Approximating large resonance parameter covariance matrices with group-wise covariance matrices for advanced nuclear fuel cycle applications

M.E. Dunn, G. Arbanas, L.C. Leal, D. Wiarda

Oak Ridge National Laboratory, P.O. Box 2008, MS6170, Oak Ridge, TN
dunnme@ornl.gov

Abstract: The large size of resonance parameter covariance matrices (RPCMs) in the actinide region often renders them problematic for dissemination via ENDF. Therefore, a method of approximating the RPCM by a much smaller group-wise covariance matrix (GWCM) is described, implemented, and examined. In this work, ^{233}U RPCM is used to generate GWCMs for the 44-group AMPX, 100-group GE, 171-group VITAMIN-C, and 240-group CSWEG. Each of these GWCMs is then used to compute group-wise uncertainties for the groups of the remaining group structures. The group-wise uncertainties thus obtained are compared with those obtained from a full RPCM, that is, without the approximation. A systematic comparison of group-wise uncertainties based on GWCMs vs RPCM, for a variety of group structures, will shed light on the validity of this approximation and may suggest which group structure(s) yield a GWCM that could be used in lieu of the RPCM.

Introduction

Complete RPCMs of ^{235}U, ^{238}U, ^{233}U, ^{239}Pu and other actinides have recently been evaluated at the Oak Ridge National Laboratory, for example [1]. Due to the large size of these RPCMs, their inclusion into ENDF files, renders these problematic for dissemination via ENDF. To illustrate, the sizes of ^{235}U, ^{238}U, ^{239}Pu, and ^{233}U RPCMs are ≈ 1.7 GB, 0.7 GB, 0.2 GB, and 0.1 GB, respectively; while the entire ENDF database is ≈ 0.5 GB in size. The proposed RPCM-to-GWCM conversion scheme is an attempt to compress the RPCM while preserving its essential information.

Methodology

A compression scheme that converts the RPCM into a group-wise covariance matrix (GWCM) is investigated for four (relatively arbitrary) group-structures: 44-group AMPX, 100-group GE, 171-group VITAMIN-C, and 240-group CSWEG. The energy boundaries of these group structures are plotted in Fig. 1. ^{233}U was chosen for this study because it has relatively few resonances, thus making computations amenable to a repetitive numerical study, and because its RPCM was recently evaluated. The analysis consists of these four steps:

1. Group-wise cross-sections and uncertainties are computed for each of the four group-structures using the ^{233}U RPCM. These computations are used as a reference for the purpose of estimating the deviations introduced by the compression scheme.
2. ^{233}U RPCM is converted into a GWCM for each of the four group structures.
3. For each group structure, cross-sections and uncertainties (standard deviations) are computed from the GWCMs of the three remaining group-structures. Namely, the 44-group GWCM is used to compute uncertainties on the 100-, 171-, and 240-group structures, the 100-group GWCM is used to do the same on the 44-, 171-, and 240-group structure, and so on.
4. Uncertainties obtained in Step 3 are compared to the reference uncertainty obtained in Step 1; large deviations would be a sign of inadequacy of a particular GWCM.

A modified PUFF-IV [2] was used to convert the RPCM, stored in ENDF File 32, into a GWCM and then to seamlessly join the GWCM with the high-energy File 33. All computations assumed a constant neutron flux. It was verified that the uncertainties obtained from GWCMs are identical to those obtained from RPCMs for the same group structure.

Results

For each group structure the total cross-section and its uncertainty were computed using RPCM and the GWCMs of the remaining three group-structures.

For each group-structure, a total cross section is plotted in the first row of Figs. 2 and 3, its standard deviations are plotted in the second row, its relative standard deviations (RSDs) are plotted in the third row, and the *relative* RSD deviations from the RPCM's RSD are plotted in the fourth row. Each group structure occupies one of the columns in Figs. 2 and 3: 44-group AMPX and the 100-group GE structures are in the left and right columns in Fig. 2, respectively; while the 171-group VITAMIN-C and the 240-group CSWEG structures are in the left and right columns in Fig. 3, respectively.

We use the RPCM computation of RSDs as a reference for determining the deviation introduced by GWCMs. This deviation is introduced when a GWCM is used to compute group-wise RSD for a group structure that is *different* from the group structure on which the GWCM was originally created. A large deviation from the RPCM RSD indicates that a GWCM may not be suitable for computations on that group structure.

The largest relative deviations of the RSD are seen when 44- and 100-group GWCMs are used to compute RSDs for the remaining three group structures: a 40–60% deviation from the RPCM RSD can be seen in narrow groups between 0.1 and 10 eV in the bottom row of plots. This may indicate that 44-group structure may not be a good candidate for a reliable GWCM.

Overall, the 240-group GWCM outperformed its counterparts on the 100- and 171-group structures. This may not be surprising because it has more grid points, which (usually) means a better approximation to the RPCM. Details of distribution of energy boundaries of a given structure may also affect the quality of GWCM computations in a specific energy range. This may explain why the 240-group GWCM had deviations comparable to those of other GWCMs on the 44-group structure, because the 44-group structure is denser than the other three below 1 eV, as seen in Fig. 1.

Conclusions

It appears that a judicious choice of energy group structure could make the RPCM-to-GWCM compression scheme viable for computations of group-wise uncertainties. A group structure with a dense grid across the entire energy range is a likely candidate. It is conceivable that a new group structure could be designed specifically to retain the most RPCM information for all common group structures. Effects of this method on uncertainties in resonance integrals and thermal cross sections, as well as on off-diagonal covariance elements, require further study.

References

[1] L. Leal et al., "ORNL Methodology for Covariance Generation for Sensitivity /Uncertainty Analysis", p.25-29 in Proceedings of the 8th Int. Conference on Nuclear Criticality Safety (ICNC 2007), Vol. II, May 28-June 1, 2007, St. Petersburg, Russia.

[2] D. Wiarda and M. E. Dunn, *PUFF-IV: A Code for Processing ENDF Uncertainty Data into Multigroup Covariance Matrices*, ORNL/TM-2006/147, Oak Ridge National Laboratory (October 2006).

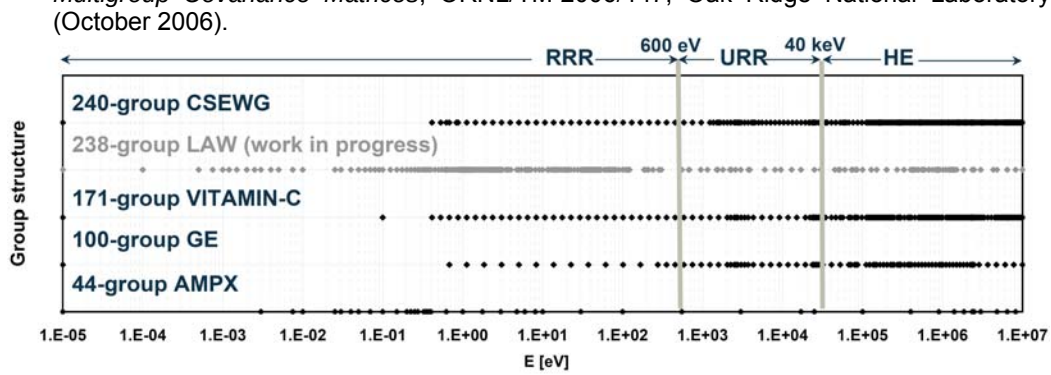

***Figure 1**. Energy grids of the four group-structures. ^{233}U energy regions are noted.*

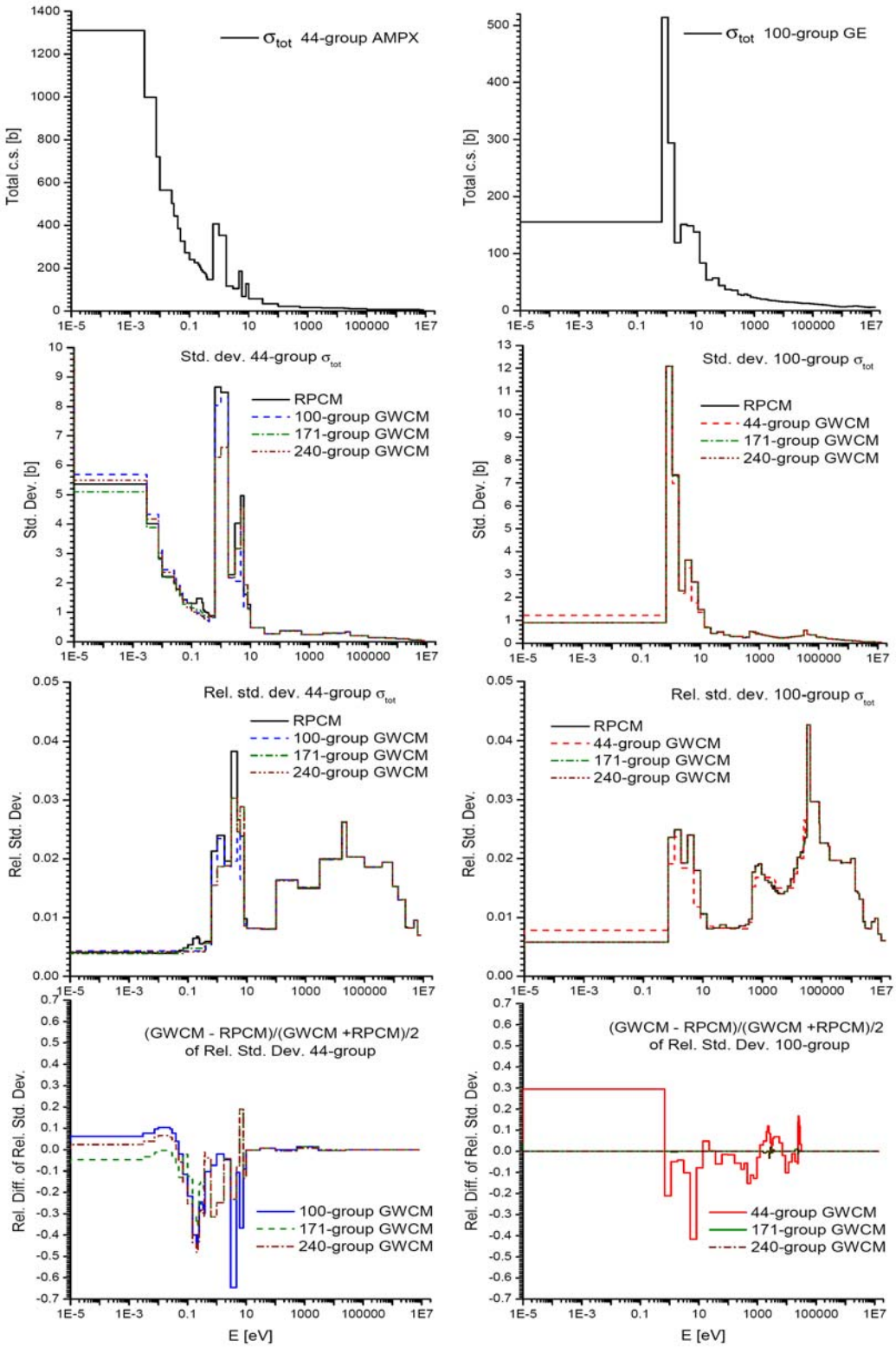

Figure 2. *Total cross section, its standard deviation, its RSD, and relative deviations from the RPCM RSD for the 44-group (left column) and the 100-group (right column).*

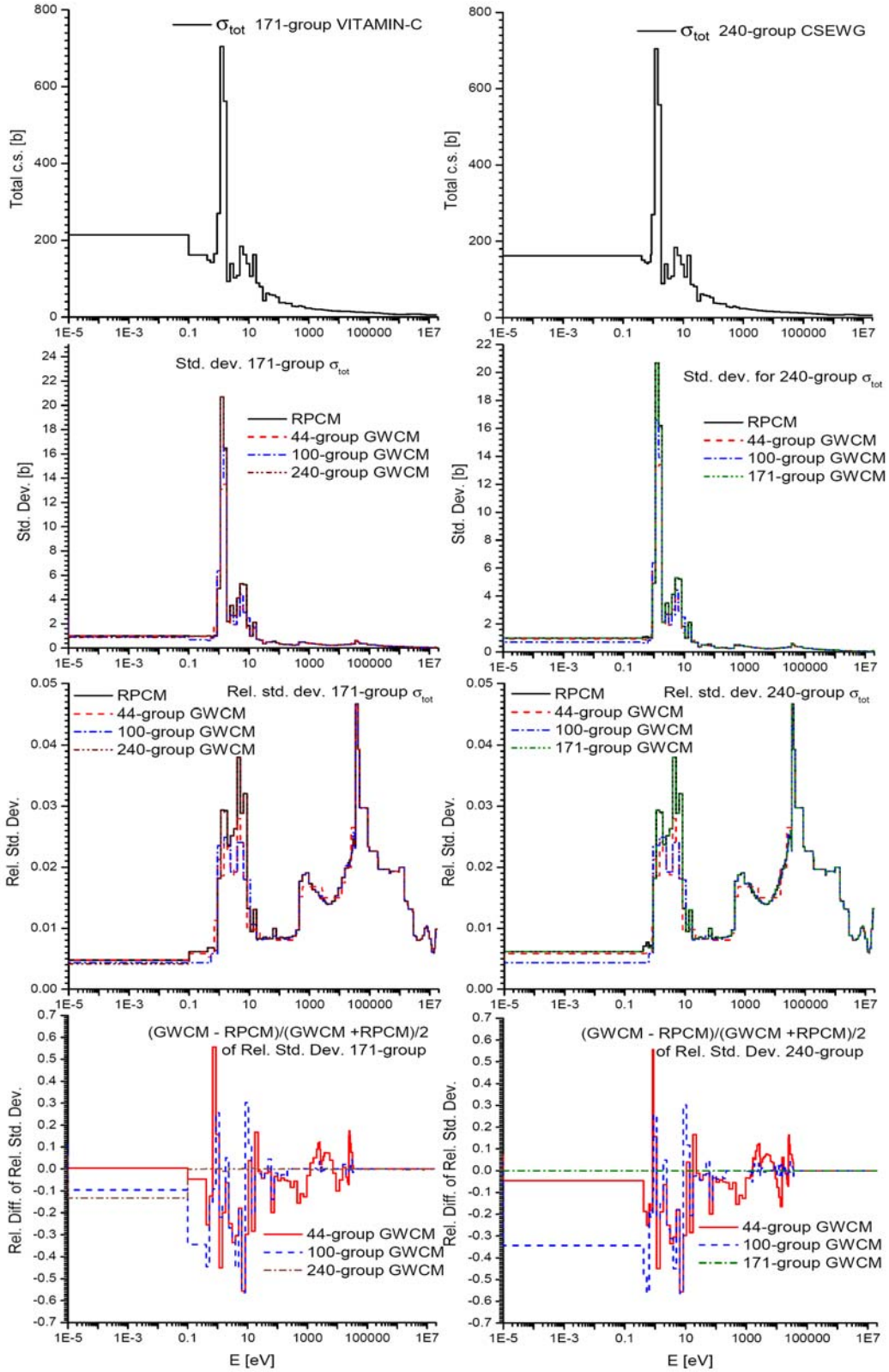

Figure 3. *Total cross section, its standard deviation, its RSD, and relative deviations from the RPCM RSD for the 171-group (left column) and the 240-group (right column).*