Covariances Obtained from an Evaluation of the Neutron Cross Section Standards

A. D. Carlson[1], S. A Badikov[2], Chen Zhenpeng[3], E. Gai[4], G. M. Hale[5], F.-J. Hambsch[6], H. M. Hofmann[7], T. Kawano[5], N.M. Larson[8], S. Y. Oh[9], V. G. Pronyaev[4], D. L. Smith[10], S. Tagesen[11], H. Vonach[11]

[1] National Institute of Standards and Technology, Gaithersburg, MD USA, [2] Central Research Institute of Management, Economics and Information, Moscow Russia, [3] Tsinghua University, Beijing, China, [4] Institute of Physics & Power Engineering, Obninsk, Kaluga Region, Russia, [5] Los Alamos National Laboratory, Los Alamos, NM, USA, [6] Institute for Reference Materials and Measurements, Geel, Belgium, [7] Erlangen-Nürnberg University, Erlangen, Germany, [8] Oak Ridge National Laboratory, Oak Ridge, TN, USA, [9] Korea Atomic Energy Research Institute, Yuseong, Daejeon, Republic of Korea, [10] Argonne National Laboratory, Argonne, IL, USA, [11] Vienna University, Vienna, Austria

Presented at The
Workshop on Neutron Cross Section Covariances
Port Jefferson, NY, June 26, 2008

NIST National Institute of Standards and Technology • Technology Administration • U.S. Department of Commerce

Outline

•Standards Evaluation Procedure.

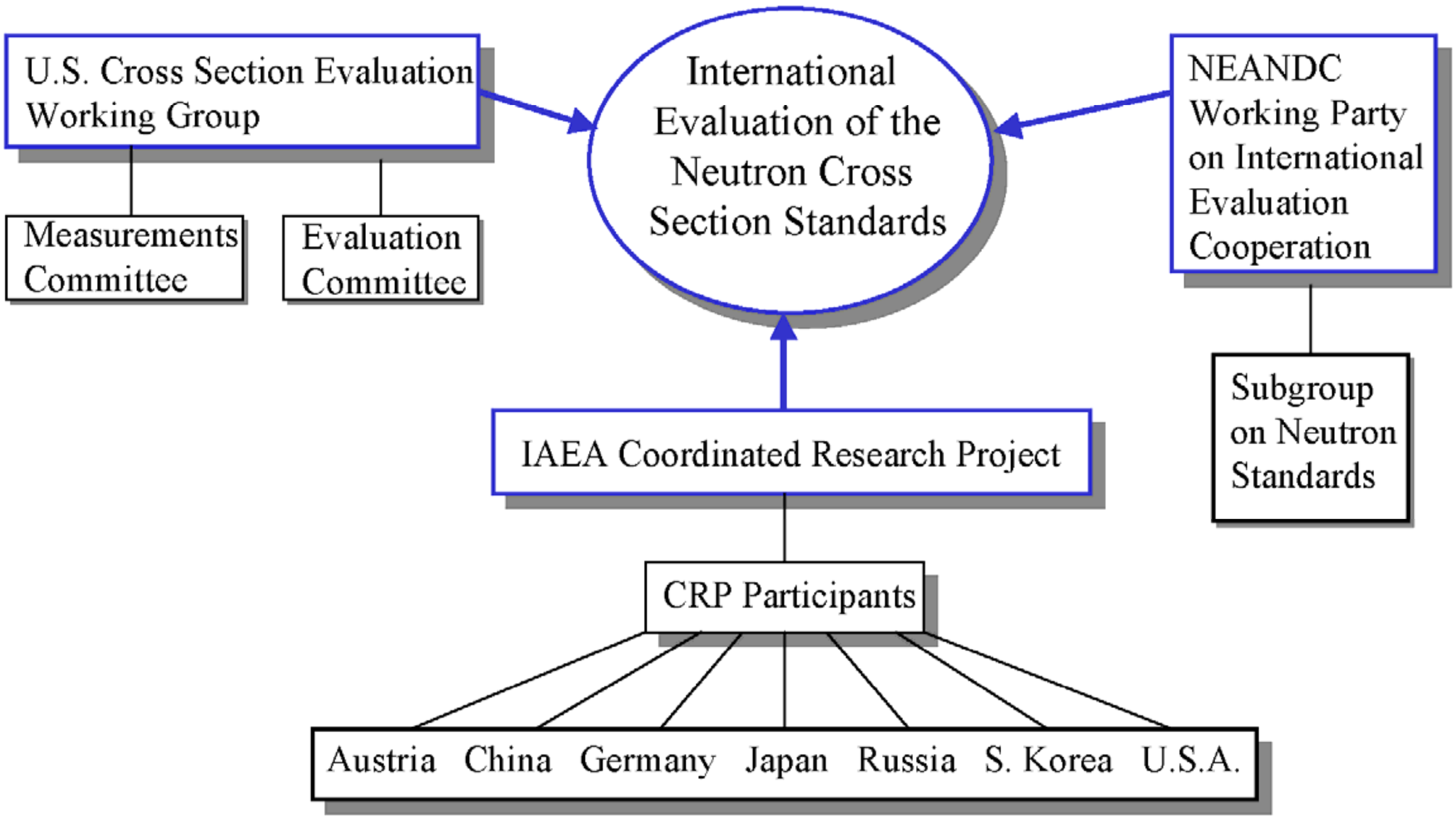
•Factors Affecting the Covariances Produced.

•The Small Uncertainty Problem.

•Results

•Summary

The Standards Evaluation



The Neutron Cross Section Standards

Reaction	Energy Range
H(n,n)	1 keV to 20 MeV
$^{3}He(n,p)$	thermal to 50 keV
$^{6}Li(n,t)$	thermal to 1 MeV
$^{10}B(n,\alpha)$	thermal to 1 MeV
$^{10}B(n,\alpha_1\gamma)$	thermal to 1 MeV
C(n,n)	thermal to 1.8 MeV
$^{197}Au(n,\gamma)$	thermal, 0.2 to 2.5 MeV
$^{235}U(n,f)$	thermal, 0.15 to 200 MeV
$^{238}U(n,f)$	2 to 200 MeV

Data Types Used in GMAP

Type	Data Type	Example
1	Absolute cross section	$\sigma_{nf}(^{235}U)$
2	Cross section shape	$c * \sigma_{n\alpha}(^{6}Li)$, c unknown
3	Absolute cross section ratio	$\sigma_{nf}(^{238}U) / \sigma_{nf}(^{235}U)$
4	Ratio shape	$c * \sigma_{nf}(^{235}U)/\sigma_{n\alpha}(^{6}Li)$ c unknown
5	Sum of cross sections	$\sigma_{tot}(^{6}Li) = \sigma_{nn}(^{6}Li) + \sigma_{n\alpha}(^{6}Li)$
6	Spectrum averaged cross section	$\sigma_{nf}(^{235}U)$ averaged over ^{252}Cf spont. fission spect
7	Absolute ratio of cross section/ sum of cross sections	$\sigma_{nf}(^{235}U) / \sigma_{n\alpha}(^{10}B)$, where $\sigma_{n\alpha}(^{10}B) = \sigma_{n\alpha_0}(^{10}B) + \sigma_{n\alpha_1}(^{10}B)$
8	Shape of Type 5 data	
9	Shape of Type 7 data	

Neutron Database

^{6}Li(n,t)

^{6}Li(n,n)

→ ^{6}Li total cross section

^{10}B(n,a$_{0}$)

^{10}B(n,a$_{1}$)

^{10}B(n,n)

→ ^{10}B total cross section

Au(n,γ)

^{235}U(n,f)

^{238}U(n,γ)

^{239}Pu(n,f)

R-matrix Evaluation Database

^{6}Li Total		^{10}B Total	
$^{6}Li(n,n)$	Integral Data	$^{10}B(n,n)$	Integral Data
$^{6}Li(n,n)$	Differential Data	$^{10}B(n,n)$	Differential Data
$^{6}Li(n,n)$	Polarization Data	$^{10}B(n,n)$	Polarization Data
$^{6}Li(n,t)$	Integral Data	$^{10}B(n,\alpha_0)$	Integral Data
$^{6}Li(n,t)$	Differential Data	$^{10}B(n,\alpha_0)$	Differential Data
$^{6}Li(n,t)$	Polarization Data	$^{10}B(n,\alpha_1)$	Integral Data
$^{4}He(t,n)$	Differential Data	$^{10}B(n,\alpha_1)$	Differential Data
$^{4}He(t,t)$	Differential Data	$^{7}Li(\alpha_0,\alpha_0)$	Differential Data
$^{4}He(t,t)$	Polarization Data	$^{7}Li(\alpha,\alpha_1)$	Differential Data
		$^{7}Li(\alpha,n)$	Differential Data

Factors Affecting the Covariances

- Database Studies
  - There are more than 430 data sets in the GMA database.
  - Each experiment was reviewed for uncertainty components.
  - The components were tabulated as a function of energy.
  - Known correlations were documented.
  - This information was used to obtain covariances for the experimental data.

Factors Affecting the Covariances (cont.)

- Discrepant data.
    - Work has been done to reduce problems with discrepant data. For the neutron database used for the GMA and RAC evaluations, an additional medium energy range correlation component was added for outliers. The length of the correlation component was determined from the energy dependency of the discrepancy. This increases the uncertainty of the results but only changes the cross section slightly.

Uncertainty Components for Set 523 in GMAP

```
5231984U5(N,F)          A.D.CARLSON ET AL.          84GEEL,PROC.
 1 1 0 1 16   67  8  0  0  0  0
 UNCERTAINTIES
 1 U5 MASS
 2 FF DET. BIAS
 3 FLIGHT PATH (GEOM.)
 4 COL. AREA (GEOM.)
 5 FF EXTRAPOLATION
 ENERGY DEP. UNCERT.
 3 STATISTICS
 4 FROM TIMING UNCERT.
 5 DUE TO TRANS. OF      MATERIALS IN BEAM
 6 DUE TO UNCERT. IN     ADC ZERO FOR BLACK DET.
 7 DUE TO UNCERT. IN     DEAD TIME CORR.
 8 FROM UNCERT. IN BD    EFFICIENCY
 9 FROM UNCERT. IN       FISSION CHAMBER BKGND
 10 FROM UNCERT IN       BD BKGND
 11 FROM UNCERT.IN SCATT. FROM MATERIAL IN F.C.
  1.2  .0  .0  .2  .5  .0  .0  .0  .0  .0 1  1  1  1  1  0  0  0  0  0
```

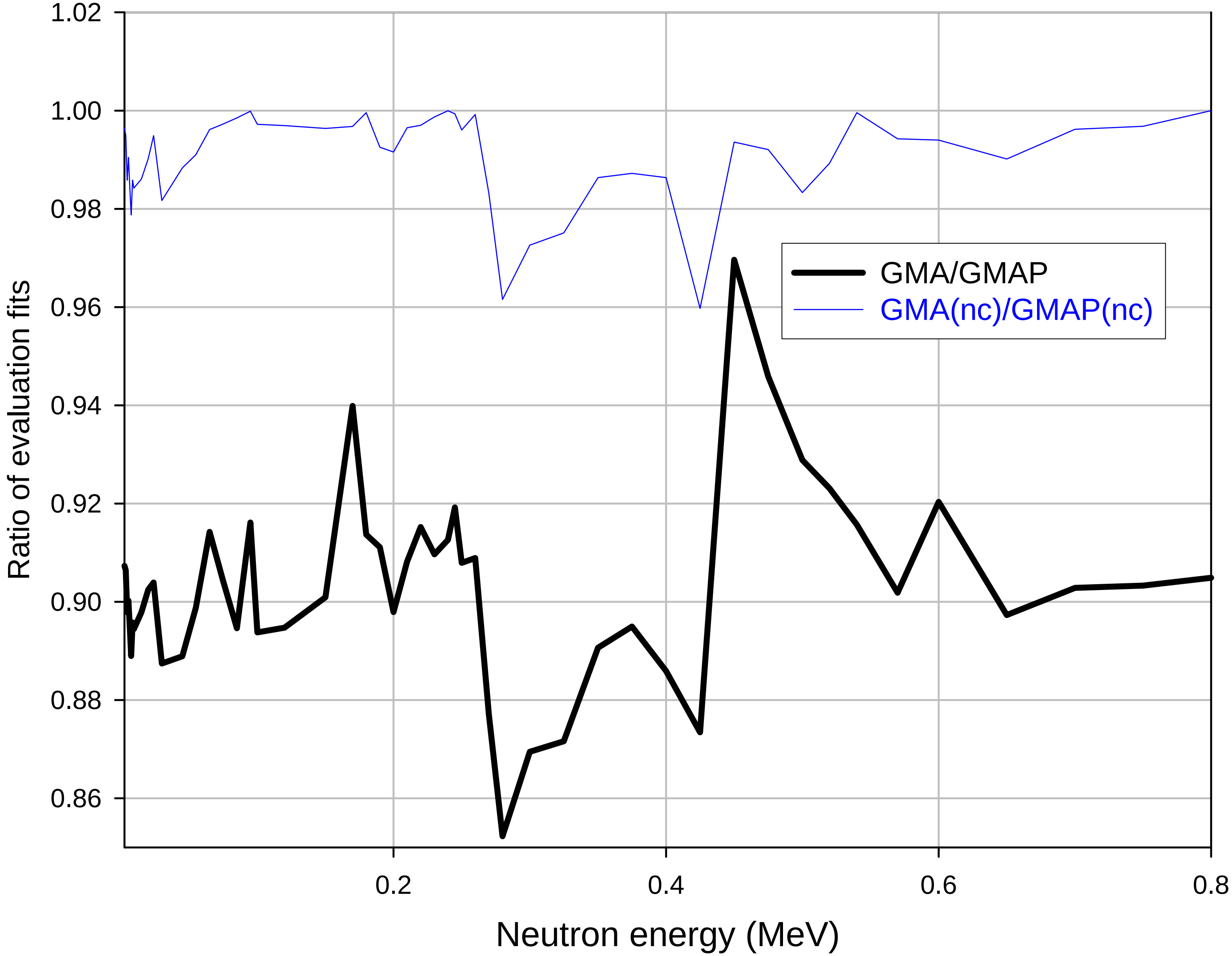
Tabulated Uncertainties in GMAP for Set 523

En	Sig	DE	Res	Stat	Tm. u.	Mat Tr	ADC 0	DTC.	BD eff	FC Bk	BD Bk	FC Sc	Tot. U.
.3097E+00	.1227E+01	.2	2.3	1.0	.4	.6	.5	.1	1.0	.3	.4	.1	2.2
.3245E+00	.1242E+01	.2	2.4	1.0	.4	.5	.5	.1	1.0	.3	.4	.1	2.2
.3391E+00	.1223E+01	.2	2.0	1.0	.3	.5	.5	.1	1.0	.3	.4	.1	2.1
.3534E+00	.1213E+01	.2	2.1	1.0	.3	.5	.5	.1	1.0	.3	.4	.1	2.1
.3686E+00	.1224E+01	.2	2.1	1.0	.1	.6	.4	.1	1.0	.3	.4	.1	2.1
.3840E+00	.1205E+01	.2	2.0	1.0	.2	.5	.4	.1	1.0	.3	.4	.1	2.1
.3996E+00	.1179E+01	.2	2.0	1.0	.1	.5	.4	.1	1.0	.3	.4	.1	2.1
.4171E+00	.1214E+01	.2	2.3	1.0	.1	.7	.4	.1	1.0	.3	.4	.1	2.2
.4367E+00	.1201E+01	.2	2.3	1.0	.4	.9	.4	.1	1.0	.3	.4	.1	2.3
.4556E+00	.1134E+01	.2	1.9	1.0	.7	.7	.3	.1	1.0	.3	.4	.1	2.3
.4727E+00	.1132E+01	.2	1.8	1.0	.7	.6	.3	.1	1.0	.3	.4	.1	2.2
.4897E+00	.1123E+01	.2	1.8	1.0	.4	.5	.3	.1	1.0	.3	.4	.1	2.1
.5065E+00	.1118E+01	.2	1.6	1.0	.4	.5	.3	.1	1.0	.3	.4	.1	2.1

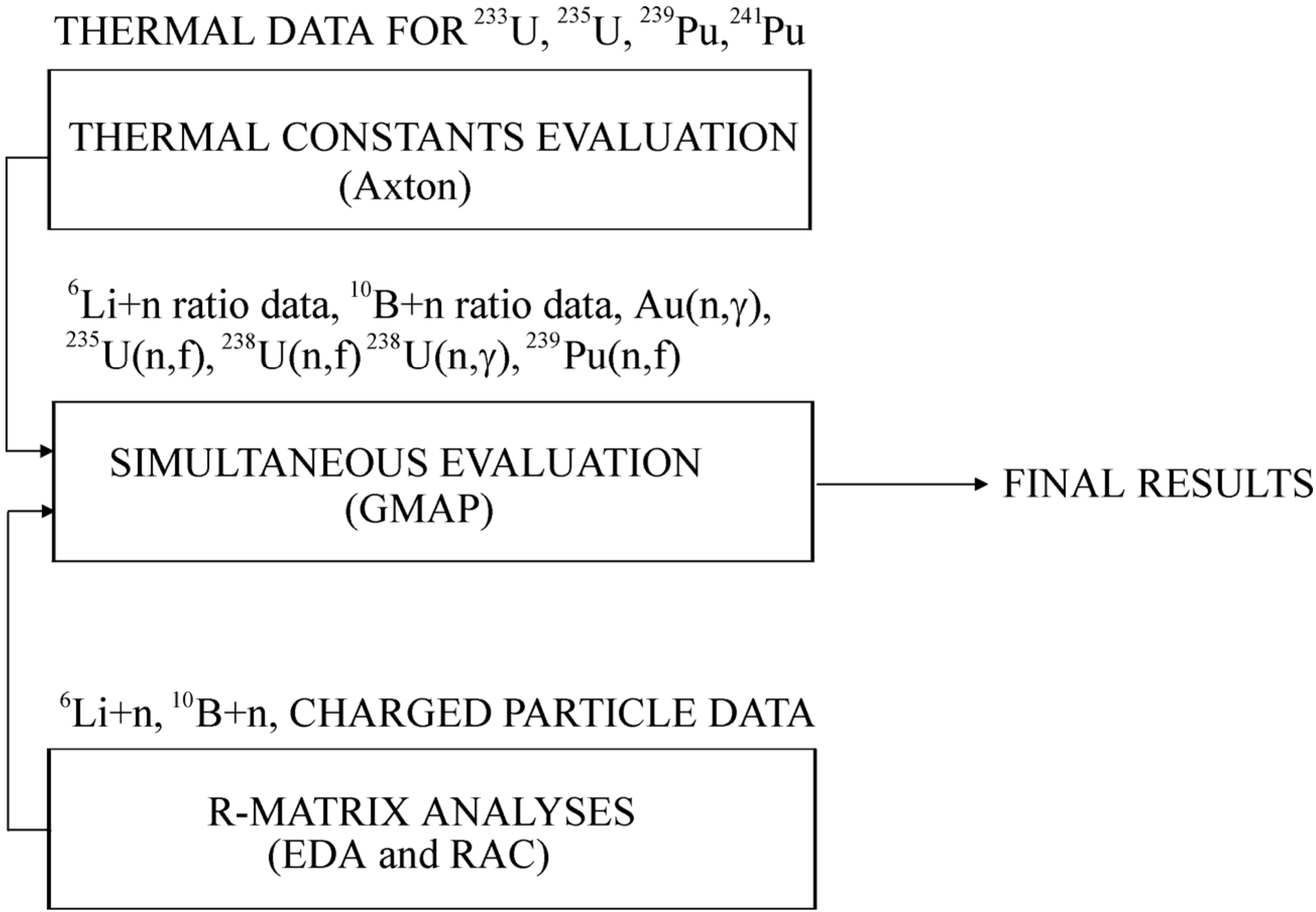
Factors Affecting the Covariances (cont.)

- Peelle's Pertinent Puzzle (PPP)
  - Noticed early in the evaluation activities.
  - Seen in model-independent LS analyses.
  - Results commonly from use of correlated-discrepant data.
  - Not present when measured primary observables (raw data) are used in the LS fitting
  - Several methods reduce the PPP effect and give similar results
    - Chiba-Smith
    - Box-Cox
    - Logarithmic transformation
  - Chiba-Smith method was used in the evaluation (in GMAP)
  - The additional uncertainty from the use of this method is small.

PPP Effect for a $^{6}Li(n,t)$ Database



New Standards Evaluation Procedure



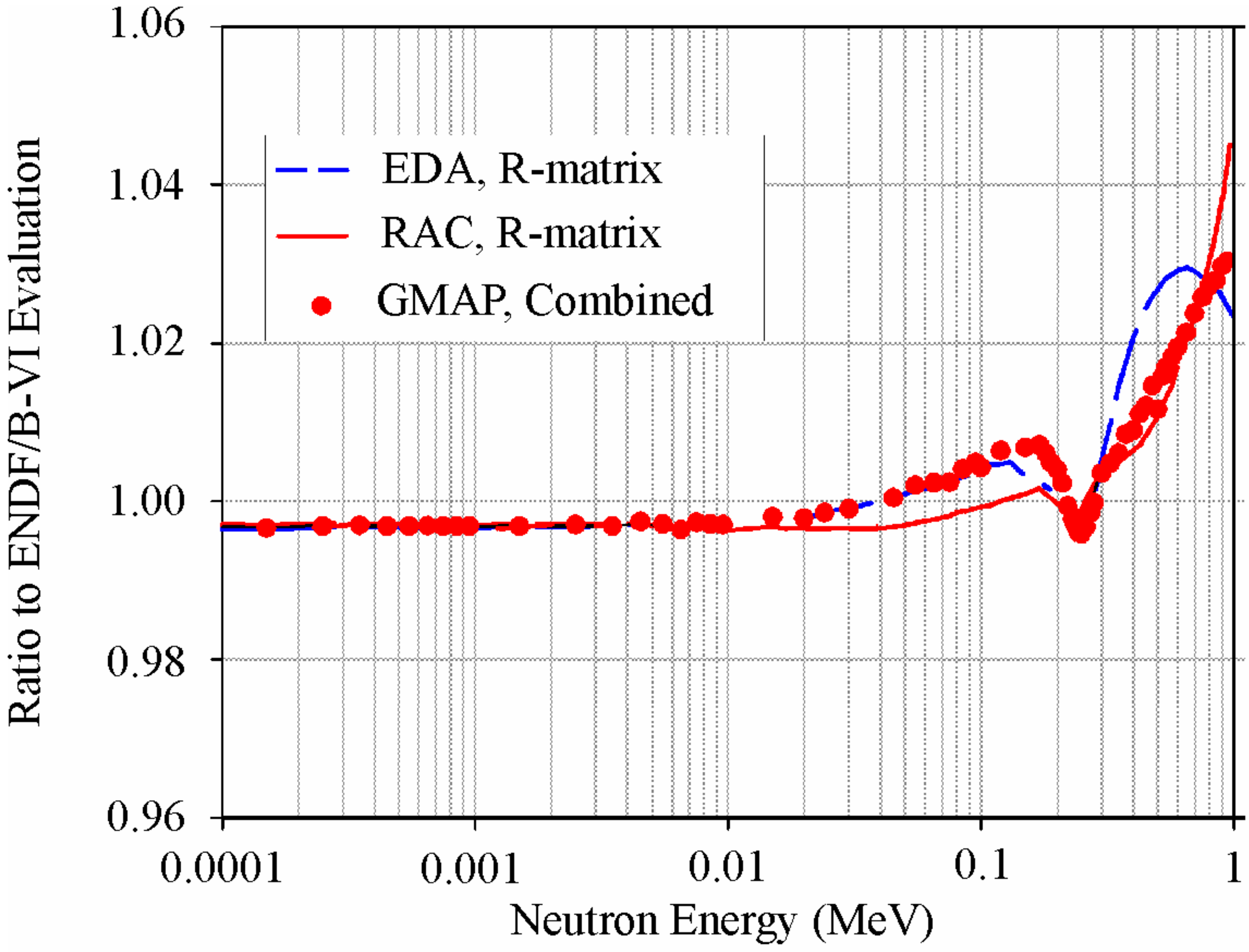
Factors Affecting the Covariances (cont.)

- The Evaluation Procedure
  - Reactions producing covariances were evaluated using GMAP.
  - There were three different sets of input data to GMAP.
    - R-matrix data (and covariances) from RAC and EDA.
    - An evaluation of the thermal constants (with covariances).
    - The portion of the GMA database containing data (and covariances) that the R-matrix codes could not use.
  - The R-matrix and GMAP databases were totally independent of each other. There were no common data sets and no data sets that have correlations between the R-matrix and GMAP databases.

Factors Affecting the Covariances (cont.)

- The Evaluation Procedure (cont.)
    - The RAC and EDA central values (cross sections) were not identical so, the average (unweighted) cross sections from these analyses were used for the R-matrix cross section input to the GMAP code. The RAC covariance matrix was used.
    - At each energy point, half the difference between the RAC and EDA results was treated as a model uncertainty which was added quadratically to the RAC total uncertainty.

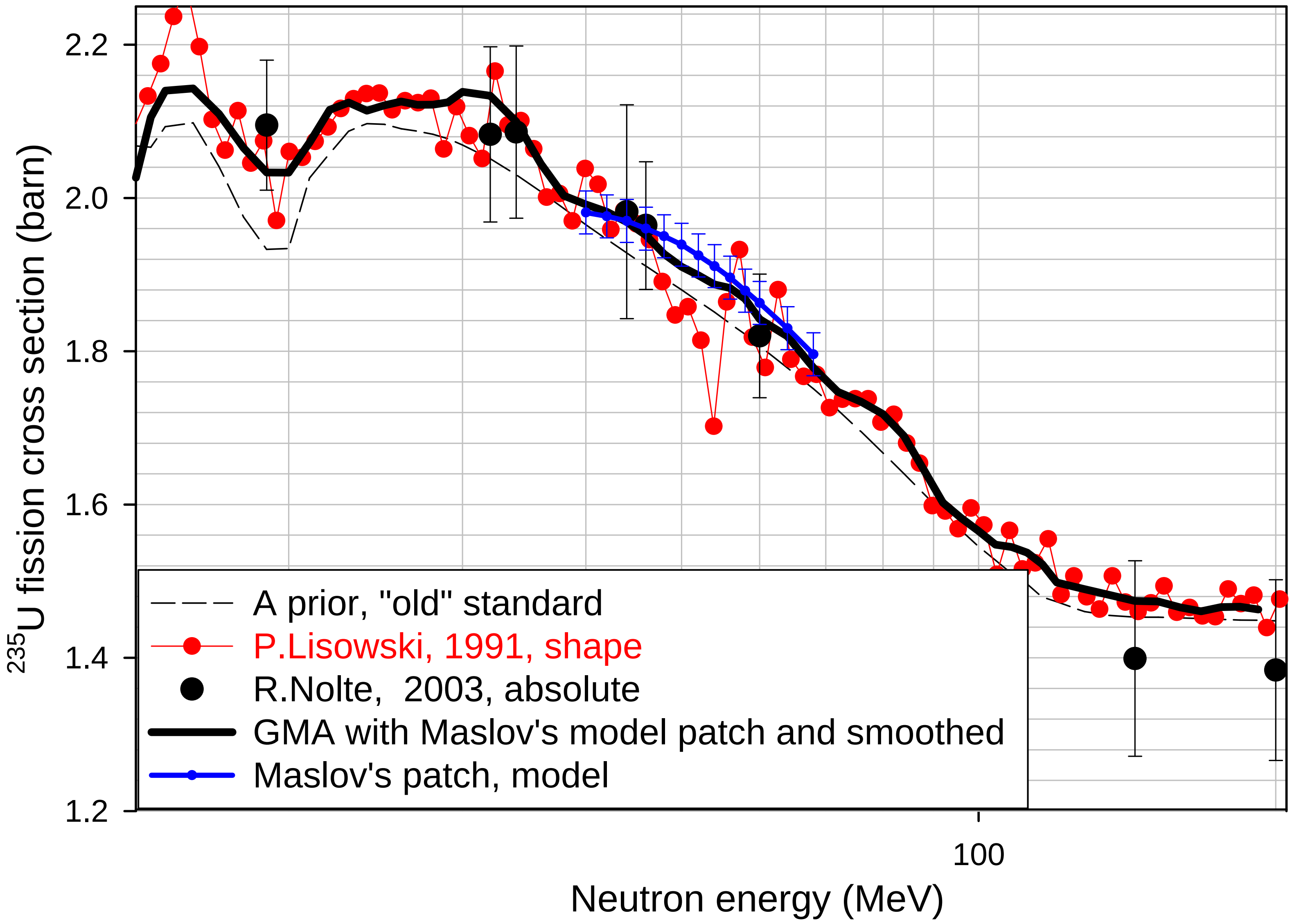
$^{6}Li(n,t)$ Cross Section Comparisons



Factors Affecting the Covariances (cont.)

- Smoothing of the Results
  - $^{6}Li(n,t)$, $^{10}B(n,\alpha)$ and $^{10}B(n,\alpha_1\gamma)$ data are basically smooth due to the dominance of the R-matrix fit.
  - Models provide insight on the shape of the data.
  - A simple smoothing algorithm was used to remove fluctuations.
  - In one case a patch using the shape of the Maslov $^{235}U(n,f)$ evaluated curve was used. For it the normalization was free and MERC and SERC were set to 2%

Smoothing of the ^{235}U(n,f) Cross Section Near 50 MeV



The Small Uncertainty Problem

- There were concerns due to the small uncertainties in the ENDF/B-VI Standards Evaluation.
  - To justify the use of the codes to be used in the evaluation, comparisons of a number of R-matrix and model-independent least squares codes were made.
    - A test data set containing various ^{6}Li+n experiments was used with no correlations among the experiments and only SERC and LERC within each experiment.
    - Model-independent codes GMA, GLUCS & SOK agree on both cross sections and covariances.

The Small Uncertainty Problem (cont.)

- Theoretical model calculations using effective NN potentials for the $^{6}Li(n,t)$ cross section were made for comparison with R-matrix results. This work provided guidance for initial values in the R-matrix work, improved the values of the parameters and aided in obtaining more realistic uncertainties in the cross sections.

- R-matrix codes EDA, SAMMY and RAC agreed on cross sections and covariances however there are some local differences due to analysis procedures.

- The R-matrix codes gave similar cross section but smaller covariances than the model-independent codes..

•Thus use of the EDA, RAC and GMA (GMAP) codes for this evaluation appeared justified.

The Small Uncertainty Problem (cont.)

- The presence of unrecognized systematic uncertainties can lead to underestimations of uncertainties in evaluations.
  - Discrepancies suggest that unknown systematic uncertainties are present in some data sets.
    - The work on MERC for the neutron database suggests that much of the problem with discrepant data has been removed there.
    - Charged-particle data used in the R-matrix analyses claim very small uncertainties. It is possible that systematic uncertainties are not fully estimated.

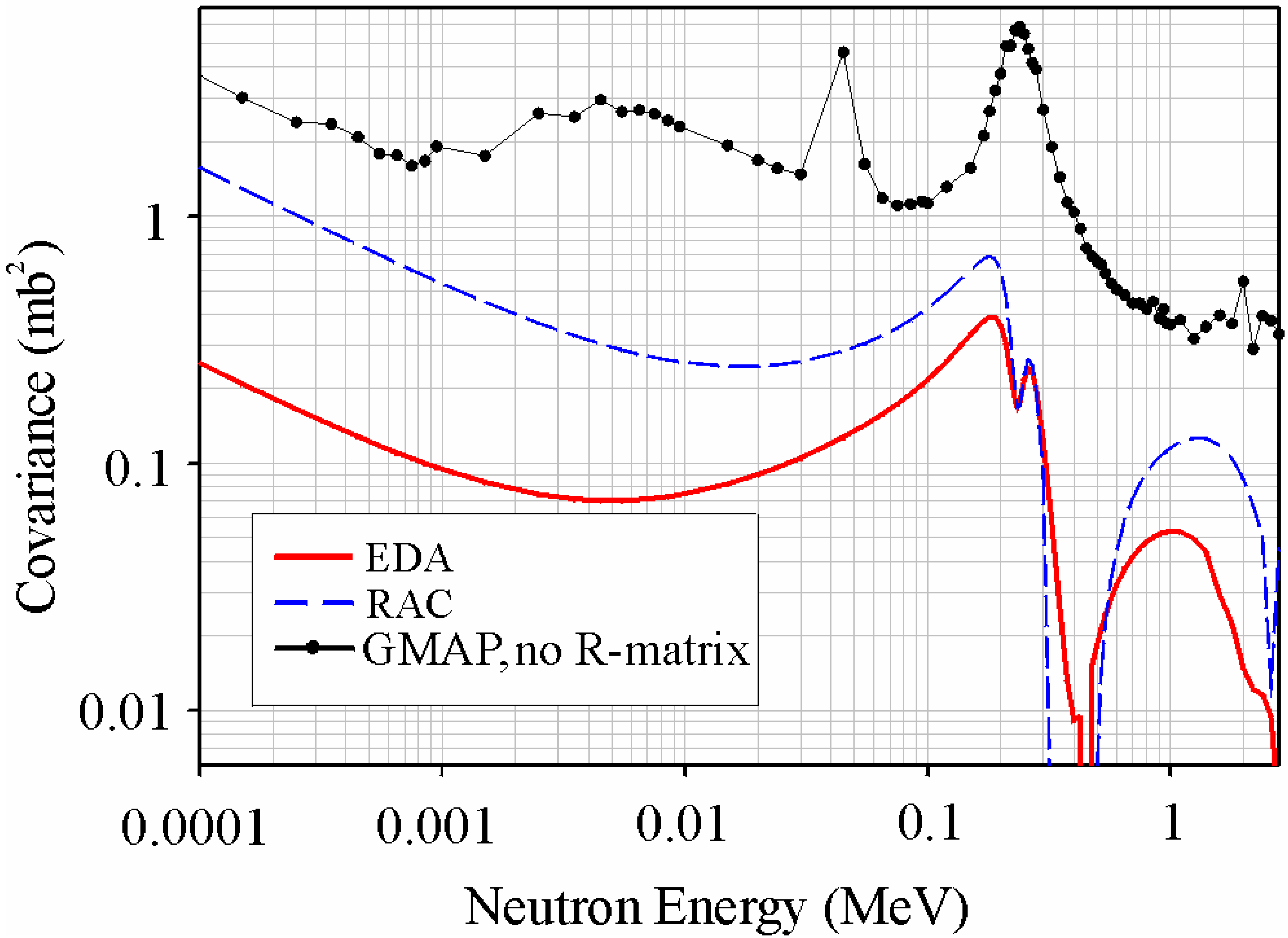
The Small Uncertainty Problem (cont.)

•For the full database used in the final evaluation differences were obtained for the EDA and RAC analyses for the ^{6}Li(n,t), ^{10}B(n,α) and ^{10}B(n,$\alpha_1\gamma$) cross sections..

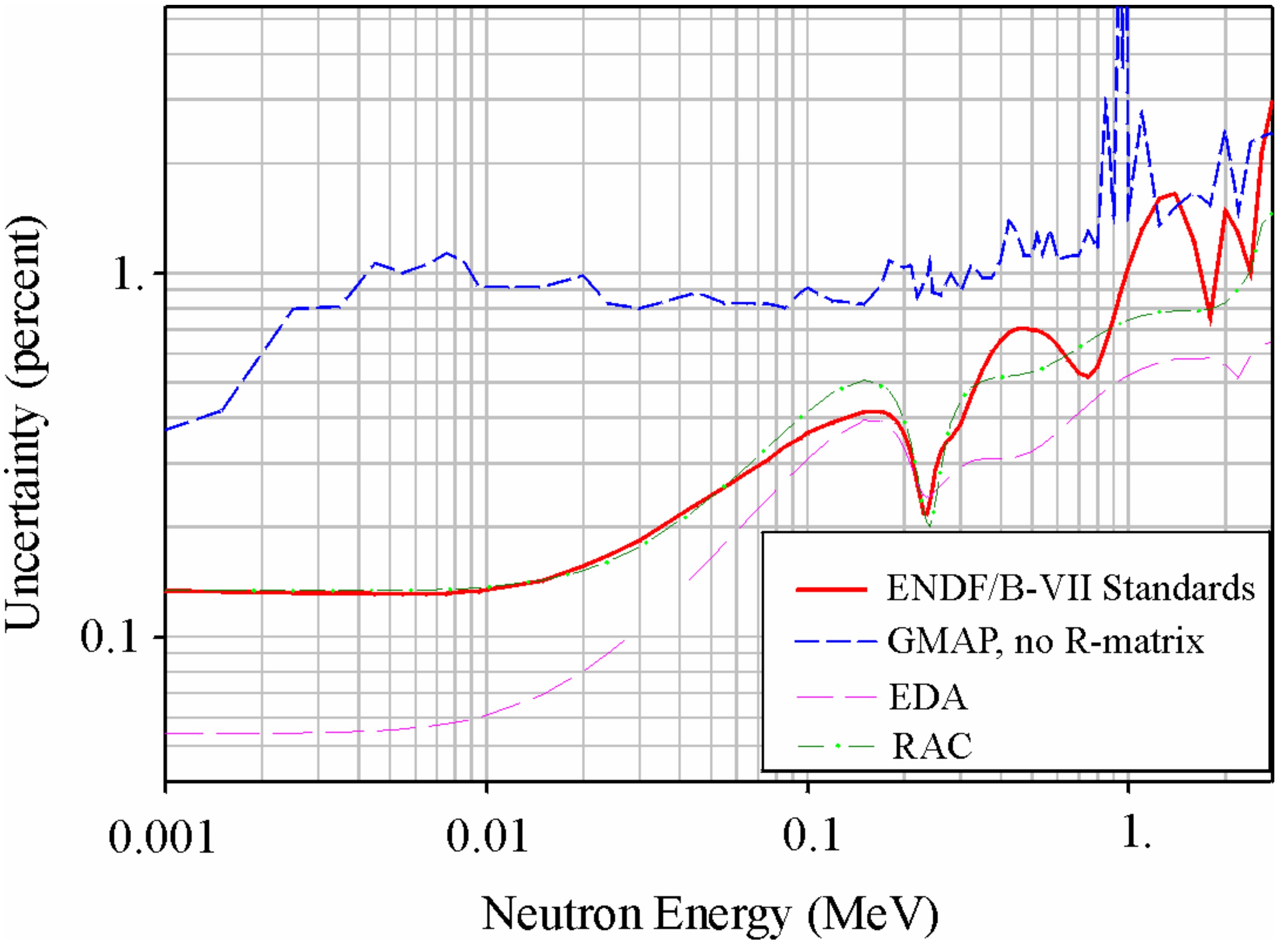
The Small Uncertainty Problem (cont.)

- Possible reasons for smaller covariances and variances with EDA vs. RAC using the full database.
  - In an effort to more properly handle the charged-particle data, the RAC analyses increased the uncertainties of outlying charge-particle data.
  - The RAC analyses also used the neutron database with the added MERC component that leads to larger uncertainty.
  - The EDA and RAC R-matrix model fits used different expressions for the χ^2 minimized function. RAC uses the full measurement covariance matrix; EDA uses the scale and normalization components.

Covariances Between the Point at 0.045 MeV and Other Energies Obtained Using All ^{7}Li Data



Uncertainties for the $^{6}Li(n,t)$ Cross Section Obtained Using All ^{7}Li Data



The Small Uncertainty Problem (cont.)

- Underestimation of correlations that may exist between different measurements causes smaller uncertainty.
  - Common samples, detectors, etc. can lead to high correlations (often 100%) for these components of the uncertainties in different measurements.
  - For the GMAP database, these correlations are taken into account where known.
  - For the charged-particle data these correlations may not be as well understood.

The Small Uncertainty Problem-Conclusion

- Based on this discussion, it can be expected that the uncertainties obtained from this work are reasonable.
- An important result is that it is essential to consider the covariances, not just the variances, in applications of cross sections to practical systems.
    - The use of models in fits leads to the redistribution of the uncertainties between variances and off-diagonal covariances of the uncertainty matrix with a reduction of the variances. As a result, the percent uncertainties are reduced but the uncertainty of the integral quantities sensitive to the evaluated data in a wide energy region is conserved in general.

Results

- A new standards sublibrary was created. It contains:
  - Cross sections for H(n,n), ^{3}He(n,p) ^{6}Li(n,t), ^{10}B(n,α_0), ^{10}B(n,α_1), C(n,n), ^{197}Au(n,γ), ^{235}U(n,f), ^{238}U(n,f) and ^{238}U(n,γ).
  - Covariances for ^{6}Li(n,t), ^{10}B(n,α_0), ^{10}B(n,α_1), C(n,n), ^{197}Au(n,γ), ^{235}U(n,f), ^{238}U(n,f) and ^{238}U(n,γ) cross sections.
  - The thermal constants data.
  - The data can be obtained from the NNDC web-site at http://www.nndc.bnl.gov/exfor/endf00.htm
- Files with full covariances (including cross-material covariances) are available from the NNDC web-site in the ENDF/A library at http://www.nndc.bnl.gov/exfor7/4web/ENDF-A/partial-evaluations/
  - ^{239}Pu(n,f) data are included in these files

Summary

•This standards evaluation is an improvement over previous ENDF evaluations of the standards in terms of the scope of the work and the covariance information.

•There is an increase in the cross sections, averaging several percent but even more than 5% in several cases compared with ENDF/B-VI.

•The importance of considering the covariances not just the variances is stressed for any practical applications.

•Unfortunately some of the covariances from this work are not available in the ENDF/B-VII library since they do not extend to 20 MeV.

•An IAEA Nuclear Data Development Project is now underway to assist in this evaluation work. Updated standards will then be available for new versions of data libraries. New experiments will be encouraged and experimental results can be investigated for use in new evaluations.