584	0.732	1.713	1.103	1.749
	1	7.230	9.049	3.752	2.945	0.804
				7.269	1.330	0.526
				9.931	2.262	0.642
				17.543	0.826	2.585

RGM calculation might yield more poles

Standard error Propagation in R-matrix Model Fitting for light elements

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Abstract. The error propagation features with R-matrix model fitting ^{7}Li, ^{11}B and ^{17}O systems were researched systematically. Some laws of error propagation were revealed, an empirical formula $P_j = U_j^c / U_j^d = K_j \cdot \bar{S} \cdot \sqrt{m} / \sqrt{N}$ for describing standard error propagation was established, the most likely error ranges for standard cross sections of ^{6}Li(n,t), ^{10}B(n,α0) and ^{10}B(n,α1) were estimated.

The problem that the standard error of light nuclei standard cross sections may be too small results mainly from the R-matrix model fitting, which is not perfect. Yet R-matrix model fitting is the most reliable evaluation method for such data. The error propagation features of R-matrix model fitting for compound nucleus system of ^{7}Li, ^{11}B and ^{17}O has been studied systematically, some laws of error propagation are revealed, and these findings are important in solving the problem mentioned above. Furthermore, these conclusions are suitable for similar model fitting in other scientific fields.

1. Data simulation

The formulas used for preparing *simulated data* are given in the reference [1,2]. In R-matrix fit, if experimental data are used to investigate the law of error propagation, there would be the following difficulties:

A. In general, experimental data involve several thousand data points, to make χ^2 minimum would involve especially tremendous calculations;

B. Usually, the experimental data measured by different laboratories are inconsistent to some extent, because some experimental errors were not recognized or were underestimated.

Therefore, it is difficult to get reliable error propagation law if experimental data are used in the study, so simulated data (SD) whose central values and errors are determined completely were adopted in this work.

Simulated data were prepared for all open reaction channels and reaction types in the energy range considered for a light nucleus system. The reaction channels are (n, ^{6}Li) and (t, ^{4}He) for ^{7}Li, (n, ^{10}B), (α_0, ^{7}Li) and (α_1, ^{7}Li*) for ^{11}B and (n,^{16}O) and (α,^{13}C) for ^{17}O. The data types include neutron total cross section σ_t, all kinds of integral reaction cross sections and differential cross section and polarization for elastic scattering. Energy ranges are E_n=0.253 $\times 10^{-7}$-1.04 (MeV), E_t=7.6-10.0 (MeV) for ^{7}Li; E_n=0.253$\times 10^{-7}$-1.04 (MeV), E_α =7.6-10.0

(MeV) for ^{11}B; $E_{n=}0.253\times10^{-7}$-6.4 (MeV), E_{α}=2.7-6.2 (MeV) for ^{17}O.

In order to investigate the dependence of the error propagation on data number *N*, 4 collections of data with different *N* (see table 2) were created for each light nuclide; there are some independent sub-collections in each collection of data. The points of each sub-collection of data are distributed uniformly in the energy range given.

The total relative error of simulated data was assigned according to practical situation. It is 2% for neutron total cross section, 4% or 5% for integral cross section, 6% for differential cross section, and 3% for polarization. In other cases, all relative errors were taken as 5%. Altogether 264 sets of data were involved in the investigation. The details of error distribution are described in reference [1].

In order to study relation between error propagation and error distribution, two collections of simulated data with 3250 data points and 4381 data points were created for ^{7}Li and ^{11}B respectively. For a given total variance U_i^2, we can define the ratio of total systematic variance to total variance $Y_i = Y_i^2/U_i^2$, and for a given total systematic variance Y_i^2, define the ratio of medium-range variance to total systematic variance $M_i = M_i^2/Y_i^2$. So let *Y* to be increase from 0.0 to 0.9999 and *M* from 0.0 to 1.0 with the step 0.05 for both, thus the combinations of all *Y* and *M* include all together 882 sets of data. In order to research the effect of Medium Energy Range Correlation (MERC) part of systematic errors, assume the correlation range follows normal distribution versus energy, and define distribution parameter *W* as the ratio of the distribution width to the whole energy range of the data. For a data set of ^{7}Li with *N*=3250 data points, 136 sets of data formed by the combination of different *Y*, *M* and W were dealt with.

In addition, the errors of a data collection with 4381 points of ^{11}B were decreased or increased in order to study the linear character of error propagation.

Simulated data were calculated according to the following formula

$$D_i^j = D_{it}[1 + (S_i/V_i)\cdot R_i + (Y_i/V_i)\cdot(-1)^j]. \qquad (1)$$

Here *j* refers to the sub-collection of the data, *i* to the data point, D_{it} to the calculated value of the data point *i* by using the R-matrix parameters taken from Chinese Evaluated Nuclear Data Library. R_i is a random numeral number generated by Monte Carlo and follows standard normal distribution. $(-1)^j$ expresses the change of sign of the systematic error contribution, to bring simulated data more close to the real case.

2. Calculation and analysis of error propagation

R-matrix Analyzing Code—RAC[1,3] was used for calculation. RAC is written according to the R-matrix formula given by A. M. Lane[4]. The kernel formulas are

$$R_{cc'} = \sum_{\lambda\mu}^{N_1} \gamma_{\lambda c} \times \gamma_{\mu c'} A_{\lambda\mu} + \sum_{\lambda}^{N_2} \frac{\gamma_{\lambda c'} \times \gamma_{\lambda c}}{E_\lambda - E} + R_{cc'}^{\infty} \ , \tag{2}$$

$$\left[A^{-1}\right]_{\lambda\mu} = \left[E_\lambda^{res} - E + \sum_c (S_c(E) - B_c)\gamma_{\lambda c}\gamma_{\mu c} - \frac{i}{2}\Gamma_{\lambda\mu}^{e} \right]\delta_{\lambda\mu} . \tag{3}$$

Parameters of R-matrix include reduced width amplitude γ, position of energy level E_λ, width of reduced channel $\Gamma_{\lambda\mu}^{e}$, boundary condition B_c, constant background of distant levels $R_{cc'}^{\infty}$, channel radius a_c. The sensitivities of all parameters were worked out through prior trial calculations. The parameters, which are not sensitive to fitted observable, are regarded as constant. The numbers of parameters of R matrix used for ^{7}Li, ^{11}B and ^{17}O are eventually determined as 18, 50 and 121 respectively.

The simulated data given above were taken as RAC code input and were fitted by adjusting the R-matrix parameters one by one to get the best parameters. In fact, for any set of data with systematic error contribution in the total error (*Y)* less than 99.99%, the initial value of χ^2 is about 1.0 and no adjusting was needed.

In calculated covariance matrix, the non-diagonal elements of covariance matrix give the information about correlation, which will be discussed in another paper. The square root of diagonal element of covariance matrix is just the standard error of each calculated data. Because the original error of simulated data was known, the information about standard error propagation can be obtained.

Relative error is averaged statistically according to following expression and then error propagation coefficient (EPC) P_j can be obtained,

$$U_j^c = \sum_l U_l^c \cdot N_j^l / \sum_l N_j^l \ , \tag{3}$$

$$P_j = U_j^c / U_j^d \ . \tag{4}$$

Here j expresses data type, summing over *l* means that there are *l* sets of j-type data and there are N_j^l data points for each set. Each data type in each simulated data collection has a corresponding error propagation coefficient. The characteristics of error propagation for (n, α) reaction, which was paid the most attention to, are discussed here. Of course, the conclusion obtained is suitable for other reaction type also.

Figs. 1, 2 are “hillock-like” pictures, which show error propagation coefficient *P(Y, M)* of ^{11}B and ^{7}Li respectively. In each figure, ordinate expresses variable *Y* and abscissa expresses variable *M* and *P (Y, M)* is shown by symbols different in size and shape. Points in the area, which is full of solid triangle, give largest *P(Y, M)*. Whole symbols look like a “hillock”, so it is called “hillock-like” picture here. In each figure, the central values of *P (Y, M)* are expressed by a corresponding symbol as shown in square box on right. In figs. 1 and 2, they are given with steps 0.004 and 0.002 for first five values and 0.01 and 0.005 for last eleven values. Both figures have some sense of three dimensions, and have a function of data table in some sense. For a given pair of *Y* and *M*, approximation of corresponding *P (Y, M)* can be read out from them.

In Fig. 3 is shown *P* (*Y, M*) curves of ^{7}Li system, the ordinate expresses error propagation coefficient *P* and abscissa is variable *M*. From figures above it can be seen that *P* (0,*M*) of ^{7}Li and ^{11}B are equal to 0.048 and 0.070 respectively when total error is entirely statistic one, *P*(0.9999,1.0) are equal to 0.024 and 0.055 respectively when total error is almost entirely MERC of systematic error, and *P*(0.9999,0.0) are equal to 0.0035 and 0.0033 respectively when total error is almost entirely LERC of systematic error. These show that with R-matrix model fitting, if only one type of error is taken into account, EPC of statistic error is larger than that of systematic error, EPC of the MERC of systematic error is larger than that of the LERC of systematic error, and all these EPC are relative small.

If total error includes both statistic and systematic error, *P (Y, M)* increases first rapidly with increasing systematic error until that systematic error is about half the total error, which can be seen clearly in fig 3. This shows that with R-matrix model fitting, neglect of systematic error would lead evaluated standard error to smaller, and this is just the main reason that makes the errors of current light nucleus standard cross section are too small.

When *Y* is smaller than 0.1, value of *M* has little influence on *P* (*Y, M*), but when *Y* is larger than 0.1, value of *M* effects error propagation considerably, which can be seen from fig 3. This shows that with R-matrix model fitting the influence of MERC of systematic error must be seriously considered, and neglect of it would lead evaluated standard error to remarkably smaller.

Fig. 4 shows the dependence of *P* (*Y, M*) on the correlation parameter *W* of MERC of systematic errors for ^{7}Li system. When the *W* increases from 0.5% at the beginning, and go through 1%, 3% and finally approach to 5%, *P* (*Y, M*) increases very rapidly and lies in highest value area already. *W* is relative to the factors such as energy resolution of detector and so on. In general, the energy resolution is several percent, so value of *W* is fixed as 5% in this work.

The propagation coefficients kept unchanged when the initial errors of simulated data were increased or decreased in proportion. There are 120 sets of ^{7}Li system simulated data whose initial errors were all 5%, are fitted by using R-matrix model, and no larger difference was found between the obtained *P* (*Y, M*) and that shown in fig 3.

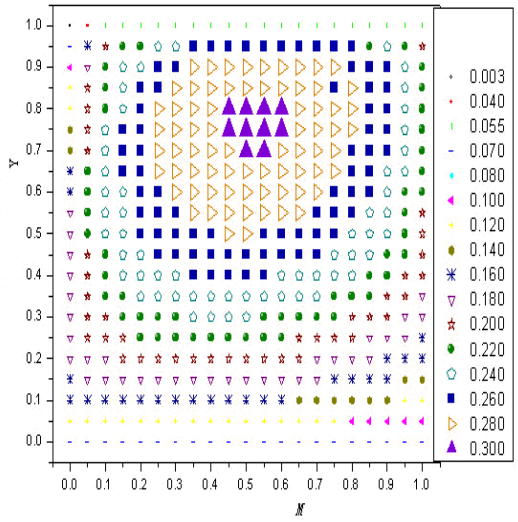

Fig. 1 Hillock-like pictures of $\sigma_{n,\alpha}$ error propagation coefficient $P(Y,M)$ for ^{11}B system.

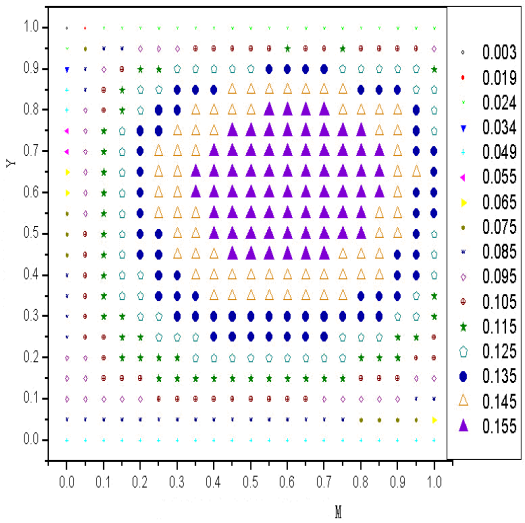

Fig. 2 Hillock-like pictures of $\sigma_{n,\alpha}$ error propagation coefficient $P(Y,M)$ for ^{7}Li system

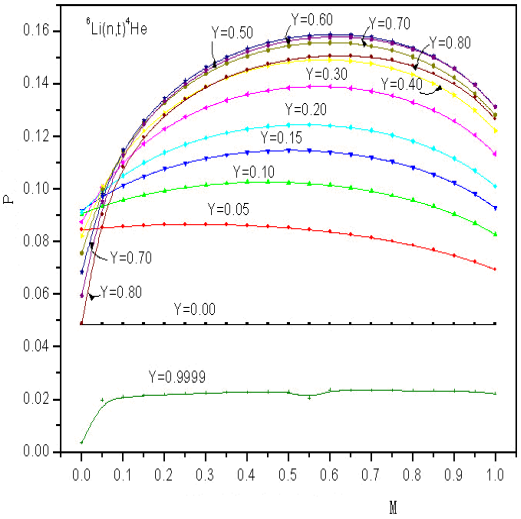

Fig. 3 Curves vs. M of $\sigma_{n,\alpha}$ error propagation coefficient $P(Y,M)$ for ^{7}Li system

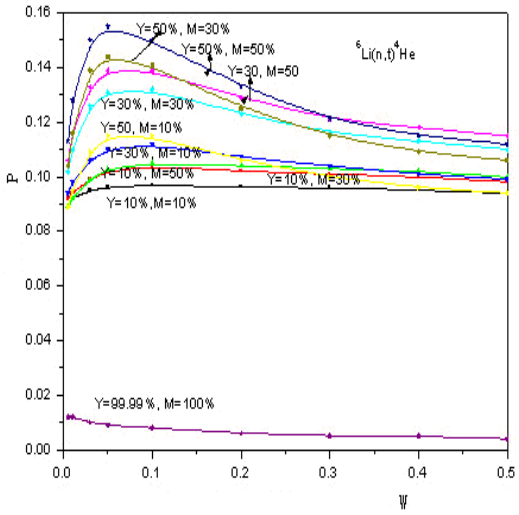

Fig. 4 Curves vs. W of $\sigma_{n,\alpha}$ error propagation coefficient $P(Y,M)$ for ^{7}Li system

In this paper the error distribution of simulated data almost covers the situation of existing available experimental data, so the calculated result can be used to estimate the range of standard error for evaluated standard cross section of ^{6}Li(n,t) ,^{10}B(n,α) and ^{10}B(n,α_1). In table 1, *P*-lower means Y=0.10 and M=0.50, *P*-higher means Y=0.50 and M=0.50. For realistic experimental data, additional errors caused by normalization and correction for non-consistent data also should be considered, and the experience indicates that these two factors could lead fairly remarkable contribution to the errors. It is possible that this make the "ideal" error increase by 50% or larger. The average of *P*-lower and *P*-higher gives the most possible value 4% and is chosen as the average of relative error of $\sigma_{n,\alpha}$ experimental data, thus the mean values of relative error of the three standard cross section mentioned above are about 0.76%, 1.2% and 1.0%. respectively.

Table 1. Estimated values of standards error for ^{6}Li(n,α), ^{10}B(n,α) and ^{10}B(n,α$_1$)

	Ideal value		Corrected value		
	p-lower	*p*-higher	*p*-lower	*p*-higher	*p*-mean
^{6}Li(n,α)	10%	15%	15%	23%	19%
^{10}B(n,α0)	15 %	26%	23%	39%	31%
^{10}B(n,α$_1$)	12.9%	20.0%	20%	30%	25%

The theoretical formulas of error propagation in model fitting are very complicated matrix operations. An empirical expression for describing standard error propagation coefficient P_j was deduced according to the results calculated systematically in this work, that is

$$P_j = U_j^c / U_j^d = K_j \cdot \bar{S} \cdot \sqrt{m} / \sqrt{N} \qquad (5)$$

Here *j* expresses the type of nuclear reaction, *m* the number of parameters, *N* the total number of the data, $\bar{S}$ the mean of absolute value of all sensitive matrix elements, and K_j is a positive real number and is called "error propagation factor" in this paper. The base of mathematics and physics for the formula is qualitatively explained as follows.

The R-matrix model fitting is essentially based on maximum likelihood method and to make the best parameter estimation from a great deal of statistical samples. $P_i \propto 1/\sqrt{N}$ comes from normal distribution of the sample statistic error. Mean $\bar{S}$ reflects character of nuclear reaction of light nuclide and is relative to the composition of the fitted data, but not to the error situation. The value of $\bar{S}$ for each data collection for the three nuclides are listed in table 2, where the unit of cross section, length and energy is b, fm and MeV respectively. The absolute value of each matrix element reflects corresponding sensitivity of a data point to a parameter. Whole sensitivity of parameters is ultimately reflected by relative error of parameter; smaller relative error means more sensitivity and stronger influence on data error propagation. Calculations shows that a parameter with relative error larger than 60% has a very small contribution to error propagation, and was treated as a constant in the calculations, so *m* in formula (5) is only the number of parameters with relative error smaller than 60%. It can be seen that the calculations of theoretical covariance need to be summed over *m* parameters, this leads to the dependence of *P* on the square root of *m*. Put P_j of each data type and corresponding $\bar{S}$, *m, N* into formula (4), the error propagation factors K_j of each data type were obtained.

Table 2. N, χ^2,m, $\bar{S}$ of simulated data and *P(Y, M),K(Y, M)* of (n,α) reaction

	No	N	χ^2	m	$\bar{S}$	P (0,0.5)	K (0,0.5)	P (0.5,0.5)	K(0.5,0.5)
^{7}L	A	1980	0.9	18	0.604	0.095	1.287	0.169	2.779
	B	2801	0.9	18	0.397	0.088	1.346	0.165	2.871
	C	3624	0.9	18	0.531	0.072	1.409	0.145	2.832
	D	4275	0.9	18	0.399	0.065	1.310	0.138	2.777
^{11}B	A	2713	0.9	50	0.142	0.097	1.904	0.308	6.025
	B	4636	0.9	50	0.145	0.074	1.852	0.277	6.994
	C	7011	0.9	50	0.197	0.058	1.555	0.232	6.193
	D	8654	0.9	50	0.170	0.051	1.510	0.220	6.435
^{17}O	A	3928	1.0	121	0.249	0.137	1.559	0.227	2.593
	B	5722	1.0	121	0.256	0.116	1.580	0.170	2.314
	C	7625	1.0	121	0.255	0.096	1.517	0.145	2.284
	D	9519	1.0	121	0.249	0.085	1.502	0.129	2.299

The values of N, χ^2, m and $\bar{S}$ of the four groups of data for each light nuclide system, and the value of *P* and *K* for the reaction (n,α) are shown in table 2. When systematic error is zero, the value of *P* and *K* is minimum. For each nuclide system the value of *P* decreases with the increasing of data number *N*. But it is an exception for the oxygen data, for which, *N* is larger, *P* is also relatively larger, this is due to more R-matrix parameters were used. There is remarkable difference among the four *P* values of each nuclide system, but the corresponding error propagation factors *K* are very close to each other; this shows that empirical expression (5) has impersonal foundation in physics and mathematics. In fact, the empirical expression (5) can be directly deduced from formulas 1 to 5, assuming that all data are not correlated, and that all sensitive matrix elements are chosen as the mean, and non-diagonal covariance matrix elements of parameters are neglected. The errors generated by above approximations are reflected in factor *K*.

Averaging the four groups of data for each nuclide system and treating $\bar{S} \times$K as a coefficient, it was obtained that $P_{n\alpha}(^{7}Li) \approx 0.34\sqrt{m}/\sqrt{N}$, $P_{n\alpha}(^{11}B) \approx 0.29\sqrt{m}/\sqrt{N}$, $P_{n\alpha}(^{17}O) \approx 0.38\sqrt{m}/\sqrt{N}$. And making approximation further, it was obtained finally that $P_{n\alpha} \approx 1/3 \cdot \sqrt{m}/\sqrt{N}$.

In experimental nuclear physics, approximation formula $P \approx 1/\sqrt{N}$ is taken to estimate relative error of measured data, which is very convenient and practical to design and plan the experiment. The above empirical formula has similar function for theoretical model fitting and experimental data evaluation. For example, when a preliminary result of fitting is obtained according to an experiment data collection, the formula (5) can be used to judge the rationality of the experiment data collection. Formula (5) also shows that in order to obtain more accurate evaluation results, the number of experiment data should be as more as possible, their errors should be as small as possible and the number of theory model parameters should be as few as possible.

3. Conclusion

A. With R-matrix model fitting, if only one kind of data errors is considered, propagation coefficient of statistic error is larger than that of systematic error; propagation coefficient of MERC of systematic error is larger than that of LERC of systematic error; and these propagation coefficients are all quite small.

B. If total error includes statistic error and systematic error at the same time, with systematic error increasing, the coefficient of error propagation increases rapidly at the beginning, and then continue to increase until systematic error is about half of the total error. This shows that with R-matrix model fitting, neglect of the systematic error must lead to the smaller evaluated standard errors. From the study of this work, the most possible mean values of relative standard error for ^{6}Li(n,α), ^{10}B(n,α) and ^{10}B(n,α_1) are about 0.76%，1.2% and 1.0% respectively.

C. When the proportion of the systematic error *Y* is less than 10%, the proportion of MERC of systematic error to total systematic error *M* has little influence on error propagation. But when *Y* is more than 10%, *M* has a very large influence on error propagation. This shows that with R-matrix model fitting, neglect of the MERC of systematic error must lead to the remarkably smaller evaluated standard error.

D. With R-matrix model fitting, theoretical expression for error propagation involves very complicated matrix operations, but standard error propagation coefficient *P* can be expressed by a very simple empirical formula $P_j = U_j^c / U_j^d = K_j \cdot \bar{S} \cdot \sqrt{m} / \sqrt{N}$. This formula may play an important role on evaluation of experimental data and is suitable for similar fields in other subjects.

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References

1. Chen Z. P.,Sun Y. Y., New function for deal with covariance matrix in RAC.
2. Smith D L. Probability, Statistics, and Data Uncertainties in Nuclear Science and Technology, American Nuclear Society, Inc. 1991, 229-232
3. Chen Z. P., Reduced R-Matrix Analysis for ^{17}O system, Atomic Energy Science and Technology, 1995,29(4): 366-371
4. Lane A M, Thomas R. G.,. R-Matrix Theory of Nuclear Reaction, Reviews of Modern Physics, 1958, 30 (2): 257

New Function for Deal with Covariance Matrix in RAC

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1. Basic formula for error propagation in Model fitting

The theoretical formula for error propagation in R-matrix model fitting [3] is as follow:

$$\vec{y} - \vec{y}_0 = D(\vec{P} - \vec{P}_0), \tag{1}$$

$$D_{ki} = (\partial y_k / \partial P_i)_0 . \tag{2}$$

Here $\vec{y}$ refers to the vector of calculated values, D to the sensitivity matrix, $\vec{P}$ to the vector of R-matrix parameters. Subscript 0 means optimized original value, *k and i* are for fitted data and R-matrix parameter subscript respectively. The covariance matrix of parameter $\vec{P}$ is

$$V_{\vec{p}} = (D^{+}V^{-1}D)^{-1} \quad , \tag{3}$$

here *V* refers to covariance matrix of the data to be fitted, and its inversion matrix can be expressed as following:

$$V^{-1} = \begin{bmatrix} V_1^{-1} & & & 0 \\ & V_2^{-1} & & \\ & & \ddots & \\ 0 & & & V_k^{-1} \end{bmatrix} . \tag{4}$$

Here $V_1, V_2 \cdots V_k$ refer to the covariance matrixes of the sub-set data, which are independent with each other. The covariance matrix of calculated values is

$$V_{\vec{y}} = DV_{\vec{p}}D^{+} \tag{5}$$

Formula adopted for optimizing of parameters with R-matrix fitting is

$$\chi^2 = (\vec{\eta} - \vec{y})^{+}V^{-1}(\vec{\eta} - \vec{y}) \Rightarrow \text{minimum}, \tag{6}$$

here $\vec{\eta}$ refers to the vector of experimental data, $\vec{y}$ refers to the vector of calculated values. All the elements of V are included in calculation.

2. Basic formula for calculation of covariance matrix

Suppose U_i^2, S_i^2, L_i^2, M_i^2 and Y_i^2 are total variance, statistical variance, long-range component (LERC) of systematic variance, medium-range component (MERC) of systematic variance and total systematic variance of *i*-th experimental data point respectively, and let $U_i^2 = S_i^2 + L_i^2 + M_i^2$, $Y_i^2 = L_i^2 + M_i^2$. For a given total variance U_i^2, we can define the ratio of total systematic variance to total variance $Y_i = Y_i^2 / U_i^2$, for a given total systematic variance Y_i^2,

define the ratio of medium-range variance to total systematic variance $M_i = M_i^2 / Y_i^2$.

For differential cross section, assume the correlation among different angles also follows normal distribution, and the distribution width is given value (degree).

The element of covariance matrix is

$$V_{ij} = C_{ij} \cdot U_i U_j \,. \tag{7}$$

The diagonal elements C_{jj} of correlation coefficient matrix C are 1 for all.

The non-diagonal elements for integral cross section are

$$C_{ij} = C_{ij}^L + C_{ij}^M \,, \tag{8}$$

here C_{ij}^L refer to the LERC of systematic errors, C_{ij}^M to the MERC of systematic errors, and

$$C_{ij}^L = L_i L_j / (U_i U_j) \,, \tag{9}$$

$$C_{ij}^M = M_i M_j / (U_i U_j) \cdot f_{ij} \,, \tag{10}$$

$$f_{ij} = Exp[-(E_i - E_j)/W]^2 / 2 \,, \tag{11}$$

here W is a distribution width parameter, E_i and E_j express energy points of the data.

The non-diagonal elements of C for differential cross section are

$$C_{ij} = (C_{ij}^L + C_{ij}^M) \cdot G_{ij} \,, \tag{12}$$

$$G_{ij} = Exp\{-[(\theta_i - \theta_j)/160]^2 / 2\} \,. \tag{13}$$

Here 160 is a distribution parameter related to angle, θ_i and θ_j are angle values.

It can be seen from the formulas given above that correlation coefficient is determined by total error and systematic error, and a larger systematic error leads to a larger correlation coefficient.

The covariance matrix of parameter was calculated with formula (3), and the sensitive matrix elements D_{ij} were calculated by using finite difference methods ,

$$D_{ij}=\{T(p+3d)-T(p-3d)+ 9[T(p-2d)-T(p+2d)]+45[T(p+d)-T(p-d)]\}/(60d) \tag{14}$$

In order to ensure reliability of calculations, the best range of the step d was studied in very detail.

Covariance matrix of theoretical value is calculated according to formula (5). Because the original error of simulated data is known, all information about standard error propagation can be obtained.

Relative error is averaged statistically according to the following expression and then error propagation coefficient (EPC) P_j can be obtained,

$$U_j^c = \sum_l U_l^c \cdot N_j^l / \sum_l N_j^l \,, \tag{15}$$

$$P_j = U_j^c / U_j^d \quad . \tag{16}$$

Here j expresses data type, summing over *l* means there are *l* sets of j-type data and there are N_j^l data points for each set. Each data type in each data collection has a corresponding error propagation coefficient.

3. Checking for positive definiteness

In physics, it is pointed that [3] 'matrices which properly represent physical uncertainties are positive definite'. So the covariance matrix V of experimental data is real symmetric and positive definite.

In mathematics it is pointed that, ' to every real symmetric matrix A an orthogonal matrix H can be found such that

$$H^{-1}AH=\lambda i, \tag{17}$$

the matrix H is sometimes called the model matrix of A'. When A is positive definite, λi is a diagonal and positive definite matrix, λi^{-1} is positive definite too. So that

$$[H^{-1}AH]^{-1}=H^{-1}A^{-1}H=\lambda i^{-1}, \tag{18}$$

It is shown that A^{-1} is positive definite, and the inverse matrix V^{-1} is positive definite.

In mathematics, there is a formula as: If $A \varepsilon R^{nxn}$ is a positive definite matrix, and the column vectors of the matrix $X \varepsilon R^{nxk}$ are linearly independent, then the matrix

$$B=X^T AX \varepsilon R^{kxk} \tag{19}$$

is also positive definite.

According to formula (19), in formula (3) $V_{\hat{p}} = (D^+ V^{-1} D)^{-1}$ and formula (5) $V_{\tilde{y}} = D V_{\tilde{p}} D^+$, if sensitivity matrix D is linearly independent, the covariance matrix of parameters and calculated cross sections will be positive definite.

The calculation of covariance matrix involves inversion of high rank matrix and numerous product adding, sometimes the number of product adding reaches several ten million. The sensitivity of data points related to energy is very high, and some troubles may easily occur when the energy of a data point is in the vicinity of 'extraordinary point' and 'vertex point'. Therefore the code was carefully designed to ensure that sensitivity matrix D is linearly independent and every kind of covariance matrix is positive definite. By getting eigenvalues of calculated covariance matrix we check it's positive definiteness.

Reference

1. Lane A. M, Thomas R G., R-Matrix Theory of Nuclear Reaction, Reviews of Modern Physics, 1958, 30 (2): 257
2. Chen Z. P., Reduced R-Matrix Analysis for ^{17}O system, Atomic Energy Science and Technology, 1995,29(4): 366-371
3. Smith D. L., Probability, Statistics, and Data Uncertainties in Nuclear Science and Technology, American Nuclear Society, Inc. 1991, 229-232

Progress Report on calculation of ^{6}Li(n,t) with RAC

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Some works on calculation of ^{6}Li(n, t) have been done with RAC, mainly in order to make comparison of GMA-fitting and RAC-fitting.

1. Data base

In RAC-fitting, the data-base used is shown in Table 1. It includes the main kinds of data in ^{7}Li system, come to total number of 1004 data. The 5 data-sets of ^{6}Li(n, t) with total number of 154 data have been studied with GMA and GLUCS. There exists rather lager discrepancy among these data.

TABLE 1 Information of data base in ^{7}Li system

AUTHER	NORM.FAC	ER-FAC		NUMBER	
'HARV-TO1'	1.000000	'F' 2.0	1.00	1	22
'HARV-TO2'	1.000000	'F' 2.0	1.00	23	85
'KITT-TOT'	1.000000	'F' 2.0	1.00	108	134
'LANE-DNN'	1.000000	'F' 2.0	1.00	242	95
'MEAD-INT'	1.000000	'F' 2.0	1.00	337	1
'RENE-INT'	1.000000	'F' 2.0	1.00	338	3
'LAMAZ-NA'	1.000000	'F' 2.0	1.00	341	51
'FORT-NA1'	1.000000	'F' 2.0	1.00	392	13
'FORT-NA2'	1.000000	'F' 2.0	1.00	405	25
'POENI-NA'	1.000000	'F' 2.0	1.00	430	19
'FRIES-NA'	1.000000	'F' 2.0	1.00	449	46
'OVEL-DNT'	1.000000	'F' 2.0	1.00	495	256
'BROW-DNT'	1.000000	'F' 2.0	1.00	751	25
'JARM-DTT'	1.000000	'F' 2.0	1.00	776	127
'JARM-YTT'	1.000000	F' 2.0	1.00	903	84
'DROSG-TN'	0.270000	'F' 2.0	1.00	987	10
'DRO-DTN2'	0.200000	'F' 2.0	1.00	997	8

2 The dependency on number of data

By changing the factor of error for a data-set, it's possible to make the data-set informative or non-informative. The calculation includes 4 situations:

1. D1004. All data are informative. By search to get a good parameter set D1004.par, this

parameter set will be taken as starting values for other cases.

2. D0155. The 5 data-sets of ^{6}Li(n, t) with total number of 154 data are informative, the data at 0.253E-07 is informative too.
3. D0154. Just 5 data-sets of ^{6}Li(n, t) with total number of 154 data are informative;
4. D0108. 4 data-sets of ^{6}Li(n, t) with total number of 108 data are informative, the data of 'FRIES-NA' is non-informative.

Table 2 shows some characteristic values of the evaluated data. The first impression is:

1. The value of D1004 is very close to the value of ENDF/B6.
2. The value of D0154 is lower then the value of ENDF/B6 obviously, and it's very near the value of DGAMS; this is just due to fit 154 data of ^{6}Li(n, t) .
3. The value of D0155 get much improvement relative to ENDF/B6, this is duo to the data of 0.253E-07 MeV is included. This explain that the data at thermal energy is very important in the evaluation of ^{6}Li(n, t). But in Table 2 it is shown that the thermal data is relative lower then that of ENDF/B6, This explain that other kinds of data have to be Considered in evaluation of ^{6}Li(n, t) when with R-matrix fit.
4. The value of D0108 is higher then all other values. This is because the data of 'FRIES-NA', which are not included, are below any others.

TABLE 2 . Comparison of calculated ^{6}Li(n,t) at some energies

En(MeV)	0.253E-07	0.25E-02	0.100	0.240	0.800
ENDF/B6	940983.	2979.1	651.5	3257.0	254.0
D1004	938933.	2979.7	670.7	3260.4	250.1
D0155	923275.	2922.1	659.3	3235.0	258.6
D0154	817995	2595.7	616.6	2995.8	248.4
GMAS		2665.9	596.3	3939.1	224.1
D0108	964407	3094.2	669.2	3220.3	252.5

3. The dependency on error of data

If for different data sets, the discrepancies exist at many points, which are larger than the errors given, then there is no any possibility to get average χ^2 close to 1.0 using original error values. Tables 3 and 4 show, that when the given error is multiplied by a factor, the calculated values of ^{6}Li(n, t) are different in the best fits. A very important data point is the value calculated at 0.253E-07 MeV which with given data is usually below 932 b in normal situations. The experimental value 941.8 b was at 0.253E-07 MeV with very small error was added in case of D1004 for test.

TABLE 3. FACTOR OF ERRORS

DATA	TOT	DIF(N,N)	(N,T)-THE.	INT(N,T)	DIF(N,T)	DIF(T,T)	DIF-(T,N)
A1004	1.0	1.0	1.0	1.0	1.0	1.0	1.0
B1004	1.4	1.4	1.0	1.0	1.0	2.5	1.0
C1004	1.0	1.0	0.4	1.0	1.0	3.5	1.0
E1004	1.0	1.0	0.4	1.0	1.5	2.5	2.0
D1004	1.0	1.0	0.1	1.0	1.0	3.5	1.0
F1004	1.0	1.0	1.0	1.0	1.5	2.5	2.0

TABLE 4. ^{6}Li(n, t) cross section(mb) at some characteristic points

En (MeV)	0.253E-7	0.0025	0.0095	0.045	0.0950	0.202	0.242	0.402	0.802
A1004	913242.8	2892.0	1496.3	756.1	671.2	2141.1	3400.1	538.4	239.7
B1004	929857.1	2951.1	1525.5	768.1	678.2	2146.9	3401.7	541.0	241.2
C1004	904872.2	2866.4	1484.3	751.9	664.3	2055.1	3280.0	520.7	259.5
D1004	938933.2	2971.1	1534.4	766.8	664.5	2007.9	3262.4	520.3	249.7
E1004	932374.1	2951.1	1525.5	768.1	678.2	2146.9	3401.7	541.0	241.2
F1004	932374.0	2951.1	1525.5	768.1	678.2	2146.9	3401.7	541.0	241.2

4. Comparison among R-matrix code

The comparison among R-matrix code EDA, SAMMY and RAC has been done. Table 5 presents the result of calculations of integral cross section of ^{6}Li(n, t) and Table 6 - the result for differential cross section of ^{6}Li(n, n) reaction. The agreement is very good. If RAC will use the relativistic kinematics the agreement between EDA and RAC will be even better.

Table 5. Comparison for calculated ^{6}Li(n, t) with same parameter

En(MeV)	SAM(mb)	RAC(mb)	EDA(mb)	(S-E)/E%	(R-E)/E%	(S-R)/R%
0.253E-07		926584.0				
0.0010		4634.231	4634.227		0.00011	0.03831
0.0020		3273.382	3273.380		0.00006	0.04009
0.0040	2314.282	2314.280	2314.280	0.00008	0.00000	0.00008
0.0060	1891.544	1891.542	1891.543	0.00008	-0.00005	0.00013
0.0080	1640.885	1640.882	1640.884	0.00007	-0.00011	0.00018
0.0100	1470.794	1470.791	1470.793	0.00007	-0.00016	0.00022
0.0150	1209.054	1209.050	1209.054	0.00004	-0.00029	0.00033
0.0200	1055.808	1055.803	1055.808	0.00002	-0.00042	0.00044
0.0250	953.426	953.421	953.426	-0.00001	-0.00056	0.00055
0.0300	879.737	879.731	879.737	-0.00003	-0.00069	0.00067
0.0350	824.173	824.166	824.173	-0.00004	-0.00083	0.00079
0.0400	780.986	780.979	780.987	-0.00006	-0.00098	0.00091
0.0450	746.763	746.755	746.763	-0.00010	-0.00113	0.00103
0.0500	719.338	719.330	719.339	-0.00012	-0.00127	0.00115
0.0600	679.601	679.591	679.602	-0.00018	-0.00161	0.00143
0.0700	654.841	654.830	654.842	-0.00023	-0.00194	0.00171
0.0800	641.646	641.633	641.648	-0.00029	-0.00228	0.00200
0.0900	638.426	638.411	638.428	-0.00034	-0.00262	0.00228
0.1000	644.724	644.707	644.726	-0.00041	-0.00294	0.00254
0.1100	660.944	660.925	660.947	-0.00046	-0.00325	0.00279
0.1200	688.296	688.275	688.300	-0.00051	-0.00351	0.00300
0.1300	728.882	728.859	728.886	-0.00055	-0.00368	0.00313
0.1400	785.907	785.882	785.912	-0.00060	-0.00376	0.00316
0.1500	864.021	863.994	864.026	-0.00061	-0.00370	0.00309
0.1600	969.789	969.761	969.795	-0.00060	-0.00349	0.00289
0.1700	1112.227	1112.199	1112.234	-0.00059	-0.00313	0.00254
0.1800	1303.120	1303.093	1303.127	-0.00053	-0.00262	0.00209
0.1900	1556.243	1556.218	1556.250	-0.00049	-0.00211	0.00162
0.2000	1883.305	1883.279	1883.313	-0.00047	-0.00181	0.00134
0.2100	2282.458	2282.421	2282.469	-0.00048	-0.00211	0.00163
0.2200	2716.121	2716.042	2716.139	-0.00067	-0.00359	0.00292
0.2300	3089.881	3089.708	3089.912	-0.00101	-0.00662	0.00561
0.2400	3275.455	3275.146	3275.505	-0.00154	-0.01097	0.00944
0.2500	3201.237	3200.806	3201.303	-0.00207	-0.01552	0.01345
0.2600	2916.738	2916.255	2916.811	-0.00249	-0.01907	0.01658
0.2700	2539.009	2538.543	2539.079	-0.00274	-0.02109	0.01835
0.2800	2163.991	2163.581	2164.052	-0.00282	-0.02176	0.01895
0.2900		1837.111	1837.506		-0.02154	
0.3000	1569.876	1569.592	1569.918	-0.00269	-0.02077	0.01808
0.3200	1185.997	1185.805	1186.026	-0.00243	-0.01862	0.01619
0.3400	941.487	941.353	941.507	-0.00214	-0.01636	0.01423
0.3600	780.245	780.148	780.259	-0.00188	-0.01434	0.01246
0.3800	669.169	669.095	669.180	-0.00167	-0.01261	0.01094
0.4000	589.423	589.366	589.432	-0.00146	-0.01113	0.00967
0.4200	530.054	530.008	530.060	-0.00130	-0.00990	0.00860
0.4400	484.451	484.414	484.457	-0.00117	-0.00887	0.00770
0.4600	448.475	448.444	448.480	-0.00106	-0.00800	0.00693
0.4800	419.435	419.409	419.439	-0.00095	-0.00726	0.00631
0.5000	395.525	395.502	395.529	-0.00090	-0.00664	0.00574
0.5500	350.874	350.857	350.877	-0.00072	-0.00544	0.00471
0.6000	319.753	319.740	319.755	-0.00062	-0.00462	0.00400
0.6500	296.620	296.609	296.621	-0.00056	-0.00406	0.00351
0.7000	278.560	278.551	278.561	-0.00049	-0.00367	0.00318
0.7500	263.910	263.903	263.912	-0.00043	-0.00340	0.00297
0.8000	251.657	251.650	251.658	-0.00044	-0.00320	0.00276

Table 6. Comparison for calculated differential ^{6}Li(n, t) with the same parameters

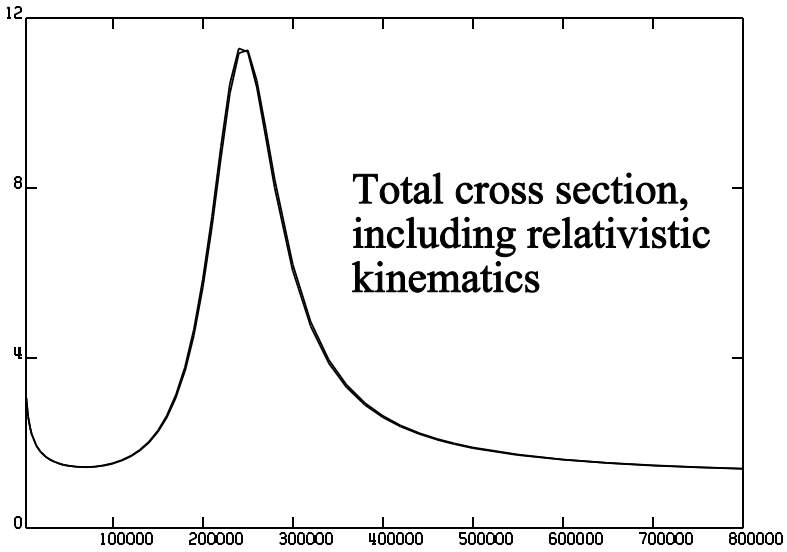
En(Lab)	------0.100 MeV------			----- 0.250 MeV ------			----- 0.800 MeV ------		
A(deg)	RAC	EDA	(R-E)/E%	RAC	EDA	(R-E)/E%	RAC	EDA	(R-E)/E%
0	27.29	27.29	-0.00449	1123.47	1123.34	0.01143	301.60	301.58	0.00469
5	27.42	27.42	-0.00444	1119.04	1118.91	0.01143	300.28	300.27	0.00469
10	27.83	27.83	-0.00428	1105.87	1105.75	0.01141	296.36	296.35	0.00466
15	28.51	28.51	-0.00403	1084.33	1084.21	0.01138	289.92	289.91	0.00462
20	29.46	29.46	-0.00369	1055.02	1054.90	0.01132	281.09	281.08	0.00457
25	30.67	30.67	-0.00328	1018.72	1018.61	0.01125	270.06	270.05	0.00450
30	32.16	32.16	-0.00281	976.45	976.34	0.01117	257.05	257.04	0.00442
35	33.90	33.90	-0.00233	929.35	929.25	0.01104	242.33	242.32	0.00430
40	35.90	35.90	-0.00182	878.71	878.61	0.01088	226.19	226.18	0.00417
45	38.15	38.15	-0.00130	825.88	825.79	0.01069	208.95	208.94	0.00402
50	40.64	40.64	-0.00079	772.28	772.20	0.01043	190.94	190.93	0.00383
55	43.36	43.36	-0.00028	719.33	719.26	0.01011	172.50	172.49	0.00362
60	46.30	46.30	0.00021	668.42	668.35	0.00971	153.97	153.96	0.00336
65	49.45	49.45	0.00068	620.84	620.79	0.00921	135.66	135.66	0.00305
70	52.79	52.79	0.00113	577.81	577.76	0.00864	117.89	117.88	0.00269
75	56.30	56.30	0.00155	540.35	540.31	0.00796	100.93	100.92	0.00226
80	59.96	59.96	0.00195	509.35	509.31	0.00721	85.02	85.02	0.00181
85	63.75	63.74	0.00233	485.46	485.43	0.00639	70.38	70.38	0.00115
90	67.63	67.63	0.00269	469.12	469.10	0.00554	57.16	57.16	0.00043
95	71.58	71.58	0.00302	460.56	460.54	0.00472	45.49	45.49	-0.00043
100	75.57	75.57	0.00332	459.74	459.73	0.00398	35.43	35.43	-0.00145
105	79.57	79.57	0.00360	466.42	466.40	0.00335	27.02	27.02	-0.00264
110	83.55	83.54	0.00386	480.11	480.09	0.00285	20.22	20.22	-0.00389
115	87.45	87.45	0.00409	500.12	500.11	0.00248	14.98	14.98	-0.00501
120	91.26	91.26	0.00432	525.59	525.57	0.00226	11.18	11.18	-0.00553
125	94.93	94.93	0.00451	555.48	555.47	0.00214	8.71	8.71	-0.00468
130	98.43	98.43	0.00469	588.66	588.65	0.00210	7.38	7.38	-0.00169
135	101.73	101.72	0.00485	623.88	623.87	0.00212	7.03	7.03	0.00292
140	104.78	104.77	0.00499	659.88	659.86	0.00219	7.44	7.44	0.00773
145	107.55	107.55	0.00511	695.36	695.34	0.00228	8.41	8.41	0.01128
150	110.02	110.02	0.00521	729.06	729.05	0.00236	9.75	9.75	0.01352
155	112.16	112.16	0.00531	759.83	759.81	0.00245	11.25	11.25	0.01476
160	113.95	113.94	0.00538	786.59	786.57	0.00253	12.75	12.75	0.01545
165	115.36	115.35	0.00544	808.41	808.39	0.00260	14.09	14.09	0.01581
170	116.38	116.37	0.00547	824.55	824.53	0.00264	15.14	15.13	0.01594
175	116.99	116.99	0.00556	834.47	834.44	0.00268	15.80	15.80	0.01599
180	117.20	117.19	0.00551	837.81	837.79	0.00268	16.03	16.03	0.01600

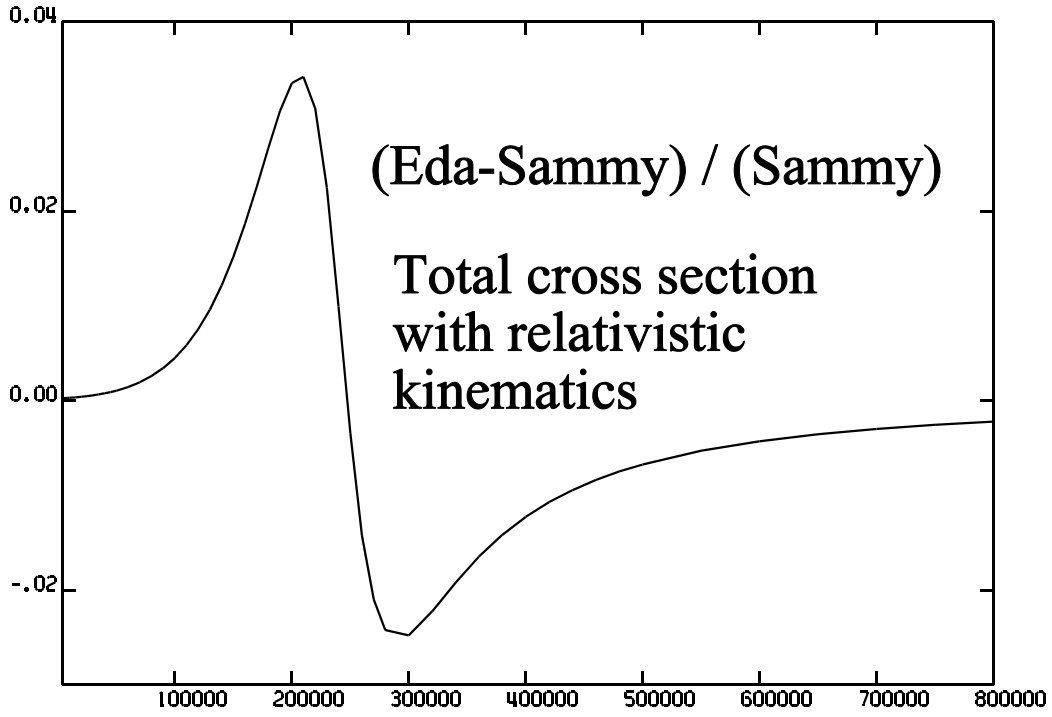
A Different Perspective on Resonance Fitting

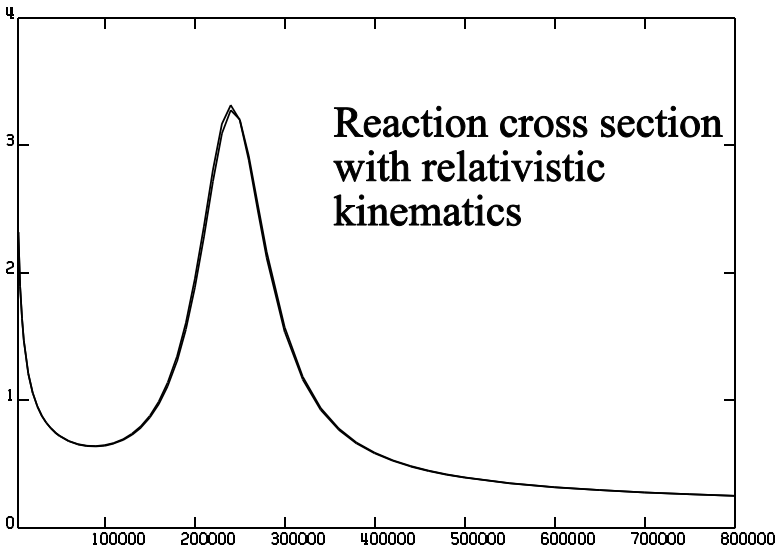
N. M. Larson
Oak Ridge National Laboratory

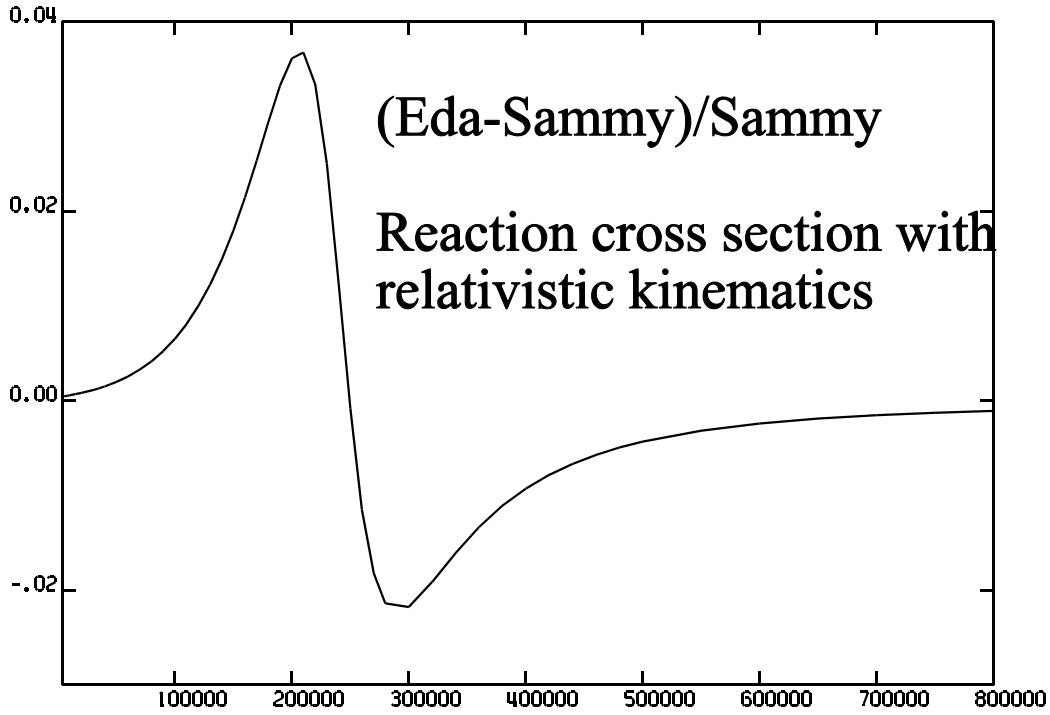
prepared for the first
Research Coordination Meeting on
Improvement of the Standard Cross Sections
for Light Elements

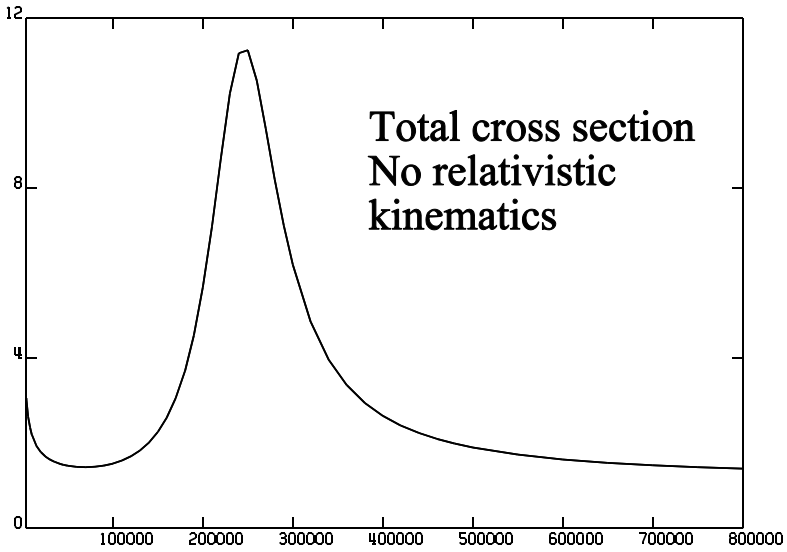
23-27 September 2002
IAEA Headquarters
Vienna, Austria

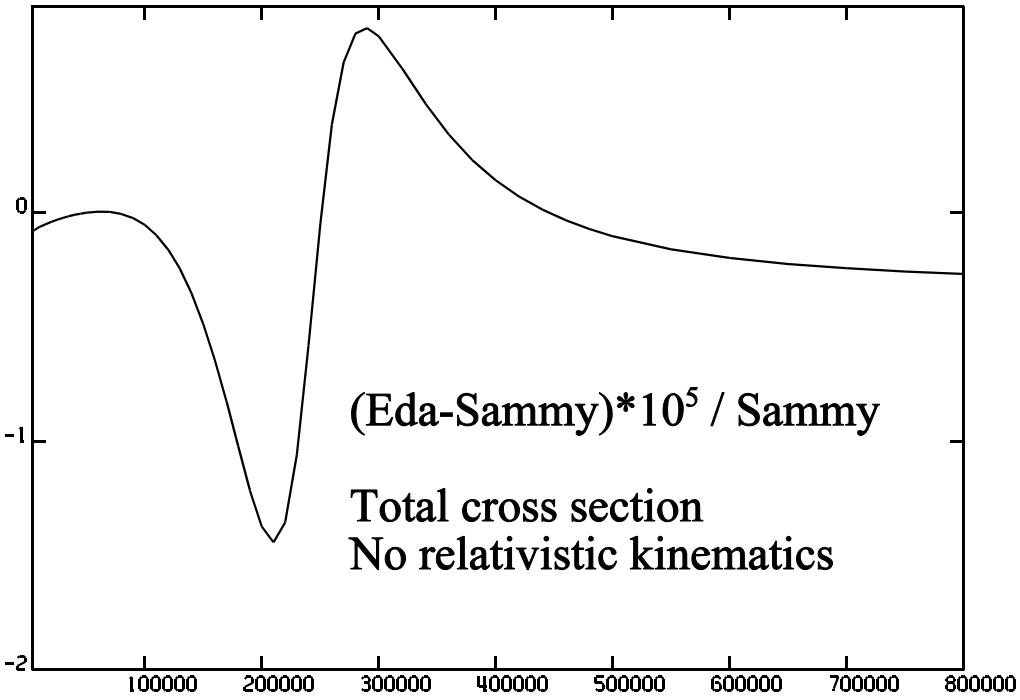

12
8
4
0
100000
200000
300000
400000
500000
600000
700000
800000
Total cross section,
including relativistic
kinematics

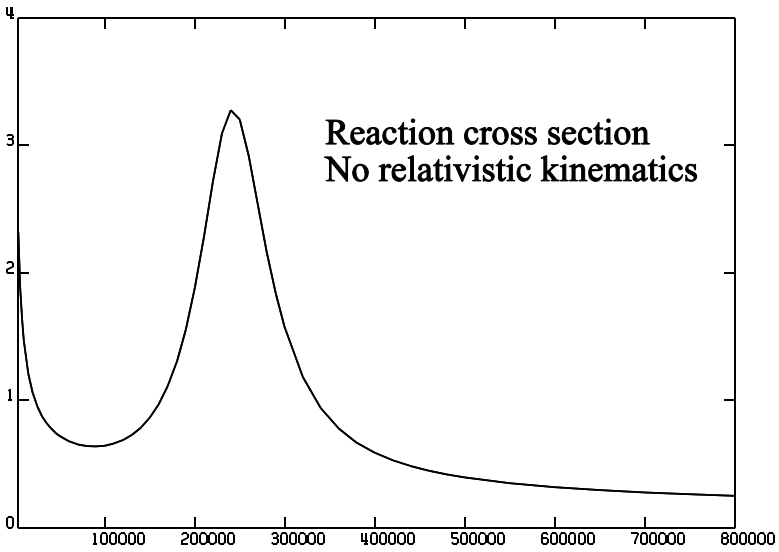

0.04
0.02
0.00
-.02
100000
200000
300000
400000
500000
600000
700000
800000
(Eda-Sammy) / (Sammy)
Total cross section
with relativistic
kinematics


Reaction cross section
with relativistic
kinematics
4
3
2
1
0
100000
200000
300000
400000
500000
600000
700000
800000


(Eda-Sammy)/Sammy
Reaction cross section with
relativistic kinematics
0.04
0.02
0.00
-.02
100000
200000
300000
400000
500000
600000
700000
800000


12
8
4
0
100000
200000
300000
400000
500000
600000
700000
800000
Total cross section
No relativistic
kinematics


0
-1
-2
100000
200000
300000
400000
500000
600000
700000
800000
(Eda-Sammy)*10^5 / Sammy
Total cross section
No relativistic kinematics


Reaction cross section
No relativistic kinematics
0
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2
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4
100000
200000
300000
400000
500000
600000
700000
800000

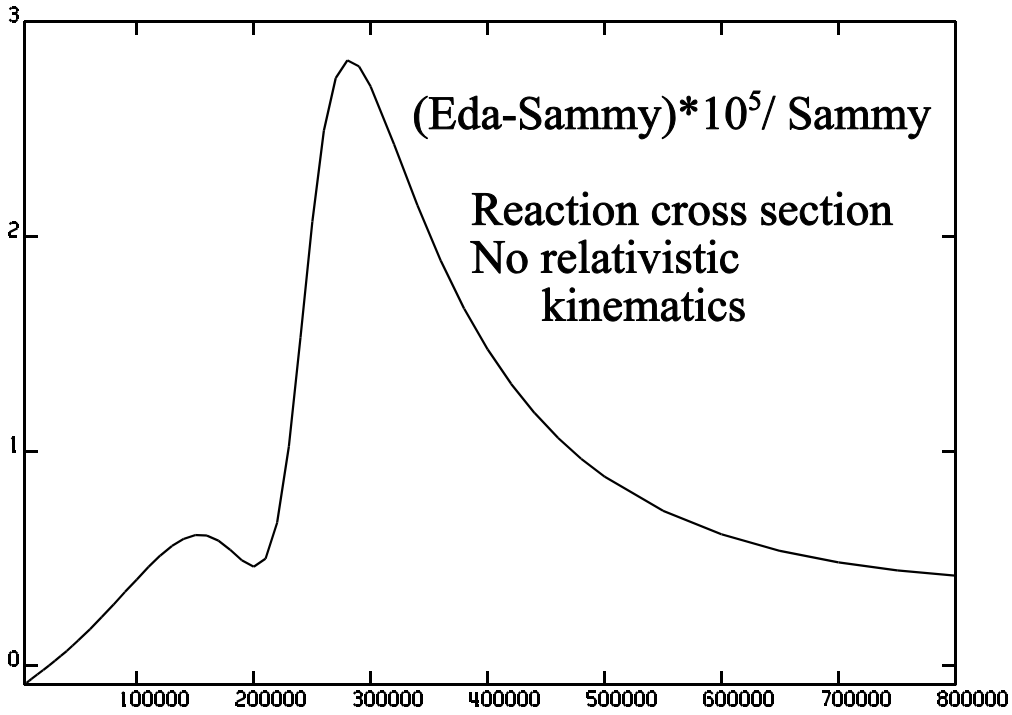

(Eda-Sammy)*10^5/ Sammy
Reaction cross section
No relativistic
kinematics
0
1
2
3
100000
200000
300000
400000
500000
600000
700000
800000

Table: Code Comparison

Feature	EDA	RAC	SAMMY
R-matrix	full	full	Reich-Moore approximation (but can "fake" full)
derivatives	analytic	numeric	analytic
kinematics	relativistic(but with an off-switch)	non-relativ	non-relativistic
reference frame	center-of-mass	com	laboratory
particles	general (spin, mass, charge)	general	general (spin, mass, charge)
range of applicability	light elements; observables with little structure		designed for heavier elements, highly structured observables
observables: cross sections (energy and energy-angle differential)	yes	yes	yes
observables: polarization, tensor analyzing power, etc.	yes	yes	no (but could be added easily ?)
observables: integral quantities	no	yes?	some
inverse reactions	yes	yes ?	yes but awkward (to be simplified eventually)
multiple nuclides in sample	no; data must be for one compound nucleus only	no	yes
Doppler broadening	no	no	FGM, HEGA, CLM
resolution broadening	yes	no	RSL, ORR, RPI, DEX, UDR, …
normalization	yes	yes	yes
background	no	no	several options (energy-dependent)

Feature	EDA	RAC	SAMMY
sample-size corrections	no	no	self-shielding and multiple-scattering, others
fitting procedure	"modified variable-metric search algorithm"	least squares	Bayes' method (generalized least squares)
multiple data sets	analyzed simultaneously	simul-taneous?	analyzed sequentially using Bayes' method; gives equivalent-to-simultaneous results
uses data covariances	no	yes	explicitly or implicitly
uses prior param covariances	no	no	yes
gives posterior parameter covariances	yes	yes	yes
post-processing	convert to Kapur-Peierls R-matrix parameters	yes	generate multi-group cross sections with covariance matrix (other options also available)
for ENDF files	convert to point-wise cross sections	yes?	provide resonance parameters in ENDF formats; also give (concise) param correlation matrix
number of resonances	no limits	no limits	as many as needed (~1000's) (no limits)
# of data points	no limits	no limits	many (~ 100,000's) (no limits)
code details	FORTRAN (not portable)	FOR-TRAN, VAX	FORTRAN, modern, maintained on Unix, VMS, Linux, pc; has been ported to most modern computer platforms
size of code			~130,000 lines
availability			via RSICC (or NEA)

SAMMY tests for ^{6}Li(n,α) data –

(Concentrate on features that are not available in other codes)

- locate (& "blindly repair") discrepant data sets
- study effects of Doppler- and resolution-broadening
- study effects of finite-size corrections
- study effects of initial data covariances

Discrepant data

Recall: SAMMY uses consecutive rather than simultaneous analyses for multiple data sets

Step a:

1. Run SAMMY with this input:

   $\{P_0, M_0\}$ (initial parameter values plus covariance matrix)

   $\{D_1, V_1\}$ (first data set plus its covariance matrix)

   to obtain this output:

   $\{P_{1a}, M_{1a}\}$ (intermediate parameter values plus covariance matrix)

   with chi-squared value:

   χ^2_{1a} (for data set 1 after one pass)

2. SAMMY + $\{P_{1a}, M_{1a}\}$ + $\{D_2, V_2\}$ => $\{P_{2a}, M_{2a}\}$ & χ^2_{2a}

. . .

n. SAMMY + $\{P_{n-1,a}, M_{n-1,a}\}$ + $\{D_n, V_n\}$ => $\{P_{na}, M_{na}\}$ & χ^2_{na}

STOP HERE ?

In the best-of-all-possible worlds, here we are done.

In the best-of-all-possible worlds, $\{P_{na}, M_{na}\}$ fit all data sets.

In the real world, we've just begun.

* Non-linearity
* Discrepant data sets
* Etc.

SO CONTINUE:

Step b:

1. SAMMY + $\{P_{n\,a}, M_{n\,a}\}$ + $\{D_1, V_1\}$ => $\{P_{1b}, M_{1b}\}$ & χ^2_{nb}
2. SAMMY + $\{P_{1b}, M_{1b}\}$ + $\{D_2, V_2\}$ => $\{P_{2b}, M_{2b}\}$ & χ^2_{2b}

. . .

n. SAMMY + $\{P_{n-1,b}, M_{n-1,b}\}$ + $\{D_n, V_n\}$ => $\{P_{nb}, M_{nb}\}$ & χ^2_{nb}

Step c: repeat.
Step d: repeat.
Step e: etc.

Eventually, either

things converge (values of χ^2 do not change very much)

or

things diverge (values of χ^2 grow excessively)

If things diverge, probably it's due to discrepant data.

Sometimes, looking at changes in χ^2 values can isolate which data set has the problem.

> [This happened when I first started looking at these data sets, which pointed to a problem with data set 4. Unfortunately those results disappeared into the abyss and I was not able to reproduce them.]

"Correcting" discrepant data

Steps for evaluator:

- Try to determine what's wrong –
  - Read the paper re the measurement
  - Contact the experimentalist
  - etc.
- Fix the mistake

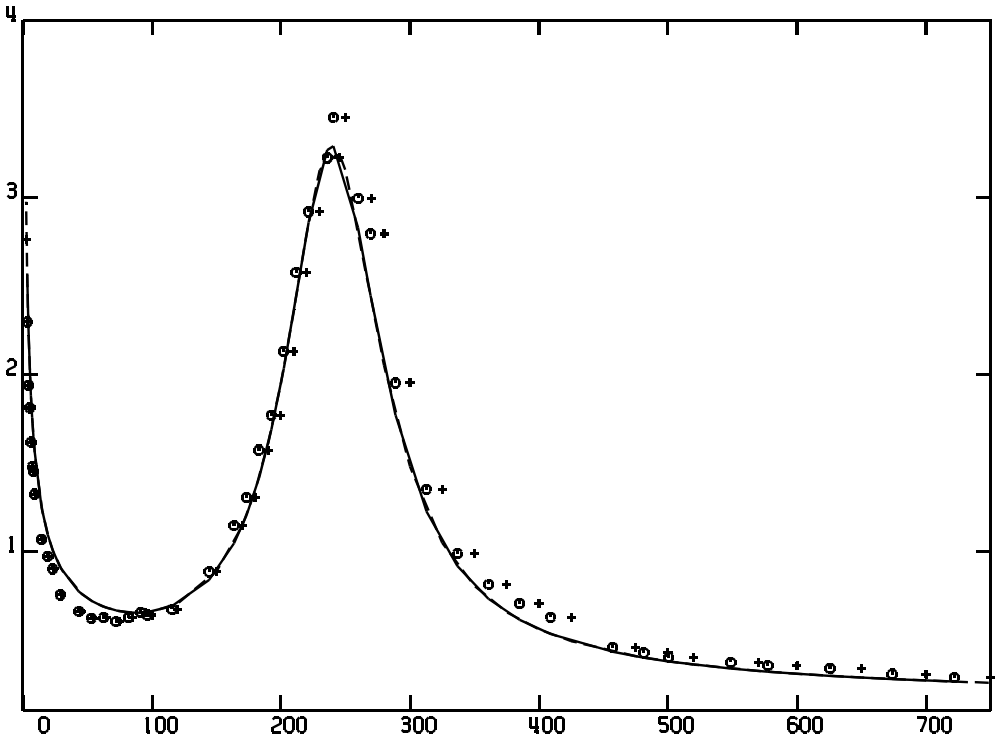
But sometimes that's not possible. Then what?

- Throw out the data, or
- Use very large uncertainties, and/or
- Make "blind" corrections

How to make blind corrections ?

- Energy scale
  - Fit highest-resolution data (usually, transmission data) to determine resonance energies
    - $\chi^2 / N =$ {0.98, 0.56, 2.4, 1.8, 0.00055, 2.1} for data sets {0,1,2,3,thermal,total} respectively
  - Keep R-matrix parameters fixed, fit flight-path-length and t-zero for other data sets
  - Modify energy-scale on those data sets to conform to the high-resolution data
  - This works well for situations with many narrow resonances, may not work so well for few broad resonances

Data set # 4 of Vladimir's



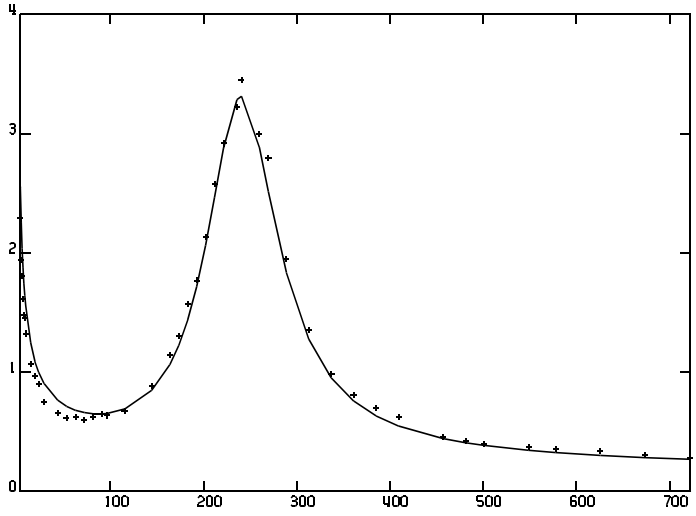
+	Original data points
o	Energy-adjusted data points
line	Curve that fits the other data sets

Initially χ^2 /N = 11.8, afterwards χ^2 /N = 8.3

- Now include data set 4 into the fitting process

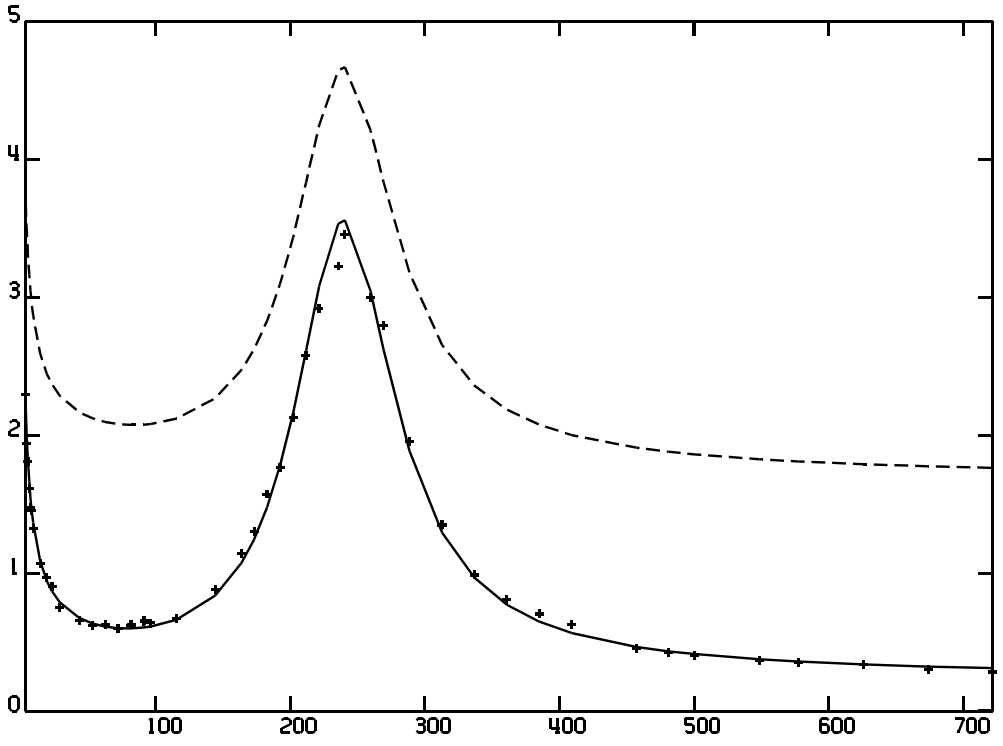
Table: χ^2 / N after energy-adjustment on data set 4

data set	excluding # 4	energy-adjusted # 4
0	0.98	2.2
1	0.56	0.70
2	2.4	2.5
3	1.8	1.7
4		6.9
thermal	0.00055	0.55
total	2.1	1.8



How to make blind corrections, continued

- Normalization and backgrounds
  - SAMMY permits fitting the following
    - normalization (no energy-dependence)
    - constant background
    - energy-dependent backgrounds
      - linear in t or $1/t$, t raised to a power, $\exp\{-bt\}$, others
  - Start with arbitrary values, vary only the normalization and background (not the resonance parameters)
    - χ^2 decreased from 2700 to 1.2



- Then adjust the data to accommodate the new normalization and background

- Now include data set 4 into the fitting process

Table: χ^2 / N after norm and background adjustment on data set 4

data set	excluding data set # 4	energy-adjusted data set # 4	# 4 with norm and background
0	0.98	2.2	1.1
1	0.56	0.70	0.62
2	2.4	2.5	2.2
3	1.8	1.7	1.8
4		6.9	1.0
thermal	0.00055	0.55	0.00065
total	2.1	1.8	2.2

- Remember: normalization and background adjustments give rise to off-diagonal data covariance matrix
- Use IDC = "implicit data covariance matrix"

Table: χ^2 / N after norm and background adjustment on data set 4, including implicit data covariance for # 4

data set	excluding data set # 4	energy-adjusted data set # 4	# 4 with norm and backgrnd	ditto with IDC
0	0.98	2.2	1.1	1.1
1	0.56	0.70	0.62	0.63
2	2.4	2.5	2.2	2.2
3	1.8	1.7	1.8	1.8
4		6.9	1.0	1.0
thermal	0.00055	0.55	0.00065	.0037
total	2.1	1.8	2.2	2.1

- Try IDC on all data sets (except thermal)

Table: χ^2 / N with IDC on all data sets except thermal

data set	omit # 4	energy-adjusted # 4	# 4 with norm & bckgrnd	IDC on # 4	IDC on all but thermal
0	0.98	2.2	1.1	1.1	2.8
1	0.56	0.70	0.62	0.63	0.47
2	2.4	2.5	2.2	2.2	2.3
3	1.8	1.7	1.8	1.8	4.5
4		6.9	1.0	1.0	1.2
th	0.00055	0.55	0.00065	.0037	0.00066
total	2.1	1.8	2.2	2.1	5.1

Interpretation?

- Maybe there is a normalization/background problem with those data sets for which χ^2 / N is large.

- The normalization is not explicitly included in either the theory or the data – so not reflected in χ^2 / N

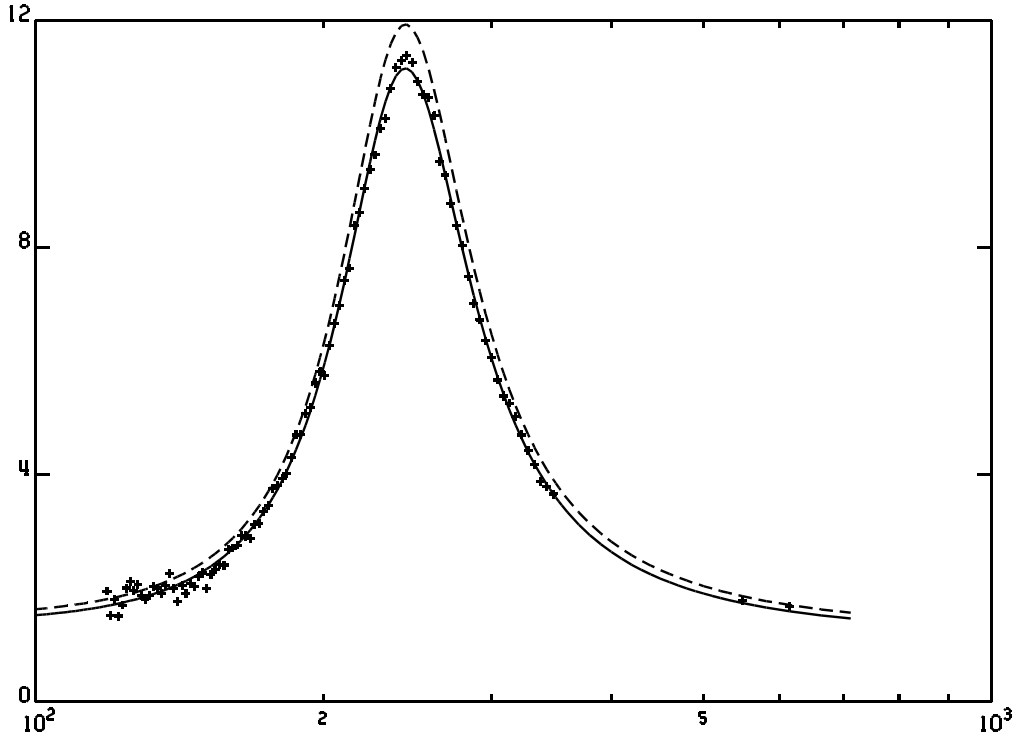
Next obvious step ... let's DO include normalization explicitly in the fitting procedure, for everything except thermal

Table: χ^2 / N with normalization on all data sets except thermal

data set	omit # 4	energy-adjustd # 4	# 4 with nrm & bkgrnd	IDC on # 4	IDC on all but therml	norm (not on therml)
0	0.98	2.2	1.1	1.1	2.8	0.56
1	0.56	0.70	0.62	0.63	0.47	0.49
2	2.4	2.5	2.2	2.2	2.3	2.4
3	1.8	1.7	1.8	1.8	4.5	1.2
4		6.9	1.0	1.0	1.2	.94
th	.00055	0.55	.00065	.0037	.00066	.000006
total	2.1	1.8	2.2	2.1	5.1	1.5

Table: Normalization on the various data sets

data set	χ^2 / N with norm	value of normalization	correlation matrix (triangular)
0	0.56	1.0212 ± 0.0045	100
1	0.49	1.0016 ± 0.0102	28 100
2	2.4	1.0268 ± 0.0081	51 18 100
3	1.2	1.0564 ± 0.0070	59 21 39 100
4	.94	1.0064 ± 0.0041	60 24 41 47 100
total	1.5	0.9351 ± 0.00 36	-50-14-36-42-37 100
th	.000006		



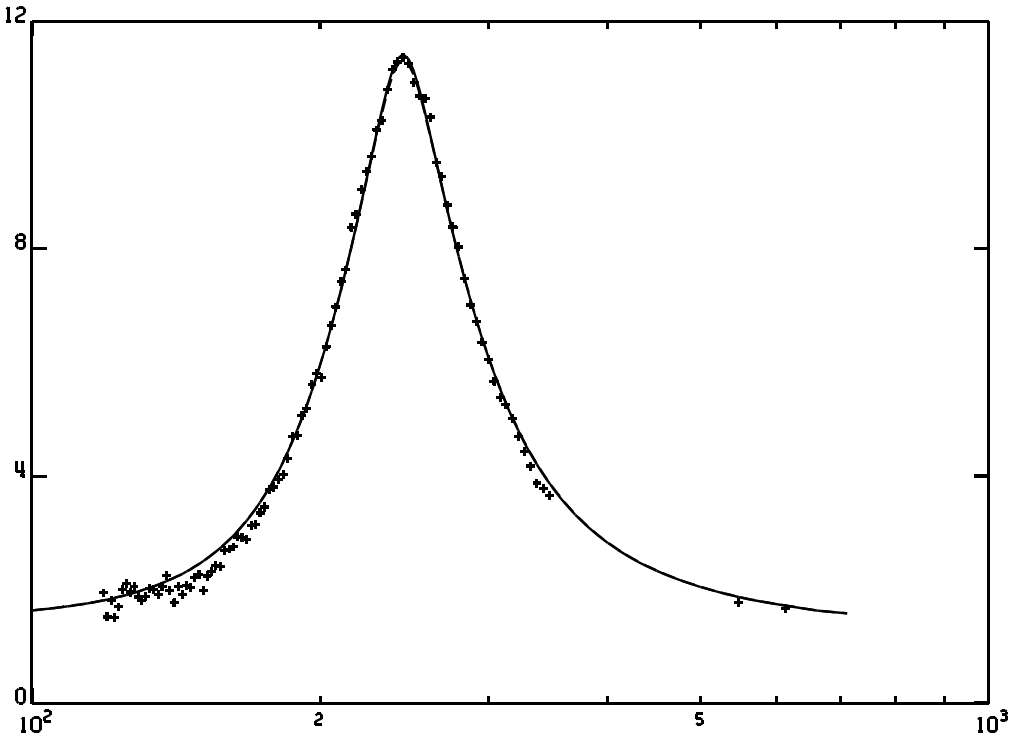
++ data

- - - no normalization

——— with normalization

What might cause normalization < 1 on total cross section?

- Doppler? No.
- Resolution? Maybe.



+ + data (total cross section)
—— resolution-broadened

Proof that Bayes and Least Squares Give Exactly Equivalent Results for Arbitrary Number of Data Sets (assuming linearity)

N.M.Larson, ORNL

December 11, 2002

prepared at request of V. Pronyaev for IAEA CRP 12027

Given:

Independent measurements (data sets) D_i with covariance matrix V_i, for $i = 1, K$. Data set i contains N_i data points.

Wanted:

The "best value" for the quantity which these data purport to measure.

Least-Squares Method:

$$P' - P = M' G^t V^{-1} (D - T)$$
$$M' = W^{-1}$$
$$W = G^t V^{-1} G$$

where

P = initial parameter value (arbitrary)
P' = final parameter value
M' = final covariance matrix for parameter value P'
D = experimental data
V = covariance matrix for experimental data
T = theoretical value
G = partial derivative of T with respect to P

The number of data points for this situation is

$$N = \sum_{i}^{K} N_i$$

Let L represent the number of parameters. Then

P and P' are vectors of length L
M' is a L x L matrix
D and T are vectors of length N
V is an N x N block-diagonal matrix
G is a L x N matrix

Explicitly

$$D = \begin{bmatrix} D_1 \\ D_2 \\ \dots \\ D_K \end{bmatrix} \qquad T = \begin{bmatrix} T_1 \\ T_2 \\ \dots \\ T_K \end{bmatrix} \qquad V = \begin{bmatrix} V_1 & 0 & \dots & 0 \\ 0 & V_2 & \dots & 0 \\ \dots & \dots & & \dots \\ 0 & 0 & \dots & V_K \end{bmatrix} \qquad G = \begin{bmatrix} G_1 \\ G_2 \\ \dots. \\ G_K \end{bmatrix}$$

where the submatrices are of different sizes: D_i and T_i are vectors of length N_i; V_i is a symmetric matrix of size N_i x N_i , and G_i is a non-square matrix of size N_i by L. The quantities needed in the least-squares equations can then be written as

$$W = G^t \, V^{-1} \, G$$

$$= \begin{bmatrix} G_1^t & G_2^t & \dots & G_K^t \end{bmatrix} \begin{bmatrix} V_1 & 0 & \dots & 0 \\ 0 & V_2 & \dots & 0 \\ \dots & \dots & & \dots \\ 0 & 0 & \dots & V_K \end{bmatrix}^{-1} \begin{bmatrix} G_1 \\ G_2 \\ \dots. \\ G_K \end{bmatrix}$$

$$= \begin{bmatrix} G_1^t & G_2^t & \dots & G_K^t \end{bmatrix} \begin{bmatrix} V_1^{-1} & 0 & \dots & 0 \\ 0 & V_2^{-1} & \dots & 0 \\ \dots & \dots & & \dots \\ 0 & 0 & \dots & V_K^{-1} \end{bmatrix} \begin{bmatrix} G_1 \\ G_2 \\ \dots. \\ G_K \end{bmatrix}$$

$$= \left[G_1^t V_1^{-1} G_1 + G_2^t V_2^{-1} G_2 + \dots + G_K^t V_K^{-1} G_K \right]$$

$$= \left[\sum_i^K G_i^t V_i^{-1} G_i \right]$$

so that the covariance matrix can be written in the form

$$M' = W^{-1} = \left[\sum_i^K G_i^t V_i^{-1} G_i \right]^{-1}$$

Hence the updated parameter value P' is found to be

$$P' - P = M' G^t V^{-1} (D - T)$$

$$= M' \begin{bmatrix} G_1^t & G_2^t & \dots & G_K^t \end{bmatrix} \begin{bmatrix} V_1 & 0 & \dots & 0 \\ 0 & V_2 & \dots & 0 \\ \dots & \dots & & \dots \\ 0 & 0 & \dots & V_K \end{bmatrix}^{-1} \begin{bmatrix} D_1 - T_1 \\ D_2 - T_2 \\ \dots . \\ D_K - T_K \end{bmatrix}$$

$$= M' \begin{bmatrix} G_1^t & G_2^t & \dots & G_K^t \end{bmatrix} \begin{bmatrix} V_1^{-1} & 0 & \dots & 0 \\ 0 & V_2^{-1} & \dots & 0 \\ \dots & \dots & & \dots \\ 0 & 0 & \dots & V_K^{-1} \end{bmatrix} \begin{bmatrix} D_1 - T_1 \\ D_2 - T_2 \\ \dots . \\ D_K - T_K \end{bmatrix}$$

$$= M' \begin{bmatrix} G_1^t V_1^{-1} (D_1 - T_1) & G_2^t V_2^{-1} (D_2 - T_2) & \dots & G_K^t V_K^{-1} (D_K - T_K) \end{bmatrix}$$

$$= \left[\sum_i^K G_i^t V_i^{-1} G_i \right]^{-1} \left[\sum_{i=1}^K G_i^t V_i^{-1} (D_i - T_i) \right]$$

QED.

Bayes Method:

$$P' - P = M' G^t V^{-1} (D - T)$$
$$M' = (M^{-1} + W)^{-1}$$
$$W = G^t V^{-1} G$$

where, as for least squares,

P = initial parameter value (arbitrary)
M = initial covariance for parameter values P
P' = final parameter value
M' = final covariance for parameter values P'
D = experimental data
V = covariance matrix for experimental data
T = theoretical value
G = partial derivative of T with respect to P

In this case we assume that the result holds for K - 1 data sets, and prove that it then holds also for K data sets. That is, we take as the prior parameter values and covariance matrix

$$P^{K-1} = M^{K-1} \left[\sum_{i=1}^{K-1} G_i^t V_i^{-1} D_i \right] \qquad M^{K-1} = \left[\sum_{i=1}^{K-1} G_i^t V_i^{-1} G_i \right]^{-1}$$

and use Bayes' Equations to determine the posterior values.

From Bayes' Equations, the updated covariance matrix is

$$M^K = ((M^{K-1})^{-1} + W)^{-1} = \left[\sum_{i=1}^{K-1} G_i^t V_i^{-1} G_i + G_K^t V_K^{-1} G_K \right]^{-1}$$

$$= \left[\sum_{i=1}^{K} G_i^t V_i^{-1} G_i \right]^{-1}$$

which is the same result as for the Least Squares case.

The updated parameter values can similarly be found from Bayes' Equations to be

$$
\begin{aligned}
P^K &= P^{K-1} + M^K G_K^t V_K^{-1} (D_K - T_K) \\
&= M^{K-1} \left[\sum_{i=1}^{K-1} G_i^t V_i^{-1} D_i \right] + M^K G_K^t V_K^{-1} (D_K - T_K) \\
&= M^K (M^K)^{-1} M^{K-1} \left[\sum_{i=1}^{K-1} G_i^t V_i^{-1} D_i \right] + M^K G_K^t V_K^{-1} (D_K - T_K) \\
&= M^K \left[\sum_{i=1}^{K-1} G_i^t V_i^{-1} G_i + G_K^t V_K^{-1} G_K \right] \left[\sum_{i=1}^{K-1} G_i^t V_i^{-1} G_i \right]^{-1} \left[\sum_{i=1}^{K-1} G_i^t V_i^{-1} D_i \right] \\
&\quad + M^K G_K^t V_K^{-1} D_K - M^K G_K^t V_K^{-1} T_K \\
&= M^K \left[\sum_{i=1}^{K} G_i^t V_i^{-1} D_i \right] + M^K G_K^t V_K^{-1} G_K M^{K-1} \left[\sum_{i=1}^{K-1} G_i^t V_i^{-1} D_i \right] - M^K G_K^t V_K^{-1} T_K \\
&= M^K \left[\sum_{i=1}^{K} G_i^t V_i^{-1} D_i \right] + M^K G_K^t V_K^{-1} \left(G_K P^{K-1} - T_K \right)
\end{aligned}
$$

At this point, we must invoke linearity: in the case where the theory in linear with respect to the parameters, the quantity in parentheses in the previous equation is zero. If the theory is not linear, then this term gives an estimate for the difference between Bayes-sequential and Least-Squares-simultaneous analyses.

QED.

Different Forms of Bayes' Equation.

Extraction from Report ORNL/TM-9179/R5 (2000)

"Updated Users Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equation"

by N.M. Larson

ORNL, USA

(available online at
http://www.ornl.gov/~webworks/cppr/y2001/rpt/108983.pdf)

II.A.1 Details of the Derivation

In Sect. II.A, we stated that Bayes' equations may be derived directly from Bayes' theorem,

$$p(P|DX) = p(P|X)\, p(D|PX) \quad , \tag{IIA1.1}$$

provided the three basic assumptions are met. These assumptions are:

i. the prior joint pdf is a joint normal. That is, the pdf for the parameters, prior to consideration of the data D, is

$$p(P|X) \quad \alpha \quad \exp\left[-\frac{1}{2} (P-\bar{P})^t \; M^{-1} \; (P-\bar{P}) \right] \quad , \tag{IIA1.2}$$

ii. the likelihood function is a joint normal. That is, the pdf for the experimental data is

$$p(D|PX) \quad \alpha \quad \exp\left[-\frac{1}{2} (D-T)^t \; V^{-1} \; (D-T) \right] \quad . \tag{IIA1.3}$$

iii. the true value is a linear function of the parameters. That is, a Taylor expansion of the theoretical values around the prior expectation values of the parameters truncates after the linear term,

$$T(P) = \bar{T} + G(P-\bar{P}) \quad , \tag{IIA1.4}$$

where the sensitivity matrix G is defined by

$$G_{ik} = \frac{\partial T_i}{\partial P_k} \quad \text{with} \quad P = \bar{P} \quad , \tag{IIA1.5}$$

and the theoretical value $\bar{T}_i$ (i.e., $\bar{T}$ for data point i) is also evaluated at $P = \bar{P}$.

Given these three assumptions, the posterior pdf $p(P|DX)$ is also a joint normal distribution and may be written

$$p(P|DX) \quad \alpha \quad \exp\left[-\frac{1}{2} \left\{ \; (P-\bar{P}')^t \; M'^{-1} \; (P-\bar{P}') \; \right\} \right] \tag{IIA1.6}$$

Substituting Eq. (IIA1.2) through (IIA1.6) into Eq. (IIA1.1) and equating the exponents yield, in matrix form,

$$(P-\bar{P}')^t \; M'^{-1} \; (P-\bar{P}') + Y \;\; = \;\; (P-\bar{P})^t \; M^{-1} \; (P-\bar{P}) \;\; + \;\; \left(D-\bar{T}-G(P-\bar{P})\right)^t \; V^{-1} \; \left(D-\bar{T}-G(P-\bar{P})\right) \quad , \tag{IIA1.7}$$

where Y represents the normalization constant and is independent of P. Setting $P - \bar{P} = P - \bar{P}' + \bar{P}' - \bar{P}$ in Eq. (IIA1.7), and rearranging terms, we obtain

$$
\begin{aligned}
&(P-\bar{P}')^t\, M'^{-1}\, (P-\bar{P}') + Y \\
&\quad = \quad (P-\bar{P}')^t \left(M^{-1} + G^t V^{-1} G \right) (P-\bar{P}') \\
&\qquad + \quad (P-\bar{P}')^t \left[\left(M^{-1} + G^t V^{-1} G \right) (\bar{P}'-\bar{P}) - G^t V^{-1} (D-\bar{T}) \right] \\
&\qquad + \quad \left[(\bar{P}'-\bar{P})^t \left(M^{-1} + G^t V^{-1} G \right) - (D-\bar{T})^t V^{-1} G \right] (P-\bar{P}') \\
&\qquad + \quad (\bar{P}'-\bar{P})^t\, M^{-1}\, (\bar{P}'-\bar{P}) \quad + \quad \left(D-\bar{T}-G(\bar{P}'-\bar{P})\right)^t V^{-1} \left(D-\bar{T}-G(\bar{P}'-\bar{P})\right) \quad .
\end{aligned}
\tag{IIA1.8}
$$

Because Eq. (IIA1.8) must hold for all values of P, we may equate terms quadratic, linear, or constant in $(P-\bar{P}')$. From the quadratic we obtain Bayes' equation for updating the covariance matrix, and from the linear we obtain Bayes' equation for updating parameter values. The constant yields the invariant "Bayesian χ^2".

We begin with the covariance matrix; the coefficients of the quadratic $(P-\bar{P}')^t \ldots (P-\bar{P}')$ in Eq. (IIA1.8) yield

$$(M')^{-1} \;=\; M^{-1} + G^t V^{-1} G \quad , \tag{IIA1.9}$$

which is the form used in the MPW inversion scheme, with $W = G^t V^{-1} G$. Algebraic manipulation of this matrix equation gives us the form used in the other inversion schemes:

$$(M')^{-1} M \;=\; M^{-1} M + G^t V^{-1} G M \;=\; I + G^t V^{-1} G M \quad ,$$

where I represents the identity matrix. Multiplying by M' gives

$$M' (M')^{-1} M \;=\; M' + M' G^t V^{-1} G M \quad ,$$

which reduces to

$$M \;=\; M' \left(I + G^t V^{-1} G M \right) \quad , \tag{IIA1.10}$$

Thus we may define Q as

$$Q \;=\; G^t V^{-1} G M \quad , \tag{IIA1.11}$$

(as in Eq. (IIA.13) and obtain from Eq. (IIA1.10) the result

$$M' \;=\; M \left(I + G^t V^{-1} G M \right)^{-1} \quad , \tag{IIA1.12}$$

which is exactly Bayes' equation for updating the covariance matrix in the IPQ inversion scheme, Eq. (IIA.12).

To obtain the NPV version of Bayes' equations for the covariance matrix, further algebraic manipulation is required. Using the identity

$$X^{-1} = Z(XZ)^{-1} \tag{IIA1.13}$$

with

$$X = I + G^t V^{-1} G M = I + Q \tag{IIA1.14}$$

and

$$Z = G^t (N+V)^{-1} G \quad , \tag{IIA1.15}$$

where

$$N = G M G^t \quad , \tag{IIA1.16}$$

gives, from Eq. (IIA1.12),

$$\begin{aligned} M' &= M G^t (N+V)^{-1} G \left(\left(I + G^t V^{-1} G M \right) G^t (N+V)^{-1} G \right)^{-1} \\ &= M G^t (N+V)^{-1} G \left(G^t (N+V)^{-1} G + G^t V^{-1} G M G^t (N+V)^{-1} G \right)^{-1} \quad . \end{aligned} \tag{IIA1.17}$$

Substituting the value for N and rearranging give

$$M' = M G^t (N+V)^{-1} G \left(G^t \left\{ (N+V)^{-1} + V^{-1} N (N+V)^{-1} \right\} G \right)^{-1} \quad . \tag{IIA1.18}$$

The quantity in curly brackets is equal to V^{-1}; making that substitution and introducing the identity $V V^{-1} = I$ into the expression give

$$M' = M G^t (N+V)^{-1} V V^{-1} G \left(G^t V^{-1} G \right)^{-1} \quad . \tag{IIA1.19}$$

Replacing V by its equivalent $N + V - N$ then gives

$$\begin{aligned} M' &= M G^t (N+V)^{-1} (N+V-N) V^{-1} G \left(G^t V^{-1} G \right)^{-1} \\ &= M G^t V^{-1} G \left(G^t V^{-1} G \right)^{-1} - M G^t (N+V)^{-1} N V^{-1} G \left(G^t V^{-1} G \right)^{-1} \quad . \end{aligned} \tag{IIA1.20}$$

When N is replaced by its definition in the second of these terms, the equation immediately collapses to the form

$$M' = M - M G^t (N+V)^{-1} G M \quad , \tag{IIA1.21}$$

which is exactly the NPV version of Bayes' equation for updating the covariance matrix, Eq. (IIA.9).

If the indices for the matrices in EQ. (IIA1.21) are explicitly displayed, the equation becomes

$$M'_{kl} = M_{kl} - \sum_{n=1}^{K} \sum_{i=1}^{L} \sum_{j=1}^{L} \sum_{m=1}^{K} M_{kn} G_{in} \left((N+V)^{-1} \right)_{ij} G_{jm} M_{ml} \quad , \tag{IIA1.22}$$

where N is given by

$$N_{ij} = \sum_{n=1}^{K} \sum_{m=1}^{K} G_{in} M_{nm} G_{jm} \quad . \tag{IIA1.23}$$

To obtain Bayes' equation for updating the parameter values, we equate the linear terms of Eq. (IIA1.8). Since the left-hand-side of that equation has no terms linear in $(P-\bar{P}')$, the coefficient of $(P-\bar{P}')$ on the right-hand side must be zero. That is,

$$\left(M^{-1} + G^t V^{-1} G \right) (\bar{P}' - \bar{P}) = G^t V^{-1} (D - \bar{T}) \quad . \tag{IIA1.24}$$

From Eq. (IIA1.9), the first quantity on the left is just M'^{-1}; we therefore have

$$\bar{P}' - \bar{P} = M' G^t V^{-1} (D - \bar{T}) \quad , \tag{IIA1.25}$$

which is the form that Bayes' equation takes in the MPW inversion scheme, Eqs. (IIA.14). Substituting for M' from Eq. (IIA1.12) gives the form used in the IPQ inversion scheme,

$$\bar{P}' - \bar{P} = M (I+Q)^{-1} G^t V^{-1} (D - \bar{T}) \quad , \tag{IIA1.26}$$

as in Eq. (IIA.11).

To obtain the expression needed for the NPV inversion scheme, replace M' in Eq. (IIA1.25) with Eq. (IIA1.22) to give

$$\bar{P}' - \bar{P} = \left(M - M G^t (N+V)^{-1} G M \right) G^t V^{-1} (D - \bar{T}) \quad , \tag{IIA1.27}$$

which reduces to

$$\bar{P}' - \bar{P} = M G^t (N+V)^{-1} (D - \bar{T}) \quad . \tag{IIA1.28}$$

Explicitly displaying the indices in this equation gives

$$\bar{P}_k' - \bar{P}_k = \sum_{l=1}^{K} \sum_{i=1}^{L} \sum_{j=1}^{L} M_{kl} G_{il} \left((N+V)^{-1} \right)_{ij} (D_j - \bar{T}_j) \quad . \tag{IIA1.29}$$

Finally, we note that the constant term in Eq. (IIA1.8) may be simplified using Eq. (IIA1.29) to give

$$Y = (D-\overline{T})^t \left[(N+V)^{-1}\, GMG^t (N+V)^{-1} + (I-(N+V)^{-1}N)\, V^{-1} (I-N(N+V)^{-1})\right](D-\overline{T}) \quad , \tag{IIA1.30}$$

which reduces to

$$Y = (D-\overline{T})^t (N+V)^{-1} (D-\overline{T}) \tag{IIA1.31}$$

In SAMMY, this quantity is referred to as the "Bayesian χ^2". In the IPQ inversion scheme, this quantity can be simplified to the form

$$Y = (D-\overline{T})^t V^{-1} (D-\overline{T}) - (D-\overline{T})^t V^{-1} GM(I+Q)^{-1} G^t V^{-1} (D-\overline{T}) \tag{IIA1.32}$$

in which the first term is the usual (least-squares) χ^2, and the second term can be viewed as a "correction" to χ^2. The Bayesian χ^2 is, in some sense, a measure of the "best fit" than can be found between this theoretical formulation and these experimental data. The goal of a Bayes fit is, essentially, to have the value of the least-squares χ^2 become as near as possible to the value of the Bayesian χ^2 .

Algebra to translate from Eq. (IIA1.27) and (IIA1.28):

Using

$$N = G M G^t \tag{IIA1.33}$$

we obtain

$$\begin{aligned}
P'-P &= (M-MG^t(N+V)^{-1}GM)\,G^tV^{-1}(D-T)\\
&= MG^tV^{-1}(D-T) - MG^t(N+V)^{-1}GMG^tV^{-1}(D-T)\\
&= MG^t[1-(N+V)^{-1}N]V^{-1}(D-T)\\
&= MG^t[1-(N+V)^{-1}(N+V-V)]V^{-1}(D-T)\\
&= MG^t[1-(N+V)^{-1}(N+V)+(N+V)^{-1}V)]V^{-1}(D-T)\\
&= MG^t[1-1+(N+V)^{-1}V)]V^{-1}(D-T)\\
&= MG^t(N+V)^{-1}VV^{-1}(D-T)\\
&= MG^t(N+V)^{-1}(D-T)
\end{aligned} \tag{IIA1.34}$$

Database Studies For The Evaluation of The Neutron Cross Section Standards

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First RCM 9-23-02

Introduction

Measurements of most neutron cross sections are made relative to neutron cross section standards. These standards are the basis for the neutron reaction cross section databases. It has been more than 15 years since the last comprehensive evaluation of the neutron cross section standards. Significant improvements have been made in the standard cross section database since that time, particularly for the H(n,n), ^{10}B(n,α), and ^{235}U(n,f) reactions. In response to the need for new evaluations for the standards, a new international evaluation is underway that will include the H(n,n), ^{3}He(n,p), ^{6}Li(n,t), ^{10}B(n,α), ^{10}B(n,α$_1$γ), Au(n,γ), ^{235}U(n,f), and ^{238}U(n,f) standard cross sections. For some of the standards, the energy region will be extended to 200 MeV to provide new standards in this emerging important energy region. Efforts will be made to investigate the need for a new thermal constants evaluation. A new evaluation will not be made for the C(n,n) cross section because little new data have been obtained since the ENDF/B-VI evaluation and what has been obtained is consistent with that work.

The new cross section standards are shown in Table 1. In addition to the cross sections shown in this Table, the ^{239}Pu(n,f) and ^{238}U(n,γ) cross sections will be evaluated as a result of the process being used.

Table 1. The new neutron cross section standards

Reaction	Expected 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,α)	0.0253 eV to 1 MeV
^{10}B(n,α$_1$γ)	0.0253 eV to 1 MeV
C(n,n)*	0.0253 eV to 1.8 MeV
Au(n,γ)	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

†ENDF Standard, not an NEANDC/INDC Standard
††Not an ENDF Standard, NEANDC/INDC Standard
* New evaluation will not be done

Status of the Database

Studies are being made of experiments under consideration for the standards database. For each experiment the documentation is checked for corrections that may need to be made and possible errors or missing information. The procedure leads to estimates of

the uncertainties and correlations within an experiment and correlations with other experiments. This information is used to form covariance matrices for the measurements so that a full covariance analysis can be performed. Recent work and data which will have an important impact on the evaluation will be the focus of this status report. A detailed list of the new experiments which have been considered for inclusion in the new standards evaluation is given in Table 2 at the end of this report. This list is not complete. Additional experiments will continue to be added which are found in the literature searches which are underway. Also published corrections to new or old experiments will be incorporated in the experimental results. Some effort will also be made to investigate certain experiments which were included in the ENDF/B-VI evaluation.

Hydrogen Scattering Cross Section

The hydrogen scattering cross section is the most accurately known of the neutron cross section standards. It is a very important standard since many measurements of other standards, in addition to other cross sections, have been made relative to this cross section. There has been considerable recent experimental activity on this cross section due to the rather large difference between its ENDF/B-V and ENDF/B-VI evaluations. Unfortunately the largest difference between these evaluations occurs at ~11 MeV and 0º in the laboratory system (180º in the center of mass system (CMS)), which is the most important angle for use of this standard. Angular distribution measurements by Nakamura, and Shirato near 14 MeV, which have small reported uncertainties, had a large impact on the ENDF/B-VI evaluation and led to these differences.

Unpublished measurements of Baba of the angular distribution at 14 MeV were made at Tohoku University. This work includes angles near 180º in the CMS and are in good agreement with the ENDF/B-V evaluation, however the uncertainties are about 3%.

Measurements were recently completed of the shape of the H(n,n) angular distribution at 10 MeV neutron energy in an Ohio University, NIST, LANL collaboration . The data have uncertainties from 0.8% to 1.7% for the angular range from 180º to 60º in the CMS. The data are in better agreement with the ENDF/B-V evaluation and the phase shift analysis of Arndt than the ENDF/B-VI evaluation. This collaboration investigated the measurements at 14 MeV referred to above, that had a large impact on the ENDF/B-VI standards evaluation. They found problems with some angular distribution data which led to corrections and expanded uncertainties for those data. Hale, who evaluated the hydrogen scattering cross section for the ENDF/B-VI evaluation, has added the precise 10 MeV data to his database and incorporated the corrections to the 14 MeV data suggested by the Ohio U.-NIST-LANL collaboration. Using this database his new evaluated results agree well with the 10 MeV data and the various 14 MeV measurements, within the uncertainties. The reduction in the quality of the database at ~14 MeV has led to the need for accurate measurements near that energy. Work is planned by the Ohio U.-NIST-LANL collaboration to satisfy that need.

Recent measurements by the Uppsala group of the differential H(n,n) cross section at 90 and 162 MeV disagree with the evaluated shape given by the Arndt VL40

phase-shift solution. The Arndt evaluation was accepted by the NEANDC/INDC as a primary standard for cross section measurements in the 20 MeV to 350 MeV range. The Uppsala data have a steeper angular shape at back angles by as much as 10% compared with the VL40 results. A similar disagreement is observed with recent Paul Scherrer Institute data.

Using a new neutron tagging facility at Indiana University, absolute measurements at 190 MeV were made of the hydrogen scattering cross section by Vigdor and collaborators. The data were obtained with ~1% accuracy in 5º CMS bins between 90º and 170º in the CMS. The uncertainty increases to ~2-3% in the two bins nearest 180º. The data are now being analyzed. This experiment, since it will yield absolute cross section data, can make an important contribution with respect to both the shape and normalization of the hydrogen scattering cross section thereby providing needed information for understanding the back angle problem.

^{10}B+n Standards

There has been significant experimental work on the $^{10}B(n,\alpha)$ and $^{10}B(n,\alpha_1\gamma)$ standards since the completion of the ENDF/B-VI standards evaluation. The relatively poor database caused problems with the ENDF/B-VI evaluation process thus leading to this experimental activity. Work has been done on the differential cross section for the $^{10}B(n,\alpha)^7Li$ reaction, the branching ratio, the $^{10}B(n,\alpha_1\gamma)$ cross section, the total neutron cross section, and the $^{10}Be(p,n)$ reaction. The use of the R-matrix allows all these types of data to be used in helping to define the $^{10}B(n,\alpha)$ cross sections.

Differential cross section measurements have recently been made by Zhang et al., and Giorginis and Khriachkov using Frisch-gridded ionization chambers. In Fig. 1, the results obtained by integrating the data from those experiments are shown compared

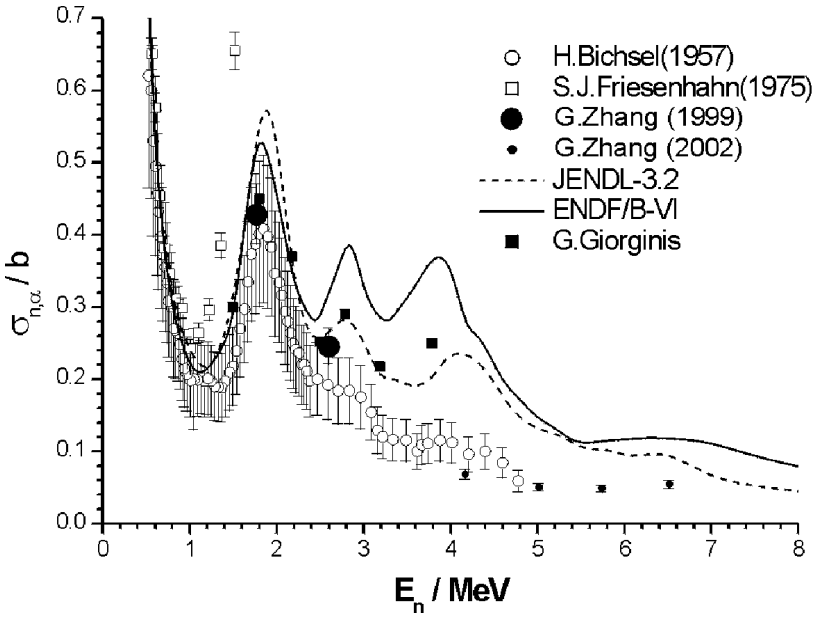

Fig. 1. Comparison of measurements and evaluations of the $^{10}B(n,\alpha)^7Li$ cross section.

with other work and evaluations. There are large differences between the various measurements and evaluations, but the greatest concern is the differences between the most recent measurements, for example near 4 MeV neutron energy. Giorginis discovered that the reason for these differences is a subtle effect he calls particle leaking. Particle leaking results when both reaction products are emitted in the forward direction. The particle identification feature which is possible with the gridded chamber treats this as a quasi $^{7}Li+\alpha$ particle. It appears in the pile-up portion of the spectrum and is rejected. Data taken without taking this into account are correct over only a limited angular range. Since particles are lost, the integrated cross section will be lower than the correct value. This agrees with the comparison between the Giorginis and Khriachkov, and Zhang et al. data sets. Zhang et al. now are correcting for this effect.

Measurements by Weston and Todd of the branching ratio, (the $^{10}B(n,\alpha_0\gamma)$ cross section/the $^{10}B(n,\alpha_1\gamma)$ cross section), are 10 % to 30 % low in the 100 keV to 600 keV energy region compared with the ratios calculated from the ENDF/B-VI cross sections. The data agree with ENDF/B-VI at the lowest and highest energies of the experiment. Preliminary measurements of this ratio have been measured by Hambsch and Bax. These data, the Weston and Todd results, and ENDF/B-VI are shown in Fig. 2. The measurements of Hambsch and Bax are in better agreement with ENDF/B-VI than the Weston and Todd measurements. The higher values obtained by

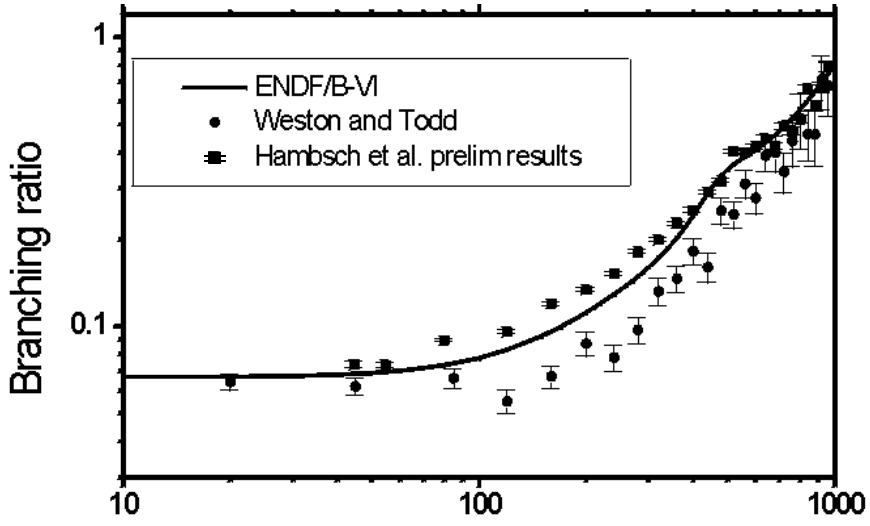

Fig. 2. Recent measurements of the ^{10}B branching ratio compared with the ENDF/B-VI evaluation

Hambsch and Bax in the hundred keV energy region are expected to be a result of backgrounds which have not been subtracted yet. These data were obtained with a

Frisch-gridded ionization chamber and require the leaking correction referred to previously. However the ratio should depend only weakly on particle leaking.

In an NIST/ORNL collaboration, Schrack et al. have made measurements of the shape of the $^{10}B(n,\alpha_1\gamma)$ cross section from 0.3 MeV to 4.0 MeV neutron energy. The cross sections obtained from this investigation, normalized to the ENDF/B-VI evaluation over the region from 0.2 MeV to 1 MeV, agree with the ENDF/B-VI evaluation below 1.5 MeV. The measured cross sections differ as much as 40 % with the ENDF/B-VI evaluation for neutron energies greater than 1.5 MeV. An additional measurement collaboration extended the cross section to lower energies so that better normalization of shape measurements could be made. The measurement covered the neutron energy range from 10 keV to 1 MeV. These data are lower than the ENDF/B-VI shape by about 5 % in the region above 100 keV.

Measurements of the ^{10}B total cross section have been made at the IRMM linac and Van de Graaff facilities. The linac work extends to 730 keV neutron energy. The present results of this work are deviations from ENDF/B-VI by ±2.5% below 10 keV, with a maximum deviation above ENDF/B-VI of 5% at 100 keV and a maximum deviation below ENDF/B-VI of 7% at 700 keV. Further work is underway. The Van de Graaff facility data are lower than ENDF/B-VI by 3-4% at 0.3 and 0.4 MeV, and by 6 to 9% from 0.6 to 1.3 MeV. They agree with that evaluation at 1.7 and 1.9 MeV. Additional work is being considered.

Wasson et al., in an NIST-ORNL collaboration have also made measurements of the ^{10}B total cross section. These data extend from about 20 keV to 20 MeV and agree with the ENDF/B-VI evaluation for neutron energies greater than about 2 MeV, but are lower by as much as 4 % between 600 keV and 2 MeV, and are greater by as much as about 5 % below 600 keV.

There is generally good agreement among the IRMM linac, IRMM Van de Graaff and NIST-ORNL measurements within the uncertainties. The data sets are still undergoing checks and corrections which are expected to improve the agreement.

Though many of the experiments are preliminary, the lower $^{10}B(n,\alpha_1\gamma)$ cross section, the lower branching ratio and the higher total cross section indicate a discrepancy in the hundred keV energy region in one or more of the measurements reported here. The preliminary work of Hambsch and Bax suggests that the problem may be the Weston and Todd data.

$^{235}U(n,f)$

The $^{235}U(n,f)$ cross section is one of the most popular standards. It is easily used in detectors such fission chambers for cross section measurements. The most recent measurements of the $^{235}U(n,f)$ cross section below 20 MeV are shown in Fig. 3. The data sets of Carlson et al., Lisowski et al., and Alkhazov et al. suggest a difference as large as about 5% compared with the ENDF/B-VI evaluation above 14 MeV. For the energy region above 20 MeV, very few measurements have been made. The recent work by Nolte et al. is shown in Fig. 4 compared with the earlier measurements. Except for the data point at 96 MeV, which Nolte et al. suggest may be a normalization problem, there is agreement within the uncertainties with the Lisowski

et al. data. This new work is an important contribution since these are the only data other than those of Lisowski et al. in this energy region that have relatively small uncertainties. 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.

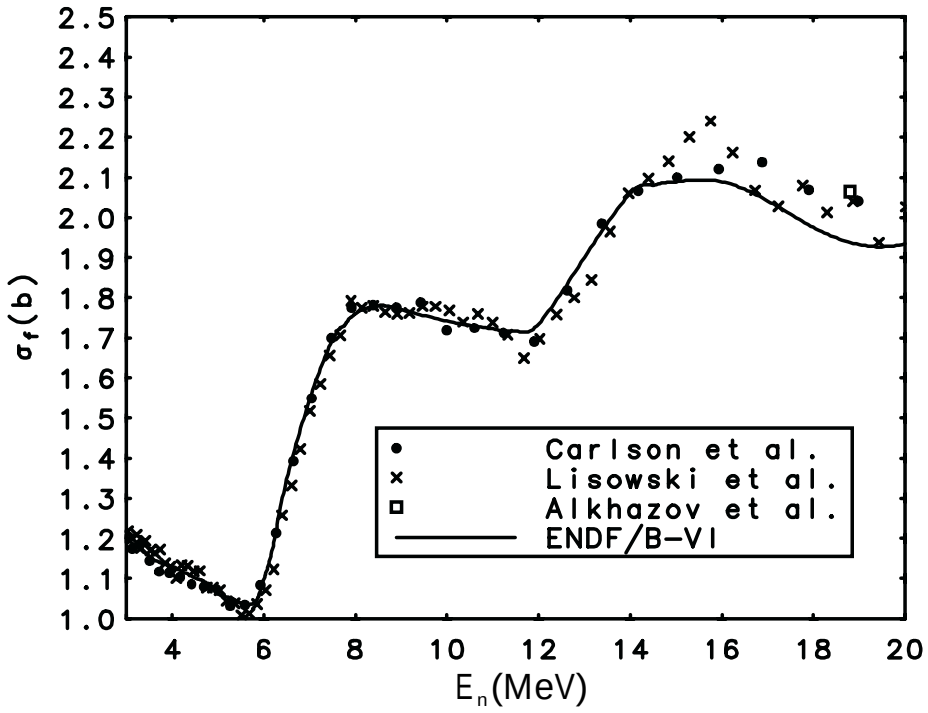

Fig. 3. Recent measurements of the ^{235}U(n,f) cross section below 20 MeV compared with the ENDF/B-VI evaluation.

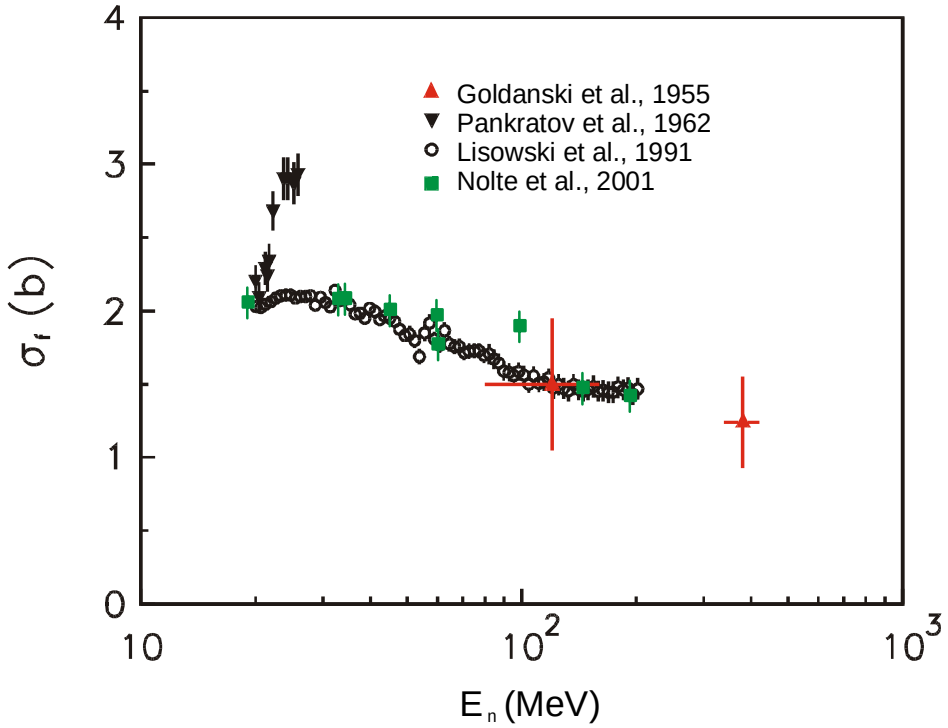

Fig. 4. Measurements of the ^{235}U(n,f) cross section above 20 MeV.

^{238}U(n,f)

The other fission standard, the ^{238}U(n,f) cross section, has an advantage over the ^{235}U(n,f) standard since its high effective threshold makes it useful where low energy neutron backgrounds are present. In Fig. 5, absolute measurements of the ^{238}U(n,f) cross section from 10 to 20 MeV are shown. The measurements of Lisowski et al., Merla et al. and Winkler et al. all indicate the ENDF/B-VI evaluation is low an average of a few percent from 15 to 20 MeV.

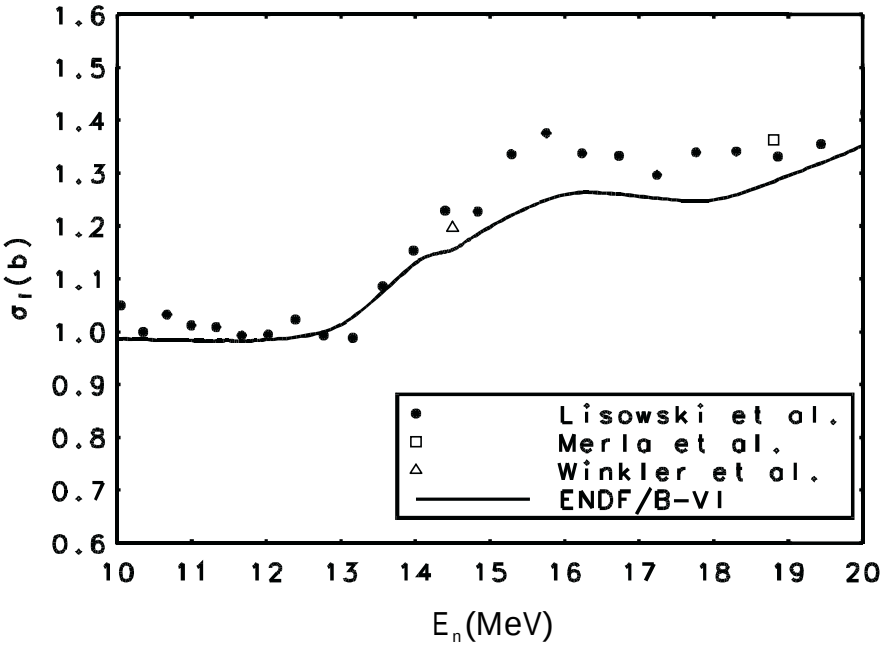

Fig. 5. Recent absolute measurements of the ^{238}U(n,f) cross section from 10 to 20 MeV compared with the ENDF/B-VI evaluation.

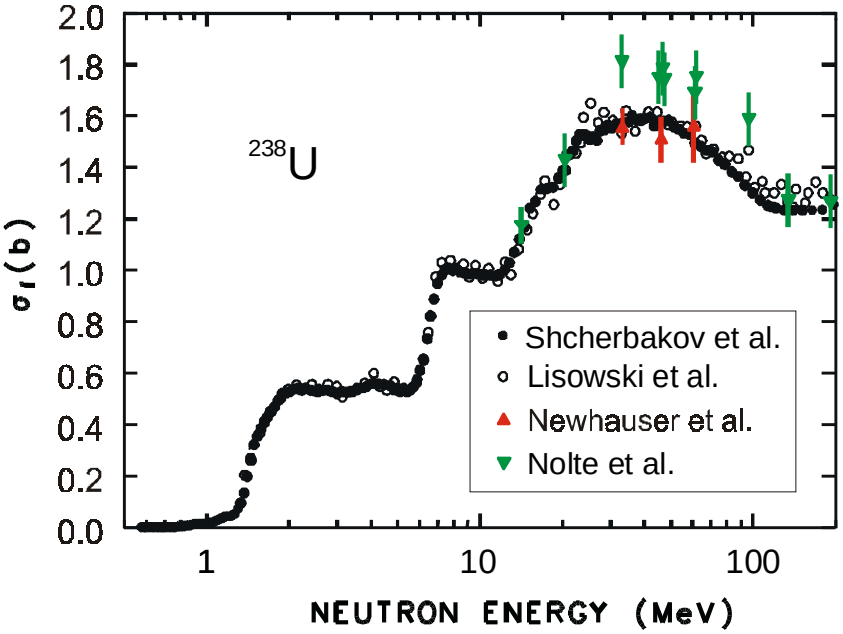

Fig. 6. Comparison of the Nolte measurements with work by Shcherbakov et al. and Lisowski et al.

In Fig. 6, recent measurements of the ^{238}U(n,f) cross section by Nolte et al. are shown compared with the results of Shcherbakov et al. and Lisowski et al. The Nolte et al. values are consistently higher than the other measurements above 20 MeV; but agree at about 14 MeV where the cross section is thought to be well defined. Also shown are the original Newhauser et al. data which required revision. The corrected results from that work have been incorporated into the Nolte work. It should however be noted that the Shcherbakov measurements are ratio measurements to the ^{235}U(n,f) cross section that were converted using the Lisowski et al. values of that cross section. Thus the good agreement between the Shcherbakov et al. and Lisowski et al. data sets up to about 100 MeV is agreement only in the shape of the cross section.

Preliminary measurements made by Eismont et al. at 22 and 75 MeV neutron energy are somewhat low compared with the Lisowski et al. work. However, there is generally good agreement with the Lisowski et al. data, within the rather large uncertainties of the Eismont et al. measurements. Additional work is being done to improve these data.

^{239}Pu(n,f)

Though this cross section is not considered a standard, there are a number of ratio measurements of standards to this cross section which are well known. There also are absolute ^{239}Pu(n,f) cross section data. Therefore these data will have an impact in the simultaneous evaluation. In Fig. 7, recent ^{239}Pu(n,f) cross section measurements are

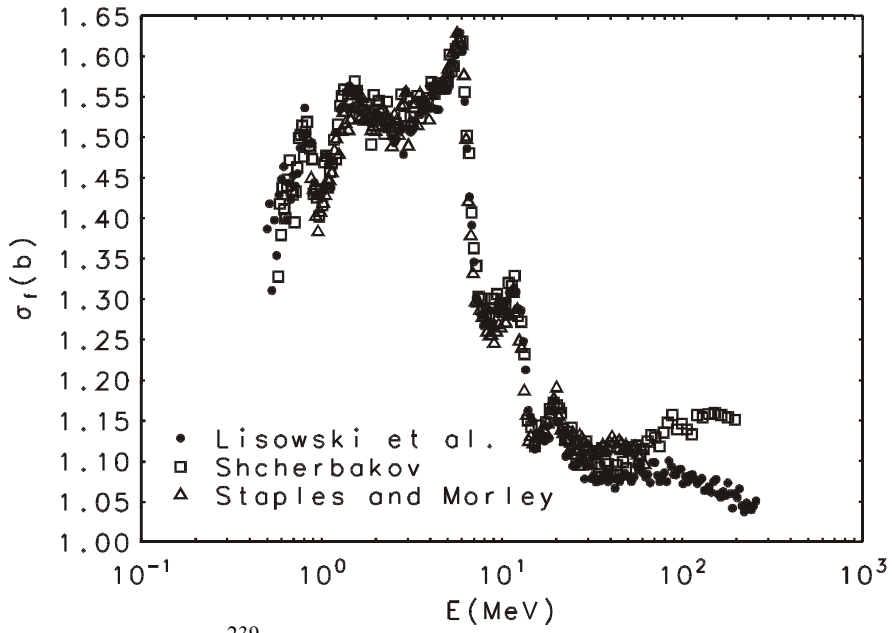

Fig. 7. Comparison of the ^{239}Pu(n,f) cross section measurements of Lisowski et al., Shcherbakov et al., and Staples and Morley.

shown. The statement, in the section on the ^{238}U(n,f) cross section above, applies to the Staples and Morley, and Shcherbakov et al. results since they are both ^{239}Pu(n,f)/^{235}U(n,f) cross section ratio measurements. The three data sets agree very well up to about 30 MeV neutron energy. Between 30 MeV and 60 MeV neutron energy, the Staples and Morley data are about 5% high compared with the other two

data sets. Above 60 MeV neutron energy, the Shcherbakov et al. and Lisowski et al. data sets gradually separate with a maximum difference of about 10% near 200 MeV.

Conclusion

Neutron cross section data continue to be reviewed and prepared for use in the new international evaluation of the neutron cross section standards.

Table 2. New Experiments for the Standards Database

$^{++}$ means the data have been reviewed and are in the library

$^{+}$means the data are available and the review process is underway

no superscript means that final data are not available (possibly final data not taken yet)

H(n,n)

$^{+}$Nakamura, J. Phys. Soc. Japan 15 (1960) 1359, 14.1 MeV; error in transformation from laboratory to CMS angles; needs correction for proton scattering, an estimate of error associated with neglecting these corrections was made; tail problems; note Table II uncertainty is statistical only (mb/sr).

$^{+}$Shirato, J. Phys. Soc. Japan 36 (1974) 331, 14.1 MeV, needs correction for proton scattering; tail problems.

$^{+}$Ryves, 14.5 MeV, $\sigma(180°)/\sigma(90°)$, Ann. Nucl. Energy 17, 657 (1990).

$^{+}$Buerkle, 14.1 MeV, angular distribution from 89.7° to 155.7°, Few-Body Systems 22, 11 (1997).

+Boukharouba, Phys Rev C 65, 014004, 10 MeV, angular distribution from 60° to 180°, additional work planned for 15 MeV.

Olsson (Uppsala group), 96 & 162 MeV, angular distribution from 70° to 180°, ND2001 & Private Comm.

$^{+}$Benck, (Louvain la Neuve), Proc. Conf. on NDST, Trieste (1997) p.1265, 28-75 MeV, angular distribution from 40° to 140°, also NP A615 (1997) p. 222.

Vigdor (IUCF) 185-195 MeV, angular distribution form 90° to 180°. Data have been obtained. A new postdoc is analyzing these data. Private Comm.

^{3}He(n,p)

$^{++}$Borzakov, 0.26 keV to 142 keV, relative to ^{6}Li(n,t), Sov. J. Nucl. Phys. 35, 307 (1982).

^{3}He total cross section

+Keith, 0.1 to 500 eV, BAPS DNP Oct 1997 paper IG.03 and thesis of D. Rich, U of Indiana.

^{6}Li(n,t)

$^{+}$NIST collaboration, thermal measurement with high accuracy using cryogenic calorimeter.

[+]Knitter, (1983) NS&E 83, 229; $^{6}Li(n,t)^{4}He$ angular distribution, 0.035-325 keV, new corrections required.

[+]Drosg, 50 keV to 4 MeV, NIM B94, p.319 (1994), using concept based on the two groups from the source reaction.

Bartle, 2 to 14 MeV, angular distribution, Proc. Conf on Nuclear Data for Basic and Applied Science, Sante Fe (1985), p. 1337 (questionable value, due to energy range and information not available).

Schwarz, 1 to 600 keV, NP 63, p.593, some based on hydrogen scattering cross section. Assumptions need study!

Koehler, 1 keV to 2.5 MeV, angular distribution data (ratio of forward and backward hemispheres responses), private comm.

Gledenov, .025 eV, ??, 87KIEV 2 237

[+]Guohui Zhang, 3.67 and 4.42 MeV, angular distribution, Comm. Of Nuclear Data Progress No.21 (1999) China Nuclear Data Center, also NSE 134, 312 (2000), new corrections required.

$^{10}B(n,\alpha_1\gamma)$

Maerten, 320 keV to 2.8 MeV, GELINA linac, relative to $^{235}U(n,f)$ and carbon standards, private comm. from H. Weigmann.

[++]Schrack, 0.2 MeV to 4 MeV, relative to Black Detector (at ORNL), NSE 114, 352 (1993).

[+]Schrack, 10 keV to 1 MeV, relative to H(n,n) prop ctr (at ORNL), Proc. Conf. on NDST, Gatlinburg (1994)p. 43.

[+]Schrack, .3 MeV to 10 MeV, relative to $^{235}U(n,f)$ ion chamber (at LANL), Private comm.

$^{10}B(n,\alpha)$ Branching Ratio

[++]Weston, 0.02 MeV to 1 MeV, Solid State detectors, NSE 109, 113 (1991).

Hambsch and Bax, ND2001, keV to MeV, Frisch gridded ion chamber, in progress.

$^{10}B(n,\alpha)$

Haight, 1 MeV to 6 MeV, angular distribution at 30°, 60°, 90° and 135°, private comm.

Hambsch and Bax, ND2001, keV to MeV, angular distribution, Frisch gridded ion chamber, in progress.

Giorginis and Khriachkov, MeV energies, angular distribution, VdG data.

[+]Guohui Zhang, 4.17, 5.02, 5.74, 6.52 MeV angular distribution, submitted for publication to NSE, new corrections required.

^{10}B total cross section

[+]Wasson, 0.02 MeV to 20 MeV, NE-110 detector, Proc. Conf. on NDST, Gatlinburg (1994), p. 50.

Wattecamps, Van de Graaff, 1 to 18 MeV, large statistical uncertainty, NE-213 detector, Proc. Conf. on NDST, Gatlinburg (1994), p. 47.

Plompen, Van de Graaff, 0.3 MeV to 1.9 MeV, NE-213 detector, 3 independent monitors, Proc. Conf. on NDST, Trieste (1997), p. 1283.

Brusegan, Linac data, 80 eV to 730 keV, Li-glass detector, Proc. Conf. on NDST, Gatlinburg (1994)p. 47, Proc. Conf. on NDST, Trieste (1997)p. 1283 and private comm.

^{10}Be(p,n) ^{10}B

Massey, E_p from 1.5 MeV to 4 MeV, data at 0°, private comm. New measurements to be made at lower energies (~.5 MeV). Also possibly ^{10}Be (p,α).

C total cross section

[+]Schmiedmayer and M. C. Moxon, Proc. Conf. Nuclear Data for Science and Technology Mito, Japan, May 30 June 3, 1988, p. 165, 50 eV to 100 keV, linac, excellent agreement with ENDF/B-VI.

[+]Kirilyuk, *et al*., Proc. of the Int. Conf. on Neutron Physics, Kiev, 1987, vol. 2, p. 298, filtered beam measurement at 2 keV,very good agreement with ENDF/B-VI.

Au(n,γ)

[+]Yamamoto, thermal, linac, NEANDC(J)-155,59,9008, 1990.

[+]Tolstikov, 0.3 to 0.7 MeV, Van de Graaff, Yad Konstanty,1994,4.

[++]Sakamoto, 23 keV and 967 keV, photoneutron source, activation experiment, NSE 109,215 (1991).

[++]Davletshin, .16 MeV to 1.1 MeV, relative to H(n,n), Sov. J. At. Energy 65, 91 (1988),
(Corrected data from Sov. J. At. Energ. 58, 183 (1985)).

[++]Davletshin, .62 MeV to .78 MeV, relative to ^{235}U(n,f), Sov. J. At. Energy 65, 91 (1988).

[+]Kazakov, Yad Konstanty, 44, 85 (1985); AE,64,(2),152,1988, Van de Graaff, 200-420 keV.

[+]Demekhin, 2.7 MeV, Proc. 36th All Union Conf. on Nuclear Data, p. 94 (1986).

[+]Voignier, ~.5 MeV to ~3 MeV, NSE, 93, 43,1986, private comm.

^{235}U(n,f)

[+]Carlson, 2 MeV to 30 MeV, relative to H(n,n), Proc. Spec. Meeting on Neutron Cross Section Standards for the Energy Region above 20 MeV, Uppsala, Sweden, 1991, Report NEANDC-305, "U", p. 165.

[+]Merla, [+]2.6, [+]4.45, [+]8.46, [+]14.7, [+]18.8 MeV ?, associated particle, Proc. Conf. on NDST Juelich (1991) p.510.

[+]Lisowski, 3 MeV to 200 MeV, relative to H(n,n), Proc. Spec. Meeting on Neutron Cross Section Standards for the Energy Region above 20 MeV, Uppsala, Sweden, 1991, Report NEANDC-305, "U", p. 177, and private communication.

[+]Nolte, 30 to 150 MeV, ND2001, and Private Comm. to increase energy range, Preliminary data.

[++]Buleeva, 0.624 MeV to 0.785 MeV, relative to H(n,n), Sov. J. Atomic Energy, 65, 930 (1988).

Grundl comment, ^{252}Cf spontaneous fission spectrum averaged cross section. NOTE; only the last NIST measurement (Schroder) should be used in the evaluation. The earlier data are improved upon with each new measurement.

[+]Kalinin, 14.7 MeV CCW, associated particle,AE,64,(3),194,8803 AE,71,(2),181,9108 (?? Merla).

[+]Carlson, 0.3 MeV to 3 MeV, relative to black detector, Proc. IAEA Advisory Group Meeting on Nuclear Standard Reference Data, Geel Belgium, p.163, IAEA-TECDOC-335 (1985).

[+]Johnson, 1 MeV to 6 MeV, relative to a dual thin scintillator, Proc. Conf. on NDST Mito (1988) p.1037.

[+]Iwasaki, 14 MeV, relative to H(n,n) and associated particle, Proc. Conf. on NDST Mito (1988) p. 87.

^{238}U(n,f)

[+]Merla, 5 MeV +?, associated particle, Proc. Conf. on NDST Juelich (1991) p.510.

[++]Winkler, 14.5 MeV, relative to Al(n,α) & ^{56}Fe(n,p), Proc. Conf. on NDST Juelich (1991), p.514.

[+]Lisowski, 0.8 MeV to 350 MeV, relative to H(n,n), Proc. Spec. Meeting on Neutron Cross Section Standards for the Energy Region above 20 MeV, Uppsala, Sweden, 1991, Report NEANDC-305, "U", p. 177, and private communication.

[+]Nolte, 30 to 150 MeV, ND2001, and Private Comm. to increase energy range, Preliminary data.

[+]Newhauser, 34, 46, and 61 MeV MeV, absolute, Proc. Conf. on NDST Juelich (1991), *removed from database.*

[+]Meadows, 14.74 MeV, CCW, ANE,15,421,8808, relative to ^{235}U(n,f).

[+]Baba, 4.6 MeV to 6 MeV, Van de Graaff relative to ^{235}U(n,f), J. Nucl. Sci. & Techn.,26,11 (1989).

[+]Shcherbakov, 1-200 MeV, relative to ^{235}U(n.f), ISTC 609-97, see also Fomichev, 0.7 MeV to 200 MeV, relative to ^{235}U(n.f), Proc. Conf. on NDST, Trieste (1997), p.1283.

[+]Li Jingwen, 14.7 MeV, CCW, CNP,11,(3),17,89.

Eismont, Trieste conf, p.494, 33.7, 46 and 60.6 MeV, relative to hydrogen scattering cross section. See also Gatlinburg conference results at 135 and 160 MeV.

[+]Garlea, 14.7 MeV, relative to ^{235}U(n,f) cross section, RRP,37,(1),19,92.

^{238}U(n,γ)

[+]Corvi. Thermal range, linac, Mito conf (1988).

[+]Macklin, linac, 1 to 100 keV, ANE,18,567,91, relative to ^{6}Li(n,t) cross section.

[+]Kazakov, Yad Konstanty, 37, (1986); Van de Graaff, 4-440 keV, liquid scintillator, VDG.

[++]Kobayashi, 0.024 MeV, 0.055 MeV, 0.146 MeV, relative to ^{10}B(n,$\alpha_1\gamma$), Proc. Conf. on NDST Juelich (1991), p. 65.

[++]Quang, 23 keV and 964 keV, photoneutron source, activation experiment, NSE 110, 282 (1992).

[++]Adamchuck, 10 eV to 50 keV, relative to ^{10}B(n,$\alpha_1\gamma$), J. Atomic Energy, 65, 920 (1989).

[++]Buleeva, 0.34 MeV to 1.39 MeV, relative to H(n,n) and ^{235}U(n,f), Sov. J. Atomic Energy, 65, 930 (1989).

[+]Voignier, ~0.5 to 1.1 MeV, NSE,93,43,1986, Van de Graaff.

^{239}Pu(n,f)

[+]Weston, linac, 0.1 keV to 20 keV, fission chamber, 10B(n,α) standard (very large # of points), NSE,111,415,9208.

[+]Weston, linac, 0.002 eV to 100 eV, fission chamber, 10B(n,α) standard (very large # of points), NSE,115,164,9310.

[+]Merla, 4.9, 8.65 and 18.8 MeV, associated particle, Proc. Conf. on NDST Juelich (1991) p.510; see also Alkhazov, YK,1986,(4),19,198612.

[+]Meadows, 14.74 MeV, CCW, ANE,15,421,8808, relative to ^{235}U(n,f).

[+]Shcherbakov, 1-200 MeV, relative to ^{235}U(n.f), ISTC 609-97 (2000).

[+]Staples, 0.5 MeV to 400 MeV, relative to ^{235}U(n,f), NSE 129, 149 (1998).

[+]Lisowski, 0.8 MeV to 250 MeV, relative to H(n,n), Proc. Spec. Meeting on Neutron Cross Section Standards for the Energy Region above 20 MeV, Uppsala, Sweden, 1991, Report NEANDC-305, “U”.

[+]Garlea, 14.7 MeV, relative to ^{235}U(n,f) cross section, RRP,37,(1),19,92.

SOME SOURCES OF THE UNDERESTIMATION OF EVALUATED CROSS SECTION UNCERTAINTIES

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ABSTRACT

The problem of the underestimation of evaluated cross-section uncertainties is addressed. Two basic sources of the underestimation of evaluated cross-section uncertainties - a) inconsistency between declared and observable experimental uncertainties and b) inadequacy between applied statistical models and processed experimental data - are considered. Both the sources of the underestimation are mainly a consequence of existence of the uncertainties unrecognized by experimenters. A model of a “constant shift” is proposed for taking unrecognised experimental uncertainties into account. The model is applied for statistical analysis of the ^{238}U(n,f)/^{235}U(n,f) reaction cross-section ratio measurements.

It is demonstrated that multiplication by sqrt(χ^2) as instrument for correction of underestimated evaluated cross-section uncertainties fails in case of correlated measurements. It is shown that arbitrary assignment of uncertainties and correlation in a simple least squares fit of two correlated measurements of unknown mean leads to physically incorrect evaluated results.

INTRODUCTION

At present there is concern on extremely low uncertainties resulting from application strict statistical methods (least squares method, Bayesian method, maximum likelihood method) to processing experimental data. In this connection 2 questions arise: 1) Is there underestimation of the uncertainties of evaluated cross-sections? 2) If this is the case, what is the value of the underestimation?

Recommended (ENDF/B-VI) and calculated (within strict statistical methods) uncertainties of the neutron standard cross-sections [1] are being often presented as most challenging example of the underestimation. Reviewers of the ENDF/B-VI standards have expressed the concern on too small calculated uncertainties of neutron standard cross-sections and expanded them in few times. For ^{235}U fission cross-section recommended uncertainties exceed calculated those in 2 – 3.3 times in the energy ranges 0.6 – 10 MeV, 14.5 – 20.0 MeV [1]. For ^{10}B(n,α_0)^{7}Li reaction cross-section exceeding is even more: 7.9 – 19 times [1]. However it would be erroneous to accept these numbers as a factor of the underestimation of the calculated neutron standard cross-section uncertainties. As follows from the comments to the ENDF/B-VI neutron standards evaluation [1] these numbers are a ratio between estimated spread for future precise cross-section measurements and the uncertainty of evaluated standard cross-sections calculated on the basis of existing measurements. So, the question on the underestimation of the uncertainties of the ENDF/B-6 neutron standard cross-sections calculated within strict statistical methods is still opened.

At the same time there exist examples where the underestimation of evaluated cross-section uncertainties was proved [2,3]. All these examples are related to cases when correlations between some components of total uncertainties recognized by experimenters have been ignored. Such simplifications have led to physically incorrect results. However, as seen today, the underestimation in cases where it really exists is mainly caused by existence of the uncertainties unrecognized by experimenters.

BASIC SOURCES OF THE UNDERESTIMATION OF EVALUATED CROSS-SECTION UNCERTAINTIES

Two basic sources of possible underestimation of evaluated cross-section uncertainties are: 1) inconsistency between declared and observable experimental uncertainties (as a rule experimental uncertainties are underestimated), 2) inadequacy between applied statistical models and processed experimental data. Both sources are interconnected and adequate statistical model must include validation of declared experimental data and their updating if necessary. To position such a model among all existing ones trace a complication of the models within strict statistical methods. Let's consider LSM (least squares method) as an example.

Within classical model **A** proposed by Gauss [4] random experimental errors ε_i^k for work k are unbiased and independent, uncertainties are constant ($\mathrm{E}\,\varepsilon_i^k=0$, $\mathrm{cov}(\varepsilon_i^k,\varepsilon_j^l)=\sigma^2\delta_{ij}\delta_{kl}$), minimized functional is a sum of squares of the deviations of the approximant from measured values - $\sum_k\sum_i(\Delta y_i^k)^2$. Developing classical model Aitken have allowed the experimental uncertainties to be different [5] and have got a model **B** (for work k random experimental errors ε_i^k are unbiased and independent, uncertainties are different - $\mathrm{E}\,\varepsilon_i^k=0$, $\mathrm{cov}(\varepsilon_i^k,\varepsilon_j^l)=(\sigma_i^k)^2\delta_{ij}\delta_{kl}$, minimized functional is a weighted sum of squares - $\sum_k\sum_i\varpi_{ik}(\Delta y_i^k)^2$). All existing neutron cross-section systematics at single energies were developed on the basis of model **B**. At next step of the complication (model **C**) correlations between experimental errors were included in statistical analysis, minimized functional has transformed from sum of squares into quadratic form (experimental errors ε_i^k are unbiased and correlated, uncertainties are different - $\mathrm{E}\,\varepsilon_i^k=0$, $\mathrm{cov}(\varepsilon_i^k,\varepsilon_j^l)=\sigma_i^k\,\sigma_j^l\,\rho_{ij}^{kl}$, minimized functional is a quadratic form - $\sum_k\sum_l\sum_i\sum_j\Delta y_i^k(V^{-1})_{ij}^{kl}\Delta y_j^l$). All the modern codes apply model **C** to statistical processing of the experimental data. Finally, now we are trying to operate with models **D** having non-zero expectation of experimental errors (ε_i^k are biased and correlated, uncertainties are different - $\mathrm{E}\,\varepsilon_i^k\neq0$, $\mathrm{cov}(\varepsilon_i^k,\varepsilon_j^l)=\sigma_i^k\,\sigma_j^l\,\rho_{ij}^{kl}$, minimized functional is a quadratic form - $\sum_k\sum_l\sum_i\sum_j\Delta y_i^k(V_1^{-1})_{ij}^{kl}\Delta y_j^l$), matrix V_1 takes biases into account either directly or effectively**.** Model **D** describes situation when difference between experimental data sets exceeds declared experimental uncertainties, i.e. there exist errors **unrecognized** by experimenters. At present we don't know a code realizing this model.

MODEL OF A "CONSTANT SHIFT" FOR TAKING UNRECOGNISED EXPERIMENTAL ERRORS INTO ACCOUNT

Model of a "constant shift" is a simplest model of the class **D**. The model is based on following idea. Having some initial approximation for the cross-section being evaluated we can estimate average shift of the measurements (for each experimental work) relative to the approximation and a spread of the measurements relative to shift's value. The spread can be interpreted as a characteristic of statistical error while the shift – as a sample value for systematic error. As initial approximation previous evaluation or LSM-estimate for measurements processed as independent can be used. Next the approximation can be successively improved. Note, that if a database includes one experimental work only unrecognized error isn't detectable. It can be estimated only in comparison with other experimental works.

In the model measured value y_i^k for experimental work *k* is assumed to be a sum of 3 values: $y_i^k = f_i + \varepsilon_i^k + \xi^k, \quad i = 1,..., N_k$ where

f_i - true value of the cross-section being estimated,

ε_i^k - random experimental errors, which are unbiased and uncorrelated - $E\,\varepsilon_i^k = 0$,

$\mathrm{cov}(\varepsilon_i^k, \varepsilon_j^l) = (\sigma^k)^2 \delta_{ij}\delta_{kl}$,

ξ^k - systematic error – constant for measurements from the work *k*,

$E(\xi^k) = \xi^k$ (averaging over distribution of random error).

Values ξ^k in dependence on k form new distribution – distribution of systematic errors. So, $\mathrm{cov}(\xi^k, \xi^l) = (\sigma_{syst})^2 \delta_{kl}$ (averaging over distribution of systematic error), N_k - number of measurements in the work *k*, *M* – number of experiments. As one of the justifications of the model we mention following fact: at any energy total cross-section error consisting of several components with different correlations (0,1,≠0) over energy can be presented as a sum of **two** components (effective statistical with correlation 0 and effective systematic with correlation 1).

The parameters of the model are the parameters of the approximant, statistical uncertainties for each experimental work - σ_k, systematic uncertainty - σ_{syst}, sample values of the systematic error - ξ^k. The parameters can be found in iterative way: a) a search of approximant, b) calculation ξ^k, σ^k and σ_{syst}:

$$\xi^k = \frac{1}{N_k}\sum_{i=1}^{N_k}(y_i^k - f_i), \quad (\sigma^k)^2 = \frac{1}{N_k - 1}\sum_{i=1}^{N_k}(y_i^k - f_i - \xi^k)^2$$

$$\xi = \frac{1}{M}\sum_{k=1}^{M}\xi^k, \qquad \sigma_{syst} = \frac{1}{M-1}\sum_{k=1}^{M}(\xi^k - \xi)^2 \Rightarrow \text{next iteration}$$

Model of a "constant shift" was applied to statistical processing of the ^{238}U(n,f)/^{235}U(n,f) reaction cross-section ratio measurements. Our evaluated curve (30 parameters) is shown in comparison with the ENDF/B-VI evaluation and the experimental data in Fig.1-3. Numerical results are summarized in Table 1. Authors of 22 experimental

Table 1. Average total and statistical experimental uncertainties estimated in the model of a “constant shift” in comparison with declared average experimental total and statistical uncertainties. Data were calculated for the measurements of the $^{238}U/^{235}U$ fission cross section ratios.

Work number	Author	Number of points	Shift, %	Declared experimental total uncertainty,%	Estimated experimental total uncertainty,%	Estim/Decl ratio for total exper. uncertainties	Declared experimental statistical uncertainty,%	Estimated experimental statistical uncertainty,%	Estim/Decl ratio for statistical uncertainties
1	Williams 46 [7]	3	-2.35	9.77	2.62	**0.27**		0.83	
2	Jarvis 53 [8]	1	1.45	1.52					
3	Lamphere 56 [9]	89	-3.83	9.90	13.9	**1.40**		13.7	
4	White 67 [10]	3	1.25	2.02	3.05	**1.50**	<2	1.77	
5	Stein 68 [11]	14	-2.40	1.02	5.32	**5.21**		4.71	
6	Poenits A 72 [12]	1	3.87	1.67			1.60		
7	Poenits B 72 [12]	2	2.23	2.03	3.07	**1.51**	1.98	1.81	0.91
8	Meadows 72 [13]	47	-0.37	2.41	5.59	**2.32**	1.21	5.01	4.14
9	Meadows 75 [14]	22	2.32	1.45	3.06	**2.11**	0.76	1.79	2.36
10	Coates 75 [15]	221	-0.34		6.42		-	5.92	
11	Cieriacks 76 [16]	73	-0.03		5.62		3.31	5.04	1.52
12	Nordborg 76 [17]	23	1.85	2.62	3.11	**1.19**	~2.5	1.88	
13	Cance 76 [18]	9	-2.25	2.88	2.88	**1.00**	0.9	1.47	1.63
14	Behrens 77 [19]	146	3.53	2.65	6.33	**2.39**	2.55	5.82	2.28
15	Fursov 77 [20]	39	1.32	1.10	3.65	**3.32**	0.51	2.68	5.25
16	Cance 78 [21]	2	-0.18	2.96	2.93	**0.99**	1.75	1.56	1.12
17	Varnagy 82 [22]	6	-0.43	5.75	2.86	**0.50**	1.3	1.43	1.1
18	Androsenko 83 [23]	52	-5.77	1.74	16.1	**9.25**	0.76	15.9	20.9
19	Goverdovsky 83 [24]	1	-0.16	1.03					
20	Goverdovsky A 84 [25]	27	-0.06	1.59	2.89	**1.81**	0.97	1.49	1.54
21	Goverdovsky B 84 [25]	5	-2.08	2.17	3.12	**1.44**	0.76	1.89	2.49
22	Meadows 88 [26]	1	3.64	1.15					

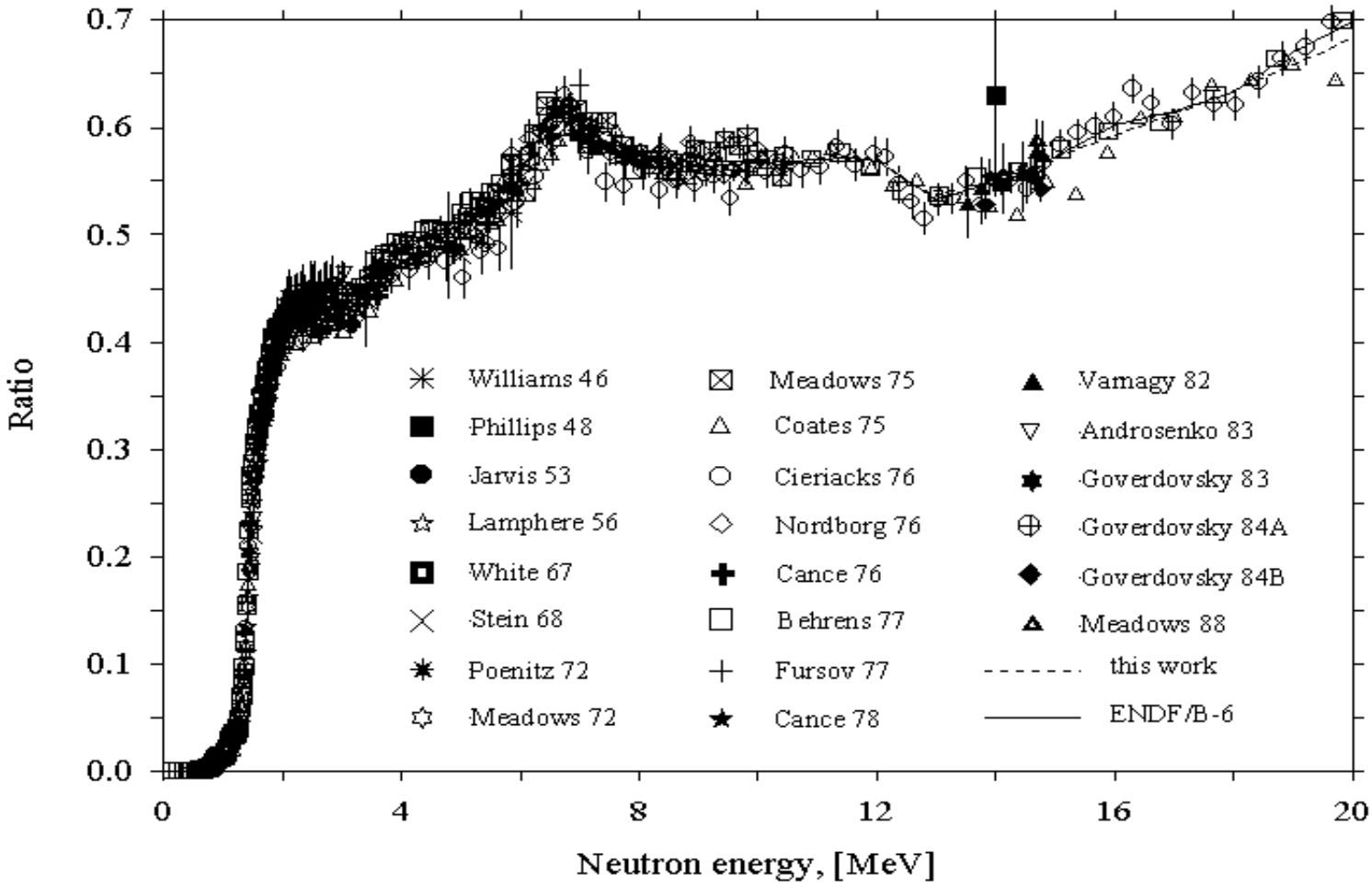

Fig.1 Evaluated ratio of the ^{238}U(n,f) reaction cross-section to the ^{235}U(n,f) reaction cross-section in comparison with the experimental data and the ENDF/B-VI evaluation.

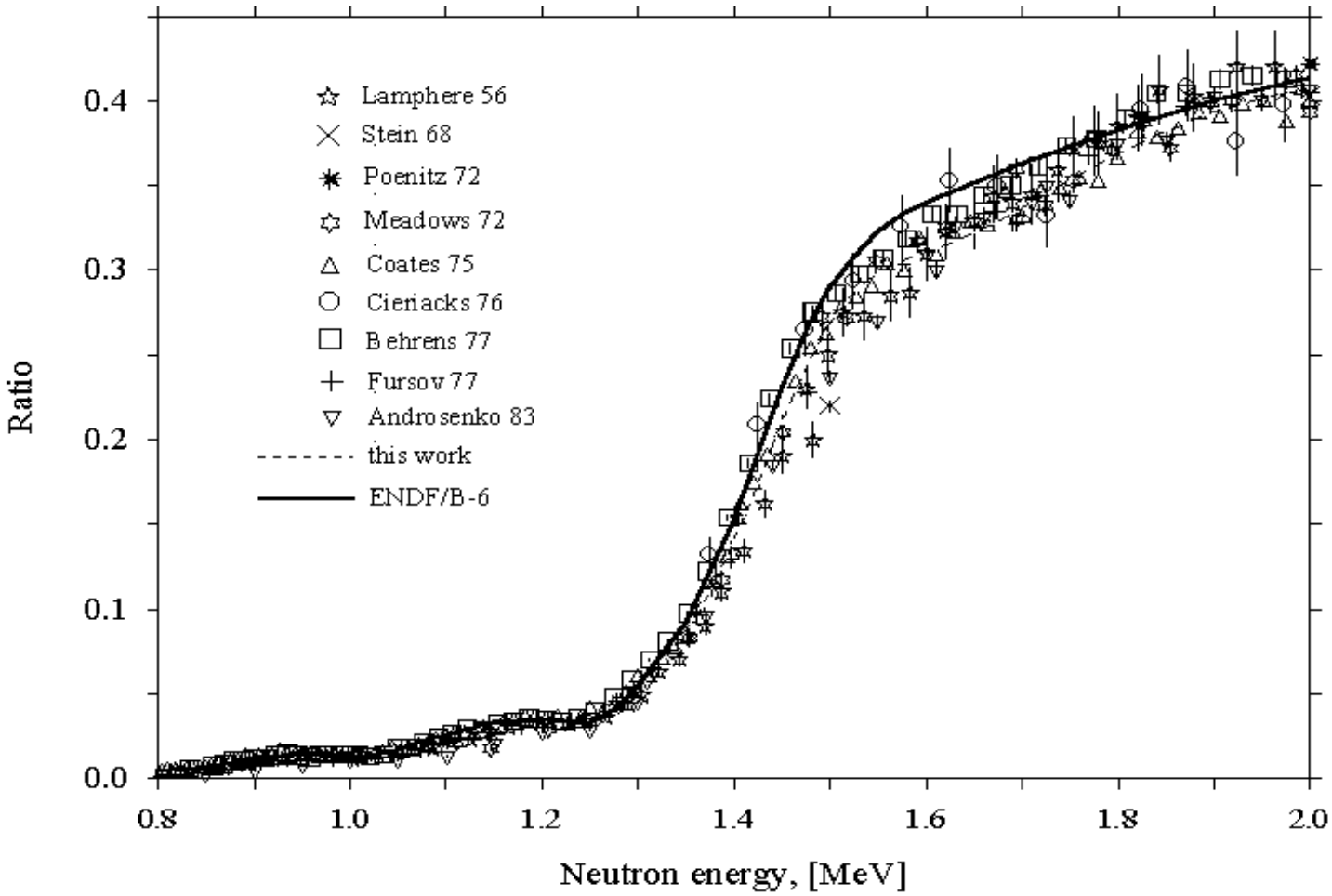

Fig 2. Evaluated ratio of the ^{238}U(n,f) reaction cross-section to the ^{235}U(n,f) reaction cross-section in comparison with the experimental data and the ENDF/B-VI evaluation. Expanded display of the neutron energy range 0.8 - 2.0 MeV.

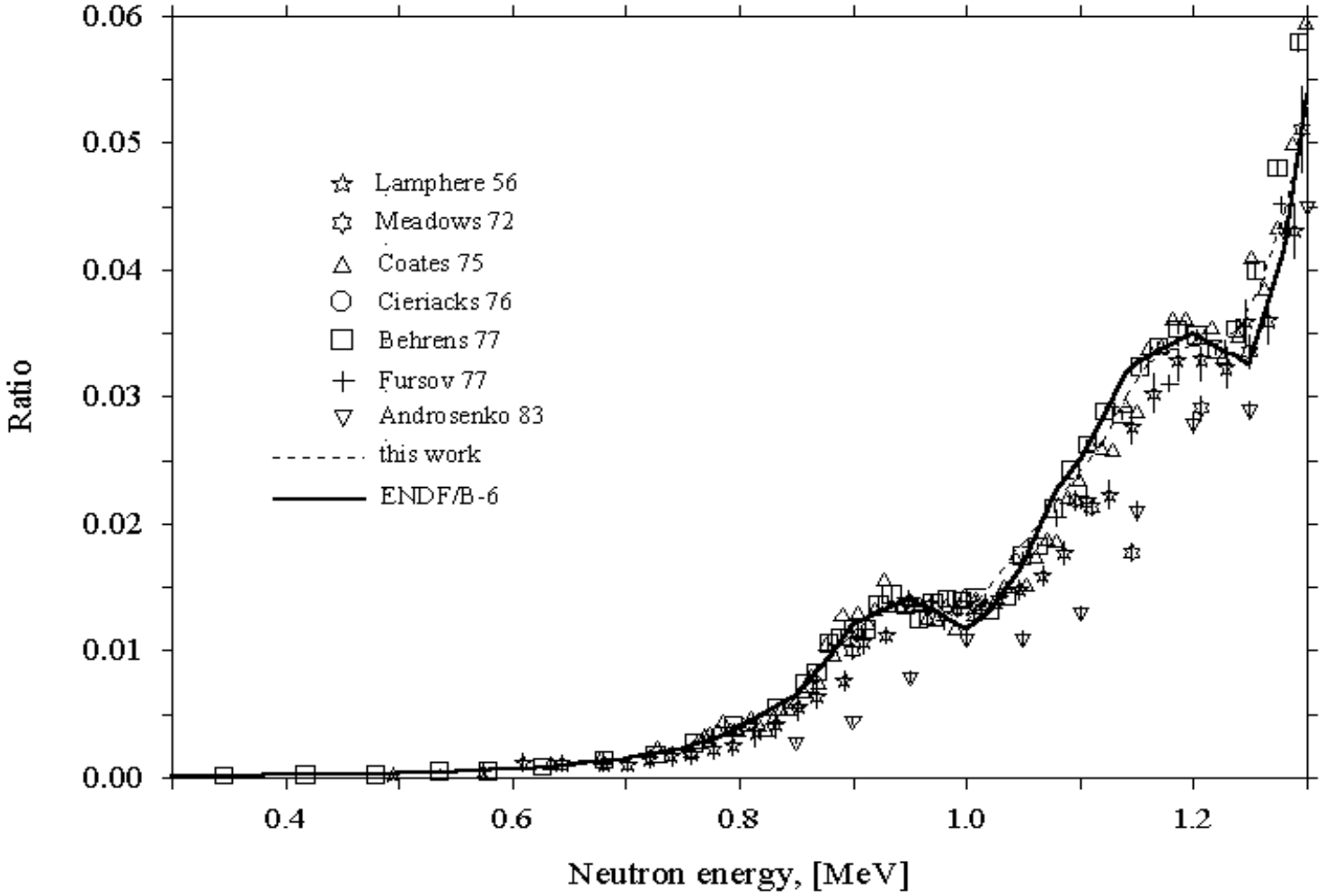

Fig.3 Evaluated ratio of the ^{238}U(n,f) reaction cross-section to the ^{235}U(n,f) reaction cross-section in comparison with the experimental data and the ENDF/B-VI evaluation. Expanded display of the neutron energy range 0.3 - 1.3 MeV.

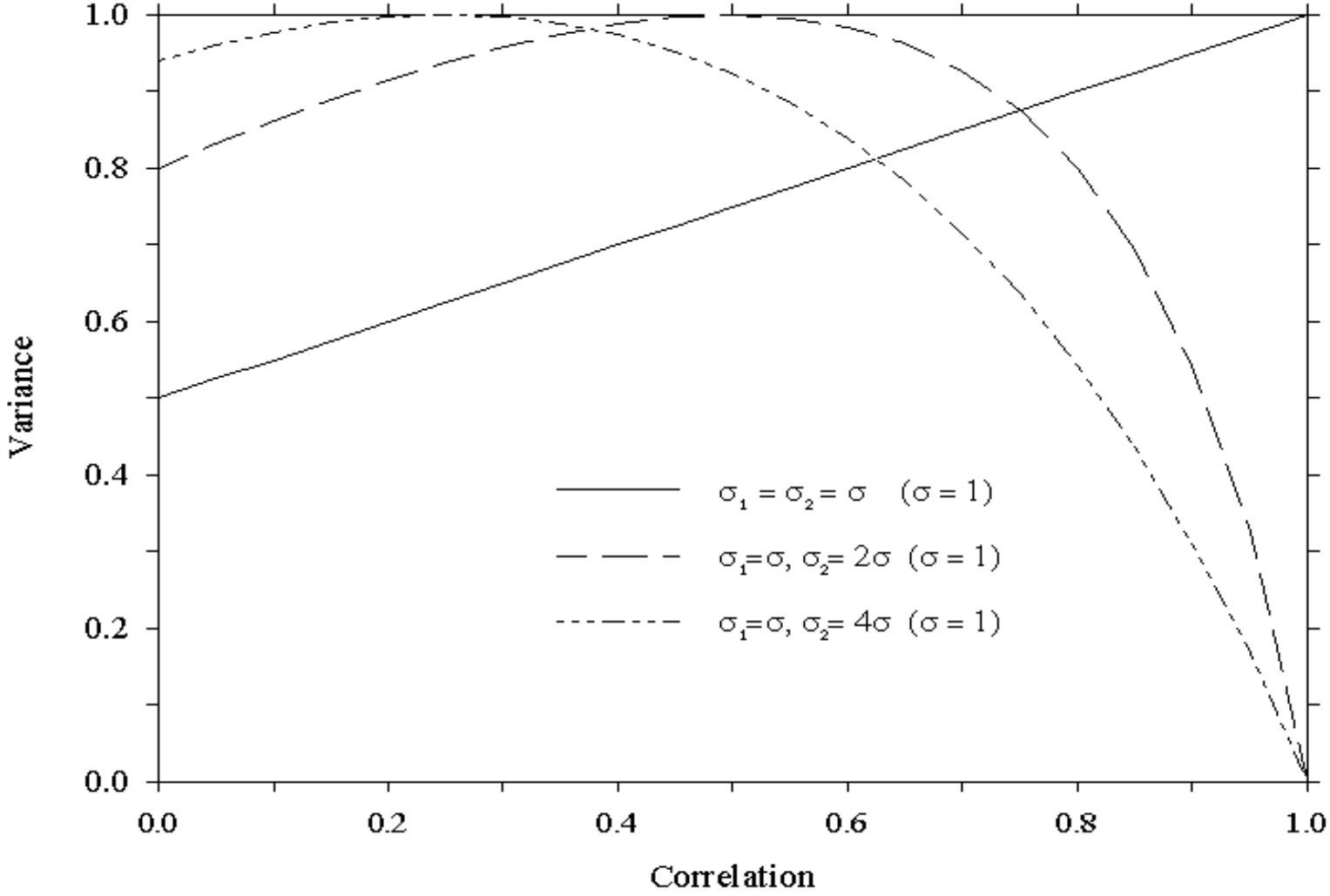

Fig.4 Variance of the LSM-estimate of unknown mean in dependence on correlation of 2 measurements.

data sets extracted from the EXFOR library are listed in column 2. Column 3 informs on the number of measurements in the experimental data sets. Average shift of the measurements relative to the approximant for each experimental data set is given in column 4. Average declared and estimated experimental total uncertainties and their ratios are presented in columns 5, 6 and 7. Columns 8, 9 and 10 include average declared and estimated statistical uncertainties of measurements and their ratio. Blank cells are given in case when the experimental data are not available or the method doesn't allow calculating corresponding values.

The calculations were carried out in relative units. Parameters of the distribution of systematic errors (in %): expectation – 0.05, standard deviation – 2.48. As follows from Table 1: 1) almost all the experimenters underestimate the total experimental uncertainty, average coefficient of the underestimation for total experimental uncertainties (excluding "outliers" – data of Williams 46, Androsenko 83) – 1.91; 2) "contributions" of statistical and systematic components to the underestimation of the total experimental uncertainties are volatile and change sharply from one experimental data set to another. Trying to interpret the values in columns 8 and 9 from Table 1 it should be kept in mind that those are not quite comparable. The experimenters list an uncertainty in the number of counts as statistical (column 8) while a value given in column 9 includes the uncertainty in the number of counts plus the uncertainties corresponding to the random parts of components (with correlations different from 0 or 1 over energy) of the total error. Group ratios, their uncertainties and correlations, comparison with corresponding values from BNAB evaluation [6] are presented in Tables 2 and 3.

Table 2. Group ratios of the ^{238}U fission cross section to the ^{235}U fission cross-section and their uncertainties calculated in the model of a "constant" shift. In last column – uncertainties of the ratios from BNAB evaluation [6].

Energy Group [MeV] to [MeV]	Group Number	Ratio	Uncertainty, [%]	Uncertainty, [%] (BNAB)
0.20 - 0.40	1	0.128E-03	4.88	1.5
0.40 - 0.80	2	0.107E-02	2.22	1.5
0.80 - 1.40	3	0.328E-01	0.92	1.5
1.40 - 2.50	4	0.367E+00	0.68	1.5
2.50 - 4.00	5	0.443E+00	0.68	1.5
4.00 - 6.50	6	0.521E+00	0.65	1.5
6.50 - 14.00	7	0.566E+00	0.71	1.5
14.00 - 20.00	8	0.615E+00	0.96	1.5

Table 3. Correlation matrix (lower triangle) of the uncertainties of group ratios of the ^{238}U fission cross section to the ^{235}U fission cross-section calculated in the model of a "constant shift". Upper triangle contains correlation matrix from the BNAB evaluation [6]. Correlations are given in %.

Energy Group [MeV] to [MeV]	Group Number	1	2	3	4	5	6	7	8
0.20 - 0.40	1	100	0	0	0	0	0	0	0
0.40 - 0.80	2	61	100	100	30	20	20	20	20
0.80 - 1.40	3	33	45	100	30	20	20	20	20
1.40 - 2.50	4	9	22	54	100	30	30	30	30
2.50 - 4.00	5	7	17	51	69	100	100	100	100
4.00 - 6.50	6	10	21	53	68	80	100	100	100
6.50 - 14.00	7	7	17	45	59	62	72	100	100
14.00 - 20.00	8	6	11	31	39	40	40	43	100

MULTIPLICATION BY SQRT(χ^2) AS INSTRUMENT FOR CORRECTION OF EVALUATED CROSS SECTION UNCERTAINTIES IN CASE OF CORRELATED MEASUREMENTS

Multiplication by sqrt(χ^2) is generally accepted procedure for the correction of evaluated cross section uncertainties calculated within strict statistical methods. Exceeding χ^2 over 1 indicates on the underestimation of declared experimental uncertainties. So, multiplication by sqrt(χ^2) is a trial to correct declared experimental uncertainties and, correspondingly, the uncertainties of evaluated cross sections. However this widely spread procedure fails in case of correlated measurements.

Let's consider exactly solvable model example. There exist N measurements y_i, i=1,…,N of a mean θ to be estimated. Unknown true statistical and systematic uncertainties of measurements - σ_{stat} and σ_{syst}, whereas assumed statistical and systematic uncertainties - $\alpha\sigma_{stat}$ and $\beta\sigma_{syst}$, here α and β are coefficients of the underestimation. What is the relationship between true and assumed (before and after multiplication by sqrt(χ^2)) uncertainty of LSM-estimates for the mean θ. Minimized functional has a form:

$$\chi^2 = \frac{1}{N-1}\sum_{i=1}^{N}\sum_{j=1}^{N}(V^{-1})_{ij}(y_i-\theta)(y_j-\theta) =$$

$$= \frac{1}{N-1}\left\{\frac{\sum_{i=1}^{N}(y_i-\theta)^2}{\alpha^2\sigma_{stat}^2} - \frac{(\sum_{i=1}^{N}(y_i-\theta))^2\beta^2\sigma_{syst}^2}{\alpha^2\sigma_{stat}^2(\alpha^2\sigma_{stat}^2+N\beta^2\sigma_{syst}^2)}\right\}$$

The LSM-estimates and their variances calculated for true and assumed uncertainties of measurements are summarized in Table 4. Note that expectation of χ^2 ($E(\chi^2) = \alpha^{-2}$) doesn't depend on the coefficient of the underestimation for systematic uncertainty.

Table 4. The LSM-estimates and their variances calculated for true and assumed uncertainties of measurements.

Experimental uncertainties	LSM –estimate	Variance of LSM-estimate
True	$\hat{\theta}_t = \frac{1}{N}\sum_{i=1}^{N} y_i$	$V(\hat{\theta}_t) = \frac{\sigma_{statt}^2}{N} + \sigma_{syst}^2$
Assumed (before multiplication by sqrt(χ^2))	$\hat{\theta}_a = \frac{1}{N}\sum_{i=1}^{N} y_i$	$V(\hat{\theta}_a) = \frac{\alpha^2\sigma_{statt}^2}{N} + \beta^2\sigma_{syst}^2$
Assumed (after multiplication by sqrt(χ^2))	$\hat{\theta}_a = \frac{1}{N}\sum_{i=1}^{N} y_i$	$V(\hat{\theta}_a) = \frac{\sigma_{statt}^2}{N} + \frac{\beta^2\sigma_{syst}^2}{\alpha^2}$

Thus, for different α, β (coefficients of the underestimation for statistical and systematic uncertainties) multiplication by sqrt(χ^2):

a) doesn't reconstruct true uncertainties of measurements unlike the case with purely statistical uncertainties of measurements,

b) reconstructs statistical component of true uncertainty of the measurements and doesn't reconstruct systematic component,
c) can result in underestimated or overestimated systematic uncertainty in dependence on β-value.

ARBITRARY ASSIGNMENT OF THE UNCERTAINTIES AND CORRELATIONS FOR EXPERIMENTAL ERRORS

Finally, we would like to pay attention to simple model example demonstrating consequences of arbitrary assignment of the uncertainties and correlations for experimental errors.

Let there exist 2 measurements y_i , i=1,2 with the uncertainties σ_1 and σ_2 of a mean θ to be estimated. The measurements correlate with coefficient ρ. Minimized functional has a form

$$S = \frac{1}{2}\,(\vec{y} - \theta)^t\, V^{-1} (\vec{y} - \theta) = \frac{1}{2}\left\{ \frac{(y_1-\theta)^2}{\sigma_1^2(1-\rho^2)} + \frac{(y_2-\theta)^2}{\sigma_2^2(1-\rho^2)} - 2\rho\frac{(y_1-\theta)}{\sigma_1(1-\rho^2)}\frac{(y_2-\theta)}{\sigma_2} \right\}$$

LSM-estimate for θ and its variance V(θ) can be written as

$$\theta = \frac{y_1\left(\frac{1}{\sigma_1^2} - \frac{\rho}{\sigma_1\sigma_2}\right) + y_2\left(\frac{1}{\sigma_2^2} - \frac{\rho}{\sigma_1\sigma_2}\right)}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2} - \frac{2\rho}{\sigma_1\sigma_2}}, \qquad V(\theta) = \frac{1-\rho^2}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2} - \frac{2\rho}{\sigma_1\sigma_2}}$$

Let's consider variances of LSM-solution corresponding to different relationship between uncertainties of measurements:

a) uncertainties of measurements equal each other: $\sigma_1 = \sigma_2 = \sigma$

$$V(\theta) = \frac{\sigma^2}{2}(1+\rho)$$

Observable effect confirms our expectations: strong correlation deteriorates quality of measurements and leads to expanding the uncertainty of estimate (see Fig.4),

b) unequal uncertainties of measurements: $\sigma_1 = \sigma$, $\sigma_2 = 2\sigma$.

$$V(\theta) = \frac{4\sigma^2(1-\rho^2)}{5-4\rho}$$

Observable effect is in contradiction with expectations: there exists range ($0.5 \le \rho \le 1$) where increasing the correlation results in decreasing the uncertainty of estimate (see Fig.4). Moreover for ρ=1 the estimate is known accurately.

The same effect we observe when the uncertainty of second measurement is 4 times more the uncertainty of first measurement: $\sigma_1 = \sigma$, $\sigma_2 = 4\sigma$.

$$V(\theta) = \frac{16\sigma^2(1-\rho^2)}{17-8\rho}$$

As seen in Fig.4, the uncertainty of the estimate decreases with the increase of correlation in the range $0.25 \le \rho \le 1$.

Thus the uncertainty of the estimate changes differently with the increase of the correlation in case of unequal uncertainties of the measurements. There are wide ranges where the uncertainty of estimate decreases with increasing ρ. Thus, arbitrary assignment of the uncertainties for two experimental errors imposes following constraints on covariance and correlation between experimental errors ε_1 and ε_2:

$$\mathrm{cov}(\varepsilon_1, \varepsilon_2) \le \min\,(V(\varepsilon_1), V(\varepsilon_2)),$$

where $V(\varepsilon_1)$ and $V(\varepsilon_2)$ – variances of the experimental errors ε_1 and ε_2;
or if $\sigma_1 = \sigma$, $\sigma_2 = k\sigma$, $k>1$ then correlation between experimental errors ε_1 and ε_2 must be:

$$\mathrm{cor}(\varepsilon_1, \varepsilon_2) \le 1/k\ .$$

It should be noted that an anomaly known as “Peelle’s Pertinent Puzzle” [27] in the interpretation of S.Chiba and D.L.Smith [28] doesn’t satisfy the latter constraints.

SUMMARY

1. As seen at present, there are two basic interconnected sources of the underestimation of evaluated cross-section uncertainties: a) inconsistency between declared and observable experimental uncertainties, b) inadequacy between applied statistical models and processed experimental data.

2. Multiplication by sqrt(χ^2) as instrument for correction of evaluated cross-section uncertainties fails in case of correlated measurements.

3. Arbitrary assignment of the uncertainties and correlations for experimental errors leads to physically incorrect evaluated results**.**

REFERENCES

1. Nuclear Data Standards for Nuclear Measurements, Ed. H.Conde, OECD, Paris, 1992.
2. S.A.Badikov, E.V.Gai, Proceedings of International Conference “Nuclear Data for Science
and Technology “ G.Reffo, A.Ventura and C.Grandi (Eds.), p.949-951, SIF, Bologna, 1997.
3. S.A.Badikov, E.V.Gai, Atomnaya Energiya V.86, N.1, p.40-45, 1999 (in Russian).
4. C.F.Gauss, Methode der Kleinsten Quadrate, Stankiewicz, Berlin, 1887.
5. A.C.Aitken, Proceedings of the Royal Society V.55, N.1, 1936.
6. L.P.Abagyan, N.O.Bazazyanz, M.N.Nikolaev, A.M.Tsibulya, Group Constants for

Calculation of Reactors and Shield, Energoizdat, 1981 (in Russian).
7. J.H.Williams, Report LA-520, Los Alamos Scientific Laboratory, 1946.
8. G.A.Jarvis et al., Report LA-1571, Los Alamos Scientific Laboratory, 1953.
9. R.W.Lamphere, Physical Review V.104, p.1654-1660, 1956
10. P.H.White, G.P.Warner, Journal of Nuclear Energy V.21, p.671-679, 1967.
11. W.E.Stein et al., Nuclear Cross Sections and Technology, Washington, DC, NBS Special Publication 299, V.I, p.627, 1968.
12. W.P.Poenits, Journal of Nuclear Energy V.26, p.483-487, 1972.
13. J.W.Meadows, Nuclear Science and Engineering V.49, N.3, p.310-316, 1972.
14. J.W.Meadows, Nuclear Science and Engineering V.58, p.255, 1975.
15. M.S.Coates et al., Nuclear Cross Sections and Technology, Washington, DC, NBS Special Publication 425, V.II, p.568, 1975.
16. S.Cieriacks et al, Proceedings of the NEANDC/NEACRP Specialists Meeting on Fast Neutron Fission Cross Sections of U-233, U-235, U-238 and Pu-239, June 28-30 1976, ANL, USA, Report ANL-76-90, p.94-113, 1976.
17. C.Nordborg, H.Conde, L.G.Stremberg, Proceedings of the NEANDC/NEACRP Specialists Meeting on Fast Neutron Fission Cross Sections of U-233, U-235, U-238 and Pu-239, June 28-30 1976, ANL, USA, Report ANL-76-90, p.141-148, 1976.
18. M.Cance, G.Grenier, Proceedings of the NEANDC/NEACRP Specialists Meeting on Fast Neutron Fission Cross Sections of U-233, U-235, U-238 and Pu-239, June 28-30 1976, ANL, USA, Report ANL-76-90, p.128-140, 1976.
19. J.W.Behrens, G.W.Carlson, Nuclear Science and Engineering V.63, p.250, 1977.
20. B.I.Fursov et al., Atomnaya Energiya V.43, N.3, p.181-186, 1977.
21. M.Cance, G.Grenier, Nuclear Science and Engineering V.68, N.2, p.197-203, 1978.
22. M.Varnagy, J.Csikai, Nuclear Instruments and Methods V.196, p.465-468, 1982.
23. Kh.D.Androsenko, G.G.Korolev, D.L.Shpak, Proceedings of All-Union Conference on Neutron Physics, October 2-6 1983, Kiev, USSR, v.2, p.153-158, Moscow, 1984.
24. A.A.Goverdovsky et al., Proceedings of All-Union Conference on Neutron Physics, October 2-6 1983, Kiev, USSR, v.2, p.159-163, Moscow, 1984.
25. A.A.Goverdovsky et al., Atomnaya Energiya v.56, N.3, p.162-165, 1984.
26. J.W.Meadows, Annals of Nuclear Energy v.15, p.421, 1988.
27. R.W.Peelle, “Peelle’s Pertinent Puzzle”, Informal memorandum dated October 13, 1987, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, 1987.
28. S.Chiba, D.L.Smith, Report JAERI-M 94-068, p.5-12, 1994.

Arbitrariness of Evaluated Covariance in Least-Squares Method

Presented at the First RCM of the IAEA CRP on
"Improvement of the Standard Cross Sections for Light Elements"
Vienna, Sept. 23 ~ 27, 2002
(*Corrected/Modified Dec. 2002*)

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1. Work Scope

- **Evaluation of standard CS's for light elements <u>using a (non-model) least-squares method</u>:**
  - study the error propagation in the least-squares method,
  - evaluate CS's and covariance matrices for H^1 (n,n), He^3(n,p), Li^6(n,t), B^{10}(n,α_0), and B^{10}(n, $\alpha_1\gamma$) reactions using GMA (and ZOTT if necessary), and
  - participate to the study of inter-comparison between model fit and non-model fit

- **Enhancement of the Bayes' Method**
  in cooperation with other participants

2. Issues

- Is the model (design matrix) utilized in the GMA almighty? Especially in terms of
  - statistical significance of the fitting and
  - justification of covariance matrix of evaluated CS's (magnitude of uncertainty as well as correlation)

- Is there any method not (or less) sensitive to a model utilized in a least squares method?

- Resolution for Peelle's Pertinent Puzzle in using GMA?

3. Statistical Significance of GMA Fitting

- A sample problem shown in Fig.1.
  - Six data on four energy points
  - Data look very linear to the energy.

- The F-test indicates that the 2^{nd} and higher order terms are insignificant.

- Evaluated CS's and their uncertainties seem to be comparable, but the resulting covariance matrices are quite different each other.

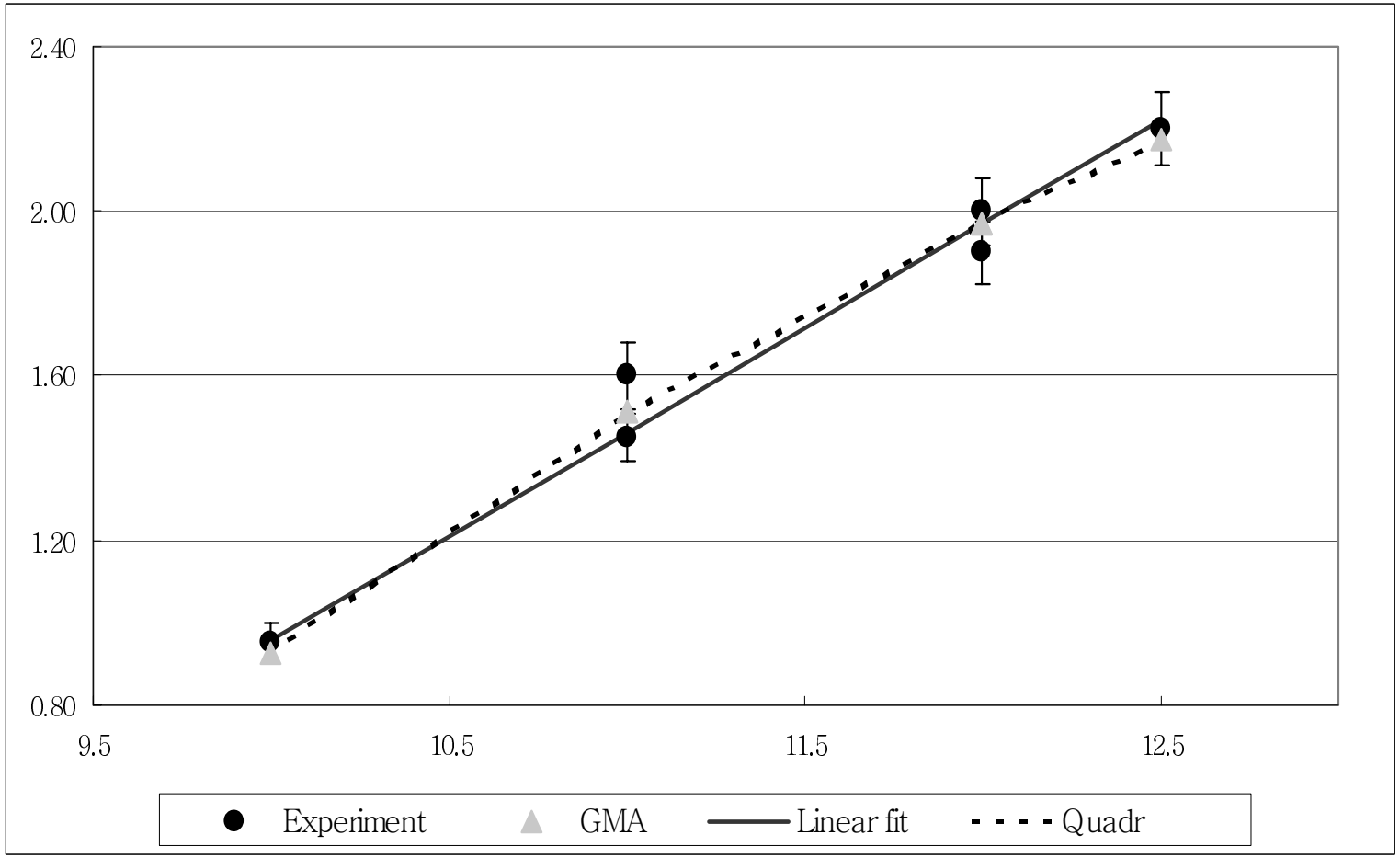

Fig.1. Examples of LSM fitting for very linear data

Data									
En (MeV)	Sig.	total (%)	syst (%)	V					
10	0.95	5	3.5	0.002256	0.00186	0	0	0	0
11	1.60	5	3.5	0.001862	0.0064	0	0	0	0
11	1.45	4	3.5	0	0	0.003	0.003375	0	0
12	1.90	4	3.5	0	0	0.003375	0.006	0	0
12	2.00	4	3.5	0	0	0	0	0.0064	0.00539
12.5	2.20	4	3.5	0	0	0	0	0.00539	0.0077
Solutions									
GMA	Sig-eval	unc	unc (%)	Correlation					
	0.924	0.043	4.7	1.00					
	1.511	0.042	2.8	0.28	1.00				
	1.972	0.052	2.6	0.17	0.59	1.00			
	2.176	0.071	3.3	0.10	0.36	0.61	1.00		
Linear Fit	y=a+b*x								
	0.958	0.039	4.1	1.00					
	1.464	0.034	2.3	0.71	1.00				
	1.969	0.049	2.5	0.18	0.82	1.00			
	2.221	0.060	2.7	0.02	0.72	0.99	1.00		
Quadr									
	0.926	0.043	4.6	1.00					
	1.509	0.041	2.7	0.32	1.00				
	1.977	0.049	2.5	0.13	0.72	1.00			
	2.168	0.066	3.0	0.17	0.31	0.86	1.00		
3rd order	**For any 4-parameters model tested, results do not alter regardless of the form of regression function.**								
	0.924	0.043	4.7	1.00					
	1.511	0.042	2.8	0.28	1.00				
	1.972	0.052	2.6	0.17	0.59	1.00			
	2.176	0.071	3.3	0.10	0.36	0.61	1.00		
Linear Fit	y=a+b/x								
	0.931	0.040	4.3	1.00					
	1.501	0.034	2.3	0.65	1.00				
	1.975	0.049	2.5	0.15	0.85	1.00			
	2.184	0.058	2.6	0.01	0.77	0.99	1.00		

4. Evaluation with Discrepant, Strongly Correlated Data

- A regression model assumes the normality of errors:

$$\mathbf{y}_{\text{meas}} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} = N(\mathbf{0}, \sigma^2 \mathbf{I}).$$

- If residuals (i.e., $y_{reg} - y_{meas}$) are distributed far from the normal distribution, the model is not appropriate.

- Then, what can we do?
  - Consider a revision of $\mathbf{V}_y$, the covariance matrix of $\mathbf{y}_{meas}$.
  - Consider a revision of the model, **X**.
  - Consider a transformation of (dependent) variable.

4.1. The PPP again

- Peelle's Pertinent Puzzle:

  For a quantity *y*, measured are

  $y_1 = 1.50 \pm 0.33$ (statistical unc. 10%, systematic 20%)

  $y_2 = 1.00 \pm 0.22$ (statistical unc. 10%, systematic 20%).

  What is the estimate of y?

- Solution by Least-Squares Method:

  $\hat{y} = 0.882 \pm 0.218$ using the design matrix of $(1 \;\; 1)^t$ and

$$\mathbf{V}_y = \begin{pmatrix} 1.5^2(0.1^2 + 0.2^2) & (1.5 \times 0.2)(1.0 \times 0.2) \\ (1.5 \times 0.2)(1.0 \times 0.2) & 1.0^2(0.1^2 + 0.2^2) \end{pmatrix} = \begin{pmatrix} 0.1125 & 0.06 \\ 0.06 & 0.05 \end{pmatrix}$$

- There are several interpretations on the origin; improper linearization, improper treatment of uncertainty of derived quantity…

4.2. Box-Cox Transformation

- Box-Cox transformation:

$$w_i = \begin{cases} \left(y_i^{\lambda} - 1\right)/\lambda, & \lambda \neq 0 \\ \ln y_i, & \lambda = 0 \end{cases}$$

- The optimum λ maximizes

$$L(\lambda) = -\frac{n}{2}\ln s^2 + (\lambda - 1)\sum_n \ln y_i,$$

where s^2 is the Residual Sum of Squares divided by n.

4.3. Box-Cox Transformation in the PPP

- Solution with the optimum $\lambda = 0$,

$$\hat{y} = 1.224 \pm 0.260$$

Cf. Other solutions (Example 11.17 of D. Smith 1991)

y ~ 1.22: mean value of skewed, non-Gaussian pdf

y ~ 1.15 or 0.88: most probable value

- The solution looks reasonable. However, does the transformation method always guarantee a reasonable solution?

4.4. Box-Cox Transformation in Example #2

Meas. Set	Energy	Measured CS	Unc. Total (%)	Unc. Syst. (%)
1	10.0	0.95	20	19
1	11.0	1.00	20	19
2	11.0	1.50	20	19
2	12.0	1.90	20	19
3	12.0	2.00	20	19
3	12.5	2.20	20	19

- What we want to investigate:
  - Sensitivity of the solution to the model
  - Covariance matrices of evaluated CS's
- *Solutions using the transformation are less sensitive to the order of model.*
- *The covariance matrices are still model dependent.*

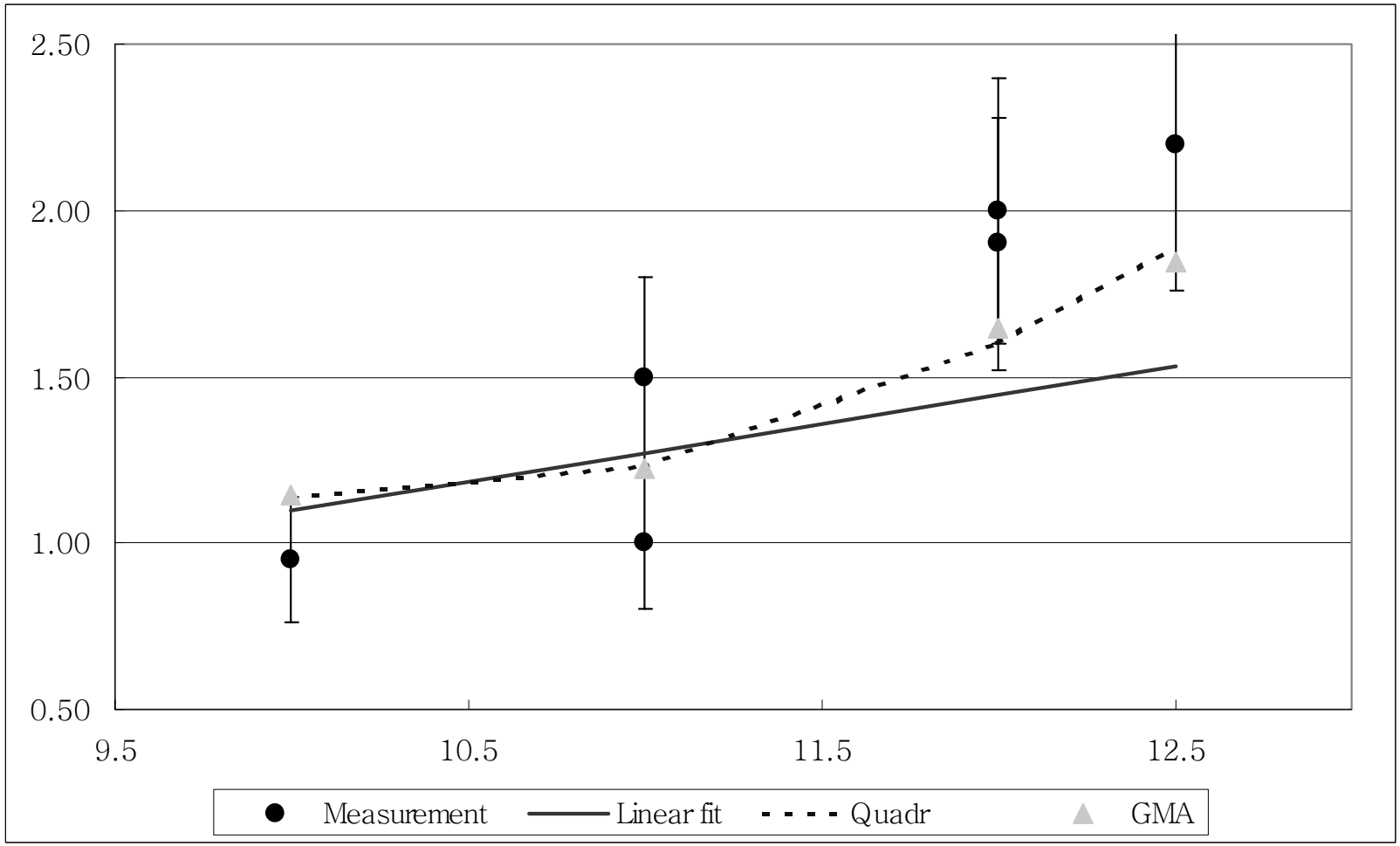

Fig.2. Solutions using Usual Least Squares Method

Data									
En (MeV)	Sig.	total (%)	syst (%)	V					
10	0.95	20.00	19.00	0.0361	0.03430	0	0	0	0
11	1.00	20.00	19.00	0.034295	0.04	0	0	0	0
11	1.50	20.00	19.00	0	0	0.090	0.102885	0	0
12	1.90	20.00	19.00	0	0	0.102885	0.144	0	0
12	2.00	20.00	19.00	0	0	0	0	0.1600	0.15884
12.5	2.20	20.00	19.00	0	0	0	0	0.15884	0.1936
Solutions									
GMA	Sig-eval	unc	unc (%)	Correlation					
10	1.142	0.154	13.5	1.00					
11	1.224	0.152	12.4	0.85	1.00				
12	1.644	0.213	12.9	0.59	0.70	1.00			
12.5	1.847	0.284	15.4	0.44	0.52	0.74	1.00		
Linear Fit	y=a+b*x								
	1.099	0.153	13.9	1.00					
	1.271	0.151	11.8	0.89	1.00				
	1.443	0.180	12.5	0.63	0.92	1.00			
	1.529	0.203	13.3	0.51	0.85	0.99	1.00		
Quadr									
	1.139	0.154	13.5	1.00					
	1.228	0.152	12.4	0.85	1.00				
	1.598	0.197	12.3	0.63	0.78	1.00			
	1.889	0.274	14.5	0.47	0.53	0.94	1.00		
3rd order									
	1.142	0.154	13.5	1.00					
	1.224	0.152	12.4	0.85	1.00				
	1.644	0.213	12.9	0.59	0.70	1.00			
	1.847	0.284	15.4	0.44	0.52	0.74	1.00		
Linear Fit	y=a+b/x								
	1.103	0.153	13.9	1.00					
	1.269	0.151	11.9	0.88	1.00				
	1.408	0.176	12.5	0.65	0.94	1.00			
	1.469	0.193	13.1	0.56	0.89	0.99	1.00		

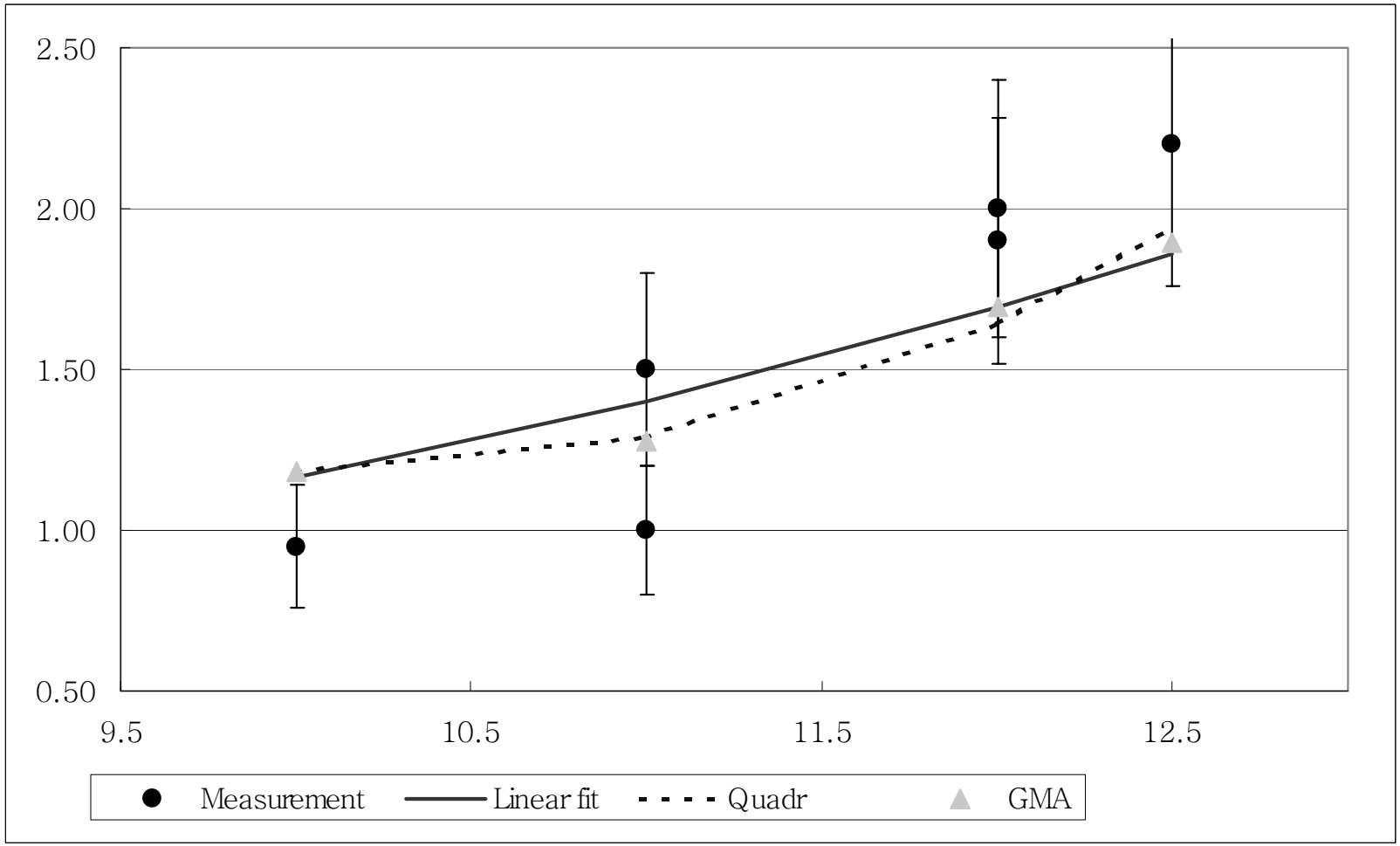

Fig.3. Solutions using Box-Cox Transformation, then Least Squares Method

Data									
En (MeV)	Sig.	total (%)	syst (%)	V					
10	0.95	20.00	19.00	0.0361	0.03430	0	0	0	0
11	1.00	20.00	19.00	0.034295	0.04	0	0	0	0
11	1.50	20.00	19.00	0	0	0.090	0.102885	0	0
12	1.90	20.00	19.00	0	0	0.102885	0.144	0	0
12	2.00	20.00	19.00	0	0	0	0	0.1600	0.15884
12.5	2.20	20.00	19.00	0	0	0	0	0.15884	0.1936
Solutions		after Box-Cox Transformation							
GMA	Sig-eval	unc	unc (%)	Correlation					
10	1.183	0.161	13.6	1.00					
11	1.274	0.156	12.2	0.82	1.00				
12	1.692	0.210	12.4	0.61	0.74	1.00			
12.5	1.893	0.273	14.4	0.47	0.57	0.77	1.00		
Linear Fit	y=a+b*x								
	1.164	0.160	13.7	1.00					
	1.402	0.161	11.5	0.92	1.00				
	1.691	0.198	11.7	0.64	0.89	1.00			
	1.858	0.237	12.8	0.46	0.77	0.98	1.00		
Quadr									
	1.181	0.161	13.7	1.00					
	1.288	0.156	12.1	0.82	1.00				
	1.641	0.194	11.8	0.63	0.83	1.00			
	1.940	0.269	13.9	0.49	0.57	0.92	1.00		
3rd order									
	1.183	0.161	13.6	1.00					
	1.274	0.156	12.2	0.82	1.00				
	1.692	0.210	12.4	0.61	0.74	1.00			
	1.893	0.273	14.4	0.47	0.57	0.77	1.00		
Linear Fit	y=a+b/x								
	1.173	0.163	13.9	1.00					
	1.432	0.164	11.5	0.90	1.00				
	1.696	0.198	11.7	0.62	0.90	1.00			
	1.829	0.229	12.5	0.47	0.80	0.98	1.00		

5. Summary and Open Questions

- Regardless of good evaluated CS's from the least-squares method, it seems the covariance (or correlation, at best) matrix of resulting CS's is arbitrary.
- Should we adopt a covariance matrix produced from the most statistically significant fitting?

- Any criteria useful in distinguishing well-evaluated covariance?
- Modification of GMA?
  - Box-Cox transformation algorithm
  - Treatment of discrepant data proposed by Drs. Smith and Chiba (already implemented in GMA-JNDC version)
  - others

Box-Cox Transformation for Resolving Peelle's Pertinent Puzzle in Curve Fitting

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Abstract

Incorporating the Box-Cox transformation into a least-squares method is presented as one of resolutions of an anomaly known as Peelle's Pertinent Puzzle. The transformation is a strategy to make non-normal distribution data resemble normal data. A procedure is proposed: transform the measured raw data with an optimized Box-Cox transformation parameter, fit the transformed data using a usual curve fitting method, then inverse-transform the fitted results to final estimates. The generalized least-squares method utilized in GMA is adopted as the curve fitting tool for the test of proposed procedure. In the procedure, covariance matrices are correspondingly transformed and inverse-transformed with the aid of error propagation law. In addition to a sensible answer to the Peelle's problem itself, the procedure resulted in reasonable estimates of ^{6}Li(n,t) cross sections in several to 800 keV energy region. Meanwhile, comparisons of the present procedure with that of Chiba and Smith show that both procedures yield estimates so close each other for the sample evaluation on ^{6}Li(n,t) above as well as for the Peelle's problem. Two procedures, however, are conceptually very different and further discussions would be needed for a consensus on this issue of resolving the Puzzle. It is also pointed out that the transformation is applicable not only to a least-squares method but also to other parameter estimation method such as a usual Bayesian approach formulated with an assumption of normality of the probability density function.

1. Introduction: Peelle's Pertinent Puzzle

The least-squares method (LSM) is a well-developed, powerful tool for curve fitting along with model parameter estimation. Nevertheless, an anomaly is observed such that the method sometimes yields strange, unacceptable estimates. In the nuclear data society, the anomaly is known as Peelle's Pertinent Puzzle (PPP), which is quoted below for completeness from a secondary source:[1]

"Suppose we are required to obtain the weighted average of two experimental results for the same physical quantity. The first result is 1.5, and the second result 1.0. The full covariance matrix of these data is believed to be the sum of three components. The first component is fully correlated with standard error of 20% of each respective value. The second and third components are independent of the first and of each other, and correspond to 10% random uncertainties in each experimental result.

The weighted average obtained from the least-squares method is 0.88 ± 0.22*, a value outside the range of the input values! Under what conditions is this the reasonable result that we sought to achieve by use of an advanced data reduction technique?"

Several studies have been devoted to investigate the reason and resolution of PPP.[1-5] Previous studies will not be reviewed here, but D. Smith's view[6] on this issue is briefly introduced. He showed seven distinct solutions to PPP and noted that each method is unique in concept and each treats the available experimental information differently. He suggested solutions from the Bayesian approach† as the rigorous one, in which quite skewed, non-normal posterior probability distribution for the quantity under evaluation is properly dealt with. His point is that the anomaly stems from the probability distribution of observable that is non-normal but implicitly assumed as normal in, say, a least-squares method. Interpretations such that PPP originates from an improper linearization[3] or from an improper treatment/calculation of the covariance of derived (or normalized in many cases of nuclear data evaluation) quantity[2,4,5] are essentially not far from Smith's viewpoint.

Unfortunately, PPP is alive in a real world; for example, in an evaluation of ^{115}In(n,n')^{115m}In cross sections.[1] During the titled CRP work, Pronyaev also reported[7] PPP in the evaluation of ^{6}Li(n,t) cross sections using GMA code[8]‡. Thus, the CRP recently decided to revisit PPP and search for a resolving method. Even though 'the Bayesian procedure (with due consideration on the governing probability distribution) is both appealing and rigorous in principle,' we face up to the question of how to deal with a real problem in a practical way because of the complexity of the real problem.[6] Chiba and Smith proposed a practical, iterative procedure for resolving PPP and implemented it into GMA.[1] That version of GMA will be referred as GMAJ[9] for convenience hereafter. Their idea looks working well in a real evaluation, but is based on a more or less subjective interpretation of the fractional uncertainties usually provided along with measured data. In their procedure, the absolute uncertainty is computed from fractional uncertainty multiplied by the 'true' value, not by measured one. Without knowing the true value, the procedure needs iterations.

2. New Procedure for Resolving the Puzzle

2.1. Outline

A least-squares method (LSM) assumes a normality of residuals, *i.e.* the differences between estimates and raw data, even though the derivation of necessary formulas does not explicitly require the normality. A distribution of residuals far from the normality implies that the fitting model, rather than the methodology, is inappropriate to such kind of raw data. Remind that PPP is perceived from biased residuals. There are three options in dealing with non-normally distributed residuals: re-interpret the covariance associated with the measurement, transform the 'independent' variable (model parameter in other words), or transform the 'dependent' variable to be a suitable type to the model. The second option is

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* Originally presented was 0.87 ± 0.23, which is essentially identical to 0.88 ± 0.22 obtained from the least-squares method. See the solution in Section 3.1 of this article.

† Methods 1 and 2 in his book are regarded as the Bayesian method. Method 2 utilizes a logarithmic transformation as the other way of obtaining the best mean value estimate, while other methods except Methods 1 and 2 give a most probable value.

‡ In this article, let GMA refer to GMAR, which is a bug-corrected version by Pronyaev of GMA sent to IAEA for this CRP.

equivalent to a revision of the model. The last one, while keeping the original model, is the approach proposed in this article.

The fitting procedure proposed is as follows: transform the measured data and their covariance matrix, fit the transformed data using a conventional method, then inverse-transform the estimates and associated covariance into the space of original data. The key of the proposal is a concept dealing with 'transformed' data in curve fitting or, equivalently, in evaluation of model parameters. The Box-Cox transformation[10] is utilized as the tool for making non-normally distributed data resemble normally distributed data.

As a tool for curve fitting itself, the generalized LSM of GMA is adopted for tests in this study. The concept, however, can be incorporated not only into a LSM method but also into any other methods such as a usual Bayesian approach and maximum likelihood method as well. It is worth to remind that PPP is invoked by the data discrepant and strongly correlated each other, not by a fitting methodology. In other words, even a Bayesian approach, if it assumes a normal distribution of the observable in its formulation, is not free from PPP. In addition to the normality assumption, an assumption of linearity of measured quantities with respect to model parameters makes the Bayesian method (with non-informative priors) be identical to the LSM.[11] It provides another basis that the concept of variable transformation can be applied to a usual Bayesian method.

2.2. Box-Cox Transformation and Associated Formulas

Box and Cox proposed a transformation[§] of dependent (response) variable y to w as

$$w_i(\lambda) = \begin{cases} \left(y_i^{\lambda} - 1\right)/\lambda, & \lambda \neq 0 \\ \ln y_i, & \lambda = 0 \end{cases}, \quad i = 1, \ldots, N, \tag{1}$$

which makes the probability density function of w rather close to the normal distribution. The transformation is performed for all N data points of a vector $\mathbf{y} = (y_1\ y_2\ \ldots\ y_N)^t$ to the vector $\mathbf{w}$. The power λ is determined to maximize the log-likelihood function

$$\ln L(\lambda) = -\frac{N}{2}\ln\left[\frac{1}{N}\sum_{i=1}^{N}\left(\hat{w}_i - w_i\right)^2\right] + (\lambda - 1)\sum_{i=1}^{N}\ln y_i\ , \tag{2}$$

where $\hat{w}_i$ is the estimate of w_i. A numerical solver, usually a grid search method, is used in determining λ since $L(\lambda)$ in Eq. (2) is a recursive function of w. The optimum λ is searched in the range of [–2, 2] usually. Note that $\lambda = 1$ implies no transformation in fact.

$\mathbf{V}_y$, the covariance matrix associated and given along with $\mathbf{y}$, is transformed to $\mathbf{V}_w$ with the aid of the law of error propagation as follows:

$$\mathbf{V}_w = \mathbf{S}\,\mathbf{V}_y\,\mathbf{S}^t, \tag{3}$$

where $\mathbf{S}$ is a diagonal sensitivity matrix whose (i, i) element is computed as

$$S_{i,i} = \frac{\partial w_i}{\partial y_i} = \begin{cases} y_i^{\lambda-1}, & \lambda \neq 0 \\ 1/y_i, & \lambda = 0 \end{cases}.$$

[§] There are several variations of the transformation function, usually more complex than this, for the same purpose. Nonetheless, the present transformation seems to be enough in dealing with PPP.

A curve fitting method, the generalized LSM here, then yields the estimate $\hat{\mathbf{w}}$ and its associated covariance matrix $\mathbf{V}_{\hat{\mathbf{w}}}$. The estimate $\hat{\mathbf{w}}$ is easily inverse-transformed into $\hat{\mathbf{y}}$ by

$$\hat{y}_i = \begin{cases} \left(\hat{w}_i \lambda + 1\right)^{1/\lambda}, & \lambda \neq 0 \\ exp(\hat{w}_i), & \lambda = 0 \end{cases} .$$

The inverse-transformation of $\mathbf{V}_{\hat{\mathbf{w}}}$ to $\mathbf{V}_{\hat{\mathbf{y}}}$ is performed similarly to Eq. (3).

3. Sample Evaluations

3.1. Peelle's Problem

Before to advance, formulas for the LSM are summarized below[**]. With respect to a model defined as

$$\mathbf{y} = \mathbf{G}\,\mathbf{p} + \boldsymbol{\varepsilon} \ , \ \boldsymbol{\varepsilon} \sim N(\mathbf{0}, \mathbf{V}\sigma^2) ,$$

the LSM provides the estimate of model parameter vector **p** and its associated covariance matrix as

$$\hat{\mathbf{p}} = \left(\mathbf{G}^t \mathbf{V}_{\mathrm{y}}^{-1} \mathbf{G}\right)^{-1} \mathbf{G}^t \mathbf{V}_{\mathrm{y}}^{-1}\, \mathbf{y} \quad \text{and} \quad \mathbf{V}_{\hat{\mathbf{p}}} = \left(\mathbf{G}^t \mathbf{V}_{\mathrm{y}}^{-1} \mathbf{G}\right)^{-1} . \tag{4}$$

G is the design matrix, **y** the measured data vector, and $\mathbf{V}_{\mathrm{y}}$ the covariance matrix of **y**. Then the estimate $\hat{\mathbf{y}}$ is obtained as

$$\hat{\mathbf{y}} = \mathbf{G}\,\hat{\mathbf{p}} ,$$

while its covariance matrix $\mathbf{V}_{\hat{\mathbf{y}}}$ is calculated from the law of error propagation as

$$\mathbf{V}_{\hat{\mathbf{y}}} = \mathbf{G}\,\mathbf{V}_{\hat{\mathbf{p}}}\mathbf{G}^t .$$

LSM Solution

PPP is modeled, with single parameter *p* representing the average of two data, as

$$\mathbf{y} = \mathbf{G}\,\mathbf{p} + \boldsymbol{\varepsilon} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \cdot p + \boldsymbol{\varepsilon} \quad . \tag{5}$$

Measured data **y** and $\mathbf{V}_{\mathrm{y}}$ are given as

$$\mathbf{y} = \begin{pmatrix} 1.5 \\ 1.0 \end{pmatrix} \quad \text{and} \quad \mathbf{V}_{\mathrm{y}} = \begin{pmatrix} 1.5^2(0.1^2 + 0.2^2) & 1.5 \cdot 0.2 \times 1.0 \cdot 0.2 \\ 1.5 \cdot 0.2 \times 1.0 \cdot 0.2 & 1.0^2(0.1^2 + 0.2^2) \end{pmatrix} = \begin{pmatrix} 0.1125 & 0.06 \\ 0.06 & 0.05 \end{pmatrix} .$$

Then the parameter *p* is estimated from Eq. (4) as $\hat{p} = 0.882 \pm 0.218$, which is outside the range of raw data of 1.5 and 1.0. This is the PPP solution.

[**] The LSM means the generalized LSM in this paper. The generalized LSM, which is called as the weighted LSM of usual, takes into account the data covariance while an ordinary LSM does not.

GMAJ Solution

The method of GMAJ is based on an assumption that the absolute uncertainties are computed in terms of fractional uncertainties from experiments and 'true' value.[1,9] Instead of $\mathbf{V}_y$, the LSM deals with $\mathbf{V}_y^*$ such that

$$\mathbf{V}_y^* = \begin{pmatrix} y_0^2(0.1^2+0.2^2) & y_0\cdot 0.2\times y_0\cdot 0.2 \\ y_0\cdot 0.2\times y_0\cdot 0.2 & y_0^2(0.1^2+0.2^2) \end{pmatrix} = y_0^2 \begin{pmatrix} 0.05 & 0.04 \\ 0.04 & 0.05 \end{pmatrix},$$

where y_0 is the true (unknown) value. Only one iteration is needed with any initial guess on y_0 because it is canceled in the evaluation of $\hat{p}$ using Eq. (4). The GMAJ solution is $\hat{p} = 1.250 \pm 0.265$.

Even though the GMAJ solution does not differ by too much from the rigorous Bayesian solution of 1.21 ± 0.30, it is argued that the method yields a most probable value instead of a mean value.[6]

Proposed Method

Let the Box-Cox solution mean the LSM solution with Box-Cox transformation hereafter. The model is same to Eq. (5), but the data that LSM deals with are different. With the optimum value $\lambda = 0$, data $\mathbf{w}$ and $\mathbf{V}_w$ are computed as

$$\mathbf{w} = \begin{pmatrix} \ln y_1 \\ \ln y_2 \end{pmatrix} = \begin{pmatrix} 0.405 \\ 0.0 \end{pmatrix} \text{ and } \mathbf{V}_w = \begin{pmatrix} 1/y_1 & 0 \\ 0 & 1/y_2 \end{pmatrix} \mathbf{V}_y \begin{pmatrix} 1/y_1 & 0 \\ 0 & 1/y_2 \end{pmatrix} = \begin{pmatrix} 0.05 & 0.04 \\ 0.04 & 0.05 \end{pmatrix}.$$

Eq. (4), *i.e.* the LSM, yields the model parameter $\hat{p} = 0.203 \pm 0.212$ so that

$$\hat{\mathbf{w}} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \cdot 0.203, \text{ then inverse-transformed } \hat{\mathbf{y}} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \cdot 1.225 \ .$$

This $\hat{y} = 1.225 \pm 0.260$ (let's use this notation to avoid a confusion with $\hat{p}$ computed with $\mathbf{w}$; $\hat{y} = \hat{y}_1 = \hat{y}_2$) looks reasonable and is same to the solution that Smith gave[6] as Method 2. Note that $\lambda = 0$ implies a logarithmic transformation. Normalization is regarded as the very origin of PPP in most relevant studies, thus taking a logarithm that eliminates the non-normality due to the quotient seems to be reasonable and promising.

Table 1 shows $\ln L(\lambda)$ and $\hat{y}$ varying with λ. Note that $\lambda = 1$, which implies no transformation, results in the smallest uncertainty of $\hat{y}$.

Table 2 presents solutions from various LSMs with the same data but different uncertainties. It is noticed that the estimate from GMAJ does not change at all regardless of the magnitude of uncertainties. The estimate from the present procedure with $\lambda = 0$ is insensitive to the magnitude of uncertainties as is shown in the table (See one different estimate only for the case with 20% systematic and 1% statistical uncertainty), but the estimate with large absolute value of λ is very sensitive (not shown here). It might be understood such that the magnitude of λ controls the degree of impact of inconsistency and correlation between data on the estimate.

Table 1. Log-Likelihood Function and Box-Cox Solution to Peelle's Problem Varying with λ

λ	$\ln L(\lambda)$	$\hat{y}$
-1.0	1.62	1.700 ± 0.421
-0.5	2.16	1.475 ± 0.327
-0.1	2.75	1.273 ± 0.271
0.0	**2.79**	**1.225 ± 0.260**
0.1	2.75	1.178 ± 0.250
0.5	2.16	1.107 ± 0.225
0.8	1.78	0.928 ± 0.219
1.0	1.62	**0.882 ± 0.218**
1.2	1.52	0.847 ± 0.221
1.5	1.44	0.776 ± 0.229

Table 2. Various LSM Solutions to Peelle's Problem with Different Data Uncertainties

Uncertainty (%)		Usual LSM	Chiba & Smith[1] (GMAJ)	Present Procedure*
Systematic	Statistical			
20	20	1.071 ± 0.278	1.250 ± 0.306	1.225 ± 0.300
20**	**10****	**0.882 ± 0.218**	**1.250 ± 0.265**	**1.225 ± 0.260**
10	10	1.071 ± 0.139	1.250 ± 0.153	1.225 ± 0.150
10	20	1.132 ± 0.202	1.250 ± 0.217	1.225 ± 0.212
10	5	0.882 ± 0.109	1.250 ± 0.133	1.225 ± 0.130
2	1	0.882 ± 0.022	1.250 ± 0.027	1.225 ± 0.026
20	1	0.036 ± 0.042	1.250 ± 0.250	1.221 ± 0.244

* Optimum λ for Box-Cox transformation is zero for all cases.
** Uncertainties in the original Peelle's problem

3.2. Evaluation of ^{6}Li(n,t) Cross Sections

The cross sections of ^{6}Li(n,t) reaction were evaluated using GMA, GMAJ, and GMA-like LSM (*i.e.* a generalized LSM) with Box-Cox transformation. Five experimental data sets were utilized: Lamaze et al. 1978, Fort and Marquette 1972, Fort 1970, Poenitz and Meadows 1972, and Friesenhahn et al. 1974. Cross sections in data sets distributed to the CRP participants are those already adjusted to total 51 energy grids from 2.5 keV to 800 keV for GMA. Each set of Lamaze and of Friesenhahn includes data over the whole energy range, but these two sets are discrepant from each other. The Friesenhahn set seems to cause PPP in this evaluation. Meanwhile, note that comparisons[7,12,13] of the LSM with the Bayesian method codes with and without physics model have been conducted. Such inter-comparisons are beyond the scope of this article, however, it is pointed out here that preliminary analysis using RAC, a R-matrix code, seems to reveal PPP, too. For the same reaction, the results from GLUCS, a non-model Bayesian code, are essentially same to those from GMA.

Table 3 and **Figure 1** compare results from three approaches, which are conceptually different from each other but utilize same tool in curve fitting itself. While the GMA solution runs below almost all experimental data points, the solution from present procedure (say, Box-Cox solution) passes through data points. The optimum λ for the transformation is determined as –0.07. Throughout the entire energy region, the Box-Cox cross sections are consistently higher than GMA cross sections by 10~15 % and than GMAJ's by 0.5~1.5%. GMAJ solution is not well distinguished from the Box-Cox solution in the Figure. The percent uncertainties in Box-Cox cross sections are consistently smaller than those from GMA by 2~6% and are comparable with those from GMAJ. However, absolute uncertainties of Box-Cox solution are larger than GMA's.

Table 4 shows covariances and correlations between the cross section, as an example, at 0.2 MeV and cross sections at any other energy grids. No significant difference in 'correlations' is found between three solutions except that Box-Cox correlations are slightly larger than those from GMA. Meanwhile, the Box-Cox 'covariances' are much larger than GMA's very consistently, by ~13 % at almost every energy point. The same trend, with magnitudes of 12~15% difference, is found from other rows of covariance matrices. Thus the univariate variance from the present procedure is larger than that from GMA by 13%. The univariate variance, as a kind of single measure of magnitude of uncertainties, is sum of all elements of covariance matrix divided by the number of elements.

The χ^2 value per degree of freedom increases from 9.7 in GMA to 11.2 in Box-Cox solution with optimum λ and to 11.0 with $\lambda = 0$, as was expected at the beginning. It is reminded, however, that the χ^2 is less meaningful when the governing probability distribution deviates from the normal distribution.

Intuitively one may adopt zero for λ to take a logarithm. It is equivalent to linearizing a quantity in a form of quotient or multiplication of two or more sub-quantities. Cross section from ratio measurement is an example of such quantity. However, in this test evaluation on ^{6}Li(n,t) reaction, the Box-Cox procedure with $\lambda = 0$ results in cross sections smaller than those with optimum $\lambda = -0.07$ by 1% consistently throughout the entire energy region. Very likely, a theoretician may prefer zero to other values near zero. Nevertheless, the 1% difference in the sample evaluation is not negligible, so it is recommended to search an optimum value that might be near zero but not zero. Two-digit precision might be enough for most applications including ^{6}Li(n,t) evaluation.

Figure 2 shows one of sensitivity calculation results. Only two data sets, Lamaze and Friesenhahn, are utilized for the evaluation. The original systematic uncertainties are 1.6% and 2.7% for Lamaze cross sections and Friesenhahn's, respectively. Evaluated cross sections from GMA and Box-Cox procedure with these two sets are not much different from those in Figure 1. Now let a test problem assume 10% systematic uncertainties to each data set. As shown by a dotted line in lower part of the figure, GMA resulted in meaningless cross sections. However, the present procedure, with the optimum $\lambda = -0.002$, produced reasonable estimates again. Indeed, it is not distinguished from the Box-Cox solution with the original uncertainty data (optimum $\lambda = -0.04$); the differences in two sets of evaluated cross sections are less than 0.3%. In short, with a λ near zero, the proposed procedure is insensitive to given data uncertainties.

Table 3. Evaluated ^{6}Li(n,t) Cross Sections

E_n (MeV)	GMA		GMAJ		Present Procedure	
	CS (b)	Unc. (%)	CS (b)	Unc. (%)	CS (b)	Unc. (%)
2.50E-03	2.568	3.4	2.835	3.4	2.873	3.1
3.50E-03	2.139	3.2	2.364	3.2	2.395	3.0
4.50E-03	1.855	3.0	2.072	3.1	2.092	2.8
5.50E-03	1.739	2.6	1.938	2.5	1.956	2.4
6.50E-03	1.577	2.5	1.770	2.6	1.783	2.3
7.50E-03	1.469	2.5	1.659	2.5	1.669	2.3
8.50E-03	1.414	2.2	1.584	2.2	1.597	2.1
9.50E-03	1.288	1.8	1.445	1.8	1.456	1.6
1.50E-02	1.045	1.7	1.172	1.7	1.181	1.6
2.00E-02	0.955	1.8	1.068	1.8	1.076	1.7
2.40E-02	0.866	1.9	0.963	1.9	0.971	1.8
3.00E-02	0.766	1.8	0.865	1.8	0.870	1.6
4.50E-02	0.670	1.8	0.751	1.7	0.755	1.7
5.50E-02	0.630	1.8	0.705	1.7	0.709	1.7
6.50E-02	0.604	1.9	0.672	1.8	0.677	1.7
7.50E-02	0.579	1.9	0.643	1.8	0.648	1.8
8.50E-02	0.608	1.4	0.674	1.3	0.679	1.3
9.50E-02	0.599	1.8	0.662	1.6	0.667	1.6
1.00E-01	0.597	1.6	0.664	1.5	0.669	1.5
1.20E-01	0.640	1.4	0.710	1.3	0.715	1.3
1.50E-01	0.795	1.4	0.881	1.3	0.887	1.3
1.70E-01	1.005	1.6	1.118	1.5	1.126	1.5
1.80E-01	1.209	1.6	1.342	1.5	1.352	1.5
1.90E-01	1.449	1.5	1.610	1.4	1.621	1.4
2.00E-01	1.727	1.6	1.920	1.4	1.932	1.4
2.10E-01	2.060	1.4	2.287	1.3	2.301	1.3
2.20E-01	2.490	1.4	2.765	1.3	2.781	1.3
2.30E-01	2.804	1.5	3.106	1.4	3.127	1.4
2.40E-01	2.942	1.8	3.254	1.6	3.271	1.7
2.45E-01	2.895	1.6	3.200	1.5	3.225	1.5
2.50E-01	2.859	1.6	3.171	1.4	3.194	1.5
2.60E-01	2.557	1.5	2.835	1.4	2.850	1.4
2.70E-01	2.313	1.7	2.605	1.4	2.619	1.5
2.80E-01	1.908	1.6	2.191	1.3	2.192	1.5
3.00E-01	1.379	1.6	1.568	1.3	1.571	1.4
3.25E-01	0.992	1.8	1.126	1.5	1.130	1.7
3.50E-01	0.760	1.8	0.853	1.6	0.858	1.7
3.75E-01	0.626	1.8	0.701	1.5	0.705	1.6
4.00E-01	0.546	2.0	0.611	1.7	0.614	1.8
4.25E-01	0.481	3.0	0.553	2.3	0.556	2.7
4.50E-01	0.387	4.8	0.432	4.6	0.434	4.4
4.75E-01	0.387	2.7	0.428	2.5	0.432	2.5
5.00E-01	0.358	3.0	0.402	2.7	0.405	2.8
5.20E-01	0.342	3.0	0.381	2.7	0.385	2.8
5.40E-01	0.323	3.3	0.354	3.0	0.356	3.0
5.70E-01	0.315	2.9	0.351	2.5	0.354	2.6
6.00E-01	0.293	2.4	0.325	2.1	0.327	2.2
6.50E-01	0.272	2.5	0.305	2.2	0.307	2.3
7.00E-01	0.256	2.4	0.284	2.2	0.286	2.2
7.50E-01	0.238	2.4	0.265	2.1	0.267	2.2
8.00E-01	0.224	2.4	0.250	2.2	0.251	2.2

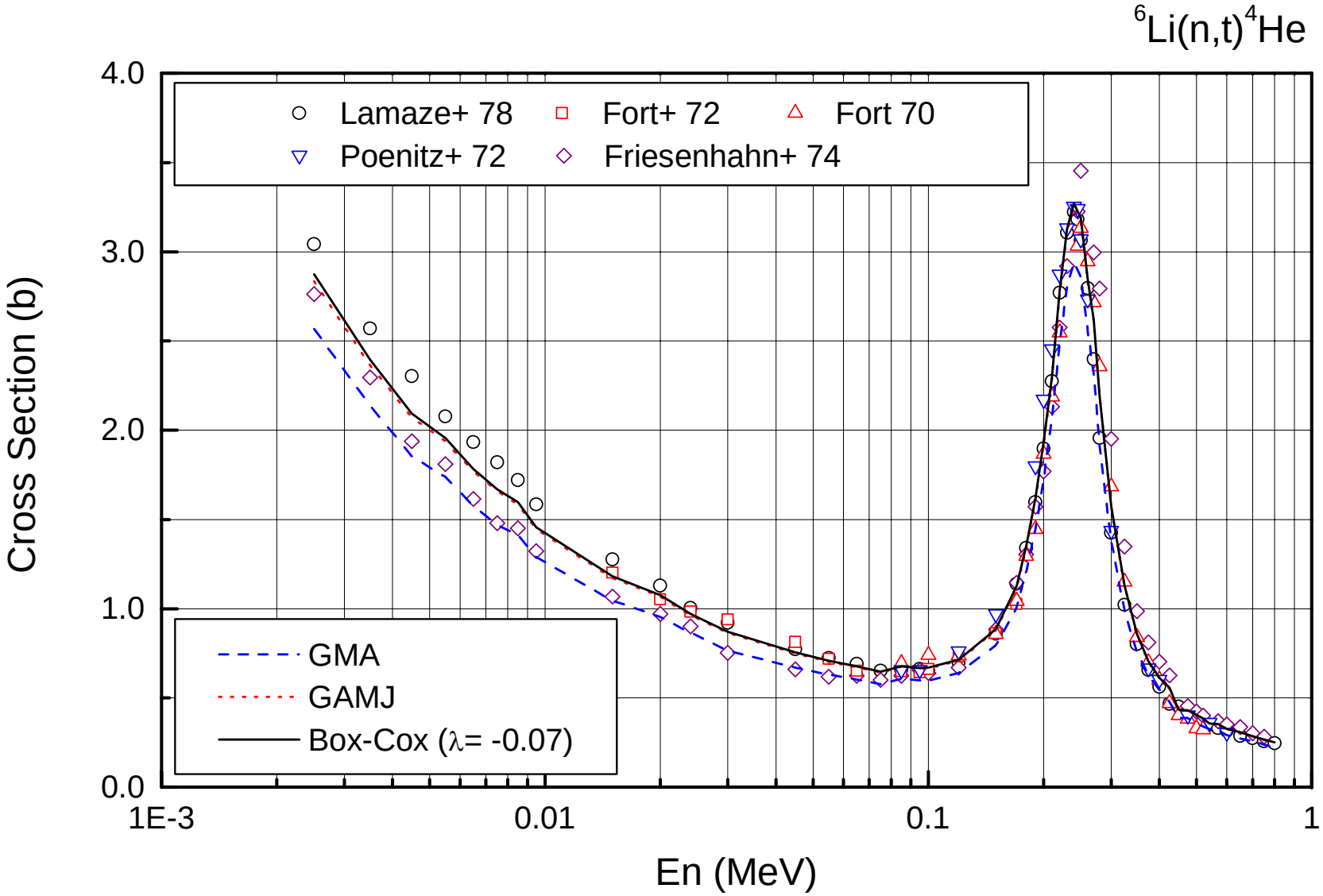

Figure 1. Evaluated ^{6}Li(n,t) Cross Sections

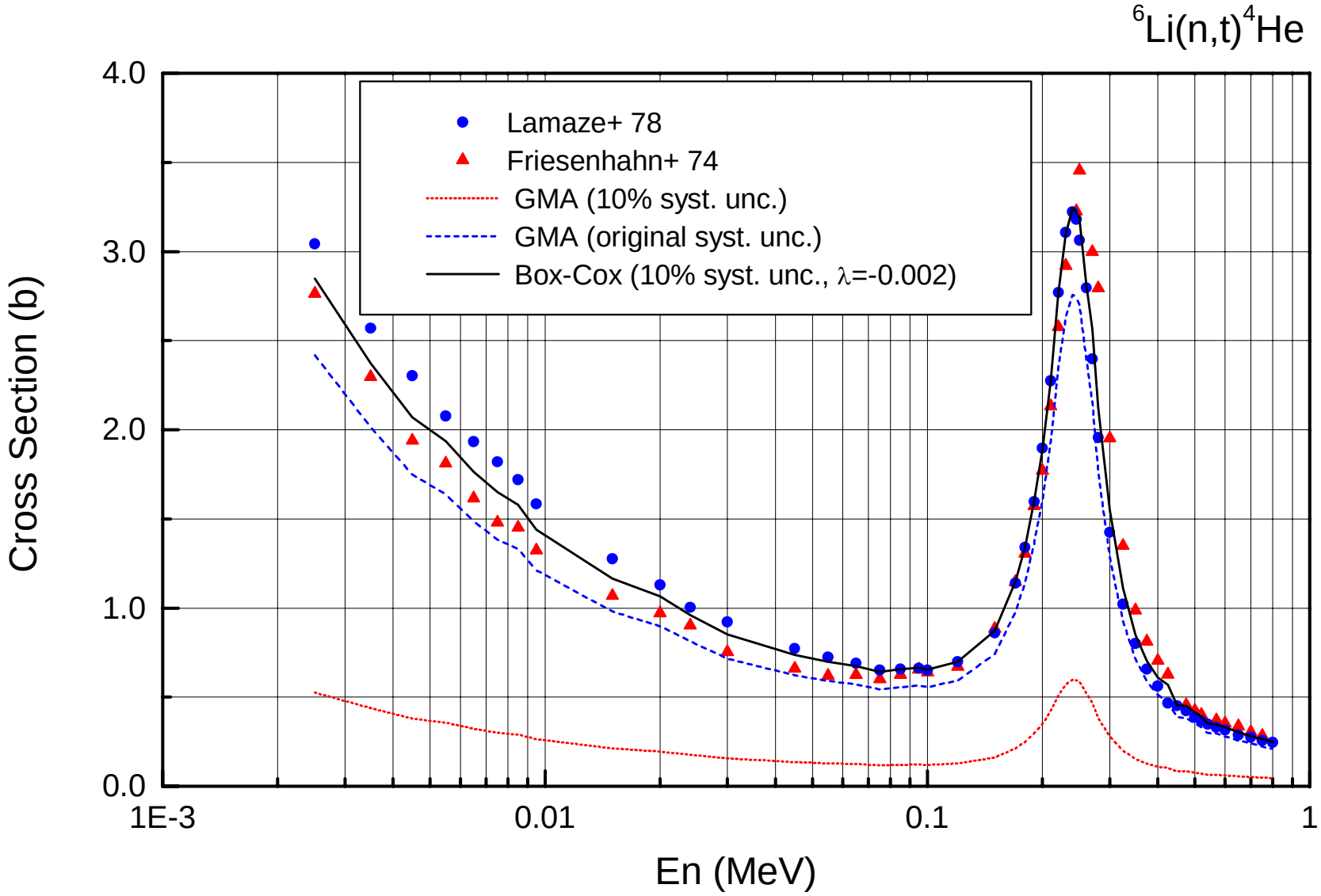

Figure 2. Results of Test Evaluation of ^{6}Li(n,t) Cross Sections using Two Data Sets

Table 4. Evaluated Covariances and Correlations between ^{6}Li(n,t) Cross Sections at 0.2 MeV and other Energy Grids

E_n (MeV)	GMA		GMAJ		Present Procedure	
	Covar. (b^2)	Correl. (%)	Covar. (b^2)	Correl. (%)	Covar. (b^2)	Correl. (%)
2.50E-03	4.68E-04	20	5.48E-04	21	5.27E-04	21
3.50E-03	3.89E-04	21	4.61E-04	22	4.39E-04	22
4.50E-03	3.38E-04	23	4.15E-04	24	3.84E-04	24
5.50E-03	3.17E-04	26	3.74E-04	28	3.59E-04	28
6.50E-03	2.87E-04	27	3.48E-04	28	3.27E-04	28
7.50E-03	2.68E-04	28	3.28E-04	29	3.06E-04	29
8.50E-03	2.58E-04	30	3.10E-04	32	2.93E-04	32
9.50E-03	2.35E-04	38	2.85E-04	40	2.67E-04	40
1.50E-02	1.90E-04	39	2.29E-04	41	2.16E-04	41
2.00E-02	1.73E-04	37	2.03E-04	39	1.97E-04	39
2.40E-02	1.57E-04	35	1.80E-04	37	1.77E-04	37
3.00E-02	1.39E-04	38	1.65E-04	40	1.59E-04	40
4.50E-02	1.21E-04	37	1.38E-04	39	1.38E-04	39
5.50E-02	1.14E-04	37	1.29E-04	39	1.29E-04	39
6.50E-02	1.09E-04	36	1.23E-04	38	1.23E-04	38
7.50E-02	1.06E-04	35	1.18E-04	37	1.19E-04	37
8.50E-02	1.09E-04	47	1.17E-04	49	1.24E-04	49
9.50E-02	1.05E-04	37	1.16E-04	39	1.19E-04	39
1.00E-01	1.08E-04	42	1.17E-04	44	1.22E-04	44
1.20E-01	1.15E-04	46	1.24E-04	48	1.29E-04	48
1.50E-01	1.42E-04	46	1.52E-04	49	1.60E-04	48
1.70E-01	1.83E-04	43	2.06E-04	45	2.07E-04	45
1.80E-01	2.21E-04	41	2.43E-04	43	2.49E-04	43
1.90E-01	2.59E-04	43	2.82E-04	45	2.92E-04	45
2.00E-01	**7.26E-04**	**100**	**7.52E-04**	**100**	**7.82E-04**	**100**
2.10E-01	3.71E-04	48	4.06E-04	50	4.18E-04	50
2.20E-01	4.48E-04	48	4.93E-04	50	5.05E-04	50
2.30E-01	5.00E-04	44	5.50E-04	46	5.63E-04	46
2.40E-01	5.16E-04	36	5.62E-04	38	5.82E-04	38
2.45E-01	5.15E-04	42	5.62E-04	44	5.80E-04	44
2.50E-01	5.09E-04	42	5.40E-04	44	5.75E-04	44
2.60E-01	4.57E-04	43	4.96E-04	45	5.15E-04	45
2.70E-01	4.23E-04	41	4.34E-04	43	4.83E-04	43
2.80E-01	3.49E-04	42	3.54E-04	44	4.04E-04	44
3.00E-01	2.46E-04	42	2.53E-04	45	2.84E-04	45
3.25E-01	1.81E-04	37	1.85E-04	39	2.08E-04	39
3.50E-01	1.39E-04	37	1.45E-04	39	1.58E-04	39
3.75E-01	1.11E-04	37	1.16E-04	39	1.26E-04	39
4.00E-01	9.57E-05	32	9.80E-05	34	1.09E-04	34
4.25E-01	8.80E-05	23	8.42E-05	24	1.02E-04	24
4.50E-01	7.12E-05	14	8.21E-05	15	8.05E-05	15
4.75E-01	6.65E-05	23	7.29E-05	25	7.56E-05	25
5.00E-01	6.54E-05	22	7.01E-05	24	7.46E-05	24
5.20E-01	6.24E-05	22	6.67E-05	24	7.08E-05	24
5.40E-01	5.28E-05	18	5.71E-05	20	5.95E-05	20
5.70E-01	5.75E-05	24	5.97E-05	25	6.50E-05	25
6.00E-01	5.09E-05	27	5.47E-05	29	5.78E-05	29
6.50E-01	4.97E-05	27	5.17E-05	28	5.64E-05	28
7.00E-01	4.67E-05	28	4.95E-05	29	5.27E-05	29
7.50E-01	4.35E-05	28	4.64E-05	30	4.91E-05	30
8.00E-01	4.10E-05	28	4.46E-05	30	4.62E-05	29
Average	2.20E-04		2.43E-04		2.47E-04	

4. Conclusion and Remarks

The CRP encountered Peelle's Pertinent Puzzle during the evaluation of ^{6}Li(n,t) cross section as one of standard cross sections of light elements. For resolving the Puzzle, proposed is a method that adopts Box-Cox transformation in combining with a usual curve fitting method. The method incorporated into a generalized least-squares code GMA shows good performance in a test, but realistic evaluation of the ^{6}Li(n,t) reaction cross section as well as in the Peelle's problem.

In addition to the principal conclusion above, several findings, along with future works, are summarized as follows.

(1) The degree of impact of inconsistency and correlation between raw data on the resulting estimate is controlled by the magnitude of λ in the Box-Cox transformation. For instance, a logarithmic transform makes the estimate be insensitive to the magnitude of uncertainties in the Peelle's problem.

(2) The optimum λ is rather small, but not zero, in ^{6}Li(n,t) cross section evaluation. Taking zero for λ may look reasonable and even physical for, for instance, normalized cross sections. However, blind taking zero is not recommended. On the other hand, further study is planned for dealing with data types other than the type of absolute cross section, such as sum of several cross sections. Then, if the CRP agrees on the necessity for the proposed method instead of or parallel to Chiba's approach, the method will be implemented to GMA.

(3) The proposed method results in smaller fractional uncertainties (but larger absolute uncertainties) than those from GMA. Regarding the expansion of 'calculated' uncertainties as one of the CRP issues, the method seems not to provide any good justification. When an evaluator encounters strange estimates, he/she will review the raw data at hands as the first action. However, doing that is beyond the role of the method proposed here: the method deals with the data sets as they are given, neither adds something to raw data nor interprets given data subjectively. As Badikov has proposed,[14] a systematic search for unrecognized, thus excluded from the reported uncertainties might be one of resolutions for PPP[††] as well as for expanding uncertainties. That approach is the other version of the first option mentioned at Section 2.1 of this article.

References

1. S. Chiba and D. L. Smith, "A Suggested Procedure for Resolving an Anomaly in Least-Squares Data Analysis Known as Peelle's Pertinent Puzzle and the General Implications for Nuclear Data Evaluation," ANL/NDM-121, Argonne National Lab. (Sept. 1991)

2. Z. Zhao and F. G. Perey, "The Covariance Matrix of Derived Quantities and Their Combination," ORNL/TM-12106, Oak Ridge National Lab. (June 1992)

3. F. H. Froehner, "On Assignment of Uncertainties to Scientific Data," Extended version of a paper in *Proc. of Int'l Conf. on Reactor Physics and Reactor Computations*, p. 287, Tel Aviv, 23-26 Jan. 1994.

[††] It is not overlooked, however, that just scaling up or down all the uncertainties does not alter the LSM solution to Peelle's problem as shown in Table 2, Section 3.1.

4. S. Chiba and D. L. Smith, "Impacts of Data Transformations on Least-square Solutions and Their Significance in Data Analysis and Evaluation," *J. Nucl. Sci. Tech.* **31**, 770 (1994)

5. G. D'Agostini, "Probability and Measurement Uncertainty in Physics – a Bayesian Primer," DESY 95-242 (Dec. 1995)

6. D. L. Smith, Probability, Statistics, and Data Uncertainties in Nuclear Science and Technology, pp. 205-209, American Nuclear Society (1991)

7. V. G. Pronyaev, "Test and intercomparison of general least squares code GMA with Bayesian code GLUCS in fitting of ^{6}Li(n,α) reaction," Presented at the first RCM held in Vienna, Sept. 2002.

8. W. P. Poenitz and S. E. Aumeier, "The Simultaneous Evaluation of the Standards and Other Cross Sections of Importance for Technology," ANL/NDM-139, Argonne National Lab. (Sept. 1997); The code GMA is available as PSR-367 from the Radiation Safety Information Computational Center, Oak Ridge National Lab.

9. S. Chiba, Private communication on Program GMA (Rev. 2, Jan. 1990), Japan Nuclear Data Center, Japan Atomic Energy Research Institute.

10. G. E. P. Box and D. R. Cox, "An Analysis of Transformations," *J. Royal Statistical Soc*., Series B, **26**, 211 (1964); Concerning the formulation, see general materials on regression, for instance, *http://www.itl.nist.gov/div898/handbook/pmc/section5/pmc52.htm*

11. N. M. Larson, "Proof that Bayes and Least Squares Give Exactly Equivalent Results for Arbitrary Number of Data Sets," Private communication within the CRP (Dec. 2002)

12. V. G. Pronyaev, "Does model fit decrease the uncertainty of the data in comparison with a general non-model least-squares fit?" Presented at the first RCM held in Vienna, Sept. 2002.

13. Chen Zhenpeng, "Preliminary results of model least squares fit obtained with R matrix code RAC implementing full error propagation law," Private communication within the CRP (Aug. 2002)

14. S. A. Badikov and E. V. Gai, "Some Sources of the Underestimation of Evaluated Cross Section Uncertainties," Presented at the first RCM held in Vienna, Sept. 2002.

Test and Intercomparisons of Data Fitting with General Least Squares Code GMA versus Bayesian Code GLUCS

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Revised, 13 January 2003

Two approaches are mainly used for non-model nuclear cross section evaluation: Gauss-Markov-Aitken general least squares formalism[1] implemented in GMA code [2] and Bayes formalism [1,3] implemented in GLUCS code [4]. There are general statements that both should led to the same result if the influence of a prior to the posterior evaluation is infinitely small (a case of so-called uninformative prior) or if as a prior, the data set which contributes in evaluation was chosen. The analytical proof of equivalence of GMA and Bayes formalism is given in paper by N.M. Larson included in this Summary Report.

Bayes approach uses iteration type of solution for posterior evaluation. At each step with inclusion of new data set, the data adjustment vector δT is presented as:

$$\delta T = T' - T = MG^{+}(GMG^{+}+V)^{-1}(R-R_T), \quad (1)$$

where: T' is a vector of posterior evaluation,

T is a prior vector,

G is a matrix of sensitivity coefficients with the matrix element $g_{ij}=\partial R_i/\partial T_j$

M is covariance matrix of prior data,

V is covariance matrix of experimental data,

R is a vector of experimental cross section and

R_T is a vector of prior cross section wit values interpolated to the point where R is given and the upper scripts (+) and (*-1*) mean transpose and inverse operation respectively.

The adjustment matrix δM which brings to the covariance matrix of posterior evaluation M' is calculated as:

$$\delta M = M' - M = -MG^{+}(GMG^{+}+V)^{-1}GM \quad (2)$$

General least squares Gauss-Markov-Aitken (GMA) formalism gives in close variables definition (see [1], equations (33.15) and (33.30)):

$$\delta T = T' - T = (G^{+}WG)^{-1}G^{+}WR = (G^{+}V^{-1}G)^{-1}G^{+}V^{-1}(R-R_T) \quad (3)$$

and

$$\delta M = M' - M = (G^{+}WG)^{-1}G^{+}WV((G^{+}WG)^{-1}G^{+}W)^{+} = \sigma^2(G^{+}WG)^{-1} = (G^{+}V^{-1}G)^{-1}, \quad (4)$$

where: W is a matrix of relative weights with $W=\sigma^2 V^{-1}$

σ^2 is a scale factor, which is determined from the sum of squared residuals.

Comparing (1) with (3) and (2) with (4), we see that GMA equations do not require the knowledge of any prior cross section and its covariance matrix if, under T in (3) we understand any experimental data set belonging to the ensemble of data which are fitted. The

same is true for Bayes formalism if as initial prior in successive iteration procedure the experimental data set belonging to the ensemble of data to be fitted is selected.

To check the performance GMA and GLUCS codes and their consistency two tests were prepared. In the first test (TEST1), five non-correlated experimental data sets for ^{6}Li(n,α) reaction covering neutron energy from 2.5 to 800 keV were used. These pseudo-experimental cross sections, given in Appendix, were taken from GMA database [4]. Central values were taken as they are given in [4] and covariance matrix was prepared from two components: systematical (or long energy range correlative component (LERC)) and statistical (or short energy range correlative component (SERC)), because some model codes, which could also participate in the intercomparison, cannot treat medium energy range correlations. The data for TEST1 with first data set treated by GLUCS as a prior are shown in Annex 4 of this Summary Report. It was found that the version of the GMA code described in [4] and submitted to the IAEA at November 1999 contains some simple bug: the nullification of the vector BM, which used for calculation of the central value adjustment vector was misplaced inside the cycle on experimental data. As result only last experimental block for each data type treated by GMA is contributed in the adjustment vector with right account of statistical weight of this data block.

The results of comparison between GLUCS code and corrected GMA code are shown in Fig. 1 together with the experimental data and R-matrix model fit with RAC code [5]. The details of RAC fitting will be discussed in another paper. Figures 2 to 4 shows the difference presented as ratio of GMA to GLUCS result more clear. As we see it has probably some stochastic nature and caused presumably pure numerical inaccuracies in the different ways of calculations (see equations (1) and (3)). As we see also from Fig. 1 the data evaluated with GMA and GLUCS lay at few per cents below majority of experimental data and their R-matrix model fit. There are no visible discrepancies in the evaluated covariance matrices as it will be shown in another paper. Lets show that this behaviour of central values is a direct consequence of the Peelle's Pertinent Puzzle (PPP) [6] (for strongly variable data when some covariances have larger value than variances). It looks like the fit of resonance curve in space of R-matrix model parameters is practically free from PPP.

As we see from (3), the central values will be not changed if we multiply at the same factor the covariance matrices of all fitted data. This was checked also numerically for GMA. By this multiplication we may always reduce the chi-square to the value of order 1. This can be done also with data for TEST1 case. But this means, that if we have some abnormalities in central values after fitting, we can not remove them by simple multiplication of covariances of all data at the same factor as well as *good (less than 1.0) chi-square can not guarantee that PPP does not contribute in the bias of evaluated cross sections*.

To show which role plays PPP in TEST1 case, the fitting with different LERC relative contribution in the same total uncertainty was done. For this the TEST1 experimental covariance data for GMA were slightly modified providing the fitting with different long-range correlation coefficients but with the same diagonal components of covariance matrices. The results of calculation are shown in Fig. 5 for 0, 14, 24, 36, 50, 66, 84, and 99% LERC correlations. Chi-square of fitting was respectively 9.2, 9.0, 9.4, 10.5, 15.0, 17.8, 21.8 and 1134. It is clearly seen how with the increase of the LERC the central values of evaluated data are decreasing. As discussed in [6] this reduction happens if covariance matrix of fitted experimental data contains elements:

$$V_{ij} > V_{kk} \qquad \text{for any } i, j, k \text{ and } i \neq j. \tag{5}$$

This often happened when data have strong variation or have strong LERC or both. $^{6}Li(n,\alpha)$ reaction has one order of magnitude variation in the fitted energy region with rather large estimated cross-energy correlations in matrices experimental data. The covariance matrix will contain elements, which satisfy (5).

The iterative approach to exclude effect of PPP was proposed in [6]. It is based on minimization procedure of modified minimized functional containing not variances, but percentage errors which are free from "top-bottom" asymmetry in the error presentation.

Because LERC are determined by the experimental conditions we have no real justification to their decrease if constructed covariance matrix of uncertainty of experimental data is a positive definite matrix. But to free from PPP we probably can use also the other approach, - transformation of the data in the form where they are more smoothed, their least-squares fitting free from PPP and then backward transformation. R-matrix model fit presents possibly a particular example of this type of transformation, when the number of parameters is changed during transformation.

It was checked that order of the data input (what is equal to the order in which data are processed) does not influence at final GMA and GLUCS results.

The second test, TEST2, was used to check numerical convergence of the results of calculations with GLUCS and GMA in conditions when more and more data are included in the fitting. TEST2 was formulated in such a way, that the result of fitting when number of included data sets will be increased to the infinity is a priori known. For this one data set (Lamaze et al. data, see Appendix 1) was taken as a prior data for GLUCS or first data set for GMA and Fort&Marquette data set was repeatedly introduced 1, 2, 4, 20, 100 or 500 times. It is evident that evaluated data (central values) should asymptotically converge to the Fort&Marquette data in the points where these data are given. The results of intercomparison where also "old" GMA fitting is presented [7] are shown in Table 1 and Fig. 6. Here we refer at "old" GMA, as a version of the code, which was updated by S. Chiba in 1990 and since this time was frozen [8]. The comparison of the part of correlation matrix evaluated with GLUCS and GMA for 1+20 data sets is shown in Table 2. Differences marked by **bold** are insignificant. Good convergence of GMA fitting to the asymptotic value is demonstrated on Fig. 7. The difference from asymptotic value for 1+500 experimental data sets is less than 0.1%.

In conclusion we can summarize that:

1. Data fitting with GMA and GLUCS gives consistent results. Difference in the evaluated central values obtained with different formalisms can be related to the general accuracy with which fits could be done in different formalisms. It has stochastic nature and should be accounted in the final results of the data evaluation as small SERC uncertainty.

2. Some shift in central values of data evaluated with GLUCS and GMA relative the central values evaluated with R-matrix model code RAC is observed for case of fitting strongly varying data and is related to the PPP. The procedure of evaluation, free from PPP, should be elaborated.

References

1. S.L. Meyer, *"Data Analysis for Scientists and Engineers"*, John Wiley & Sons, NY (1975).

2. W.P. Poenitz, S.E. Aumeier, *"The Simultaneous Evaluation of the Standards and Other Cross Sections*", Report ANL/NDM-139 (1997).

3. D.L. Smith, "*Probability, Statistics and Data Uncertainties in Nuclear Science and Technology"*, publ. by American Nuclear Society, Inc., LaGrange Park, Illinois 60525, USA, 1991.

4. D.M. Hetrick and C.Y. Fu, *"CLUCS: A Generalized Least-Squares Program for Updating Cross Section Evaluations with Correlated Data Sets"*, Report ORNL/TM-7341 (1980).

5. Chen Zhenpeng, "Preliminary results of model least squares fit obtained with R-matrix code RAC implementing full error propagation law", Priv. communication, August 2002. See also report "Error Propagation in R-matrix Model Fitting" presented at the IAEA First Research Co-ordination Meeting on "Improvement of the Standard Cross Sections for Light Elements", IAEA Headquarters, Vienna, Austria, 23–27 September 2002.

6. S. Chiba and D.L. Smith, *"A Suggested Procedure for Resolving an Anomaly in Least-Squares Data Analysis Known as "Peelle's Pertinent Puzzle" and the General Implications for Nuclear Data Evaluation"*, Report ANL/NDM-121 (1991).

7. K. Shibata, "Results of TEST2 for "old" GMA", Priv. communication, (April 2002).

8. S. Chiba, *"GMA Documentation",* Priv. communication, (January 1990).

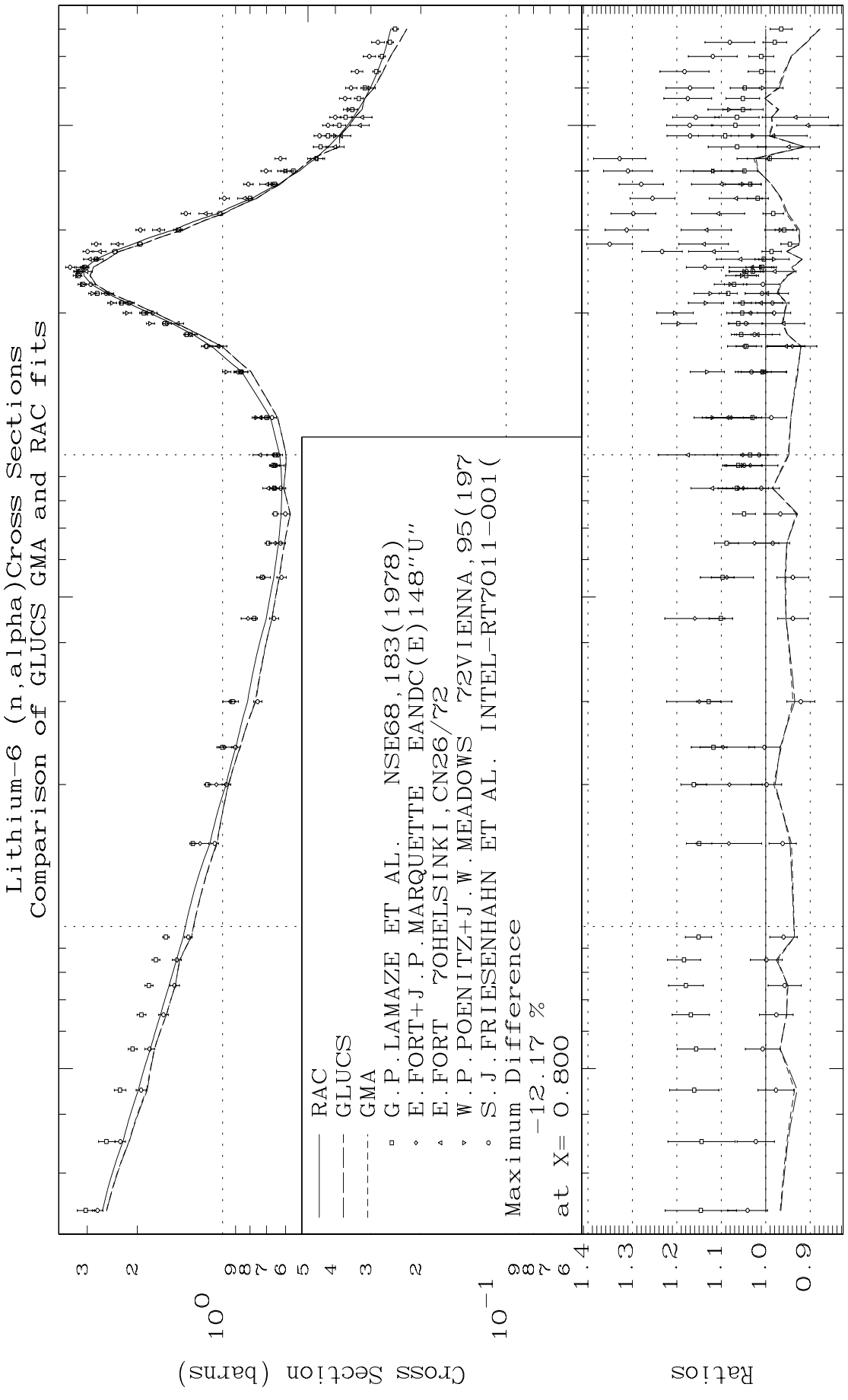

Fig.1. Intercomparison of GMA, GLUCS and RAC fitting of five data sets in TEST1 case. Ratio to the RAC result is shown in the lower part of the Figure.

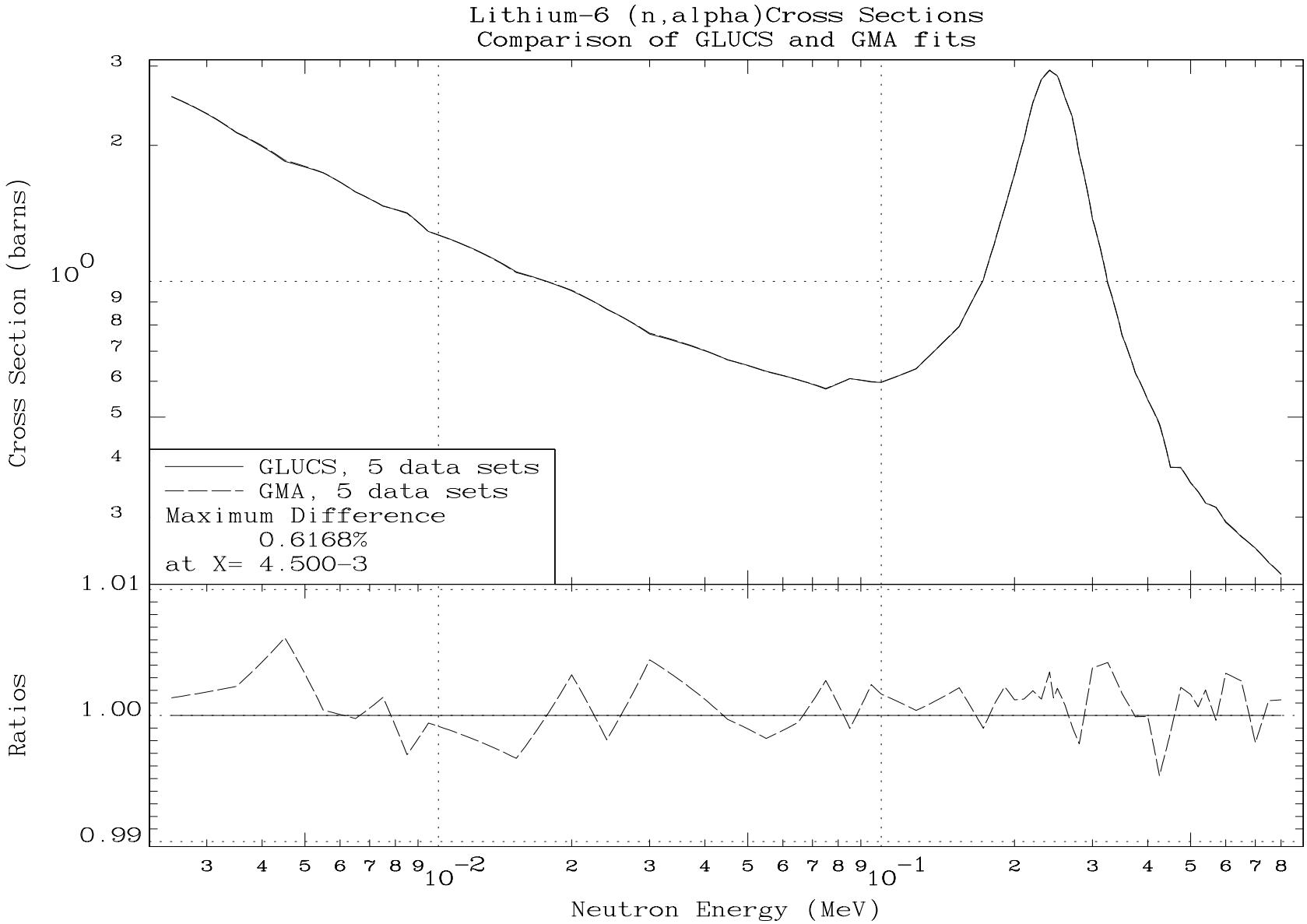

Fig.2. Intercomparison of GMA and GLUCS fitting for five data sets in TEST1 case. Ratio to the GLUCS result is shown in the lower part of the Figure.

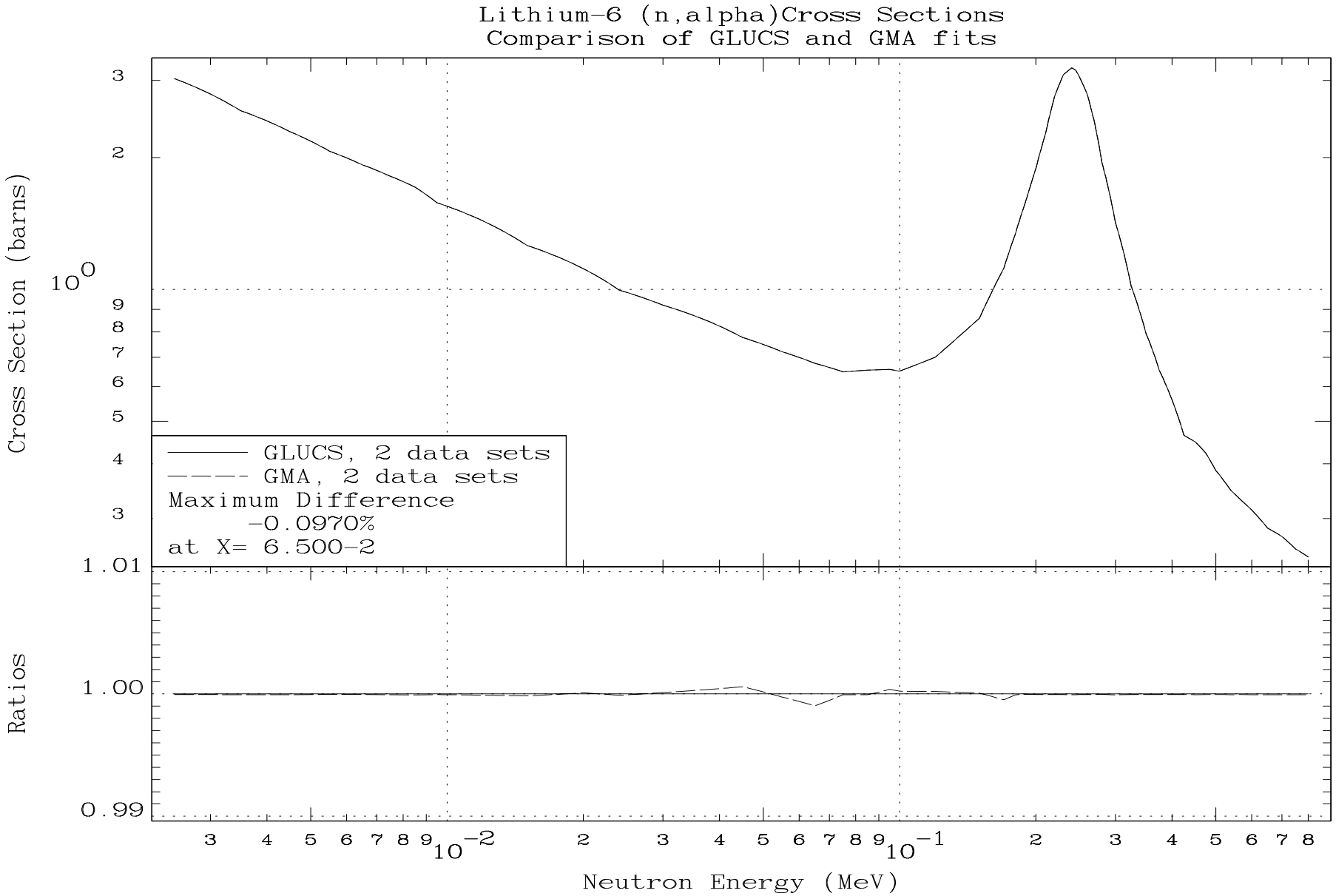

Fig.3. Intercomparison of GMA and GLUCS fitting for two data sets in TEST1 case. Ratio to the GLUCS result is shown in the lower part of the Figure.

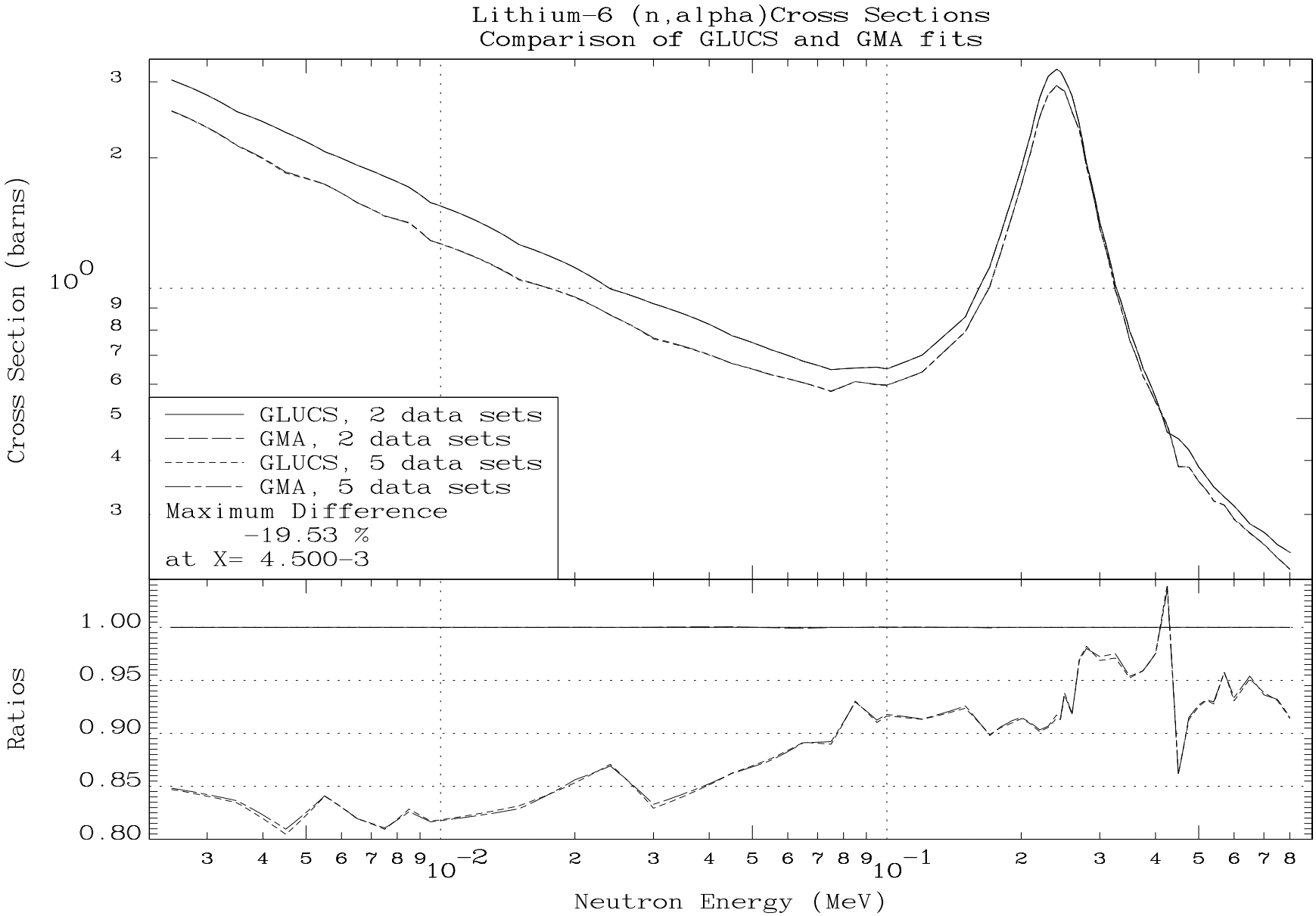

Fig. 4. Intercomparison of GMA and GLUCS fitting for two and five data sets in TEST1 case. Ratio to the GLUCS result (2 data sets) is shown in the lower part of the Figure.

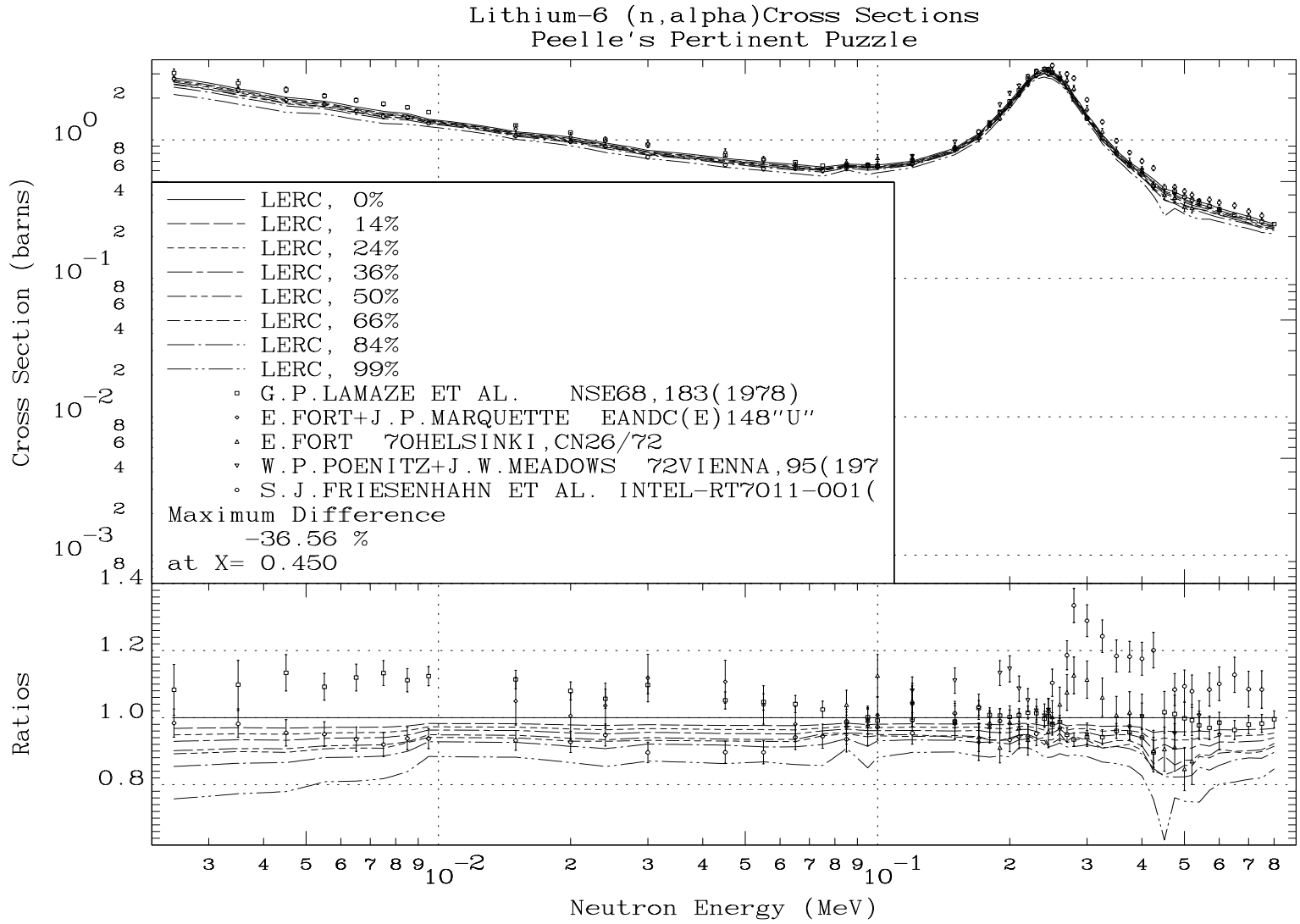

Fig. 5. GMA least-squares fit for five data sets in dependence from LERC component of the uncertainty. Ratio to the GLUCS (LERC=0%) result is shown in the lower part of the Figure.

Table 1. Results of TEST2 intercomparison of GLUCS, GMA and “old” GMA runs for fitting of 1+20 data sets.

Energy, MeV	Prior cross section, b	GLUCS cross section, b	GLUCS uncert., %	“old” GMA cross section, b	“old” GMA uncert., %	GMA cross section, b	GMA error, %	Asymptotic cross section
0.1500E-01	1.2750E+00	1.2130E+00	1.3	1.216	1.3	1.21287357	1.3	0.1201E+01
0.2000E-01	1.1300E+00	1.0651E+00	1.3	1.068	1.3	1.06535440	1.3	0.1052E+01
0.2400E-01	1.0030E+00	9.8248E-01	1.3	0.9835	1.3	0.98247242	1.3	0.9835E+00
0.3000E-01	9.2170E-01	9.2937E-01	1.2	0.9295	1.2	0.92967401	1.2	0.9390E+00
0.4500E-01	7.7240E-01	8.0081E-01	1.1	0.8000	1.1	0.80146843	1.1	0.8134E+00
0.5500E-01	7.2400E-01	7.1557E-01	1.1	0.7160	1.1	0.71542517	1.1	0.7176E+00
0.6500E-01	6.9080E-01	6.5287E-01	1.1	0.6544	1.1	0.65250817	1.1	0.6509E+00
0.8500E-01	6.5780E-01	6.4752E-01	1.1	0.6482	1.1	0.64753796	1.1	0.6490E+00
0.9500E-01	6.6190E-01	6.4476E-01	1.2	0.6460	1.2	0.64512242	1.2	0.6449E+00
0.1000E+00	6.5140E-01	6.5620E-01	1.0	0.6559	1.1	0.65644364	1.0	0.6617E+00
0.1200E+00	6.9840E-01	7.1957E-01	1.0	0.7170	1.0	0.71979811	1.0	0.7309E+00
0.1500E+00	8.6130E-01	8.5719E-01	1.0	0.8573	1.0	0.85736460	1.0	0.8620E+00
0.1700E+00	1.1400E+00	1.0465E+00	1.1	1.051	1.1	1.04592191	1.1	0.1027E+01

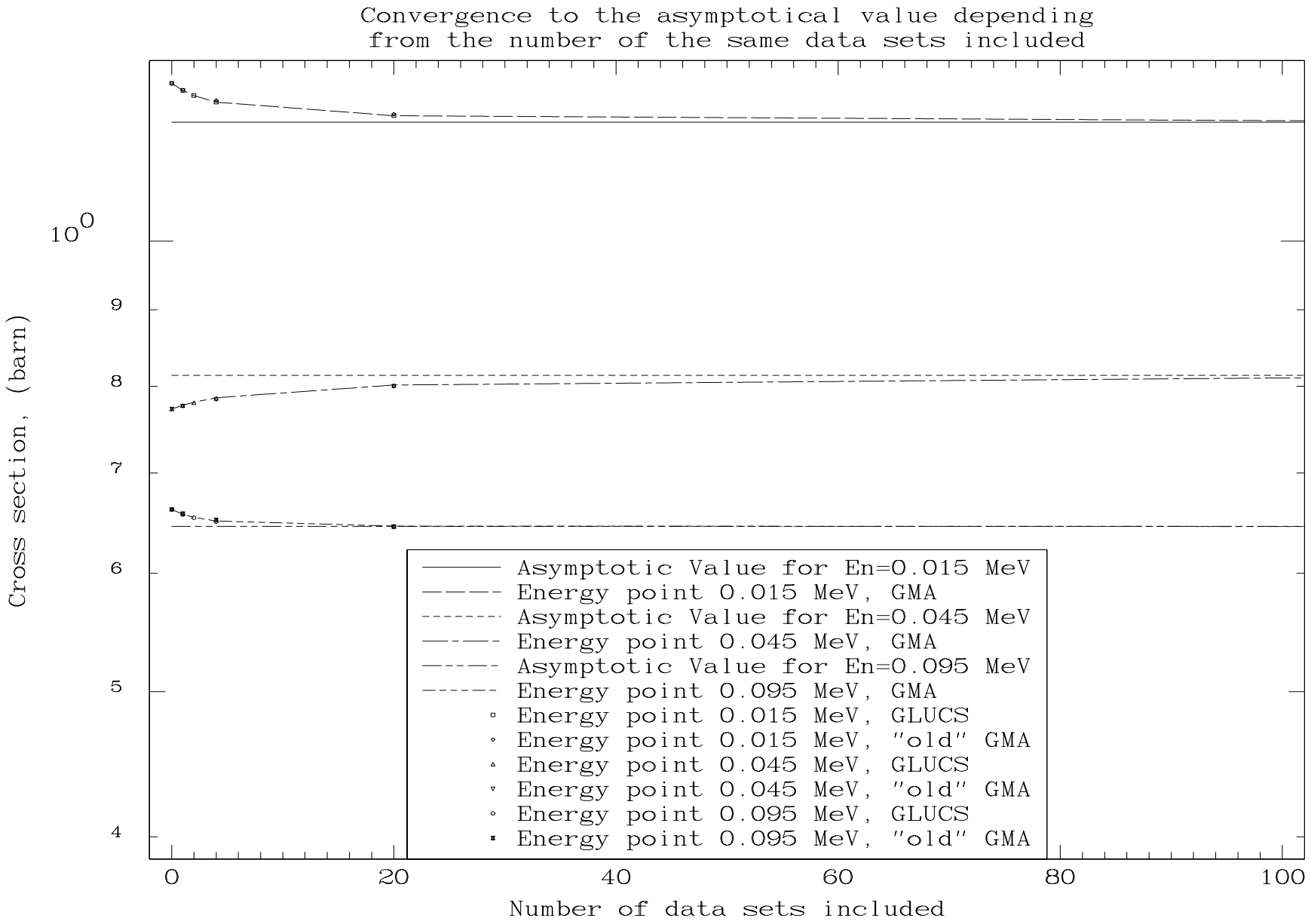

Fig.6. Convergence of GMA, “old” GMA and GLUCS evaluated cross sections to their asymptotical values for three energy points.

Table 2. Comparison of the correlation coefficients obtained with GMA and GLUCS in TEST2 for fitting of 1+20 data sets.

Code	Pt#	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
GMA	9	8	8	12	16	16	**18**	19	24	100											
GLUCS	9	8	8	12	16	16	**17**	19	24	100											
GMA	10	8	8	12	16	16	**18**	19	24	42	100										
GLUCS	10	8	8	12	16	16	**17**	19	24	42	100										
GMA	11	8	8	12	16	16	**18**	19	24	**42**	**42**	100									
GLUCS	11	8	8	12	16	16	**17**	19	24	**43**	**43**	100									
GMA	12	8	9	12	16	17	**19**	20	26	44	44	**45**	100								
GLUCS	12	8	9	12	16	17	**18**	20	26	44	44	**44**	100								
GMA	13	9	9	13	**17**	18	20	**21**	**27**	**47**	**47**	48	50	100							
GLUCS	13	9	9	13	**18**	18	20	**22**	**28**	**48**	**48**	48	50	100							
GMA	14	9	10	14	18	19	21	**22**	29	**50**	50	51	53	**57**	100						
GLUCS	14	9	10	14	18	19	21	**23**	29	**51**	50	51	53	**58**	100						
GMA	15	9	10	14	18	19	**21**	22	**29**	51	51	52	54	58	61	100					
GLUCS	15	9	10	14	18	19	**20**	22	**28**	51	51	52	54	58	61	100					
GMA	16	9	10	14	19	19	21	23	29	**51**	**51**	52	**55**	59	62	**63**	100				
GLUCS	16	9	10	14	19	19	21	23	29	**52**	**52**	52	**54**	59	62	**62**	100				
GMA	17	8	9	13	17	18	19	**20**	**27**	46	46	47	49	53	**56**	56	57	100			
GLUCS	17	8	9	13	17	18	19	**21**	**26**	46	46	47	49	53	**55**	56	57	100			
GMA	18	10	10	14	19	20	**22**	23	30	52	52	53	55	**59**	62	63	64	57	100		
GLUCS	18	10	10	14	19	20	**21**	23	30	52	52	53	55	**60**	62	63	64	57	100		
GMA	19	10	11	15	20	21	22	**24**	31	54	54	55	57	**61**	65	**66**	67	60	67	100	
GLUCS	19	10	11	15	20	21	22	**25**	31	54	54	55	57	**63**	65	**65**	67	60	67	100	
GMA	20	10	**10**	15	20	**20**	22	24	31	**53**	**53**	54	56	**60**	64	**65**	65	59	66	**68**	100
GLUCS	20	10	**11**	15	20	**21**	22	24	31	**54**	**54**	54	56	**61**	64	**64**	65	59	66	**69**	100
GMA	21	9	9	13	18	18	20	**21**	28	48	48	**49**	**51**	55	58	**59**	59	53	60	62	61
GLUCS	21	9	9	13	18	18	20	**22**	28	48	48	**48**	**50**	55	58	**58**	59	53	60	62	61

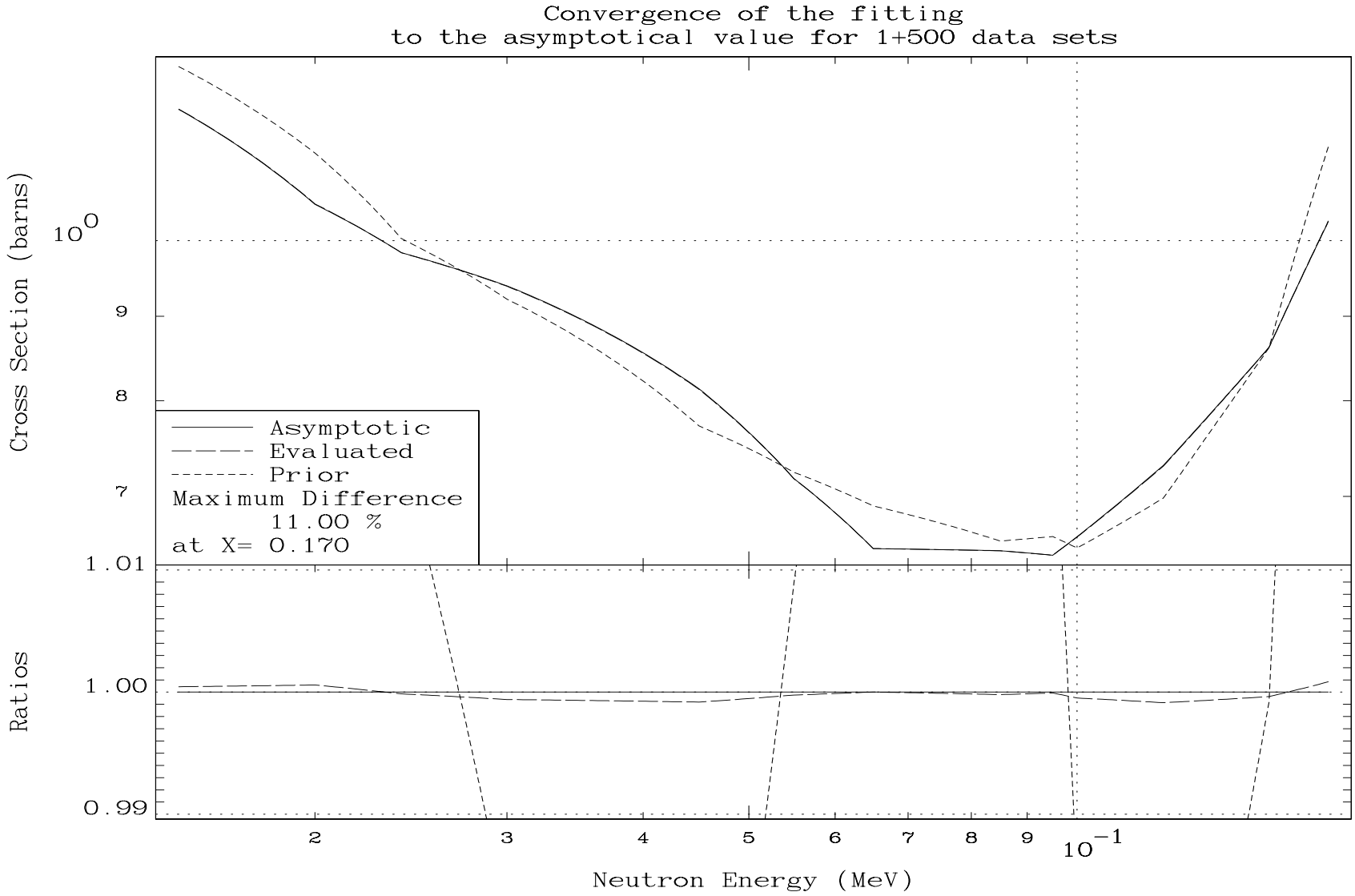

Fig.7. Convergence of GMA evaluated cross sections to their asymptotical values for fit of (1+500) experimental data sets. Ratio to the “asymptotic” (Fort&Marquette) data is shown in the lower part of the Figure.

Does model fit decrease the uncertainty of the data in comparison with a general non-model least squares fit?

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The quantitative answer at this question may depend from the *measure*, to be chosen by us for characterization of the uncertainty.

Information entropy as a measure of our knowledge about the object

It was shown by C.E. Shannon [1], that convenient generalized measure of our knowledge about the object can be an information entropy H, determined for any univariate probability distribution function as:

$$H = -\sum_i p_i \ln p_i \qquad (1)$$

if $p_1,\ldots,p_n$ is a discrete probability distribution function with $\sum_i p_i = 1$, and

$$H = -\int_{-\infty}^{+\infty} p(x) \ln p(x) dx \qquad (2)$$

if $p(x)$ is a continuum density distribution function with $\int_{-\infty}^{+\infty} p(x)dx = 1$.

Logarithmic base e is chosen here for convenience. We should remember also that the information entropy is not a directly observed (measurable) quantity. It is introduced as some *measure of knowledge* about the data characterized by particular probability distribution function. Value of information entropy H_0 is equal zero when the probability distribution function p_k=1 and p_i=0, $i \neq k$ for discrete and $H_0 \rightarrow -\infty$ for $p(x) \rightarrow \delta(x-x_k)$ where δ is a Fermi delta function for continuum probability distribution. For all other cases H is grater than H_0.

We will limit our consideration below by continuous normal (Gaussian) probability distribution function. This is because the statistical component of the uncertainty in the nuclear data measurements related with the number of counts by detector has this distribution. Many other components of the uncertainty may have different nature and characterized by non-normal probability distribution function. Because of large number of these components having different probability distributions and wide spread in the uncertainty, the total non-statistical component of the uncertainty according the central limit theorem will be well approximated by the normal distribution function.

One-dimensional (univariate) normal (Gaussian) probability distribution function has a form:

$$p(x) = \frac{e^{-\frac{(x-x^0)^2}{2\sigma^2}}}{\sqrt{2\pi}\sigma} \tag{3}$$

with normalization:

$$\int_{-\infty}^{+\infty} p(x)dx = 1\,. \tag{4}$$

Average (most probable) value x^0 is determined by the first momentum of the probability distribution function:

$$x^0 = \int_{-\infty}^{+\infty} p(x)(x - x^0)dx \tag{5}$$

and dispersion σ is determined as a square root from the second momentum of the probability distribution function:

$$\sigma^2 = \int_{-\infty}^{+\infty} p(x)(x - x^0)^2 dx \tag{6}$$

Information entropy H for univariate normal probability distribution function has the value:

$$H = \ln(\sqrt{2\pi}\sigma) \tag{7}$$

Comparing information entropy H for discrete (1) and continuum normal probability distribution function (7) we immediately see the difference. For discrete distribution, H gives the absolute measure the entropy with H=0 if p_i=1 for all $i \neq k$ and H>0 for all other cases. For continuum normal probability distribution function H gives [1] relative (the coordinate system) value with H=-∞ when $\sigma \to 0$, H=0 when σ=$1/\sqrt{2\pi}$ and H=+∞ when $\sigma \to +\infty$. This is because discrete p_i is dimensionless but continuum $p_i(x)$ is a density function, dimension of which depends from scale of the axis. Because here we will be interested only by changes in the relative values of information entropy this feature of continuum distribution is considered as unimportant.

These formulas can be generalized for case of multivariate probability distribution function [2,3]. Let consider N data values x_1, x_2, ..., x_N which can be correlated or not, but characterized by generalized N-dimension Gaussian (normal) probability distribution function:

$$p(x_1, x_2, ..., x_N) = \frac{e^{-\frac{\sum_{i,j=1}^{N} |\mathbf{C}_{ij}| (x_i - x_i^0)(x_j - x_j^0)}{2|\mathbf{C}|^{\frac{1}{2}}}}}{(2\pi)^{\frac{N}{2}} |\mathbf{C}|^{\frac{1}{2}}} \tag{8}$$

where

$\mathbf{C} = \begin{vmatrix} c_{11}\, c_{12} \ \ldots\ c_{1N} \\ c_{21}\, c_{22} \ \ldots\ c_{2N} \\ \cdot\ \ \cdot\ \ \ \cdot \\ \cdot\ \ \cdot\ \ \ \cdot \\ \cdot\ \ \cdot\ \ \ \cdot \\ c_{N1} c_{N2} \ldots c_{NN} \end{vmatrix}$ - is the covariance matrix with elements defined as:

$$C_{ij} = \int_{-\infty-\infty}^{+\infty+\infty} \ldots \int_{-\infty}^{+\infty} p(x_1, x_2, \ldots, x_N)(x_i - x_i^0)(x_j - x_j^0) dx_1 dx_2 \ldots dx_N, \quad C_{ii} = \sigma_i^2 \tag{9}$$

and $\left|\mathbf{C}_{ij}\right|$ in the nominator (8) is determinant of adjoint matrix obtained from covariance matrix **C** by deleting *i*-th row and *j*-th column and multiplying by $(-1)^{i+j}$. The multivariate probability distribution function is normalized at 1:

$$\int_{-\infty-\infty}^{+\infty+\infty} \ldots \int_{-\infty}^{+\infty} p(x_1, x_2, \ldots, x_N) dx_1 dx_2 \ldots dx_N = 1 \tag{10}$$

Lets evaluate *H* for multivariate case:

$$H = -\int_{-\infty-\infty}^{+\infty+\infty} \ldots \int_{-\infty}^{+\infty} p(x_1, x_2, \ldots, x_N) \ln p(x_1, x_2, \ldots, x_N) dx_1 dx_2 \ldots dx_N \tag{11}$$

Then

$$-\ln p(x_1, x_2, \ldots, x_N) = \ln((2\pi)^{\frac{1}{2}} \left|\mathbf{C}\right|^{\frac{1}{2}}) + \frac{\sum_{i,j=1}^{N} \left|\mathbf{C}_{ij}\right| (x_i - x_i^0)(x_j - x_j^0)}{2\left|\mathbf{C}\right|^{\frac{1}{2}}} \tag{12}$$

Substituting (12) in (11) and taking into account (9) and that $\sum_{i,j=1}^{N} \left|\mathbf{C}_{ij}\right| C_{ij} = N\left|\mathbf{C}\right|$, we will get after integration:

$$H = \ln((2\pi)^{\frac{N}{2}} \left|\mathbf{C}\right|^{\frac{1}{2}}) + \sum_{i,j=1}^{N} \frac{\left|\mathbf{C}_{ij}\right| C_{ii}}{2\left|\mathbf{C}\right|} = \ln((2\pi e)^{\frac{N}{2}} \left|\mathbf{C}\right|^{\frac{1}{2}}), \text{ or } H = \frac{N}{2}(1 + \ln(2\pi)) + \ln\left|\mathbf{C}\right|^{\frac{1}{2}} \tag{13}$$

Last presentation of *H* gives separation at pure "phase space" and "covariance" contributions. But "covariance" contribution is presented by the determinant of rank N is clearly depended from details (N, number of points) with which data are presented.

Let see the properties of *H*. If **C** is covariance matrix of data uncertainties it should be symmetric and positive definite matrix. The last requirement means that it can be transformed in diagonal form where all diagonal elements (eigenvalues) are positive. The determinant of this matrix, which should be equal to the determinant of the primary matrix (because the unitary transformation is used for reduction to the diagonal form) is just the product of all diagonal elements. Let show that the generalization of *H* to multivariate case (13) with possible interpretation it as a *measure of uncertainty* contradicts to our common sense in understanding of uncertainty.

Consider a simple two-point (bivariate) case with a central values equal to 10 at each point and covariance matrix with the values on major diagonal – variances (1, 1) and out of

diagonal – covariances (0.5, 0.5). Then the determinant will be equal to D_2=1*1-0.5*0.5=0.75 and *H*=2.694. The sign of the off-diagonal elements, which determines the existence of either correlations (+) or anti-correlations (-) between points, does not play any role for bivariate case. Lets keeping variances unchanged reduce correlations between two points to 0. Then D_2=1 and *H*=2.838. If we increase correlations to 1, we will have D_2=0 and $H=-\infty$. This means that the data with the same variances but with largest correlations between points will have the lowest information entropy. It does not contradict to our feelings, if we interpret *H* as *a measure of knowledge* about the object, which includes simultaneously the details with which we know the object and uncertainty in these details. Hundred per-cent correlation between points means that although there is an error at each point, there is no any uncertainty in the shape. Zero per-cent correlation between points means that in addition to the error at each point we have some freedom in the shape. Data in last case are clearly less informative then in previous one. But if we will interpret *H* as *a measure of uncertainty*, then increasing of covariances can be interpreted as increasing of uncertainties and should led to the increase of the information entropy, but we see just opposite behavior.

Reduced univariate variance as a common measure of uncertainty

Let introduce a *measure of uncertainty*, which does not depend from details with which data are presented. This could be so-called one-group uncertainty var*U* obtained through collapsing (reduction, averaging) multivariate distribution to the univariate one. According the error propagation law [4], if we have multivariate correlated data set $x_1, x_2, \ldots, x_N$ with covariance matrix $\mathrm{cov}(x_i,x_j)$ and would like to collapse it in one-group (univariate) value through simple arithmetic avarege $U=(x_1+x_2+\ldots+x_N)/N$, the variance of this one-group value will be:

$$\mathrm{var}U = \frac{1}{N}\sum_{i,j=1}^{N}\frac{\partial U}{\partial x_i}\frac{\partial U}{\partial x_j}\mathrm{cov}(x_i,x_j) \qquad (14)$$

In reality the equation for *U* can be more complex, accounting the widths of the energy bin or weight of each data point but for our demonstration purposes we use the simplest form for *U*. Because $\frac{\partial U}{\partial x_i}=1$ for any *i* we will get the simplest estimation:

$$\mathrm{var}U = \frac{1}{N}\sum_{i,j=1}^{N}\mathrm{cov}(x_i,x_j) \qquad (15)$$

The following one-group uncertainties can be obtained for two-point (bivariate) example given above. For hundred per-cent correlation case the collapsed one-group variance is var*U*=(1+1+1+1) /4=1 (no reduction of uncertainty). For zero per-cents correlation case the reduced one-group variance will be var*U*=(1+1+0+0)/4=0.5. For fifty per-cents correlation case the one-group uncertainty will be var*U*=(1+1+0.5+0.5)/4=0.75. If we have negative off-diagonal elements (-0.5, -0.5) (fifty per-cents anti-correlations between points), var*U*=(1+1-0.5-0.5)/4=0.25. For hundred per-cents anti-correlations between points, var*U*=0 with a full cancellation of uncertainties. This measure does not depend from the number of points, in which data are presented and can be considered as a generalized *measure of uncertainty* of the data obtained in different least squares fits.

Covariances in the model versus non-model least square fits

The comparison of the covariance matrices obtained in the model and non-model fits of the same experimental data is based on preliminary results obtained by Chen Zhenpeng [5] with

R-matrix code RAC and by V. Pronyaev [6] with the general least square code GMA and Bayesian code GLUCS. The same five sets of experimental data for ^{6}Li(n,α) reaction were used for tests and intercomparisons. All codes have shown their good performance and close results in evaluation of central values [6]. Here we discuss mainly some differences in covariance matrixes obtained in the model versus non-model least square fits having relation to the model influence. In all cases when additional (to five selected data sets) data were needed for unambiguous run of any code, they have been added mostly as an uninformative prior.

Let consider first the simple case of one experimental data set by G.P. Lamaze et al. [8], which is fitted by R-matrix model code RAC (see Table 1). The model fit smoothed the central values of the evaluated cross sections according to the shape predicted by the model. But what we also see is the substantial reduction of the errors, or more strictly speaking variances, in

Table 1. Comparison of experimental data with their model R-matrix fit.

Point #	Energy, MeV	Experimental cross section, b	Model eval. cross section, b	Experimental error, %	Model eval. error, %
1	0.2500E-02	3.0420E+00	0.30559E+01	6.9957E+00	2.2686
2	0.3500E-02	2.5700E+00	0.25828E+01	6.6189E+00	2.1389
3	0.4500E-02	2.3020E+00	0.22786E+01	4.7697E+00	2.0451
4	0.5500E-02	2.0780E+00	0.20622E+01	3.6797E+00	1.9751
5	0.6500E-02	1.9340E+00	0.18983E+01	3.5651E+00	1.9216
6	0.7500E-02	1.8210E+00	0.17687E+01	3.3466E+00	1.8805
7	0.8500E-02	1.7200E+00	0.16630E+01	3.0901E+00	1.8485
8	0.9500E-02	1.5850E+00	0.15747E+01	2.5673E+00	1.8236
9	0.1500E-01	1.2750E+00	0.12621E+01	2.4534E+00	1.7584
10	0.2000E-01	1.1300E+00	0.11018E+01	2.4823E+00	1.7445
11	0.2400E-01	1.0030E+00	0.10131E+01	2.6829E+00	1.7420
12	0.3000E-01	9.2170E-01	0.91723E+00	2.4000E+00	1.7401
13	0.4500E-01	7.7240E-01	0.77713E+00	2.3537E+00	1.7244
14	0.5500E-01	7.2400E-01	0.72446E+00	2.2694E+00	1.7086
15	0.6500E-01	6.9080E-01	0.69022E+00	2.4724E+00	1.6948
16	0.7500E-01	6.5160E-01	0.66929E+00	2.3956E+00	1.6858
17	0.8500E-01	6.5780E-01	0.65910E+00	2.1861E+00	1.6822
18	0.9500E-01	6.6190E-01	0.65855E+00	2.3962E+00	1.6828
19	0.1000E+00	6.5140E-01	0.66180E+00	2.1048E+00	1.6841
20	0.1200E+00	6.9840E-01	0.70032E+00	1.9945E+00	1.6910
21	0.1500E+00	8.6130E-01	0.86362E+00	1.9540E+00	1.6964
22	0.1700E+00	1.1400E+00	0.10968E+01	2.1799E+00	1.6981
23	0.1800E+00	1.3410E+00	0.12772E+01	2.1074E+00	1.6978
24	0.1900E+00	1.5970E+00	0.15178E+01	2.1239E+00	1.6956
25	0.2000E+00	1.8970E+00	0.18314E+01	2.1239E+00	1.6919
26	0.2100E+00	2.2750E+00	0.22194E+01	1.8839E+00	1.6897
27	0.2200E+00	2.7700E+00	0.26487E+01	1.8841E+00	1.6929
28	0.2300E+00	3.1070E+00	0.30272E+01	1.9925E+00	1.7003
29	0.2400E+00	3.2220E+00	0.32197E+01	2.1840E+00	1.7034
30	0.2450E+00	3.1810E+00	0.32154E+01	2.1838E+00	1.7019
31	0.2500E+00	3.0620E+00	0.31439E+01	2.1843E+00	1.6996
32	0.2600E+00	2.7970E+00	0.28482E+01	2.0246E+00	1.6988
33	0.2700E+00	2.3980E+00	0.24582E+01	2.2136E+00	1.7068
34	0.2800E+00	1.9560E+00	0.20760E+01	2.1401E+00	1.7198
35	0.3000E+00	1.4250E+00	0.14834E+01	2.1145E+00	1.7448
36	0.3250E+00	1.0220E+00	0.10417E+01	2.2847E+00	1.7752
37	0.3500E+00	8.0020E-01	0.79387E+00	2.2694E+00	1.8155
38	0.3750E+00	6.5610E-01	0.64519E+00	2.4249E+00	1.8608
39	0.4000E+00	5.6240E-01	0.54945E+00	2.8432E+00	1.9018
40	0.4250E+00	4.6660E-01	0.48398E+00	5.1118E+00	1.9338
41	0.4500E+00	4.5120E-01	0.43693E+00	6.0860E+00	1.9569
42	0.4750E+00	4.2480E-01	0.40173E+00	5.5462E+00	1.9738
43	0.5000E+00	3.8770E-01	0.37451E+00	5.0813E+00	1.9875
44	0.5200E+00	3.6840E-01	0.35684E+00	4.6797E+00	1.9973
45	0.5400E+00	3.4890E-01	0.34192E+00	4.2591E+00	2.0063
46	0.5700E+00	3.3090E-01	0.32344E+00	3.5721E+00	2.0162
47	0.6000E+00	3.1530E-01	0.30846E+00	3.0707E+00	2.0178
48	0.6500E+00	2.8670E-01	0.28890E+00	3.0035E+00	1.9884
49	0.7000E+00	2.7420E-01	0.27399E+00	2.8460E+00	1.9237
50	0.7500E+00	2.5680E-01	0.26221E+00	2.7457E+00	1.9205
51	0.8000E+00	2.4630E-01	0.25264E+00	2.6171E+00	2.2400

the model fit. The reduction of variances is not enough to come to the conclusion about the reduction of uncertainty. Table 2 shows how the covariances between chosen points (we select points #1 and 25) and all other points are changed in the model fit. Taking into account that although in R-matrix fit all data for exclusion of 51 data points by Lamaze et al. [7] were treated practically as uninformative (with assigned large uncertainties), because of their large number, they may contribute to a few per-cents covariances reduction in the model fit.

Table 2. Covariances (in b^2) for point #1 and #25 with variances marked by **bold**

Point #	Point #1		Point#25	
	Experimental	Model fit	Experimental	Model fit
1	**0.04516**	**0.00481**	0.00145	0.00141
2	0.00216	0.00383	0.00123	0.00121
3	0.00187	0.00320	0.00111	0.00107
4	0.00162	0.00274	0.00101	0.00097
5	0.00147	0.00243	0.00095	0.00090
6	0.00141	0.00217	0.00083	0.00083
7	0.00138	0.00196	0.00083	0.00079
8	0.00121	0.00179	0.00077	0.00075
9	0.00101	0.00123	0.00061	0.00060
10	0.00089	0.00097	0.00054	0.00052
11	0.00075	0.00083	0.00048	0.00048
12	0.00071	0.00070	0.00045	0.00043
13	0.00059	0.00054	0.00038	0.00036
14	0.00057	0.00050	0.00035	0.00033
15	0.00055	0.00049	0.00033	0.00032
16	0.00050	0.00048	0.00032	0.00030
17	0.00052	0.00049	0.00032	0.00030
18	0.00051	0.00051	0.00032	0.00030
19	0.00050	0.00052	0.00032	0.00032
20	0.00053	0.00057	0.00034	0.00042
21	0.00066	0.00072	0.00041	0.00044
22	0.00090	0.00090	0.00055	0.00055
23	0.00103	0.00102	0.00066	0.00066
24	0.00123	0.00120	0.00078	0.00079
25	0.00146	0.00142	**0.00163**	**0.00096**
26	0.00173	0.00172	0.00111	0.00115
27	0.00211	0.00208	0.00135	0.00135
28	0.00238	0.00243	0.00150	0.00147
29	0.00255	0.00262	0.00157	0.00149
30	0.00252	0.00262	0.00155	0.00147
31	0.00243	0.00255	0.00149	0.00142
32	0.00214	0.00228	0.00135	0.00121
33	0.00190	0.00195	0.00117	0.00112
34	0.00150	0.00161	0.00096	0.00096
35	0.00109	0.00113	0.00070	0.00071
36	0.00086	0.00080	0.00050	0.00050
37	0.00064	0.00064	0.00039	0.00038
38	0.00050	0.00054	0.00032	0.00031
39	0.00044	0.00048	0.00027	0.00026
40	0.00035	0.00043	0.00023	0.00023
41	0.00035	0.00039	0.00022	0.00020
42	0.00035	0.00036	0.00021	0.00019
43	0.00029	0.00033	0.00019	0.00017
44	0.00029	0.00031	0.00018	0.00017
45	0.00029	0.00030	0.00017	0.00016
46	0.00025	0.00026	0.00016	0.00015
47	0.00025	0.00025	0.00015	0.00014
48	0.00022	0.00022	0.00014	0.00013
49	0.00021	0.00020	0.00013	0.00012
50	0.00020	0.00020	0.00012	0.00012
51	0.00019	0.00021	0.00012	0.00011
Sum	0.09522	0.06293	0.03314	0.03176
Ratio, model to non-model	**0.66**		**0.96**	

Then the comparison of the results of the model and non-model fits was done for five data sets [8] (see Annex 4). Central values and variances obtained are given in the Table 3 and shown in Fig. 1. Table 4 shows the comparison of the covariances obtained in general least squares fit (GMA code) [6] with R-matrix model fit (RAC code) [5] the same five sets of experimental data. All other data needed for unambiguous R-matrix fit were treated practically as uninformative (with extremely large uncertainties assigned). As we see from direct

Table 3. Comparison of model with non-model least squares fit of 5 experimental data sets for ^{6}Li(n,α) reaction.

Energy, MeV	Cross section (central values), b			Error, %		
	GLUCS Bayesian non-model fit	GMA general least squares non-model fit	RAC R-matrix model fit	GLUCS Bayesian non-model fit	GMA general least squares non-model fit	RAC R-matrix model fit
0.2500E-02	2.5643E+00	2.56791130	0.265435E+01	3.4736E+00	3.4	1.4952
0.3500E-02	2.1340E+00	2.13894272	0.224569E+01	3.2550E+00	3.2	1.3900
0.4500E-02	1.8435E+00	1.85487058	0.198312E+01	3.0100E+00	3.0	1.3163
0.5500E-02	1.7385E+00	1.73921302	0.179651E+01	2.5948E+00	2.6	1.2631
0.6500E-02	1.5777E+00	1.57732333	0.165529E+01	2.5518E+00	2.5	1.2244
0.7500E-02	1.4669E+00	1.46900573	0.154373E+01	2.4718E+00	2.5	1.1960
0.8500E-02	1.4182E+00	1.41379212	0.145280E+01	2.2237E+00	2.2	1.1754
0.9500E-02	1.2888E+00	1.28802753	0.137692E+01	1.8064E+00	1.8	1.1606
0.1500E-01	1.0487E+00	1.04513353	0.110908E+01	1.7278E+00	1.7	1.1330
0.2000E-01	9.5192E-01	0.95499096	0.972498E+00	1.8265E+00	1.8	1.1359
0.2400E-01	8.6783E-01	0.86615244	0.897389E+00	1.9348E+00	1.9	1.1403
0.3000E-01	7.6349E-01	0.76628620	0.816803E+00	1.7740E+00	1.8	1.1429
0.4500E-01	6.6971E-01	0.66950549	0.701441E+00	1.8026E+00	1.8	1.1279
0.5500E-01	6.3158E-01	0.63043012	0.659942E+00	1.7502E+00	1.8	1.1120
0.6500E-01	6.0471E-01	0.60438930	0.634664E+00	1.8674E+00	1.9	1.0988
0.7500E-01	5.7693E-01	0.57853288	0.621291E+00	1.9369E+00	1.9	1.0907
0.8500E-01	6.0873E-01	0.60810755	0.617734E+00	1.4020E+00	1.4	1.0873
0.9500E-01	5.9780E-01	0.59926541	0.623171E+00	1.7722E+00	1.8	1.0869
0.1000E+00	5.9648E-01	0.59749230	0.629247E+00	1.5888E+00	1.6	1.0872
0.1200E+00	6.3976E-01	0.64001517	0.678214E+00	1.4318E+00	1.4	1.0877
0.1500E+00	7.9289E-01	0.79463003	0.854758E+00	1.4012E+00	1.4	1.0836
0.1700E+00	1.0061E+00	1.00507612	0.109228E+01	1.5597E+00	1.6	1.0828
0.1800E+00	1.2084E+00	1.20947152	0.127076E+01	1.6308E+00	1.6	1.0826
0.1900E+00	1.4454E+00	1.44870074	0.150399E+01	1.5343E+00	1.5	1.0816
0.2000E+00	1.7253E+00	1.72745634	0.180166E+01	1.5556E+00	1.6	1.0802
0.2100E+00	2.0577E+00	2.06036584	0.216218E+01	1.3899E+00	1.4	1.0810
0.2200E+00	2.4852E+00	2.49007621	0.255463E+01	1.3842E+00	1.4	1.0861
0.2300E+00	2.8005E+00	2.80415714	0.290012E+01	1.4850E+00	1.5	1.0930
0.2400E+00	2.9316E+00	2.94171942	0.308564E+01	1.7320E+00	1.8	1.0950
0.2450E+00	2.8906E+00	2.89460753	0.309124E+01	1.5753E+00	1.6	1.0938
0.2500E+00	2.8530E+00	2.85914450	0.303681E+01	1.5706E+00	1.6	1.0925
0.2600E+00	2.5546E+00	2.55676583	0.278391E+01	1.5635E+00	1.5	1.0956
0.2700E+00	2.3155E+00	2.31343201	0.242963E+01	1.6837E+00	1.7	1.1086
0.2800E+00	1.9120E+00	1.90770162	0.206822E+01	1.6422E+00	1.6	1.1259
0.3000E+00	1.3738E+00	1.37898444	0.148622E+01	1.5593E+00	1.6	1.1524
0.3250E+00	9.8769E-01	0.99184917	0.103940E+01	1.7859E+00	1.8	1.1734
0.3500E+00	7.5831E-01	0.75962702	0.785950E+00	1.7949E+00	1.8	1.2007
0.3750E+00	6.2623E-01	0.62617165	0.633946E+00	1.7922E+00	1.8	1.2349
0.4000E+00	5.4585E-01	0.54580942	0.536660E+00	2.0282E+00	2.0	1.2666
0.4250E+00	4.8323E-01	0.48092828	0.470728E+00	2.9850E+00	3.0	1.2897
0.4500E+00	3.8710E-01	0.38657206	0.423875E+00	4.7772E+00	4.8	1.3035
0.4750E+00	3.8596E-01	0.38682004	0.389265E+00	2.7247E+00	2.7	1.3113
0.5000E+00	3.5704E-01	0.35763385	0.362873E+00	3.0459E+00	3.0	1.3180
0.5200E+00	3.4137E-01	0.34160385	0.345974E+00	3.0316E+00	3.0	1.3256
0.5400E+00	3.2214E-01	0.32279109	0.331882E+00	3.2962E+00	3.3	1.3368
0.5700E+00	3.1541E-01	0.31529003	0.314719E+00	2.8556E+00	2.9	1.3611
0.6000E+00	2.9205E-01	0.29302733	0.301110E+00	2.3312E+00	2.4	1.3905
0.6500E+00	2.7146E-01	0.27220681	0.283922E+00	2.5621E+00	2.5	1.4259
0.7000E+00	2.5607E-01	0.25551707	0.271434E+00	2.4689E+00	2.4	1.4123
0.7500E+00	2.3794E-01	0.23822164	0.262131E+00	2.4283E+00	2.4	1.4248
0.8000E+00	2.2406E-01	0.22433707	0.255110E+00	2.5081E+00	2.4	1.8872

comparison of covariances given in Tables 2 and 4 and sum of covariances, which as we think is a good measure of uncertainty, the model, as seems, does not reduce the uncertainty in the fit. What model does, it introduces rather strong short and medium range correlations, which keep the shape of the model function used for fit and as result reduces the variances with simultaneous and compensating increases of the neighbor covariances. This is seen also from Fig. 2 and 3, if we take into account that more than 900 uninformative data points in the R-matrix fit (including thermal value) may have some influence at the uncertainty reduction.

Table 4. Covariances (in b^2) for point #1 and #25 with variances marked by **bold** for model and non-model least squares fits of five sets of experimental data

Point #	Point #1		Point#25	
	GMA non-model fit	RAC R-matrix model fit	GMA non-model fit	RAC R-matrix model fit
1	**0.00775**	**0.00158**	0.00047	0.00044
2	0.00076	0.00123	0.00039	0.00038
3	0.00064	0.00102	0.00034	0.00034
4	0.00051	0.00086	0.00031	0.00031
5	0.00050	0.00076	0.00029	0.00029
6	0.00048	0.00067	0.00027	0.00027
7	0.00042	0.00060	0.00025	0.00025
8	0.00038	0.00055	0.00023	0.00024
9	0.00032	0.00036	0.00019	0.00020
10	0.00028	0.00027	0.00017	0.00018
11	0.00025	0.00023	0.00016	0.00016
12	0.00022	0.00019	0.00014	0.00015
13	0.00020	0.00015	0.00012	0.00012
14	0.00018	0.00014	0.00011	0.00011
15	0.00017	0.00014	0.000109	0.000109
16	0.00017	0.00015	0.000106	0.000104
17	0.00016	0.00015	0.000109	0.000103
18	0.00016	0.00016	0.000106	0.000104
19	0.00017	0.00017	0.000108	0.000105
20	0.00018	0.00019	0.00011	0.00012
21	0.00022	0.00024	0.00014	0.00016
22	0.00028	0.00029	0.00018	0.00022
23	0.00033	0.00032	0.00022	0.00026
24	0.00039	0.00038	0.00026	0.00031
25	0.00047	0.00044	**0.00072**	**0.00038**
26	0.00056	0.00053	0.00037	0.00045
27	0.00067	0.00064	0.00045	0.00051
28	0.00075	0.00074	0.00050	0.00055
29	0.00075	0.00080	0.00051	0.00054
30	0.00076	0.00082	0.00052	0.00053
31	0.00075	0.00080	0.00051	0.00050
32	0.00065	0.00071	0.00046	0.00045
33	0.00064	0.00061	0.00043	0.00040
34	0.00052	0.00051	0.00035	0.00035
35	0.00038	0.00036	0.00024	0.00026
36	0.00027	0.00026	0.00018	0.00019
37	0.00021	0.00021	0.00014	0.00014
38	0.00017	0.00018	0.00011	0.00012
39	0.00014	0.00015	0.000094	0.000097
40	0.00014	0.00014	0.000089	0.000083
41	0.000098	0.00012	0.000070	0.000073
42	0.000102	0.00012	0.000065	0.000066
43	0.000106	0.000104	0.000065	0.000061
44	0.000100	0.000098	0.000061	0.000059
45	0.000075	0.000092	0.000052	0.000057
46	0.000087	0.000083	0.000058	0.000054
47	0.000079	0.000076	0.000050	0.000052
48	0.000079	0.000068	0.000050	0.000050
49	0.000071	0.000064	0.000047	0.000048
50	0.000065	0.000064	0.000043	0.000045
51	0.000063	0.000067	0.000041	0.000041
Sum	0.023875	0.019656	0.011163	0.011191
Ratio, model to Non-model	**0.82**		**1.002**	

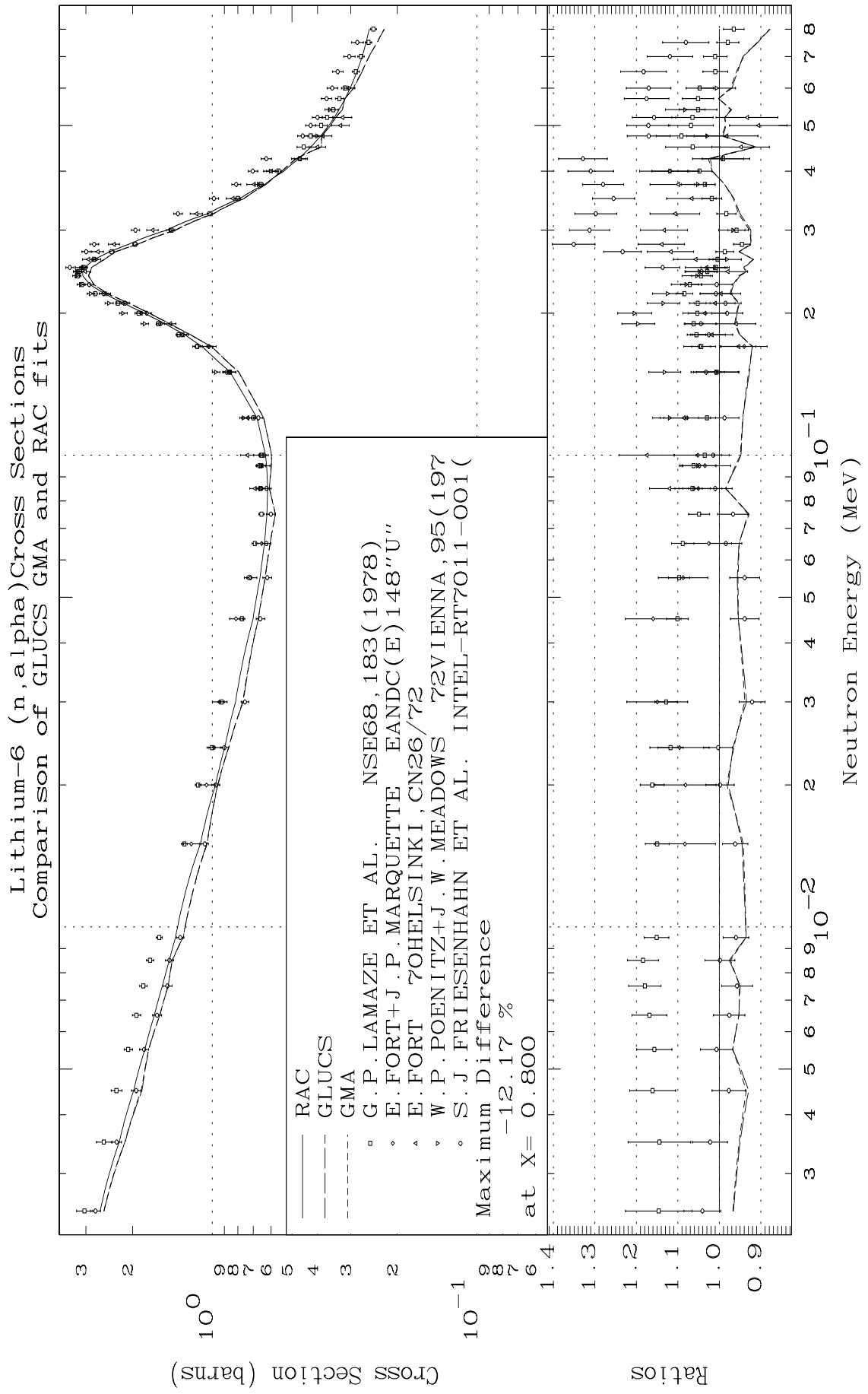

Fig.1. Intercomparison of GMA, GLUCS and RAC fitting of five data sets. Ratio to the RAC fit is shown in the lower part of the Figure.

Fig. 1

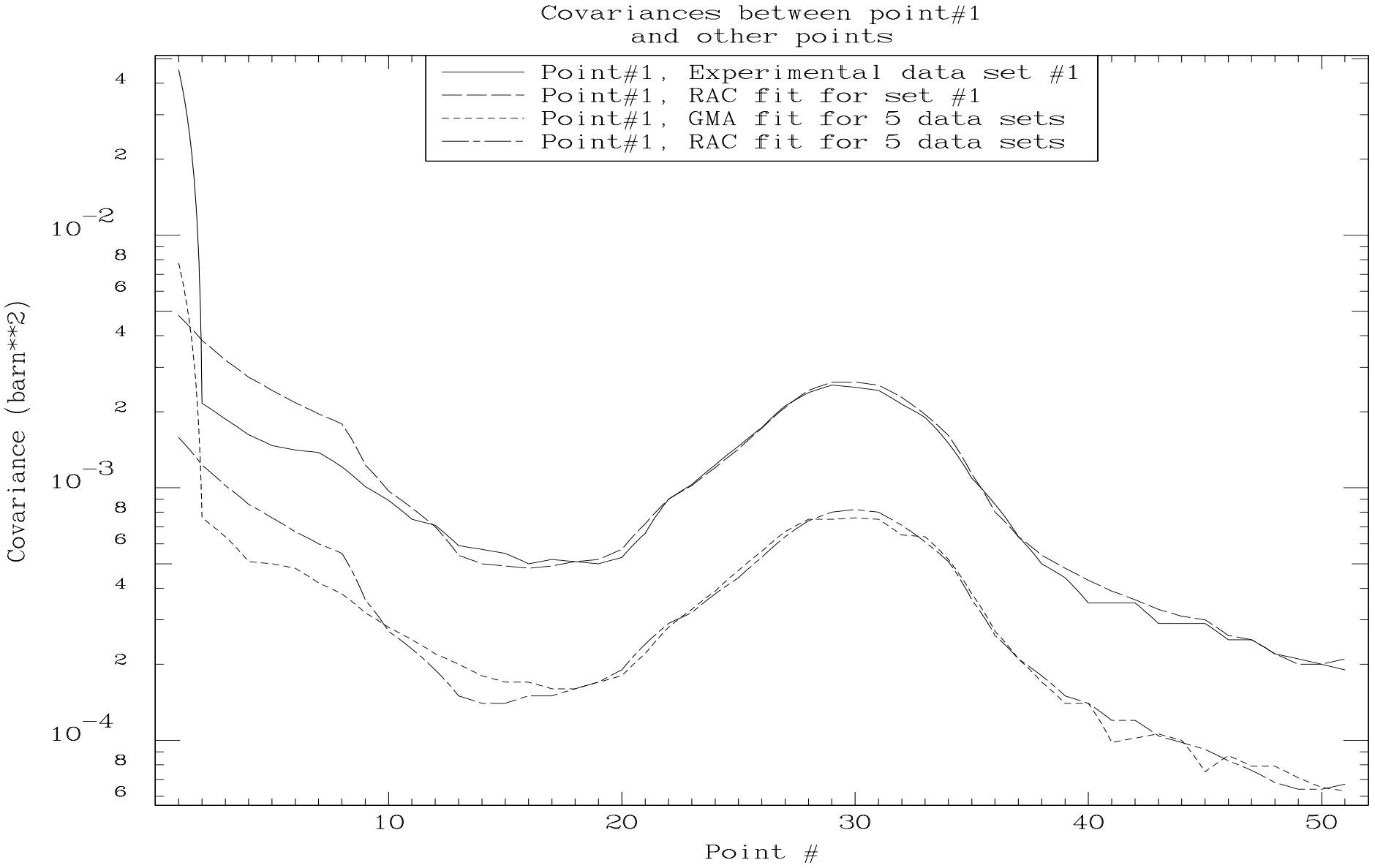

Fig.2. Intercomparison of GMA and RAC evaluated covariances between point 1 and other points.

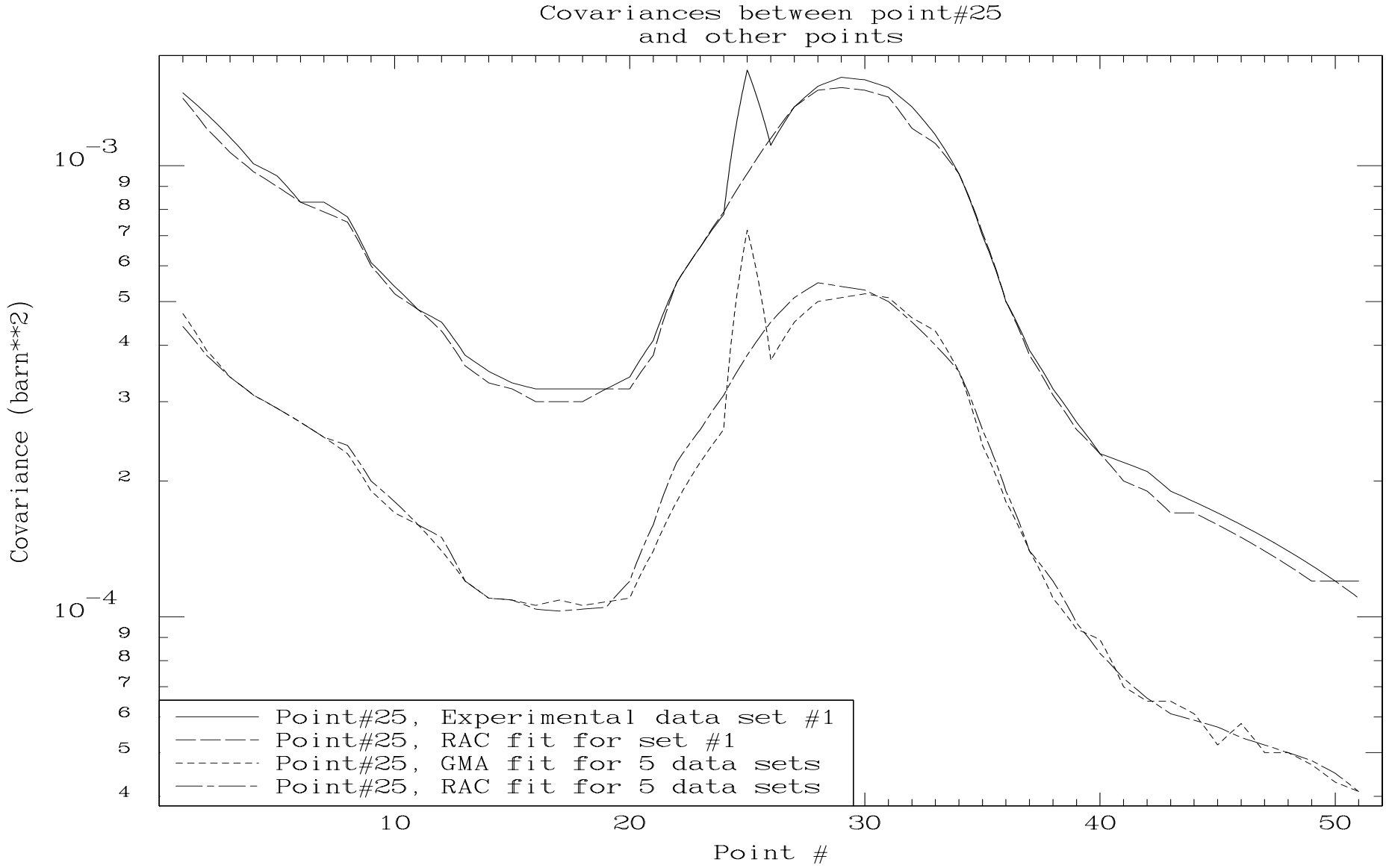

Fig.2. Intercomparison of GMA and RAC evaluated covariances between point 25 and other points.

References

1. C.E. Shannon, *"A Mathematical Theory of Communication"*, The Bell System Technical Journal, Vol.27, pp. 379-423, 623-656 (1948) as downloaded from WWW in form "reprinted with corrections".

2. J.S. Bendat, A.G. Piersol, "Random Data: Analysis and Measurement Procedures", John Wiley&Sons, Inc., 1986.

3. F.H. Fröhner, "Evaluation and Analysis of Nuclear Data", Jeff Report 18, NEA OECD, 1996.

4. D.L. Smith, "*Probability, Statistics and Data Uncertainties in Nuclear Science and Technology"*, publ. by American Nuclear Society, Inc., LaGrange Park, Illinois 60525, USA, 1991.

5. Chen Zhenpeng, "Preliminary results of model least squares fit obtained with R-matrix code RAC implementing full error propagation law", Privat communication, August 2002. See also report "Error Propagation in R-matrix Model Fitting" presented at the IAEA First Research Co-ordination Meeting on "Improvement of the Standard Cross Sections for Light Elements", IAEA Headquarters, Vienna, Austria, 23–27 September 2002.

6. V.G. Pronyaev, "Test and intercomparison of general least squares code GMA with Bayesian code GLUCS in fitting of 6Li(n,a) reaction", Privat communication, August 2002. See also report "GMA and GLUCS Tests and Covariance Matrices of Model and Non-model Least Squares Fits" presented at the IAEA First Research Co-ordination Meeting on "Improvement of the Standard Cross Sections for Light Elements", IAEA Headquarters, Vienna, Austria, 23–27 September 2002.

7. Experimental reaction cross sections and variances for 5 data sets given in Appendix were taken from GMA database (W.P. Poenitz, S.E. Aumeier, report ANL/NDM-139 (1997)). Covariance matrices were prepared as consisting only from 2 components – statistical and systematical errors.

Peelle's Pertinent Puzzle: Way of Solution

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Effect of evident bias of evaluated data below the majority of experimental data observed in general least-squares model fitting of these data was called as Peelle's Pertinent Puzzle (PPP). It was shown (at least in two-variate case) that this bias happens when covariance matrix of experimental data contains the non-diagonal element(s) V_{ij} which are larger than diagonal V_{kk}:

$$V_{ij} > V_{kk} \text{ for any } i, j, k \text{ with } i \neq j \quad (1)$$

This is often happen when the data are strongly varied in the range of evaluation or when contribution of Long Energy Range Component (LERC) in the total uncertainty is high. To overcome this the iteration procedure with minimization of the functional with percent errors characterizing uncertainties was proposed. Other approach can be based on transformation of the data to the form in which they will have no large variations. For example, if data have exponential growth or decrease, logarithm of this data will be a constant. Reaction ^{6}Li(n,α) in the energy region where it is used as the standard has an exponential decrease at low energy and a resonance at higher energy. If R_i presents this data we can transform it to the Y_i:

$$Y_i = ln(R_i + C), \quad (2)$$

where C is a constant that is not always needed.

Then the general scheme of solution free from PPP will be:

1. Prior and experimental data (central values and covariances) transformation based on relation (2).
2. List-squares fitting of transformed data.
3. Back transformation of evaluated data based on inverse relation to the (2).

As we see from (2) the transformation of the central values is trivial. Let see how the transformation of covariance matrices can be done.

The most general form of propagation errors law for linear transformations which is presented through transformation matrix A with elements A_{mn} and $m=1,...,M$, and $n=1,...,N$ can be written as:

$$Cov(Y_{ij}) = \sum_{n=1}^{N} \sum_{l=1}^{N} A_{in} Cov(R_{nl}) A_{lj}^{+} \quad (3)$$

This is exactly the form, which is used in R-matrix analysis for transformation of the covariance matrix of N evaluated parameters to the covariance matrix of the M evaluated values of cross sections. In our case (2), we have M=N. If number of points, in which data are determined, is large enough for good presentation of the data by linear interpolation between points, linear approximation to the calculation of elements of matrix A is used. With M=N and only diagonal elements being non-zero, we will have:

$$A_{ii} = \partial Y_i / \partial R_i = 1/(R_i + C) \quad (4)$$

and

$$Cov(Y_{ij}) = A_{ii}Cov(R_{ij})A^{+}_{jj} = (1/(R_i + C))Cov(R_{ij})(1/(R_j + C)) = \frac{R_i}{R_i + C} Rlc(R_{ij}) \frac{R_j}{R_j + C} \qquad (5)$$

Obtained result is very interesting, because $Rlc(R_{ij})$ is relative covariance matrix, $\sqrt{Rlc(R_{ii})} \times 100\%$ is just "percent" error. As we also see if we put $C=0$ then in fitting of Y_{ij} we will work with relative covarariances.

To check, how it works numerically, take example, given as PPP in the report ANL/NDM-121.

A) $R_1=1.5$
$R_2=1.0$
$Cov(R_{11})=R_{11}=0.1125$
$Cov(R_{22})=R_{22}=0.05$
$Cov(R_{12})=R_{12}=Cov(R_{21})=R_{21}=0.06$

On error propagation law evaluated value T' will be:

$$T'=((R_{22}-R_{12})R_1+(R_{11}-R_{12})R_2))/((R_{11}-R_{12})+(R_{22}-R_{12}))$$

and T'=0.88 - below the values of R1 and R2. Using transformation (1) with C=0 we get:

B) $Y_1=04055$
$Y_2=0.$
$Y_{11}=0.05$
$Y_{12}=Y_{21}=0.04$
$Y_{22}=0.05$

and

$T'=1.224$

This value is within the expected limits 1.0 and 1.5 but slightly below expected "true" value 1.25 which for this particular case of equal weight of both values is just T'=(1.5+1.0)/2. Using (1) we have for evaluated transformed value Y'=(ln1.5+ln1.0)/2=0.2027, or for T'=1.224.

Standards Database Extension: New Results Since 1997

(data, which are not included in ANL/NDM-139, 1997)

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(10 September 2002)

^{6}Li(n,t)

Set #	Data type	Year	Reference	# Data Values	Energy Range	Comments	Data Source and Status
	Shape ratio to ^{10}B(n,a)	1985	A.D. Carlson, 85 Santa Fe, p. 1451		1.89 to 36.75 eV	Non-inform. Ratio =1	X4: 10946
		1985	C.M. Bartle, 85 Santa Fe, p. 1337		2.16 to 14 MeV	Angular distribution	Graphs at 2.16 MeV and graphs of Legendre coeff. b1 - b4 for other energies
			Koehler		1 keV to 2.5 MeV	Angular distribution data	Private communication to A. Carlson
			Yu.M. Gledenov et al., Kiev87, v.2, p.237 (1988)		Therm.	Methodical work with no data	CINDA

^{6}Li(n,total)

Set #	Data type	Year	Reference	# Data Values	Energy Range	Comments	Data Source and Status
	Absolute	1954	C.T. Hibdon, A. Langsdorf, ANL-5175 (1954)		0.99 to 340 keV	No uncertainties, “old” data	X4: 11002
	Absolute	1974	J.A. Harvey,N. Hill,ORNL-4937,187(1974)	3309	185 to 530 keV	Should be included in R-matrix fit	X4: 13771
	Absolute	1952	DOK,110,963 (1956)	18	10 to 450 keV	“old” data	X4: 41317
	Absolute	1972	W, J.A. Harvey (1972)		4 runs, 0.008 eV to 32 MeV	Should be included in R-matrix fit	X4: 13772, few thicknesses and resolutions.

^{10}B(n,α) Branching ratio

Set #	Data type	Year	Reference	# Data Values	Energy Range	Comments	Data Source
	Shape ratio $^{10}B(n,\alpha_0)/^{10}B(n,\alpha_1\gamma)$	2001	Hambsh&Bach C, Tsukuba2001		keV to MeV	Frisch grided iron chamber	Abstracts, final experimental data are in preparation

^{10}B(n,α$_1$γ)

Set #	Data type	Year	Reference	# Data Values	Energy Range	Comments	Data Source
	Relative H(n,n)	1994	Schrack C, Gatlinburg93, p.43 (1994)		10 keV to 1 MeV		Proceedings; data are reviewed (A. Carlson)
	Shape ratio to ^{235}U(n,f)		Schrack		0.3 to 10 MeV		Private communication to A. Carlson; data are reviewed (A. Carlson)

^{10}B(n,α)= ^{10}B(n,α$_0$)+^{10}B(n,α$_1$γ)

Set #	Data type	Year	Reference	# Data Values	Energy Range	Comments	Data Source
			R. Haight		1 to 6 MeV	Angular distribution at 30, 60, 90 and 135 degrees	Private communication to A. Carlson
		2001	Hambsh& BachC, Tsukuba2001		keV to MeV	Frisch grided ionisation chamber	Conf. abstracts, final experimental data are in preparation
			Georginis& Khriachkov, C, 10-th Int. Seminar on Interaction of Neutrons with Nuclei		1.5 to 3.8 MeV	Angular distributions and cross sections, gridded ionisation chamber, particles leaking is studied	Private communication to A. Carlson
			Tang Guoyou et al., INDC(CPR)-053, (2001)	4	4 to 6.5 MeV	Angular distributions and cross sections, gridded ionisation chamber	Data are given in the INDC(CPR-053), p. 1

$^{10}B(n,tot)=^{10}B(n,\alpha_0)+^{10}B(n,\alpha_1\gamma)+^{10}B(n,n)$

Set #	Data type	Year	Reference	# Data Values	Energy Range	Comments	Data Source
			Wasson, Gatlinburg93, p. 50 (1994)		0.02 to 20 MeV	NE-110 detector	CINDA
			A. Plompen, Gatlinburg93, p.47 (1994); Trieste97, p. 1283 (1997)		0.3 to 18 MeV	LiI and Li-glass detector	CINDA
			Brusegan Gatlinburg93, (1994); Trieste97, (1997)		80 eV to 730 keV	Li-glass detector	CINDA

^{197}Au(n,γ)

Set #	Data type	Year	Reference	# Data Values	Energy Range	Comments	Data Source
		1993	Koehler, Gatlinburg93, p. 179 (1994)		0.01 eV to 50 keV	LANSCE	CINDA
		1993	Block, Gatlinburg93, p. 81 (1994)		0.01 to 100 eV	LINAC	CINDA
		1987	Bao, AND, 36, p. 411 (1987)		30 KeV maxwellian		CINDA
	Shape ratio to ^{10}B(n,α)		S.Yamamoto, INDC(JPN)-142,59 (1990)		0.013 to 0.89 eV	Can be interpolated to thermal point as ratio	X4: 22196003
	Shape ratio to ^{10}B(n,α) from 0.1 to 8 eV, and ^{nat}Sm(n,γ) at thermal		S.Yamamoto, NST, 33, (11), 815 (1996)		0.013 to 8.03 eV	Can be interpolated to thermal point ?	X4: 22370
			A.N. Davletshin, YK,,(1),41 (1992)	4	813 to 2435 keV	Check correlations with X4: 41183,41190	X4: 41121
	Shape ratio to ^{6}Li(n,α) below 100 keV and ^{10}B(n,α) above 100 keV		L.E. Kazakov, YK, 85, (2), p. 44 (1985)		3 to 420 keV	Group averaged cross sections	X4: 40890003
	Shape ratio to ^{235}U(n,f)		A.N. Davletshin, YK,,(1), 13 (1993)	5	370 to 1000 keV	Check correlations with X4: 41121,41190	X4: 41183
	Shape ratio to ^{235}U(n,f)		V.A. Tolstikov, YK,,(4), 46 (1995)	5	486 to 692 keV	Check correlations with X4: 41183,41121	X4: 41190
			Demekhin, in Proc. of 36-th All Union Conf, p. 94 (1996)		2.7 MeV		Conf. abstracts
			J. Voignier, NSE, 93, p.43, (1986)	5	0.5 to 3.0 MeV	Longcounter with BF3 counters	X4: 22006031

^{238}U(n,γ)

Set #	Data type	Year	Reference	# Data Values	Energy Range	Comments	Data Source
	Cross section shape?	1991	R.L. Macklin, ANE, 18, p. 567 (19991)	25	0.3 to 100 keV	Given as group averaged cross sections for 2 thicknesses. Reduction to 0 thickness is needed	X4: 13526002, 003
			J. Voignier, NSE, 93, p.43, (1986)	4	0.5 to 1.1 MeV	Longcounter with BF3 counters	X4: 22006049
	Shape ratio to ^{10}B(n,α)		K. Kobayashi, Juelich91, p.65 (1991)	3	24 to 150 keV	Neutron filters, preliminary data shown on Fig.	CINDA
			Akiyama, ANE, 14, p. 543 (1987)		14 MeV		CINDA
	Shape ratio to H(n,n)		N. Buleeva, AE, 65, p. 348 (1988)		0.34 to 1.39 MeV		X4: 40969005
	Relative ^{nat}Pb(n,n) elastic scattering		V. Vertebnyy, 80Kiev,2, p. 249, (1980)		24.5 keV	Obtained as difference tot-elastic, neutron filters	X4: 40839022

^{238}U(n,f)

Set #	Data type	Year	Reference	# Data Values	Energy Range	Comments	Data Source
	Relative ^{58}Ni(n,p)	1996	L.W. Meadows et al., ANE, 23, p.877 (1996)	1	10. MeV	Monitor reaction is an outsider	X4: 13586011
	Shape ratios ^{238}U to ^{237}Np	1989	J.W. Meadows et al., ANE, 16, p. 471 (1989)		1.92 to 2.55 MeV	A search for possible structure in the ^{238}U(n,f) cross section near 2.3 MeV.	X4: 13169
	Shape ratio to H(n,n)		Lisowski, NEANDC-305, p. 117 (1991?)		0.8 to 400 MeV		Data are available, private comm.. to A. Carlson
		1999	Johns, C, St.and99, p. 174		2 to 180 MeV	Preliminary data	CINDA
		1989	Block, C, Washington89, p. 354		1.4 eV to 100 keV		CINDA
	^{27}Al(n,p) reaction as a monitor	1968	C. Barrall, AFWL-TR-68-134 (1969)		14.6 MeV	Registration of fission fragments in Lexan	CINDA
			Pepelink, NIMB, 40, p. 1205 (1989)		14 MeV		CINDA
			Akiyama, ANE, 16, p.307 (1987)		14 MeV		CINDA
			Kovalenko, IP, 21, p. 344 (1985)		15 MeV	2% acc. data	CINDA
	Shape ratio to ^{235}U(n,f)		Kh.D. Androsenko et al., Kiev83, v. 2, p. 153 (1983)		0.85 to 3.72 MeV		X4: 40629002

	Shape ratio to $^{235}U(n,f)$		Fomichev, Juelich91, p. 734 (1991) Fomichev, C, Trieste97, p. 1283 (19997) Shcherbakov, C, JAERI-C-98-016 (1998) and ISTC 609-97		0.7 to 100 MeV		CINDA, Data available, privat comm.. to A. Carlson
			Goverdovskiy, JINR-E3-00-192 (2000)		1.1 to 4.0 MeV		CINDA
			Boykov, ANE, 21, p. 585 (1994)		2.9 to 15 MeV		CINDA
	Shape ratio to $^{235}U(n,f)$		Baba, J. Nucl. Sci.&Techn., 26, p. 11 (1989)		0.5 to 7 MeV, 14 MeV		No data, privare comm.. to A. Calson

^{235}U(n,f)

Set #	Data type	Year	Reference	# Data Values	Energy Range	Comments	Data Source
	Shape ratio to ^{10}B(n,α)		Weston&Todd, NSE, 111, p. 415 (1992)		0.1 keV to 2 keV	High resolution (10187 points) Linac data. Should be reduced to "poor" resolution and then interpolated	X4: 13488002
	Absolute, detector calibration with associated particle method at 2.45 and 14 MeV		R.G. Johnson, W, Carlson (1991)	19	1.066 to 5.985 MeV	Dual thin scintillator	X4: 12924002
	Absolute cross section		V.A. Kalinin et al., At. En. 71, (2), p. 181 (1991)	2	1.88 MeV 2.37 MeV		X4: 41112, data in X4=40963 are revised (?)
	Relative to black detectorl		A. Carlson, IAEA-TECDOC-335, p. 163 (1985)		0.3 to 3.0 MeV		X4: 10987002
	Relative H(n,n)		A. Carlson, NEANDC-305, p.165 (1991)		2 to 30 MeV		Data are available, A. Carlson priv. comm..
	Relative H(n,n)		T. Iwasaki et al., C, Mito88, p.87 (1988)	5	13.51 to 14.9 MeV		X4: 22091002
	Relative H(n,n)		Lisowski, NEANDC-305, p. 177 (1991?)		3 to 200 MeV		Data are available, private comm. to A. Carlson

			Rapaport, LA-11078 (1987)		0.6 to 750 MeV		CINDA
			Duvall, DOE-NDC-36, -43, -47, -49 (1985-1989)		2.5 MeV	Ass. part. method	CINDA
	Shape ratio to $^{10}B(n,\alpha)$		R.A. Schrack, C, Mito88, p. 101 (1988)		15.2 keV to 1.4 MeV	High resolution (7958 points) Linac data. Should be reduced to "poor" resolution and then interpolated	X4: 13198002
			Wasson, RE, 96, 9 (1986)	1	14.7 MeV		CINDA
	Shape ratio to $^{10}B(n,\alpha)$		Wagemans, INDC(EUR)-19, p. 6 (1985)		0.025 eV to 30 keV		CINDA
	Shape ratio to $^{6}Li(n,\alpha)$		Wagemans, C, Mito88, p. 91 (1988)		0.02 to 20 eV eV		X4: 22080003
			Zhang, IAEA-336, p.343 (1985)		0.02 to 0.3 eV		CINDA
			Kovalenko, IP, 21. p. 344 9(1985)		8.7 MeV	TUD/KRI collaboration, data for 2.6 MeV were revised by Merla – see comments in #591	X4: 30558002 – probably the data should be also revised as done by Merla

^{239}Pu(n,f)

Set #	Data type	Year	Reference	# Data Values	Energy Range	Comments	Data Source
	Shape ratio to ^{235}U(n,f)		P. Staples, K. Morley, NSE, 129, p. 149 (1988)		0.85 to 61.8 MeV	Err-S is given as no-dim. – wrong - probably it is given in %	X4: 13801002
	Shape ratio to ^{10}B(n,α)		Weston&Todd, NSE, 111, p. 415 (1992)		0.1 keV to 20 keV	High resolution (22139 points) Linac data. Should be reduced to "poor" resolution and then interpolated	X4: 13488003
	Relative ^{235}U(n,f)		Donets, JINR-E3-98-212 (1998); JINR-E3-00-192 (2000) Shcherbakov, C, JAERI-C-98-016 (1998) and ISTC 609-97		1 to 200 MeV		CINDA, Data available, privat comm.. to A. Carlson
	Relative H(n,n) (or relative ^{235}U)		Lisowski, NEANDC-305, p. 177 (1991?)		0.8 to 350 MeV		CINDA (rel. ^{235}U) Data are available, private comm. to A. Carlson
	Shape ratio to ^{235}U		Iwasaki, JAERI-M-88-065 (1988) Hirakawa, C, Mito88, p. 119 (1988)	12?	0.6 to 7.0 MeV		CINDA, To request data
	Shape ratio to ^{6}Li(n,α)		Wagemans, C, Mito88, p. 91 (1988)		0.02 to 20 eV eV	No use (shape ratio in point?)	X4: 22080003

Status of data for TUD/KRI collaboration

Reaction	Energy, MeV	Preliminary value (b), Source	Final value (b), Source **Data were revised because the correction on fission product absorption was underestimated**
^{235}U(n,f)	1.88	1.260, X4=40927002 (1986) 1.257, X4=40963002 (1988)	1.280, X4=41112002 (1991)
	2.37	1.251, X4=40963002 (1988)	1.270, X4=41112002 (1991)
	2.56	1.214, X4=40911002 (1983) 1.215, X4=41013003 (1988)	1.240, X4=22304006 (1991), GMA DB 1.238, X4=41013004 (1988)
	4.45	1.057, X4=30706002 (1985) 1.057, X4=40927002 (1986) 1.057, X4=41013003 (1988)	1.094, X4=22304002 (1991), GMA DB 1.093, X4=41013004 (1988)
	8.46	1.801, X4=40911002 (1983) 1.801, X4=41013003 (1988)	1.855, X4=22304002 (1991), GMA DB 1.853, X4=41013004 (1988)
	8.7	1.801, X4=30558002 (1985)	
	14.7	2.086, X4=40911002 (1983) 2.085, X4=41013003 (1985)	2.096, X4=22304006 (1991); GMA DB 2.094, X4=41013004 (1988)
	18.8	1.999, X4=30706002 (1985) 1.999, X4=40927002 (1986) 1.999, X4=41013003 (1988)	2.068 X4=22304002 (1991), GMA DB 2.065 X4=41013004 (1988)
^{239}Pu	1.92	2.010, X4=40927005 (1986)	
	4.9	1.740, X4=40927005 (1986) 1.740, X4=30706004 (1986)	1.773, X4=22304005 (1991), GMA DB
	8.65	2.350, X4=40927005 (1986) 2.350, X4=30706005 (1986)	2.395, X4=22304005 (1991), GMA DB
	14.7	2.620, X4=40547009 (1977) 2.309, X4=40911007 (1983) 2.394, X4=30475005 (1985)	2.449, X4=22304005 (1991)
	18.8	2.487, X4=30706006 (1985) 2.487, X4=40927005 (1986)	2.473, X4=22304005 (1991), GMA DB

^{238}U	4.8		0.562, X4=22304003 (1991), GMA DB
	5.1&5.0	0.542, X4=41013002 (1988)	0.554, X4=22304003 (1991), GMA DB
	8.2		1.041, X4=22304003 (1991), GMA DB
	14.7&14.6	1.209, X4=40256002 (1973) 1.207, X4=40547007 (1977) 1.166, X4=30475003 (1981) 1.166, X4=40911005 (1983) 1.178, X4=40911005 (1983)	1.228, GMA DB
	18.8		1.363, X4=22304003 (1991), GMA DB

Open problems

1. What do if monitor reaction is an “outsiders” (do not belong to the currently evaluated set of reactions)?

2. For assigning of the values of the cross sections in the nodes, the DAT code interpolates the values to the node and averages them with their statistical weights. This is different for group cross section presentation, when data first reduced to the resolution of order the width of the energy group, then group-averaged taking into account the error propagation law. This procedure can be used for treatment of high resolution data.

3. Final Khlopin Radium Institute (KRI) and Technical University of Dresden (TUD) high precision results obtained with an associated particle method should be selected through consultations with authors.

4. Some data are given for the resonance region or varying strongly with energy. This may cause different problems related with reduction to zero sample thickness, or self-shielding, “Peelle’s puzzle”, non-linearity,… . Should we limit our consideration only by region of smoothed cross sections?

5. High priority should be given to the latest shape, shape ratio and absolute cross section measurements with an associated particles method. It means that uncertainty of the “old” data should be increased in cases when we are not sure that either all needed corrections are introduced or calculation of corrections was done with approximations (without using of Monte Carlo method, especially for closed geometry, …).

6. Some measurements were done relative H(n,n) cross section. Primary standard, H(n,n), evaluated in R-matrix approach should be included in GMA database.

7. Recommended characteristics of decay radiation for standard reactions (with that the evaluation of cross sections was done) should be given.

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