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INDC International Nuclear Data Committee

Summary Report

Technical Meeting on

Neutron Cross Section Covariances

IAEA Headquarters
Vienna, Austria

27-30 September 2010

Prepared by

A. Trkov
Jozef Stefan Institute
Ljubljana, Slovenia

D.L. Smith
Argonne National Laboratory
USA

R. Capote Noy
IAEA Nuclear Data Section
Vienna, Austria

January 2011

IAEA Nuclear Data Section, Vienna International Centre, A-1400 Vienna, Austria

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Abstract

A summary is given of the Technical Meeting on *Neutron Cross Section Covariances*. The meeting goal was to assess covariance data needs and recommend appropriate methodologies to address those needs. Discussions on covariance data focused on three general topics: 1) Resonance and unresolved resonance regions; 2) Fast neutron region; and 3) Users' perspective: benchmarks' uncertainty and reactor dosimetry. A number of recommendations for further work were generated and the important work that remains to be done in the field of covariances was identified.

January 2011

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ANNEXES

1. Executive Summary

It has long been recognized by the nuclear data community that the inevitable uncertainties in nuclear data, be they in experimental, model calculated, or evaluated values, should be important considerations in assessing the safety, reliability, and cost-competitive advantages of nuclear power in comparison to other energy sources. This has recently given rise to a renewed interest in this information in user communities. The users of nuclear data are those experts who strive to ensure that existing power plants can be operated even more safely than in the past, to extend their usable lifetimes, and to design improved systems for the future. Interest in the nuclear power option languished for more than two decades following the understandable negative view of the public in many countries towards the advancement of nuclear power in the aftermath of the Three Miles Island and Chernobyl nuclear plant accidents. Also, there are ongoing concerns about the threat of proliferation of nuclear weapons if weapons grade materials were more plentiful and possibly more easily accessible. Furthermore, the ability of the user community to consider covariances in their applications has, in many cases, only relatively recently been refined to the point of practicality.

This technical meeting on “Neutron Cross Section Covariances” was organized by the IAEA Nuclear Data Section with the objective of bringing together a group of experts who represent the cross section measurement, modeling, and evaluation communities as well as a few key user communities, and who, as a collective group, have a great interest in improving the status of providing reliable covariance data and seeing them used in practical applications associated with nuclear power production. Twenty six experts attended this meeting; the list of participants can be found in Appendix B to this document. The meeting was organized along three main lines: i) the resolved and unresolved resonance region, ii) the fast neutron region, and iii) discussions of user data requirements. The detailed Agenda for this meeting is also attached as Appendix A. Considerable time during this meeting was dedicated to issues related to the formatting and archiving of nuclear data as well as efficient retrieval of numerical values, mainly for the purpose of facilitating the evaluation of nuclear data. The role and importance of uncertainty information generated from nuclear modeling was acknowledged and addressed with vigor. This is a relatively new development since the methodologies to produce covariances in this manner have only recently experienced major advancements. These were discussed and some of the advantages of each approach were mentioned. Furthermore, there was agreement that such comparisons of methods should continue. It was also reconfirmed that nuclear data measurers need to pay more attention to the issue of uncertainty. This topic is generally not adequately addressed in the training of nuclear scientists, and there exists an imbedded cultural view that uncertainties are not so important to consider. Furthermore, the pressures to publish in journals to advance careers, and the limitations of content that can be included in journal articles, were acknowledged by the group.

This Technical Meeting generated a number of recommendations for further work (see Section 3). By identifying the important work that remains to be done in the field of covariances, the group hopes to give impetus to the nuclear science community to undertake such projects and offer guidance to international organizations, in particular to the IAEA, in organizing dedicated projects such as data development projects (DDP) or coordinated research projects (CRP) that will stimulate and facilitate future collaborations of interested and knowledgeable scientists to undertake this important work.

The meeting was opened with a welcome address by R.A. Forrest, followed by introductory remarks of the Technical officer of the meeting, R. Capote. D. Smith was elected chairman and A. Trkov rapporteur. The Agenda was adopted with the remark that additional short presentations would be included within the discussions of individual topics.

2. Meeting Narrative

2.1. Topical Area 1: Resonance covariances

D. Smith presented introductory remarks, mentioning the renaissance of covariance analytical techniques and data development after twenty years of dormancy. The present challenge is to identify the relative strengths and weaknesses of each method. A “stress-test” should be devised to which the methods would be subjected. Further development is also needed to include cross-correlations between energy-regions, which at present are analyzed independently (e.g. resolved, unresolved resonance region and the fast neutron energy region). It is generally felt that cross-reaction and cross-material covariances are important, but the importance is difficult to assess. He also stressed the importance of treating the errors due to nuclear models used in the evaluation process. Improvements in the EXFOR database were mentioned, such as the removal of errors, but there remains the need for refinement in compilation techniques and the compilation of adjustments to the data to correct for unaccounted errors.

O. Iwamoto described the work on covariances for the JENDL-4 evaluated nuclear data library. The resonance parameters for the major actinides were evaluated with the SAMMY code while the evaluations for the minor actinides were mainly based on the variance of the published resonance parameters and cross section covariances. The fission cross sections of the major actinides were evaluated through simultaneous evaluation with the SOK code, and for minor actinides the GMA generalised least-squares code was used. Other reactions were evaluated with the CCONE-KALMAN code system, where estimated correlations between experiments were included during the evaluation process (80% for data points of the same author, 40% between data of different authors). In this context it was noted that, at the IAEA, the development of a system is under way to automatically retrieve experimental data in computational format including normalization to modern standards, correction for known deficiencies, etc. Extension to include correlations is also needed. Several interesting examples of specific nuclide evaluations were presented. All actinides in the JENDL-4 library include covariance information, including cross-material correlations for the fission cross sections in the major actinides.

In the general discussion following the presentation no serious processing problems of the JENDL-4 covariances were reported. A general recommendation was made that evaluators should state precisely what assumptions were made about the uncertainties and correlations. Ignoring unknown uncertainties and correlations is not acceptable. This includes correlations between different experiments, which are currently not included in databases such as EXFOR. In this regard, the work on JENDL-4 represents a reasonable attempt to do this.

P. Schillebeeckx talked about resonance evaluations and the sources of uncertainty. Under ideal conditions the achievable uncertainties in transmission measurements can go down to 0.5 % and in fission and capture (of non-fissile nuclides) cross-section measurements to 2 %. They mainly arise from the target characterization, background estimation (mitigated by the use of background filters), powder grain size (if present, resulting in the underestimation of the measured resonance width), gamma-ray attenuation, normalization, etc. Having both, capture and transmission measurements, greatly improves the accuracy of the evaluation. The importance of a good documentation of the experimental observables was stressed, particularly the need to have different contributions to the uncertainty broken down explicitly.

C. de Saint-Jean described current resonance evaluation procedures, which aim at taking "all" uncertainties into account. General recipes allow "mass production" of evaluations, which are low-fidelity, unless specific characteristics of individual experiments are considered. Common complaints by users are that integral experiments are not taken into account early enough, leading to unexpected discrepancies between the measured and calculated integral observables and doubts about the credibility of the covariances. He defined "nuisance parameters", which do not appear explicitly in the nuclear reaction models, but are used to account for model deficiencies, and missing or un-measurable information for modeling an experiment (normalisation, background, etc.). He also warned about the use of the full covariance information, which in certain cases may lead to biases due to non-linearity and high correlations in the evaluation process, and described the "marginalization" procedure to avoid it.

M. Herman described the genesis of the kernel approximation[1] pointing out its advantages: simplicity and transparency. It accounts for systematic uncertainties through level-level and potential scattering correlations, avoids *ad hoc* adjustments to reproduce the uncertainty in the thermal region, etc. Its main disadvantage is its inherent approximate nature, but it seems to work well for capture and somewhat less well for elastic cross sections. Comparison of the estimated uncertainties obtained by means of the kernel method with those obtained from the information in ENDF Files 32 suggests that in several evaluations the scattering radius uncertainties and/or various correlations are missing, which leads to an underestimation of the uncertainties.

A. Trkov discussed the impact of the resonance covariance representation on the self-shielded resonance integral uncertainty. He showed that when resonances are correlated, the resonance integral uncertainty strongly depends on the level of self-shielding. Thus, replacement of resonance covariances in ENDF File 32 with cross section covariances in File 33 is not advisable because the two are not equivalent. This has implications for dosimetry applications, where as a rule, cross-section covariances are used. For further details readers are referred to a recent publication[2].

The ensuing discussion on resonance covariances addressed several issues:

- To a certain degree quality assurance on covariance information is needed to make sure that the covariances are "reasonable", meaning that the covariance matrix is at least semi-positive definite and that the uncertainties of broad-group average cross sections are close to the uncertainties of the experimentally-measured values. These include thermal cross section, resonance integrals and ^{252}Cf spontaneous fission spectrum averaged cross sections as well as other spectrum-averaged cross sections measured in well-characterized irradiation facilities. Additional constraints for defining reasonable uncertainties can refer to covariances on a denser energy grid, checking on minimum and maximum variance and large jumps in the variance. Required mathematical properties of the covariance matrices should be checked on the evaluator's energy grid. In the case of resonance covariances, the criterion refers to the resonance covariance matrix and not the cross section covariance matrix derived from it.
- The kernel method for generating cross-section covariances in the resonance range has the advantage of being simple and transparent and, in many cases, produces

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[1] P. Oblozinsky, Y.-S. Cho, C.M. Mattoon, and S.F. Mughabghab, "Formalism for neutron cross section covariances in the resonance region using kernel approximation". Technical report **BNL-91287-2010**, Brookhaven National Laboratory, Upton, NY, USA, April 2010.

[2] G. Zerovnik, A. Trkov, R. Capote, and D. Rochman, "Influence of resonance parameters' correlations on the resonance integral uncertainty; ^{55}Mn case", Nucl. Instr. & Meth. in Physics Research **A632** (2011) 137–141.

reasonable uncertainties, although it is no substitute for a more elaborate resonance analysis that provides information on correlations, particularly when resonance self-shielding effects are important.

- The format for resonance covariance representation in the unresolved resonance range is too restrictive because it allows for only a single uncertainty component for each parameter. At least the energy-dependence of parameters should be allowed. Alternatively, covariances of the unresolved resonance parameters could be substituted by resonance covariances in ENDF File 33, but the impact on self-shielded cross sections should be investigated.
- It was acknowledged by ORNL and IRMM that many experimental data sets had been lost due to changes of computer platforms, hardware for reading magnetic media becoming obsolete, etc. This could have been avoided if the data had been archived in some internationally maintained data base such as EXFOR. Unfortunately, adequate formats for archiving such information in EXFOR were not available at the time. The procedure was defined only recently, and a template was proposed by IRMM and IAEA, which allows the archival of sufficient information to repeat the resonance analysis with codes such as SAMMY or REFIT. Every effort should be made to ensure that existing experimental data are entered into the EXFOR database. A consensus exists at ORNL and IRMM to archive the data from new measurements according to the new format. Part of the work of WPEC SG-36, a group formed recently, addresses the issue of archiving the uncertainty information in EXFOR. We encourage the SG-36 to co-ordinate their activities with the IAEA effort regarding enhancements to the EXFOR format for archival of time-of-flight experimental data. Unfortunately, no measured data were released so far from the n_TOF facility that would allow an independent resonance analysis to be carried out, and that could enable these data to be archived in this way. It now seems clear that the mere reporting of resonance parameters and uncertainties obtained from analysis of experimental data, while ignoring the consideration and reporting of correlations, is inadequate for many applied purposes even though this has been the common practice for a long time.
- There is a general desire to extend the resolved resonance range to higher energies, but this may lead to a large increase in volume of the resonance covariance matrices. Assuming that energy dependence of the unresolved resonance parameter covariances was to be implemented, it might be possible to extend the URR covariances into the RR range, thus reducing the volume of data for the RR covariances.
- It was discussed that in addition to the limited uncertainty information available in the EXFOR data base, the complete absence of information on correlations at all energies is a deficiency that is unlikely to be remedied in any reasonable way in the foreseeable future, if at all. It was concluded that some evaluator estimates of these correlations will certainly lead to more acceptable results than simply assuming them to be zero, but such estimates would unavoidably be *ad hoc*, introduced for practical reasons, and therefore very difficult to defend in any rigorous manner. In this regard, documentation of these assumptions by the evaluators is essential to ensure traceability in the future.

2.2. Topical Area 2: Fast neutron covariances

R. Capote stressed the importance of properly-weighted contributions of carefully selected (and adjusted, if needed) experimental data and nuclear reaction modeling results in the evaluation process of the reaction cross sections and their covariances. Great care should be taken to apply the Bayesian iteration approach only with data sets that are truly independent; otherwise the correlations between data sets are neglected. He discussed differences between deterministic, stochastic and hybrid evaluation methods, and introduced a new formulation of the Unified Monte Carlo method in which each randomly-sampled set of parameters is assigned a weight that depends on the quality of the fit of the experimental data, including correlations. The rejection method is a subset of this new method, when the weights take binary values of zero or one. The new method is very well suited for application in the Total Monte Carlo technique (TMC).

A. Koning described the TALYS code system and its role in the implementation of TMC, library cloning (allowing the possibility to make existing libraries complete and consistent) and searching for optimal solutions. An application of the system is the TENDL library, which is finding its place with data users as a shadow-library for backup when dedicated evaluations are not available. Koning also outlined the broader capabilities of the analysis system developed at Petten and identified several areas of application where benefits might accrue in the feature, e.g., in understanding the effects of cross reaction and cross material correlations, evaluating the impact of approximations and deficiencies in the ENDF-6 covariance formats, non-linearity, etc. The capabilities for benchmarking of traditional methods of sensitivity and uncertainty analysis were emphasized. This system continues to be under development, not only for evaluation purposes but for system analysis applications.

M. Herman reported on the activities of the WPEC SG-24. Different methods of generating covariance data were compared. The comparison helped to understand the differences in the results, emphasizing the importance of correlations (and particularly correlations between different experiments), as well as model deficiencies. One of the outcomes of this study was a general, though not comprehensive, re-affirmation of the fact that the venerable GLSQ method, which in one form or another remains the most commonly applied approach to nuclear reaction data evaluation in the fast region, renders results which tend to agree quite well with more sophisticated approaches under the most common situations encountered in the evaluation of nuclear data. The importance of correlations in the input data and proper treatment of model defects was stressed in avoiding excessively small uncertainties. Only when non-linear effects or more complicated data, such as ratios, are encountered, is there likely to be a need for applying the more advanced techniques.

The ensuing discussion on fast neutron covariances addressed the following:

- It was suggested to explore the possibility of an IAEA activity to further elaborate the comparison of the various proposed evaluation methods.
- The possibility of reducing the number of available options to represent cross-section covariances in ENDF-6 formats might indeed simplify the processing codes. However, each of the existing options has some specific advantage; the benefits of the removal of specific options can hardly be justified at present. The present scheme allows different contributions to the covariance matrix to be given in separate blocks, which adds to the traceability of the data.
- V. Pronyaev explained how the Standards evaluations were prepared, particularly the evaluations for the light nuclides.
- The issue of complete absence of any provisions to specify uncertainties of the thermal scattering law data was raised. There is a strong need to define formats and

prepare a test covariance evaluation. Very few laboratories in the world are active in this area.

- A. Koning suggested that different nuclear models be sampled in the evaluation process of the cross sections and their covariances. The idea is similar to the one proposed by A. Konobeev a couple of years ago. The idea does not provide an indication of the uncertainty of the models, but it provides some indication of the spread in the cross sections that different models predict.
- G. Manturov showed a few slides on the minimum uncertainties to be expected by comparing data from different evaluated libraries. He acknowledged that in many cases the data in some of the new evaluations are not independent, and this was taken into account in the source data selection.
- A. Koning presented the work of WPEC SG-30, which addressed the corrections and adjustments to the EXFOR database, including fixing of errors and collecting other adjustments in a separate database together with documentation for the justification of the adjustments.

2.3. Topical Area 3: Use of covariance information in applications

P. Griffin gave a review of the use of covariance information in reactor dosimetry. Some of the requirements that were identified were for interference reactions such as ^{237}Np(γ,f) and ^{103}Rh(γ,γ’). In order to calculate “dpa”, the uncertainties in recoil spectra are needed. The reactor community needs reliable dosimetry data and there is a need for an authoritative body to review these data. The IAEA has provided good service in this regard and should continue to monitor user requirements and recent developments in nuclear data evaluation, and maintain the dosimetry library.

G. Manturov presented the application of covariances for the analysis of reactor systems, illustrating the procedures for analyzing correlations between integral experiments and folding-in the covariances of nuclear data to obtain adjusted data sets by means of which the uncertainties in the calculated integral parameters can be reduced. Uncertainties in nuclear data should be checked to make sure they are reasonable (as discussed above). Users need sufficient covariance data to enable them to perform reasonable data adjustment. The covariances should be given not only for the cross sections but also for the angular distributions and the fission spectra.

O. Cabellos talked about various applications for uncertainty analysis including decay and transmutation that require fission product yields and decay data uncertainties in addition to the reaction data. Target accuracies were listed for ADS applications. The nuclear data community can expect that specific requests for format extensions will arise for use in inventory codes, particularly regarding correlations.

D. Muir briefly mentioned the features of the Global Assessment of Nuclear Data Requirements (GANDR), including the mathematical basis. The focus was on a formalism that enables assessing the impact of a single item of data on total system uncertainty, in the case where all data are correlated.

V. Zerkin presented the current status of software for on-line display of covariance information from the IAEA web server. He mentioned that, unfortunately, the information on experimental covariances is rather scarce. In addition, some information was lost during the migration of the database to a different platform. User-needs and the software developments in progress were listed in the presentation.

S. Simakov presented an example of the use of experimental data covariances to calculate spectrum-averaged nu-bar and the strong bias introduced if experimental correlations are neglected. Further development of the EXFOR database is needed. Guidance to the experimentalists on how to provide the information must be provided.

N. Otsuka described the current effort by the NRDC network to address the storage of partial uncertainties (split by the different sources and types), ratio data, time-of-flight spectra and old experimental covariances (when available). Formats for more elaborate covariance representation are being developed.

S. Ganesan discussed the ongoing effort in India to utilize covariance information in their nuclear data application programs, and to educate the scientific community there on the importance of covariance data in both nuclear data evaluations and applications. To this end, a workshop on covariances is held at Vel-Tech University in December 2010, and additional workshops on both covariances and evaluation methodology are being contemplated for the future. It was pointed out that India has the manpower to assist in the worldwide experimental data compilation effort under the auspices of EXFOR.

V. Maslov pointed out the importance of knowing and dealing with the uncertainties in fission neutron spectra when assessing the overall uncertainties of calculated integral fission data and before undertaking data evaluations and adjustments based on cross section uncertainties alone. Several examples were given to illustrate this issue.

The ensuing discussion on the application of covariances addressed the following:

- Documentation and instructions to authors of experimental data on how to prepare uncertainty information must be easily accessible (e.g. on the Web). Instructions should include practical examples. It was noted that a collaborative project to produce a journal article for *Nuclear Data Sheets* along this line is in progress, to be submitted for publication by 2012.
- The EXFOR formats should be flexible enough to accommodate information as provided by the experimenters. They should be extended to accommodate the full explicit covariance matrix, if provided by the authors or, alternatively, data required by a recipe for constructing covariance matrices based on providing partial error and correlation components.
- Authors of experimental data are urged to provide partial components of the uncertainties as well as correlations that can enable generation of a full covariance matrix.
- Authors of experimental data are urged to provide the data that they actually measure as the primary data (e.g. ratios) in addition to the final quantity (e.g. cross section) and the monitor data numerical values (e.g. reference cross sections).
- NRDC compilers should be instructed that it is mandatory to seek and compile uncertainty components and covariance information in computer-retrievable form.
- There is a need to search and assess systematic uncertainties for existing entries in the EXFOR database and enter them into the database in computer-retrievable form. The first step is to check the consistency of keyword usage for partial components, second to code the information available in free text, third to scan the original literature for information that was provided but not coded, and fourth to take remedial action when sufficient information is not available.
- The present computational format (C4) should be extended to accommodate partial uncertainty information consistent with that available in EXFOR. In addition, a new format should be developed, capable of accommodating experimental covariance information.

- In the ENDF File 40 it is not possible to define cross-reaction and cross-material correlations, which might be a problem in some activation libraries. This problem needs to be addressed.
- In order to calculate the uncertainties in dpa, the uncertainties in the recoil spectra are needed. When recoil spectra are given in the evaluations, they do not exhibit angular dependence, therefore their uncertainties can be given in ENDF File 35, but so far this possibility has not been exploited. This might be needed in the future. The evaluators should consider evaluating MF35 for particle and recoil emission spectra.

3. Summary of Recommendations

1. The covariances produced in the evaluation process must be reasonable, which implies that the covariance matrix must fulfill the following conditions:
    - The covariance matrix must be at least semi-positive definite on the evaluator’s energy grid. In the case of resonance covariances, the criterion refers to the resonance covariance matrix and not the cross section covariance matrix derived from it.
    - Uncertainties of broad-group average cross sections should be consistent with the uncertainties of the relevant experimentally-measured values, when available. These include thermal cross section, resonance integrals and ^{252}Cf spontaneous fission spectrum averaged cross sections and other spectrum-averaged cross sections measured in well-characterized irradiation facilities.
    - Additional constraints for defining reasonable uncertainties can refer to covariances on a denser energy grid, checking on minimum and maximum variance and large jumps in the variance.

2. Energy-dependence of unresolved resonance parameters should be allowed. This requires an ENDF-6 format extension for File 32.

3. Time-of-flight measurements should be archived in EXFOR according to the procedures proposed by IRMM and IAEA and reviewed by the Organization for Economic Co-operation and Development WPEC SG-36.

4. The IAEA should consider organizing an activity to further elaborate the comparison of the various proposed evaluation methods.

5. The issue of complete absence of any provisions to specify uncertainties of the thermal scattering law data raises a strong need to define formats and prepare a test covariance evaluation for testing them.

6. The IAEA should continue to support activities to correct errors and to complete uncertainty information in the EXFOR database, in the spirit of the work of the Organization for Economic Co-operation and Development WPEC SG-30.

7. The IAEA should continue to monitor user requirements and recent developments in nuclear data evaluation pertaining to radiation dosimetry, and to maintain the international dosimetry library.

8. Documentation and instructions to authors of experimental data on how to prepare uncertainty information should be drafted and made easily accessible (e.g. on the IAEA website). Instructions should include practical examples.

9. The EXFOR formats should be flexible enough to accommodate information as provided by the experimenters. The EXFOR format should be extended to accommodate the full explicit covariance matrix, if provided by the authors or, alternatively, data required by a recipe for constructing covariance matrices based on providing partial error and correlation components.

10. Authors of experimental data are urged to provide partial components of the uncertainties and correlation information as needed to generate the full covariance matrix.

11. Authors of experimental data are urged to provide the data that they actually measure as the primary data (e.g. ratios) in addition to the final quantity (e.g. cross sections) and the monitor data numerical values (e.g. reference cross sections).

12. The NRDC compilers should be instructed that it is mandatory to seek and compile uncertainty components and covariance information in computer-retrievable form.

13. The activity to assess systematic uncertainties for existing entries in EXFOR database and enter them into the database in computer-retrievable form should continue.

14. The present computational format (C4) should be extended to accommodate partial uncertainty information consistent with that available in EXFOR. In addition, a new format should be developed, capable of accommodating experimental covariance information.

15. The possibility of defining cross-reaction and cross-material correlations in ENDF File 40 should be addressed.

16. Evaluators should consider evaluating MF35 for particle and recoil emission spectra.

Annex A

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Technical Meeting on
Neutron Cross-Section Covariances

IAEA Headquarters, Vienna, Austria
27 – 30 September 2010
Meeting Room A0742

Preliminary AGENDA

Monday, 27 September

08:30 – 09:30 **Registration** (IAEA Registration Desk, Gate 1)

09:30 – 10:00 **Opening Session**
- Welcome: NDS Section Head R.A. Forrest
- Meeting logistics and general remarks: R. Capote
- Election of Chairman and Rapporteur
- Discussion and adoption of the Agenda (Chairman)

10:00 – 10:45 *Coffee break and administrative matters*

10:45 – 12:45 **Session 1: Introduction and Overview**
- Introductory Remarks: (D. Smith, 30 min)
- Evaluations for the JENDL-4 Library (O. Iwamoto, 60 min)
- Discussion

12:45 – 14:00 *Lunch*

14:00 – 15:30 **Session 2: Resonance and unresolved resonance region**
- P. Schillebeeckx (20 min)
- C. de Saint-Jean (20 min)
- M. Herman (20 min)
- Discussion

15:30 – 16:00 *Coffee break*

16:00 – 18:00 **Session 2 (cont'd): Resonance and unresolved resonance region**
Discussion

Tuesday, 28 September

09:00 – 10:30 **Session 3: Fast neutron region**
- R. Capote (20 min)
- A. Koning (20 min)
- Discussion

10:30 – 11:00 *Coffee break*

11:00 – 12:45 **Session 3 (cont'd)**: **Fast neutron region**
Discussion

12:45 – 14:00 *Lunch*

14:00 – 15:30 **Session 3 (cont’d): Fast neutron region**
Discussion

15:30 – 16:00 *Coffee break*

16:00 – 18:00 **Session 3 (cont’d): Fast neutron region**
Discussion

19:00 ***Dinner at a Restaurant***

Wednesday, 29 September

09:00 – 10:30 **Session 4: Users’ perspectives**
- P. Griffin (20 min)
- G. Manturov (20 min)
- O. Cabellos (20 min)
- Discussion

10:30 – 11:00 *Coffee break*

11:00 – 12:45 **Session 4 (cont’d): Users’ perspective**
- D. Muir (20 min)
- Visual tools for uncertainties @ IAEA/NDS (V. Zerkin, 15 min)
- Nu-bar Data Uncertainties (S. Simakov, 10 min)
- Discussion

12:45 – 14:00 *Lunch*

14:00 – 15:30 **Session 4 (cont’d): Users’ perspective**
Discussion

15:30 – 16:00 *Coffee break*

16:00 – 18:00 **Session 4 (cont’d): Users’ perspective**
Discussion

Thursday, 30 September

09:00 – 10:30 **Session 5: Drafting of the technical document**

10:30 – 11:00 *Coffee break*

11:00 – 12:45 **Session 5 (cont’d): Drafting of the technical document**

12:45 – 14:00 *Lunch*

14:00 – 15:00 **Session 5 (cont’d): Drafting of the technical document**
15:00 – 16:00 **Session 6: Conclusions and closing of the meeting**

ANNEX B

Technical Meeting on
“Neutron Cross Section Covariances”
IAEA, Vienna
27 – 30 September 2010

LIST OF PARTICIPANTS

AUSTRIA
Helmut LEEB
Atominstitut, TU Wien
Wiedner Hauptsatrasse 8-10
A-1040 Vienna
Tel: +43 1 58801 14258
E-mail: helmut.leeb@tuwien.ac.at

BELARUS
Vladimir MASLOV
Joint Institute for Power and Nuclear Research-Sosny
99 Academician
A.K. Krasin Str.
Minsk BY-220109
Tel: +375 17 2994441
E-mail: maslov@bas-net.by

CHINA
GE ZHIGANG
China Institute of Atomic Energy
China Nuclear Data Center
PO Box 275-41
Beijing 102413
Tel: +86 10 69357275
E-mail: gezg@ciae.ac.cn

XU RUIRUI
China Institute of Atomic Energy
China Nuclear Data Center
PO Box 275-41
Beijing 102413
Tel: +
E-mail: xuruirui@ciae.ac.cn

FRANCE
Eric BAUGE
DPTA/SP, CEA-Centre
Ile-de-France, Bruyeres-le-Chatel
91297 Arpajon Cedex
Tel: +
E-mail: eric.bauge@cea.fr

Cyrille DE SAINT JEAN
CEA Cadarache
13108 St Paul lez Durance Cedex
Tel: +33 04 42257000
E-mail: cyrille.de-saint-jean@cea.fr

Gilles NOGUERE
CEA de Cadarache
DEN/DER/SPRC/LEP
13108 St Paul lez Durance Cedex
Tel: +33 44 2252777
E-mail: gilles.noguere@cea.fr

GERMANY
Alexander KONOBEEV
Institut für Neutronenphysik und Reaktortechnik
Forschungszentrum Karlsruhe
Postfach 3640
76021 Karlsruhe
Tel: +49 724782 2638
E-mail: konobeev@inr.fzk.de

INDIA

Srinivasan GANESAN
Nuclear Data Section
Reactor Physics Design Division
5th Floor, Central Complex
Bhabha Atomic Research Centre (BARC)
Theoretical Physics Division
Trombay, Mumbai-400085
Tel: +91 22 25505151 and 25595002
E-mail: ganesan@barc.gov.in

JAPAN

Osamu IWAMOTO
Japan Atomic Energy Research Institute
2-4 Shirakata, Tokai-mura, Naka-gun
Ibaraki-ken 319-1195
Tel: +
E-mail: iwamoto.osamu@jaea.go.jp

NETHERLANDS

Arjan KONING
NRG Nuclear Research and
Consultancy Group
Westerduinweg 3
PO Box 25
1755 ZG Petten
Tel: +31 224 564051
E-mail: koning@nrg.eu

RUSSIA

Gennadi MANTUROV
Institute of Physics and Power Engineering
Bondarenko Sq. 1
Obninsk 249033
Kaluga Region
Tel: +
E-mail: mant@ippe.ru

SLOVENIA

Andrej TRKOV
Jožef Stefan Institute
Java 39
1000 Ljubljana
Tel: +386 1 5885324
E-mail: andrej.trkov@ijs.si

SPAIN

Oscar CABELLOS
Universidad Politecnica de Madrid
Nuclear Engineering Department
C/Jose Gutierrez Abascal 2
Madrid 28006
Tel: +34 913363108
E-mail: cabellos@din.upm.es

USA

Michal HERMAN
National Nuclear Data Center
Brookhaven National Laboratory
Bldg 197 D
P.O. Box 5000
Upton, NY 11975-5000
Tel: +1 631 344 2802
E-mail: mwherman@bnl.gov

Douglas MUIR
9229 Rosewater Lane
Jacksonville
FL 32256
Tel: +1 904 647 7534
E-mail: douglasmuir@comcast.net
dwmuir@mailaps.org

Patrick GRIFFIN
Sandia National Laboratories
PO Box 5800
Albuquerque
NM 87185
Tel: +1 505 845 9121
E-mail: pjgriff@sandia.gov

Luiz LEAL
Oak Ridge National Laboratory
Nuclear Data Group
Nuclear Science and Technology Division
Building 5700, Mail Stop 6170
PO 2008, OAK RIDGE
TN 37831-6170
Tel: +1 865 547 5281
E-mail: leallc@ornl.gov

INTERNATIONAL ORGANIZATION

Peter SCHILLEBEECKX
EC-JRC-IRMM
Neutron Physics Unit
Retieseweg 111
2440 GEEL
Tel: +
E-mail: peter.schillebeeckx@ec.europa.eu

CONSULTANT

Don SMITH
Nuclear Engineering Division
Argonne National Laboratory
1710 Avenida del Mundo #1508
Coronado, California 92118-3073
USA
Tel: +1 619 435 6724
E-mail: Donald.l.smith@anl.gov

Vladimir PRONYAEV
Centr Jadernykh Dannykh
Fiziko-Energeticheskij Institut
Ploshchad Bondarenko
249 033 Obninsk, Kaluga Region
RUSSIA
Tel:
E-mail: pronyaev@ippe.ru

IAEA

Roberto CAPOTE NOY
Nuclear Data Section
Division of Physical and Chemical Sciences
Wagramer Strasse 5
1400 Vienna
Tel. +43-1-2600 21713
Fax +43-1-2600 7
E-mail: r.capotenoy@iaea.org

IAEA (cont'd)

Stanislav SIMAKOV
Nuclear Data Section
Division of Physical and Chemical Sciences
Wagramer Strasse 5
1400 Vienna
Tel. +43-1-2600 21717
Fax +43-1-2600 7
E-mail: s.simakov@iaea.org

Viktor ZERKIN
Nuclear Data Section
Division of Physical and Chemical Sciences
Wagramer Strasse 5
1400 Vienna
Tel. +43-1-2600 21714
Fax +43-1-2600 7
E-mail: v.zerkin@iaea.org

Svetlana DUNAEVA
Nuclear Data Section
Division of Physical and Chemical Sciences
Wagramer Strasse 5
1400 Vienna
Tel. +43-1-2600 21727
Fax +43-1-2600 7
E-mail: s.duneava@iaea.org

Naohiko OTSUKA
Nuclear Data Section
Division of Physical and Chemical Sciences
Wagramer Strasse 5
1400 Vienna
Tel. +43-1-2600 21715
Fax +43-1-2600 7
E-mail: n.otsuka@iaea.org

ANNEX C

Summary Reports

1. Covariances on Nuclear Reaction Model Parameters: General Description and focus on URR

*C. De Saint Jean, G. Noguere, P. Archier, B. Habert, L. Leal**
CEA, DEN, CEA Cadarache, F-13108 Saint Paul lez Durance, France
**Oak Ridge National Laboratory, USA*

A recurrent puzzle for nuclear data evaluators is to take into account all uncertainties (including experimental ones) and propagate them to nuclear reaction model parameters or cross sections. In addition, mass production techniques developed for adding uncertainty information in all Evaluated Nuclear Data Files induced a lack of confidence in what are sometimes called low fidelity covariances. Furthermore, a major drawback found by reactor physicists is that most of the time integral experiments were not taken into account sufficiently soon in the evaluation process, giving rise to unexpected discrepancies.

In the energy range of interest for reactor applications, cross-section data are based on nuclear reaction models (R Matrix, Optical Model, Transmission models) with parameters not always predicted by theory. These model parameters are evaluated, as well as their uncertainties, by using a-priori guesses such as model knowledge, literature information, and systematic data uncertainty together with the use of experimental data. These experiments may give rise to statistical and systematic uncertainties due to experimental parameters, such as for example normalisation, background reduction, etc which are referred to as nuisance parameters.

In the process of evaluating model parameters correlations based on experimental data adjustments a great deal of work is devoted to the treatment of these nuisance parameters. Various mathematical techniques were developed such as retroactive analysis, marginalisation (Analytical or Monte-Carlo) in various analysis codes (Sammy, Refit and Conrad) to properly account for the nuisance parameters in the data evaluation process. The proper treatment of these uncertainties gives rise to quite high level of uncertainties on modelling the cross sections (a few percent). An additional possibility is thus to use clear and dedicated semi-integral (thermal cross sections measurements) or integral experiments (Minerve, Eole, Masurca, Profil in Phenix reactor). Conrad and partly Sammy are able to treat in the same mathematical framework both microscopic and semi-integral or integral experiments.

Additional difficulties arise when treating the unresolved resonance range:

- Resolved and unresolved resonance range connection → from a statistic of parameters to average parameters,
- Unresolved resonance and continuum range connection → Bad knowledge of average parameters give rise to wrong self-shielding corrections,
- Endf format deficiencies → no energy dependant average parameters covariances, l dependant scattering radius with no uncertainty.

For actinides, in addition, one may think of lowering the unresolved resonance range limit for uncertainty evaluations. Average parameters may thus be used as vectors of uncertainties even in some part of the resolved resonance range.

2. Total Monte Carlo and related applications of the TALYS code system

Arjan Koning, NRG

The possibilities of the TALYS code system were presented. A high degree of automation and reproducibility enables to approach various nuclear data issues in an efficient way. An important one is covariance data, and the two main outlets of the code system for this are the TALYS Evaluated Nuclear Data Library, TENDL, and Total Monte Carlo.

TENDL is a complete nuclear reaction database for all projectiles and basically all nuclides in the nuclide chart. A complete representation of covariance data is given in TENDL for MF31-35. The global approach does not allow to perform too detailed studies on a nuclide-by-nuclide level, and general models for uncertainties for TALYS parameters and resonance parameters are used. A similar approach is performed for fission quantities such as the pfns and nubar. However, for many nuclides a set of adjusted model parameters + uncertainties + "non-physical evaluation actions" is stored to be used in future versions of TENDL. Implementation of Unified Monte Carlo is a remaining challenge.

Total Monte Carlo means that the random variation of TALYS and resonance parameters, experimental data, ENDF-6 data file creation, processing and applied reactor calculation is seen as a single loop in a Monte Carlo process. This entirely avoids the issue of determining and storing covariance data of cross sections and other quantities in the ENDF-6 format. The only correlations that need to be established are the ones at the beginning of the loop: parameter correlations and correlations of experimental data. Of course, correlations between e.g. k-eff, power rates, and any other quantity will emerge at the end of the process. Full uncertainty propagation examples were given for ICSBEP criticality benchmarks and the sodium cooled fast reactor (SFR), with probability distributions for k-eff, the void coefficient and final inventories.

A short demonstration of a third possibility was given: variation of cross sections within their assigned uncertainties allows performing a Monte Carlo search for the best possible library with respect to integral data. The method was presented for Pu-239, and merely demonstrates current computational possibilities; since it is too early to claim that the found "best" library is indeed better than the existing ones.

3. Summary for Covariance Evaluation in China Nuclear Data Center

Xu Ruirui, Ge Zhigang
China Nuclear Data Center, China Institute of Atomic Energy, Beijing, China

• Introduction to the current covariance evaluation in China Nuclear Data Center

To determine the uncertainty of neutron cross sections for modern nuclear data application, a new evaluation system, COVAC, is being developed at China Nuclear Data Centre (CNDC) to achieve the covariance files **mainly for structure and fission nuclides** in CENDL. In this system, experimental data including their errors were firstly pre-analyzed and handled via some available tools. It is worth mentioning that different approaches were developed to deal with the data and errors from different experimental techniques, such as activation method and TOF; at the same time, the various reaction data were also treated in different ways. Secondly, one subsystem－SEMAW, was especially designed to calculate sensitivity matrices of various theoretical model parameters for different nuclear reaction codes (the UNF code series, DWUCK and ECIS are currently incorporated in SEMAW). The final covariance could be obtained through the generalized least-squares method (GLS) and Bayesian method, and the uncertainties and correlations from experimental evaluation and theoretical calculation process were integrated by COVAC and matrices formatted in ENDF-6. As an example, the covariance files for n+^{48}Ti have been evaluated with high fidelity to check COVAC, and it will serve producing covariance for more nuclides in CENDL in the near future.

So far, our methodology can be applicable to the fast neutron range; the resonance range is under investigation.

• Future plan

1. The covariance evaluation system for the whole mass region is being constructed in CNDC. The middle-heavy and fission nuclei can be obtained by COVAC. As for the light nuclei, another system based on the R-matrix theory will be completed to evaluate the nuclear data and relevant covariance, and the experimental data evaluation can share the similar methods with COVAC. In addition, we will introduce new codes in the middle-high energy region, such as MEND by Nankai University, to achieve more complicated reaction mechanisms in the current covariance evaluation.
2. Related tools used to evaluate and analyze the covariance information from experimental data are being improved and used in the practical evaluation. The evaluated covariance files for some nuclei will be released in the future version CENDL.
3. Apart from the integral experimental benchmark, a standard from the microscopic physical analysis and measurements for reactions is also necessary to verify the obtained covariance files. The nuclear data process codes used for covariance file will be improved and the benchmark and validation for the evaluated covariance file will be performed.

4. Covariance Evaluation for Actinide Nuclear Data in JENDL-4

Osamu Iwamoto
Japan Atomic Energy Agency

The JENDL-4.0 [1, 2] was released in March 2010. It provides neutron nuclear data for 79 actinides from Ac to Fm. All of the actinides include covariance data. The covariance data were evaluated for reaction cross sections, resonance parameters, angular distributions of elastic scattering, average number of neutrons per fission, and prompt fission neutron spectra. They were deduced basically based on the consistent methodologies with the nuclear data evaluations. Statistical processing of experimental data sometimes gives unacceptably small uncertainty compared with experimental data. They may arise from ignoring unknown errors and correlation of experimental data and also from the modeling errors. The covariance data obtained from statistical estimation using the least-squares method were sometimes modified to be reasonable taking account of consistency with dispersion of experimental data, which may reflect the uncertainties of the data.

For the fast neutron fission cross sections of 6 major actinides of ^{233,235,238}U and ^{239,240,241}Pu were evaluated simultaneously using both cross section and their ratio data with the least-squares fitting code SOK. It gave the covariance matrices that have cross correlations between different nuclei included in the analyses. For the minor actinide, the least-squares fitting code GMA was used for fission cross section evaluation for fast neutrons. The covariance data were obtained from the calculations at the same time. For other reaction cross sections, covariance matrices were evaluated using CCONE-KALMAN code system. Sensitivities to model parameters were calculated by CCONE code and used to estimate covariance matrices of the parameters with KALMAN code. Covariance matrices for other data such as resonance parameters and average numbers of fission neutrons were also evaluated based on experimental data. The evaluated covariance data were compiled to the ENDF-6 format files and included in JENDL-4.

[1] K. Shibata, O. Iwamoto, T. Nakagawa *et al.*, “JENDL-4.0: A new library for nuclear science and engineering”, *J. Nucl. Sci. Technol.* (2011) in press.

[2] O. Iwamoto, T. Nakagawa, N. Otuka, S. Chiba, “Covariance evaluation for actinide nuclear data in JENDL-4”, Proceedings of the International Conference on Nuclear Data for Science and Technology, April 26-30, 2010, Jeju Island, Korea (ND2010).

5. Experimental Data Covariances: impact on nuclear responses and comparison with models. Example: ^{237}Np(n,f) prompt fission neutron yield

S.P. Simakov, V. Zerkin, N. Otsuka, S. Dunaeva

The goal of the present contribution was to demonstrate the impact of experimental data covariances on the derived nuclear responses and validation of the hypotheses. For this purpose the prompt neutron production yield ν_p for ^{237}Np(n,f) reaction has been selected as an example. Among seven known measurements in the energy range 1 to 20 MeV only authors of work [1] have estimated the covariances. ν_p for ^{237}Np has been measured relative to ^{252}Cf using two fission chambers located inside the polyethylene cylinder with sixteen ^{3}He detectors to slow down and count fission neutrons. The incident neutron beam was produced via T(p,n) and D(d,n) reactions and collimated by the hole in the shield.

Due to the measurement relative to ^{252}Cf, the authors had to correct the final results for: dependence of detector efficiency on ν_p energy spectra, positions and sizes of fission layers, dead time of counters, fission fragment registration efficiency and its dependence on energy and emission angle, etc. In total nine corrections and their uncertainties were estimated and classified either as stochastic (energy independent, e.g., statistical) or correlated (energy dependent, e.g., systematic). Finally 31×31 energy-energy correlation matrix was produced by the authors and compiled in EXFOR (Entry #40664). It could be retrieved and visualized by ZVView system [2] from IAEA/NDS web page http://www-nds.iaea.org/exfor/exfor.htm .

The stochastic and systematic uncertainties as well as ν_p for ^{237}Np measured at individual incident neutron energies are shown in the Figure below. Many applications require the calculation of functionals such as energy averaged neutron yield $\langle\nu_p\rangle$ with uncertainty $\Delta\langle\nu_p\rangle$. This essentially reduces stochastic component of $\Delta\langle\nu_p\rangle$ but preserves the systematic one at level of individual points if strong energy-energy correlations do exist, see Figure below. Artificial neglecting of correlations (i.e., non diagonal elements) results in a three times lower uncertainty for $\langle\nu_p\rangle$ weighted with a Maxwellian spectrum in interval 0.98 - 5.9 MeV:

$\langle\nu_p\rangle = 2.969 \pm 0.007\ (0.22\%)$, neglecting energy-energy correlations for experimental data
$\langle\nu_p\rangle = 2.969 \pm 0.022\ (0.76\%)$, using whole empirical covariance matrix

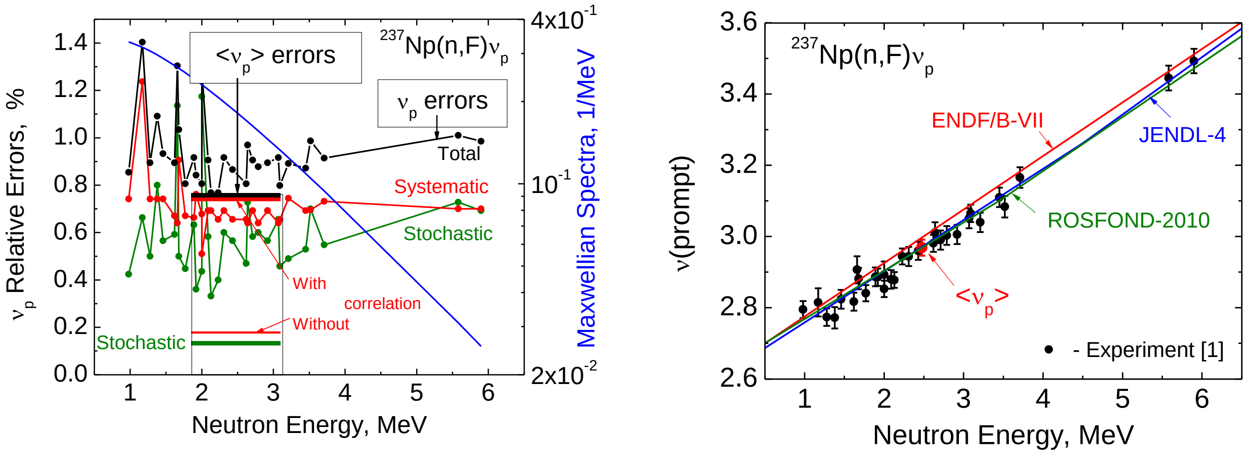

Figure: Relative uncertainties (left) and prompt neutron yield (right) for ^{237}Np(n,F) reaction versus incident neutron energy.
Points – experiment [1], histogram - $\langle\nu_p\rangle$, curves – evaluated data.

Covariances may impact on the hypothesis selection based on χ^2 criteria, if correlations are neglected or underestimated. Table shows χ^2 calculated with three different evaluations for $^{237}Np(n,F)\nu_p$. Ignorance of experimental energy-energy correlations (only diagonal elements) makes JENDL and ROSFOND more preferable over ENDF/B-VII, whereas taking into account the whole correlation matrix makes a choice among three evaluations practically equal.

Table. χ^2 for Evaluation vs. Experim. [1]

Evaluation	Whole Matrix	Only diag. Elements
ENDF/B-VII	7.2	4.2
JENDL-4	6.3	1.6
ROSFOND-2010	6.4	1.6

References

[1] V.G. Vorobyova, B.D. Kuzminov, V.V. Malinovskiy et al., INDC-CCP-0156, p. 44; EXFOR # 40664.

[2] V. Zerkin, "Multi-platform EXFOR-CINDA-ENDF", IAEA-NDS, Vienna, 1999-2010.

6. The Contribution of Individual Correlated Parameters to the Uncertainty of Integral Quantities

D. W. Muir
Argonne National Laboratory

A common application of neutron cross-section covariances is in calculating the variance, due to cross section uncertainties, of a calculated integral quantity z. Beyond this single number, it is often of interest to inquire as to the magnitude of the contributions to the variance of z arising from various portions of the data field. For example, one may want to know the impact of uncertainties in the full excitation function σ(E) for the ^{16}O(n,p) reaction on the uncertainty of k_{eff} in some reactor. Knowing this contribution would clearly be helpful in judging the benefit of performing a new measurement, calculation, or evaluation of σ(E).

Here we propose a procedure that is appropriate for determining the contribution from an identified parameter, or group of parameters, to the variance of z. Unlike alternative methods, this procedure can be applied without problems even when the data set is fully correlated.

Suppose that there are k parameters (i.e., cross sections). We begin with the simple case where there are no correlations present in the covariance library. If we neglect higher order derivatives, the total variance D(z) of an integral quantity z can be written

$$D(z) = S_1^2\, D(a_1) + S_2^2\, D(a_2) + \ldots + S_k^2\, D(a_k)\text{ , where} \tag{1}$$

$$S_i = \partial z / \partial a_i \tag{2}$$

In the uncorrelated case, the contribution of the uncertainty of one of the parameters, say a_i, to D(z) is simply the i-th term in the sum in Eq. (1).

The situation becomes considerably more complex when there are non-zero correlations in the data. The corresponding sum in this case has k^2 terms:

$$D(z) = \sum_{\substack{i=1,k \\ j=1,k}} S_i\, S_j\, \mathrm{cov}(a_i, a_j) \tag{3}$$

Here, it is not at all clear which term or terms should be identified as providing "the contribution of the i-th parameter to D(z)." Some reactor physicists have reacted to this situation by employing the idea of the "uncertainty profile,"

$$L(z, i) = \sum_{j=1,k} S_i\, S_j\, \mathrm{cov}(a_i, a_j) \tag{4}$$

If one forms a k x k square matrix **U**, with elements $u_{ij} = S_i\, S_j\, \mathrm{cov}(a_i, a_j)$, then L(z, i) is the sum of the elements of the i-th row of **U**.

This is an attractive approach for three reasons: First, the uncertainty profile L(z, i) is straightforward to calculate. Secondly, it provides a useful indicator of where the "action" is in the variance summation. Finally, the L(z, i) do actually sum up to the variance D(z). That is,

$$D(z) = \sum_{i=1,k} L(z, i) \tag{5}$$

These advantages, however, are offset by a serious disadvantage. Although L(z, i) has the units of variance, it is not a variance. For this reason, it cannot be guaranteed to be a positive quantity. The square root of L(z, i) is not a standard deviation and can even be imaginary. For a recent example of difficulties of this sort, see Ref. 1.

In the following, we propose an alternative to the uncertainty profile approach. This approach fits with the common sense definition of "contribution" and, at the same time avoids the mentioned mathematical problems. In particular, we propose to quantify the contribution of the uncertainty in a_k to the variance of z in terms of the "variance penalty" associated with our present, less-than-perfect knowledge of a_k. The variance penalty concept is closely related to the need to identify the parameters have the most leverage in improving the accuracy of our knowledge of z.

For the present purposes, it is helpful to partition the parameter column-vector **a** into n "passive" parameters **v** and m "active" parameters **w** (the parameters of particular interest), where n + m = k.

$$\mathbf{a}^{\mathbf{T}} = [\ \mathbf{v}^{\mathbf{T}}\quad \mathbf{w}^{\mathbf{T}}\ ] \tag{6}$$

The procedure we propose is the following:

1. Calculate the current value of the variance D(z) based on the current parameter covariances D(**a**).
2. Assume that the parameters of interest, **w**, are now re-measured with near-perfect precision.
3. Employ the covariance matrix of this near-perfect re-measurement as input to a calculation of the updated variance D(z') using the generalized method of least squares. (See, for example, Ref. 2.)
4. Calculate the variance penalty as P(z,**w**) = D(z) – D(z').

In carrying out this four-step procedure, straightforward application of the method of least squares leads to the following result:

$$P(z,\mathbf{w}) = \mathbf{S}\,\mathbf{H}\,\mathbf{S}^{T} \tag{7}$$

where **S** is the sensitivity vector defined in Eq. (2), and

$$\mathbf{H} = \begin{bmatrix} \mathrm{cov}(\mathbf{v},\mathbf{w})\ D^{-1}(\mathbf{w})\ \mathrm{cov}(\mathbf{w},\mathbf{v}) & \mathrm{cov}(\mathbf{v},\mathbf{w}) \\ \mathrm{cov}(\mathbf{w},\mathbf{v}) & D(\mathbf{w}) \end{bmatrix} \tag{8}$$

It is easy to show that variance penalty, thus defined, is itself a variance and, therefore, always positive. Since P(z,**w**) is positive, we can also define a standard deviation penalty as

$$\Delta(z,\mathbf{w}) = P(z,\mathbf{w})^{1/2} \tag{9}$$

We note from Eq. (8) that the variance penalty associated with the prior uncertainties in the data subset **w** involves, as expected, the entire covariance submatrix D(**w**). More interesting is the fact that the variance penalty also depends on the inverse of this matrix $D^{-1}(\mathbf{w})$ and on the covariance data occupying the off-diagonal blocks of D(**a**), namely, cov(**v**,**w**) and cov(**w**,**v**).

Recall that the uncertainty profile L(z, i) is computed simply as a weighted sum of k covariances. In contrast, the calculation of the variance penalty P(z,**w**) requires a matrix inversion and several matrix multiplications. However, the mathematical clarity of the variance-penalty approach, with its guarantee of a positive result, makes it attractive for general use in characterizing the contribution of uncertainty in data subset **w** to the variance of z.

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Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna
Austria

e-mail: services@iaeand.iaea.org
fax: (43-1) 26007
telephone: (43-1) 2600-21710
Web: http://www-nds.iaea.org