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NJOY

A Comprehensive System for the Processing of ENDF Formatted Nuclear Data

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Abstract: An introduction to the program system NJOY is given which processes data files of evaluated neutron nuclear data coded in ENDF format. NJOY is primarily used for neutron and photon transport calculations for nuclear power reactor design. The NJOY code is not available from the IAEA Nuclear Data Section but may be obtained from the Reactor Shielding Information Center, Oak Ridge, USA.

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INTRODUCTION

The NJOY Nuclear Data Processing System (Refs. 1-3) is intended to serve as a general-purpose link between ENDF-formatted evaluated nuclear data files and important applications, as discussed below. NJOY is currently compatible with ENDF versions 3, 4, 5 and, with only minor exceptions, 6.

"Important" applications can be defined here as those practical engineering tasks that motivated the actual production of the major ENDF-formatted data files. Neutronic design of the core of a fast-breeder reactor is one clear example. However, in recent years attention has increasingly turned to other applications, such as shield design, thermal-reactor core design, fusion-reactor blanket design and radiotherapy facility design, as well as many others.

Data for neutron and photon transport are clearly still important, but increasing emphasis is now placed on the computation of special "response functions" that characterize the local effects of the transported radiation, such as the production of radioactivity, nuclear heating and material damage. Another trend is the emergence of new fields, such as perturbation-based sensitivity analysis, which require entirely new kinds of processed data, such as covariance matrices for multigroup cross sections.

HISTORY

The NJOY system has been under continuous development at the Los Alamos National Laboratory since 1974 (Ref. 4). During this period it has gone through a number of versions, in response to the development of new ENDF formats, in order to add new processing capabilities, in response to changing computer systems and in order to fix errors. The precise version of NJOY used in the computer exercises conducted at this Trieste Workshop was NJOY 89.31, which was released by the code developers just prior to the course, in late 1989. This version includes a number of recent changes (Ref. 5) designed primarily to permit access to data presented in the ENDF-6 format (Ref. 6), which is used, for example, in both the ENDF/B-VI and the JEF-II nuclear data libraries.

PROGRAMMING PHILOSOPHY

In developing NJOY as a FORTRAN program with the ambitious goal of communicating most of the data types of ENDF to most of the important applications, several general design principles have always been emphasized:

(1) Different "elementary" functions (for example, the reading and writing of a single type of ENDF data record) are kept separated in different subroutines.

(2) Different "complex" functions (for example, resonance reconstruction) are kept separated in different modules, a "module" being a named suite of subroutines.

(3) Data communication between different modules is permitted only by means of the writing and reading of sequential files. This makes each module, in effect, a separate program.

(4) Where programming trade-offs are necessary, clear and concise FORTRAN coding is preferred over the achievement of ultimate execution speed, and increased speed is preferred over reduction in disk storage.

(5) All FORTRAN coding has been written in a uniform style and is heavily commented.

All of these features combine to form a system that is reasonably easy to expand and modify, in spite of its large size (approximately 50 000 FORTRAN records). That is, changes to one subroutine usually do not require changes to other subroutines, and large-scale changes to one module usually do not require changes to the other modules. This ease of modifying the system largely accounts for the sucess the code developers have had in adapting to the rather rapid evolution of nuclear-data processing needs over the past 15 years.

The same attention to fundamental design has made it straightforward to implement the code system on a wide variety of computer types. The subset of FORTRAN 77 employed in NJOY 89 is compatible with compilers on CDC, Cray, IBM, VAX, CONVEX, Sun and numerous other computer systems.

It is possible to execute individual NJOY modules even on personal computers, but for traditional production operation, a fast mainframe-type computer, accessing a several-hundred-megabyte disk-storage facility, is almost essential. It was for this reason that the NJOY exercises at the 1990 Trieste Workshop were conducted on the large CONVEX C210, rather than on personal computers.

A feature that distinguishes NJOY from some other processing systems is that it provides neutron interaction data libraries in a consistent manner to both continuous-energy Monte-Carlo and discrete-ordinates transport codes. This consistency is guaranteed by the fact that NJOY always begins the processing operation by producing an explicit, linearly interpolable table of cross-section values for all reactions (via resonance reconstruction and linearization) at a large number of energy "points". These cross sections are saved in a point-ENDF (PENDF) format on disk files. A slight reformatting and optional "thinning" of a PENDF file produces a library for point Monte-Carlo codes. An integration over energy of the data in the very same PENDF file produces group-averaged data for discrete-ordinates codes.

The fact that the data are produced as <u>linearly</u> interpolable tables adds to the size of the PENDF files, but permits coding simplification and increased computational speed in all subsequent operations, such as Doppler broadening, Monte-Carlo sampling, energy-group integrations and plotting of the data.

It is useful at this point to list the modules of the NJOY system by name and explain briefly the purpose of each:

<u>NJOY</u>

The NJOY module is the driver program that calls in other modules on request, and it also contains a "toolbox" of common subroutines used by the other modules.

RECONR

The RECONR module is used to reconstruct explicitly the energy-dependent cross-section functions $\sigma(E)$ from ENDF resonance parameters and nonlinear interpolation laws. The energy values for all reactions are members of a single, unionized energy grid. The results are written out to a PENDF file.

BROADR

The BROADR module Doppler broadens the cross sections on the input PENDF file and writes the results onto a new PENDF file. The accurate kernel broadening method is used, and the results are independent of the particular resonance representation used. In addition, smooth cross sections and resonance-region backgrounds are correctly broadened.

UNRESR

The UNRESR module uses an analytic method to compute selfshielded point cross sections (tabulated versus temperature T and background cross section σ_0) and writes them onto the output PENDF file using a specially defined section of File 2.

HEATR

The HEATR module computes the heat-production and damage-energy production cross sections (proportional to displacements per atom - DPA) and adds them to the PENDF file. This calculation has been a problem for previous ENDF versions, because the format lacked the detailed energy-angle distributions for neutrons and charged-particles needed to get good results at higher energies and because many of the evaluations had severe energy-balance problems (Ref. 7). A number of the new features of the ENDF-6 format were added specifically to alleviate these problems. As a result, the NJOY 89 version of HEATR has many changes.

THERMR

The THERMR module is used to compute neutron scattering at low thermal energies where the binding of the scatterer in a material or the motion of atoms in a gas is important. The results are written on the PENDF file using reaction MT numbers in the range 221 to 250 in Files 3 and 6. The THERMR-output File-6 format differs from the actual ENDF File-6 format.

GROUPR

The GROUPR module is used to generate selfshielded multigroup cross sections using the Bondarenko method and transfer matrices for neutrons, photons, and charged particles. There are massive changes in the 89 version of this module. The most noticeable ones have to do with reaction and particle selection, File-6 processing, and charged particles. The output of GROUPR is stored in an ENDF-like group-data (GENDF) format.

GAMINR

The GAMINR module is used to compute cross sections for gamma-ray interactions with atoms. The output of GAMINR is also stored in the GENDF format.

ERRORR and COVR

The ERROR and COVR modules are used to compute and format multigroup covariances. The output of ERRORR is stored in the "ERRORR-output" format. The library output format of COVR is called BOXR.

MODER

The MODER module is used to convert back-and-forth between coded file modes (that is, ASCII, BCD, EBCDIC, etc.) and the NJOY blocked-binary format. It can also be used to build a new ENDF, PENDF, or GENDF file containing materials selected from several input files.

DTFR

The DTFR module is used to generate transfer matrices for transport codes that can accept the DTF format. It also has a capability for plotting the edit cross sections, the neutron or photon transport matrix, and the photon production matrix. This plotting capability was made available to the Trieste participants.

CCCCR

The CCCCR module is used to generate the CCCC standard interface files, ISOTXS, BRKOXS and DLAYXS, using output from GROUPR.

MATXSR

The MATXSR module is used to convert multigroup data from GROUPR into the MATXS format. With ENDF-6 data, a MATXS library can contain cross sections for all reactions and transfer matrices for neutrons, photons, and charged particles. Once the information exists in MATXS format, it can be manipulated in many ways using the stand-alone program TRANSX-CTR (Ref. 8), in order to produce input libraries for specific transport codes.

ACER

The ACER module is used to produce libraries in the ACE (A Compact ENDF) format for the MCNP continuous-energy Monte-Carlo code (Ref. 9). At this time, MCNP and ACER have only been updated to handle one of the File 6 formats; namely, "Law 1" tabulations in the center-of-mass frame using the Kalbach angular distribution systematics.

POWR

The POWR module is used to generate multigroup libraries for the Electric Power Research Institute codes EPRI-CELL and EPRI-CPM. Several thermal-reactor research groups have developed modifications of POWR or special post-processors, in order to service the WIMS reactor cell code. One such post-processor is the WIMSLIC program (Ref. 10).

PLOTR

The PLOTR module is used to generate plots of ENDF, PENDF, or GENDF cross-sections, or of experimental data. Multiple curves from any of these sources can be overplotted, and the data points can have error bars. All the normal combinations of scales are provided, and curves can be labeled. Implementation of this module requires the DISSPLA proprietary plotting software package, which was not available on the CONVEX C210.

The flow of data from module to module and then on to the application programs is illustrated in the accompanying figure. Note that the names shown in parentheses refer to various application programs, which are not distributed as part of the NJOY system.

The interested reader is referred to the NJOY manuals (Refs. 1-3) for a rather complete description of the physics algorithms of individual modules. These documents also present explicit input and printed code output from many typical test cases.

The exact (and current) input instructions for each module are contained as comment lines in the NJOY source code, at the beginning of the given module (SUBROUTINE RECONR, for example). These input lines should always be consulted, in preference to input instructions in printed documentation, because any printed instructions are very likely to be out-of-date at any given point in time.

A complete code package (PSR-171) for NJOY 89 is available from the Radiation Information Center at the Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831, USA.

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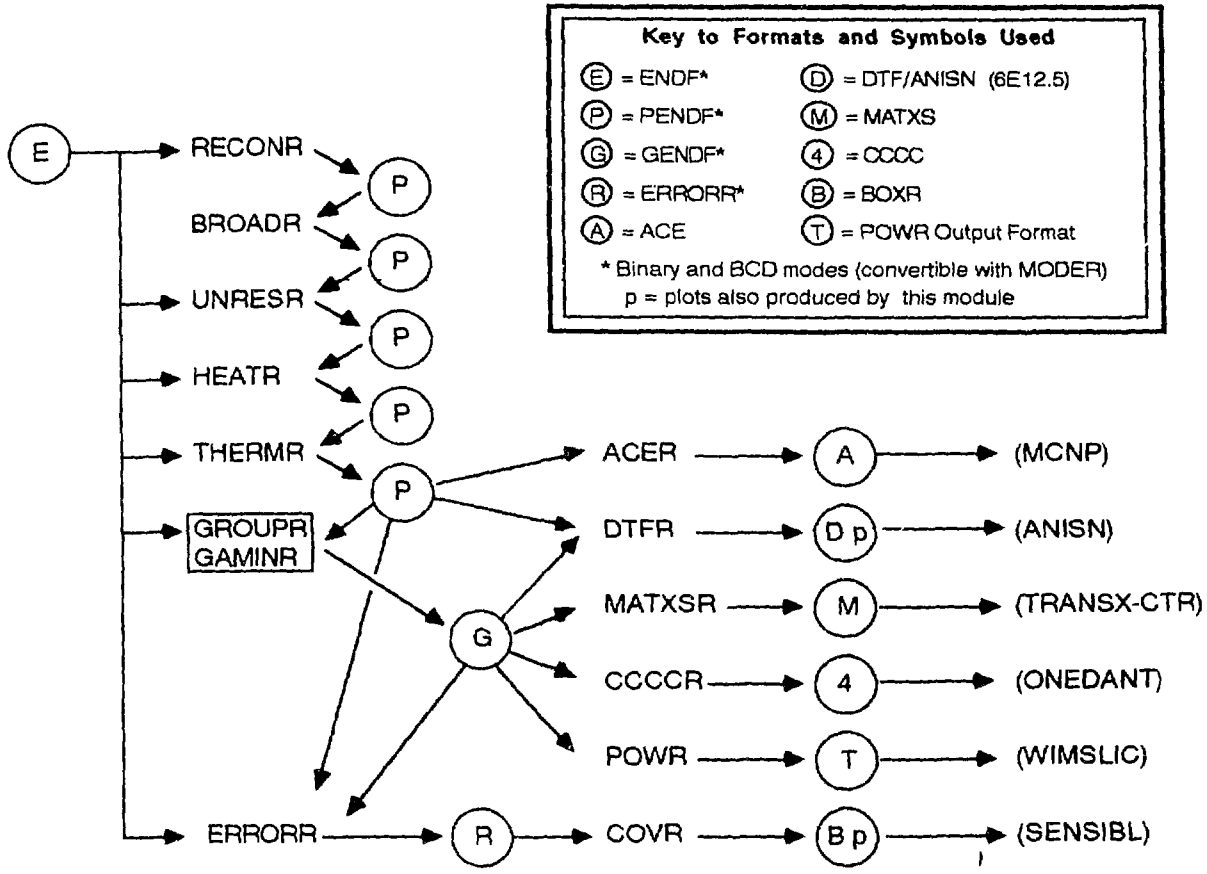

Fig. 1. Flow of Data in NJOY System