WPEC Subgroup Proposal
May 4-5, 2006

Title: Processing Covariance Data for the Resonance Region

Short Justification for the Subgroup:

The implementation of safe, efficient and optimized fissile material operations is increasingly dependent upon the use of radiation transport methods with accurate nuclear cross-section data. Moreover, covariance data that are provided in the evaluated nuclear data libraries are essential for assessing the impact of cross-section uncertainty data for nuclear fuel cycle analyses, reactor design, criticality safety analyses, etc. In WPEC/SG20, significant progress has been made to increase the availability of uncertainty data by developing new methods for covariance data evaluation and new evaluation formats to transmit the covariance data to the processing codes. The purpose of this subgroup is to build upon the work completed by WPEC/SG20. The objective is to develop the requisite processing methods that are needed to process the resonance parameter covariance data, generate cross-section covariance data files and demonstrate the use of covariance data in radiation transport analyses.

Subgroup Monitor:

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List of Subgroup Participants:

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Definition of the Project:

The project will be separated into three phases: 1) develop the resonance-parameter covariance processing methods, 2) preparation and testing of new evaluations with resonance-parameter covariance data and 3) generate cross-section covariance data for demonstration in sensitivity and uncertainty (S/U) analyses.

Because the new subgroup will build upon the work of WPEC/SG20, the accomplishments of SG20 should be highlighted in the discussion for the new subgroup. The SG20 final report will be published in the spring of 2006, and the complete report will describe the SG20 work activities in more detail. As part of the SG20 activities, the subgroup achieved the following milestones:

- Covariance data were produced for materials such as Gd, Rh (ENDF/B), and Fe (JENDL);
- The new evaluations include resonance-parameter covariance data in addition to covariance data in the higher energy ranges above the resonance region;
- The SAMMY code has been updated with a new capability to retroactively generate resonance-parameter covariance data, and the resonance parameter covariance data for the new evaluations were produced using SAMMY;
- A covariance processing code ERRORJ, which is a modified version of the ERRORR module in NJOY, has been improved to process the existing ENDF/B-VI resonance parameter covariance formats;
- A covariance processing code PUFF-IV, has been developed at ORNL;
- The new evaluations have been processed with the ERRORJ and PUFF-IV module, and SG20 demonstrated that the covariance data can be converted to group constants;
- The "Compact Covariance Format" (CCF) has been developed and approved for ENDF/B-VII. The CCF is needed to transmit resonance-parameter covariance data for isotopes having a large number of resonances (^{235}U, ^{238}U, etc.).

In WPEC/SG20 the evaluation and format issues were addressed for preparing new cross-section evaluations with resonance-parameter covariance data. However, the corresponding covariance processing methods have not been sufficiently developed and publicly disseminated for producing covariance data files for use in transport applications. Prototypic versions of the cross-section processing software have been developed to process the latest covariance formats, but additional work is needed to finalize the processing methods for distribution to the user community. The first phase of the project will focus on the development of the needed covariance processing methods and the implementation of the new processing methodology in widely used cross-section processing systems (e.g., NJOY, AMPX, etc.).

The second phase of the project will be performed concurrently with the first phase. Specifically, new evaluations will be prepared with resonance-parameter covariance data for selected nuclides. In particular, covariance data files will be generated for ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu. This phase will follow directly from the work of WPEC/SG20, and the new evaluations will be generated using the new methods and formats that were developed in WPEC/SG20.

Once the new resonance-parameter covariance processing methods are sufficiently developed, cross-section covariance data files will be generated in the third phase for use in radiation transport analyses. In addition, the newly generated covariance data files will be used in S/U analyses to demonstrate the propagation of the covariance data to specific radiation transport applications.

Justification of the Project:

Many resonance nuclide evaluations have been released with the Reich-Moore (RM) resonance parameter formalism which is essential to model the resonance-resonance interference effects that cannot be modeled with the single-level Breit Wigner (SLBW) or multi-level Breit Wigner (MLBW) formats. Recognizing the need for improved resonance parameter covariance formats, evaluation formats have been developed to permit the transmittal of RM resonance-parameter covariance data. However, the existing RM resonance-parameter covariance formats are not completely sufficient to transmit resonance-parameter covariance data for all nuclides. With the advent of improved computing capabilities coupled with improved data measurement and evaluation capabilities, resonance parameter evaluations will be generated that tax the existing

resonance-parameter covariance formats. For example, the ENDF/B-VI Release 5 evaluation for ^{235}U has 3193 resolved resonances. Each resonance is defined by at least 5 parameters; thus, there are 15,965 parameters for the entire resolved region. Consequently, the resonance-parameter covariance matrix is 15,965 x 15,965 (i.e., ~255 million numbers). As a result, the ENDF/B-VI resonance-parameter covariance formats are not efficient or adequate for addressing a RM nuclide with a large number of resonances. In coordination with WPEC/SG20, a new Compact Covariance Format has been developed by N. M. Larson (ORNL) that can be used to transmit resonance-parameter covariance data for special cases such as ^{235}U. The new Compact Covariance Format is approved for implementation in ENDF/B-VII. With the development of the Compact Covariance Format in addition to the existing resonance-parameter covariance formats, evaluation formats are now available to efficiently transmit the RM resonance-parameter covariance data for all nuclides.

Although improvements have been made in the covariance evaluation procedures, the major cross-section processing systems (e.g., AMPX, NJOY, PREPRO, etc.) have not been completely updated to process the RM resonance-parameter covariance formats and the new Compact Covariance Format. Recently, a prototypic version of the AMPX covariance processing module has been developed to process the existing RM resonance-parameter formats and the new Compact Covariance Format. The new AMPX processing capability needs to be finalized for distribution to the user community. In addition, work is currently in progress to update the NJOY covariance processing methods. More recently, the JENDL community has embraced the RM resonance-parameter covariance formats. As a result, a modified version of the NJOY covariance processing module (ERRORR) has been developed by the Japan Nuclear Cycle Development Institute (JNC). Although JNC's ERRORJ code is not officially part of NJOY, the code can be used to process RM resonance parameter covariance formats.

Concurrent to the methods development for performing covariance data evaluations, adjoint-based S/U methods have been developed to propagate cross-section covariance data to calculated quantities of interest such as k_{eff} for criticality safety analyses. Moreover, there is an ever-increasing demand from nuclear analysts to include cross-section covariance data in the radiation transport analyses of fissionable systems.

As a result, the work of WPEC/SG20 has established the requisite covariance evaluation methods, and recent radiation transport developments have provided the computational tools that are needed to propagate the cross-section covariance data to calculated quantities of interest. However, the cross-section processing methods have not been sufficiently developed to process the evaluated covariance data and generate covariance data libraries that can be used in existing S/U radiation transport methods. Therefore, the purpose of the new subgroup is to develop and implement the covariance processing methods needed to generate cross-section covariance data libraries.

Objectives of the subgroup:

Develop covariance testing methods and cross-section processing methods for processing resonance-parameter covariance data

> Although some progress was made on this effort under WPEC/SG20, the work of SG20 mainly addressed the evaluation and formatting issues. The main focus of this new subgroup is to develop the resonance-parameter covariance processing methods and implement the methodology in the cross-section processing systems. Once fully implemented, the cross-section processing methods can be distributed to the user

community. Note that the evaluation checking codes need to be updated to test the covariance data evaluations prior to distribution by nuclear data centers. Therefore, as part of the proposed subgroup, the checking codes will also be updated to test the evaluations as part of the task for updating the cross-section processing codes.

Produce resonance-parameter covariance data evaluations for important nuclides

Evaluations with resonance-parameter covariance data must be developed before the covariance processing methods can be used and demonstrated. Initially, the subgroup will work to develop evaluations with resonance-parameter covariance data for "high-priority" nuclides. Specifically, resonance-parameter covariance data evaluations will be produced for ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu. The evaluation checking codes will be used to test the new evaluations that are generated as part of this task.

Investigate the generation and use of resonance-parameter covariance data

There are two elements to this objective: 1) Once new resonance-parameter covariance processing methods are sufficiently developed, cross-section covariance data will be generated by using the new methods to process the resonance-parameter covariance data; 2) Subsequently, existing S/U methods will be used to demonstrate the use of the cross-section covariance data in various radiation transport applications.

Relevance to Evaluated Data Files:

Currently, resonance-parameter covariance data formats are available for evaluators to transmit RM covariance data for all nuclides in the various evaluated libraries: BROND, ENDF/B, JEFF, and JENDL. However, covariance processing tools are not widely available to process all the resonance-parameter covariance data and generate cross-section covariance data for radiation transport codes. Until the processing issues are addressed, the resonance-parameter covariance data cannot be used in radiation transport applications. Development of the requisite processing methods will permit the use of the new covariance information and will provide motivation for evaluators to develop covariance data for nuclides that currently do not have covariance information.

Deliverables:

- Cross-section evaluations with covariance data for important nuclides (i.e., ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu)
- Implementation of methods to test and process covariance data
- Generation of covariance data libraries for use in S/U analyses
- Demonstration calculations using the newly processed covariance data in (S/U) analyses

Time Schedule and Milestones:

2006—2007

- Perform resonance-parameter covariance data analyses for ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu, and prepare covariance-parameter data in existing or new ENDF formats for these isotopes

- Perform resonance-parameter covariance processing methods development in concert with resonance parameter covariance evaluation work for ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu
- Update evaluation checking codes to test new covariance formats

2007—2008

- Complete covariance data evaluations by combining the resonance region covariance data with high-energy covariance evaluations obtained in WPEC Subgroup 24 “Covariance Data in the Fast Neutron Region”
- Test new evaluations with checking codes
- Process covariance data and generate cross-section covariance data files using newly development processing methods
- Perform demonstration S/U calculations with cross-section covariance data files

2008—2009

- Prepare final formal report of the subgroup activities during the period 2006-2009