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The AMPX-2000 Operating System for Producing Continuous Energy and Multi-Group Cross Sections from Basic Data Libraries Using the ENDF/B-6 Formats

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The AMPX-2000 Operating System for Producing Continuous Energy and Multi-Group Cross-Sections from Basic Data Libraries using the ENDF/B-6 Formats

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AMPX-2000 is a modular system of FORTRAN computer programs that relate to nuclear analysis with a primary emphasis on tasks associated with the production and use of multigroup and continuous energy cross-sections. AMPX-2000 accepts basic cross-section data from ENDF/B libraries. As opposed to previous versions of AMPX, the current version processes the latest ENDF/B version VI formats. AMPX-2000 can be used to generate a variety of multigroup libraries that can be used with modern transport codes to perform nuclear analyses. Continuous energy or "point" cross-section libraries can be produced for use in Monte Carlo codes and other applications. In addition, AMPX has an internal multigroup format that can be read by various AMPX modules as well as codes outside the system.

KEYWORDS: multigroup, continuous energy, Evaluated Nuclear Data Files (ENDF/B), cross-section processing, nuclear energy, nuclear physics, radiation shielding, resonance self-shielding

I. Introduction

The AMPX[1)] system was developed in the early 1970's at the Oak Ridge National Laboratory (ORNL) to produce multigroup neutron and gamma-ray cross-section libraries, based on data taken from the Evaluated Nuclear Data Files (ENDF/B). The formats and procedures employed in the ENDF/B[2)] files have evolved from their first version distributed in the mid 1960's to the present collection, designated as Version VI. (Note that Roman numerals refer to a collection of evaluated data, while Arabic numerals refer to the format level). Because there are obvious advantages for using the same data format in cross-section libraries developed in different countries, the ENDF/B, JENDL,[3)] JEF,[4)] CENDL,[5)] and BROND[6)] files, developed in the USA, Japan, Europe, China, and Russia, respectively, now all employ this format. The only processing system that can completely process ENDF formats is the NJOY[7)] system developed at the Los Alamos National Laboratory (LANL), and it is universally used to process the various data collections previously mentioned. The AMPX system, last released in 1992,[8)] has a comprehensive collection of processing capabilities up through format level 5; however, the substantial differences between format level 6 and earlier levels makes it impractical to simply upgrade many of the major processing codes in this system.

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The U.S. Nuclear Regulatory Commission (NRC) has supported the development and maintenance of the SCALE[9)] system for analyzing spent fuel shipping casks and other radiation safety problems. Most SCALE cross-section libraries have been produced by AMPX. SCALE uses integral-transport methods for self-shielding resolved resonances, as opposed to the Bondarenko[10)] method used in NJOY. Because of the SCALE needs and the need for an independent code system that can process ENDF data, the NRC has sponsored a 5–6 person year effort to upgrade AMPX.

The effort was initiated in 1994, and the resulting code system has been written and is being tested, with a release expected early in 2002. The AMPX-2000[11)] package includes a complete re-write of some of its major processing codes. These new codes use some novel procedures to process the new level 6 formats. As an example, a single set of integration routines is used to produce group-averaged data and scattering matrices for all particles and all nuclear processes. This feature was implemented by requiring the codes that read the ENDF/B libraries to produce a tabular "kinematics" data file. Use of this tabular kinematics file precludes the code that makes multigroup data from requiring any knowledge of the basic physics or particle type associated with the nuclear reaction being treated.

This paper describes the design characteristics and capabilities of AMPX-2000.

II. System Design Characteristics

The upgrade to AMPX began with a review of what it would require to make it process version VI to satisfy the needs of SCALE. This review revealed at least 3 obvious options: 1) existing codes could be modified to make them process the new formats—this is an obvious approach, since AMPX was perceived to adequately address specified internal cross-section processing needs; 2) a more forward-looking approach would be to discard several of the older and less accurate modules of AMPX, and write new coding that would take advantage of lessons-learned from years of working in this area; or 3) the NJOY system could have been selected, as has been done in the rest of the world.

The first option was considered and quickly discarded. Though quite functional, many of the modules in the existing system are 30–40 years old, and have been repeatedly patched to allow them to keep abreast with the ENDF/B format changes. Furthermore, simple operations, such as numerical integration, vary in different modules, making it very difficult to assign an estimate of the precision of processed results.

The third option was seriously considered, but was not selected for two reasons. The major reason was the recognition that the complexity of the physics and programming together with the importance of processed data warranted two independent systems. Feedback from the domestic and international community supported this evaluation by ORNL. This affords the ability to compare different approaches for processing, and will provide different methods to perform very important procedures, such as resonance self-shielding. Secondly, there are serious concerns with using the Bondarenko method for multigroup resonance self-shielding, which is the only procedure provided in NJOY. This method is based on the narrow resonance approximation, which is not adequate for many of the analyses performed with SCALE.

The second option was selected for the reasons hinted at above. It was decided that the new code system could be designed with the idea of having modules that could produce multigroup neutron cross-sections, or gamma-ray cross-sections, or gamma-ray yields, or whatever, in the same coding, using the same integration routines and procedures for all situations.

This upgrade has been accomplished by using three ideas: 1) tabular cross sections are determined and stored for all particle types and nuclear processes—this is not a new idea; NJOY creates a file it calls a PENDF file that is equivalent to this. 2) Process the ENDF/B angular and energy distribution data to produce and store tabular "kinematics" information. The tabular kinematics concept is new, because all previous approaches either use raw ENDF/B data to treat kinematics or explicitly program for the type of reaction involved. 3) Create multigroup parameters with AMPX using the tabular data collections mentioned in items 1 and 2. Note that these processing routines have no knowledge of the physics of any reaction.

There are several advantages: 1) it fits well with quality assurance requirements because all particles and processes are handled by the same procedures; 2) both tabular data and kinematics data can be saved thereby substantially (in some cases) reducing the time needed for processing, and 3) new format changes and new reactions or particles are easier to accommodate because the basic processing code does not deal directly with the ENDF/B files.

The tabular kinematics file requires that the data employ a single, uniform structure that can describe the most complicated situation one will encounter; i.e., a process can vary with temperature, angle, and source and sink energies. Additional levels of dependence can be treated in the kinematics file. As an example, ENDF/B has a "subsection" variation that is used in a variety of ways to accommodate the emission of different particles, multiple scattering distributions, multiple discrete photons, etc.

An important note: all processes must specify all 5 types of variation. Most processes do not vary with temperature, or emit multiple particles. In AMPX-2000, all processes have at least one temperature, at least one particle emission, at least one level of angular variation (even when the process is isotropic), etc. This uniform structure makes it much easier to write coding that does not require the treatment of a myriad of special situations. The simplest process is treated just as is the most complicated process. The overhead in data storage and efficiency is trivial because one temperature involves a single loop with a temperature value of zero being stored in the files. An analogous observation is made for isotropic scattering processes or single particle emission.

Another important characteristic of the new system is to calculate average cross-sections and group-to-group transfer matrices at the same time. As a result, both types of parameters are calculated to the same precision.

The routines that calculate group-to-group scattering matrices always consider a source group structure and an independent sink group structure even if they are identical. The kinematics data are used in conjunction with the point cross-sections and a weighting function to tell how particles interacting in source energy space scatter to sink energy space. Thus, the same routines calculate neutron-to-neutron group parameters, gamma-to-gamma group parameters, or neutron-to-gamma group parameters (i.e., gamma yields from neutron reactions).

III. Major AMPX-2000 Capabilities

There are more than 80 modules in AMPX-2000, ranging all the way from very simple, small codes, to very complicated, multi-thousand line codes.

AMPX is a modular code system. All of the modules can be executed standalone, and new codes can be added to the system without modification to other modules or the AMPX driver program.

Within AMPX, POLIDENT is a module that reads an ENDF/B library, extracts resonance parameters, determines an accurate energy mesh to use in re-constructing the cross-sections, combines these with point data, and generates a point cross section library for neutron data. In

this respect, it is analogous to the RECONR module in NJOY. Another module, called MAKPEN, can use POLIDENT's file to create an NJOY PENDF file, which can then be used in NJOY's ACER module to create a library for MCNP[12].

Y12 is a new module that reads an ENDF/B library and makes the tabular kinematics files for both neutrons and gamma-rays.

JERGENS is a module that creates weighting functions. In addition to the usual Maxwellian—1/E—fission spectrum standard options, JERGENS can access the point data files produced by POLIDENT to construct $1/E\Sigma_t$ or more complicated functions.

X10 is a module that performs the integration procedures for constructing multigroup libraries. X10 is used for neutron, gamma-ray, or coupled neutron-gamma-ray libraries.

CENTRM is a 1-D continuous-energy discrete-ordinates code that provides the capability for performing a one-dimensional calculation involving an arbitrary number of mixtures and nuclides, with a good treatment of anisotropic scattering. It is used for resonance self-shielding of resolved resonances.

PRUDE/TABU/FABULOUS are codes that can be used to produce Bondarenko data for either the unresolved energy region or the complete energy range. The Bondarenko factors are then used in the BONAMI module for resonance self-shielding.

KRYSTAL is a new module that is a modified version of the ANL WHOPPER[13] code. It accesses Reich-Moore resonance parameters and constructs multi-pole parameters that can be used to reconstruct resolved resonances to give results equivalent to those obtained with Reich-Moore data. Its primary advantages are calculational efficiency, combined with a clever method for avoiding the costly numerical procedures for Doppler broadening point data derived from processing Reich-Moore resonance data. The multi-pole parameters are processed in the NITAWL-3 module for resonance self-shielding in the resolved resonance region.

PUFF-III[14] is a module that processes the latest covariance data formats to generate multigroup cross-section covariance data..

PURM[15] is a module that uses Monte Carlo techniques for calculating probability tables for the unresolved energy range.

Several utility modules are provided to convert between library formats for different codes. One of the more useful code is the SMILER module that reads GENDF files produced by NJOY and converts these to the AMPX master library format.

Note that the above codes are only a few of the modules available in AMPX-2000. Additional modules are available for numerous applications. Collectively, AMPX-2000 provides a comprehensive collection of capabilities that allows a user to use, manipulate and modify multigroup and point cross-section data for a variety of applications.

IV. Usage

The principal justification for the modular programming philosophy is to eliminate or minimize duplicate and redundant programming. Important functions (e.g., copying, combining, processing a particular class of data, testing, plotting, etc.,) are isolated to a single module. As a result, modules can be executed in a sequential manner to accomplish a particular task. AMPX-2000 is such a modular system. AMPX can execute NJOY as a "module" without requiring any changes to NJOY or AMPX.

As noted previously, more than 80 modules are available in AMPX-2000. Note that AMPX does not provide predefined calculational sequences for performing a specific application (e.g., generate multigroup cross-section libraries); however, AMPX can be used efficiently to perform repetitive cross-section calculations.

As an example, consider the task of producing a multigroup library based on ENDF/B data. The sequence to process a nuclide involves considerable input that is similar for all nuclides with some slight variation. Certain parameters will always be unique. For example, each nuclide has an identifier for the data on the ENDF/B file, and another for the data to be written to an AMPX master library. A "title" is needed, that succinctly spells out what the data are and where they came from. A nuclide may have special processing requirements. For example, unless it has unresolved resonance data, there is no need to request processing these data. If it has Reich-Moore resolved resonance data, a module to produce multipole parameters must be called. Other situations require similar decisions.

A two-stage procedure has been developed to automate library production tasks. A special program has been written that scans all of our ENDF/B-VI files and creates a concise directory that summarizes the contents of each evaluation. Subsequently, an additional program reads the concise directory file, selects the latest evaluation (some nuclides have 5–10 modifications), determines the modules to execute for a nuclide, and generates the AMPX-2000 input data in the order necessary to process the nuclide. In addition, an executable script file is also generated. The script file contains the AMPX-2000 execution command for each nuclide to be processed. Consequently, executing the script file can generate the entire library. Although the procedures simplify the library production tasks, the new procedures do not replace the tasks for testing a cross-section library; however, the automation procedures allow the user to generate multiple AMPX-2000 input files in an efficient manner. The automation procedures have been successfully used to process more than 300 ENDF/B-VI evaluations and generate multigroup and continuous-energy cross-section data for neutron libraries. As new cross-section processing tasks are encountered the automation procedures can be updated to generate the appropriate AMPX-2000 calculational sequences.

V. Summary

A new system, AMPX-2000, has been developed to process nuclear data evaluations in the ENDF/B formats through Version 6. In addition, AMPX-2000 provides several enhancements relative to previous version of AMPX (e.g., improved resonance self-shielding capabilities, cross-section uncertainty processing, continuous-energy library production, etc.). AMPX-2000 is a robust and modular cross-section system than can be used for a myriad of cross-section processing applications.

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