OECD/NEA Data Bank and Radiation Safety Information Computational Center (RSICC)

**WORKSHOP on NJOY-2001 and USER GROUP MEETING,**

Aix-en-Provence, France, 15 May 2001

## Summary

NJOY is a comprehensive nuclear data processing computer code system for producing continuous-energy and multi-group neutron, photon, and charged particle cross sections from ENDF format evaluated nuclear data.

***Objective of the workshop:***

Bring together the author of NJOY and its users

- for the presentation of ongoing developments and future evolution of NJOY
- for discussing feedback from its use with state of the art evaluated nuclear files and for different applications
- for presenting new developments or independent approaches by others for partial or full processing of nuclear data (e.g. CALENDF, AMPX)
- for proposing further developments arising from the production / release of data with expanded features or scope
- for continued international cooperation in this field of expertise

The meeting was jointly organised by the OECD/NEA Data Bank and the Radiation Safety Information Computational Center (RSICC) and hosted by CEA Cadarache. The principal author (R.E. MacFarlane) and a former co-author (D. Muir) attended the workshop.

Participants were welcomed to the meeting by the sponsoring and local organisations. It was attended by 25 participants from 11 countries (see list of participants). The workshop programme was reviewed and approved. The text of the presentations are available as a PDF file via hyperlinks from the programme of the workshop. A brief summary of the presentations and discussions is presented in the following.

## NJOY-2001

Robert E. MacFarlane, presented ***NJOY-2001***. His presentation covered:

- ***NJOY 2001 design and development.*** NJOY 99 is used as the base to which a modern subset of F90/95 features have been applied to improve maintainability and transportability. Method changes are limited to allow for easier testing of the results with the new code. Features used comprise modules, allocatable arrays, and modernised coding style. Testing was carried out on a number of UNIX platforms.
- ***Status of NJOY 99****:* NJOY99 was developed during the summer of 1999 based on NJOY97. The main goal was to incorporate cleanly a large number of changes needed for

high-energy data (150 MeV), outgoing and incident charged particles, and photo-nuclear data for MCNP4C. A large set of files based on ENDF/B-VI.5 was released and processed with multiple temperatures. Also a large subset of JENDL-3.2, and some JEF-2.2 and preliminary JEFF materials were processed by the author for testing. A selection of benchmark tests were performed with good results. The latest release at the time of the workshop is NJOY99.50.

- ***Software Quality Engineering*** was addressed as the next item. This aspect receives increased attention today also for some NJOY uses. Today's ideas are based on successful safety management programs and require a *risk assessment* for the software project. However the level of risk in NJOY is classified as low, which means that a *basic level* of formality applies. The goal of the *basic level* is to "stabilise the software, prevent its degradation with time, allow it to survive losses of staff or capability, and to provide a basis to advance to higher levels of formality if needed." The elements of SQA introduced comprise currently

    - Version control of software components
    - Issue tracking and requirements management
    - Automated build process
    - Regression testing and user-level testing
    - Application release process
    - Code documentation
    - Documentation of processes and coding practices

  Issue tracking has been introduced and is accessible via Internet. Problems encountered by users are shared through an electronic user forum with archiving of the problem discussions. This is one way to identify the issues for which the tracking is implemented. Concerning testing of NJOY *User Acceptance Testing* is the activity of determining if the code satisfies the needs of the users. For NJOY, this consists of running very large sets of real processing jobs to find as many special cases as possible. NJOY results are fed into selected application codes to check that the interfaces perform as expected and that the answers are as expected by the users.

- ***NJOY Info on Internet:*** Past and present corrections are all accessible via Internet. Links to other Internet web pages are also maintained, thus facilitating exchanges between author and users (see specific presentation).

***Discussion:*** the current version of NJOY-2001 is based essentially on NJOY99.0. Therefore the version that will eventually be released will contain updates at the same level as NJOY99.50 or beyond if further changes need to be applied.

**Experience and Feedback from Users on NJOY97 and 99**

Three presentations reporting problems encountered and proposed solutions were made:

Dieter Leichtle presented the ***processing of the Intermediate Energy Activation File IEAF-2000*** with GROUPR. It was carried out within a co-operation between FZK, Karlsruhe, and INPE, Obninsk. It concerns activation and transmutation cross sections for elements Z=1..84 up to 150 MeV including product nuclides with half-lives above 10 hours. Modifications to GROUPR to process mf6/mt5 multiple particle production data were presented. Automatic processing of all particle subsections is now available. Some selected results were presented. It would appear that GROUPR (NJOY99.32) is not capable of treating MT5 multiple particle subsections given in

MF6, therefore a solution is proposed that would solve the problem. This solution was checked when preparing a 256-group structure with regard to completeness of nuclide production yields (including isomeric states) and reproduction of the original data. The full library processing was successful.

***Discussion***: Sublet mentioned that there is another approach to store isotope production reaction cross-sections using the MF=8 file option. This approach allows handling individual reaction paths but is currently not compliant to ENDF-6 format rules. A proposal to allow for the required format change has been submitted to CSWEG but not yet approved. Fischer stressed that the MF=6/MT=5 (LAW=0) approach is in full accordance with the existing ENDF-6 format rules and, therefore, NJOY should be capable of processing a file prepared in this way. Further, this approach is a straightforward way to represent the large variety of open reaction channels above 20 MeV. The only drawback is the lumping of reaction channels leading to the same product isotope. This may cause problems for some activation codes relying on such data. MacFarlane will check if both options can be supported with NJOY or if one option is preferred.

Dieter Leichtle, then reported on the status of the ***$^{9}$Be-EFF-3.0/NMOD=3 data processing with ACER***.:

Pecularities of $^{9}$Be(n,2n) reaction channels as supplied in MF6/MT875-890 were discussed. It concerns a recent evaluation for EFF-3 by V.Pronyaev, S. Tagesen, H. Vonach. It includes energy-angle distributions (and covariances) and 16 channels for neutron emission, 17 for alpha emission. These partial cross sections are given as MT875 to MT890. In this presentation the (n,2n)-cross section (MT16) is redundant and should be derived as a fully consistent sum of the individual channels. The use of individual neutron emission channels in MC transport and sensitivity calculations is important in this case. However the present coding in NJOY/RECONR and ACER does not allow treating these data. Appropriate schemes to modify ACER were presented. The resulting ACE file was checked.

***Discussion***: concerning MT=16/MT=875-890 MacFarlane will check on possible double-counting on MT16. Checking should also be carried out if this is operational for the path producing cross sections for deterministic codes.

Ivo Kodeli, presented experience with ***EFF-3 cross-section processing using the ERRORR*** module:

EFF-3 Covariance Matrix Processing Comparison of the EFF-3 cross section covariance matrices processed using the modules ERRORR/NJOY and ANGELO (part of the ZZ-VITAMIN-J/COVA package) were presented, indicating a possible problem in ERRORR in case of covariance matrix processing for threshold reactions. ERRORR seems to non-physically reduce the standard deviation in the user energy group containing the threshold when the corresponding lower energy group boundary extends below the threshold energy.

Recent EFF-3 covariance data include few non-standard MT numbers such as (MT > 800, e.g. in $^{9}$Be, MT 875-890, in Ni-58, Ni-60 and Fe-56 MT 851-854). Patches for NJOY modules GROUPR, ERRORR and COVR were prepared, which allow processing of these data. $^{9}$Be covariance matrices were processed into VITAMIN-J 175 groups by NJOY and ANGELO codes. They compare very well, except for the threshold group (possibly an averaging problem).

***Discussion:*** The proposed patches are available.

**Further issues** discussed are as follows:

- ***QA and small numbers***: most problems were solved in the NJOY97 version. These arise from differences of many large numbers, which can generate "random" results. Some procedures truncate them to zero. Problems arose with processing (d,t) reactions and special patches take care of this.
- ***Recoil spectra produced by GROUPR:*** differences in PKA spectra were found depending on the computational path used in GROUPR. Explicit instructions used should be transmitted to MacFarlane for tracking the problem.
- ***Processing of application energy range for intermediate energy data:*** processing is carried out to the upper energy limit of the material file. If the application library is needed only for a lower energy range it would be convenient to have the possibility to stop processing when the desired upper energy limit is reached.
- ***Photo-nuclear data:*** these data can now be processed, but there are still problems in the data, in particular from JENDL-3. The KAERI & LANL evaluations can be processed correctly. BROND data were modified to enable processing and sent to the IAEA. An example of good representation of (γ,n) cross sections and processing performance is Gerald Hale's deuteron break-up cross section. Now full matrices can be derived

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|---|---|
| (n,n) | (γ,n) |
| (n,γ) | (γ,γ) |

## CALENDF-2001

Pierre Ribon made a brief ***presentation on CALENDF-2001*** and showed some problems:
CALENDF generates sets of resonance parameters in the unresolved resonance region (URR), it treats this URR the same way as the resolved resonance region (RRR), it calculates Probability Tables (PT) and finally after further computational steps group cross sections.

Two basic methods are used:

1. *Cubic Interpolation***:** it's the basic mode of interpolation. It is of interest for shortening of computing time and for wider meshes. A careful check of point-wise data is required in order to avoid erroneous interpolation by a cubic leading to non-physical cross-sections in particular when Doppler broadening.
2. *Padé Approximants And Gauss Quadrature***.** Moments, orthogonal polynomials, Padé approximants and Gauss quadrature are closely related.

Several approaches for generating *Cross Sections Probability Tables* exist: the two oldest ones being those by L. B. Levitt (1971) where the range of cross section is divided into regular intervals , and the one of M. N. Nicolaev et al. (1970) also called the sub-group method; the PT is established in order to fit at best the effective cross sections.

CALENDF uses recommended procedures for interpolating the URR: it interpolates the average resonance parameters, and calculates their mean value over the described energy range, it uses the suitable approximation for multilevel effects (BWMN or RM). As concerns resonance parameters these are R-matrix parameters and the appropriate method for their processing (Reich-Moore method or another approximation) depends on these parameters and the required accuracy. The approximation recommended by the evaluator is used. As it is very likely that the actual distribution of partial widths is not exactly an integer equal to the number of open channels, it is suggested to use a real number for the degrees of freedom. More examples are provided in the presented paper.

In conclusion, CALENDF-2001 is an informatic revision of CALENDF (Fortran 90, clarification of coding, and test of compilers). Several options, defined inside the code, have been made modifiable by external users. A few routines have been improved: these concern the energy mesh for a better description of high energy resonances, the linearisation (in fact, "cubitisation") of pointwise cross-sections.

There are still a few branches, which have to be tested: for example, there are now 2 methods for PT interpolation, they have to be compared in order to determine the best choice according the case.

Jean-Christophe Sublet presented CALENDF-2001, ***The User Point of View.***:

The CALENDF approach is based on Gauss quadrature as a probability table definition. This approach introduces mathematical rigorousness, procuring a better accuracy and some treatments that would be prohibited under other table definition such as group condensation and interpolation.

It has been applied to the ECCO group library scheme and the CALENDF PTs are used by the neutronic codes ERANOS, APOLLO and TRIPOLI. It is used in connection with NJOY 97-114 and 99-50. The new version CALENDF 2001 is written in Fortran 90/95 (SUN, IBM, MS Window and DEC alpha), an HTML user manual is in preparation and strict QA procedures are applied. The resonance energies samplings range from 600 to 1100, an improved resonance grid is used as well as an improved Gaussian quadrature table, finally two micro flux weightings per group are used. Several test cases were run with a diverse set of group boundaries (33 to1968). Comparison of probability table and effective cross sections have been carried out. The Beta test version of CALENDF-2001 will be distributed this summer.

The full release of this improved version is scheduled for autumn 2001 through the OECD/NEA and RSICC.

***Discussion:*** The comparisons between CALENDF and NJOY in the unresolved energy range show big differences, but CALENDF is showing fluctuations for a limited energy range while NJOY is showing averages over wider energy ranges for a large number of different ladders. Future comparisons of probability tables would be useful.

## AMPX-2000

John E. White presented a paper by Michael E. Dunn and Maurice Greene on ***the Status of the AMPX-2000 Cross-Section Processing System.***

AMPX was initially released more than 25 years ago. Several versions have been used and the most recent one is AMPX-2000. Its development started in 1995 and a possible release is scheduled for early 2002. The U. S. Nuclear Regulatory Commission has lately provided support. The objectives for its recent development are to provide an independent, state-of-the-art cross section processing capability, to process the latest ENDF formats, to support sensitivity uncertainty (s/u) methods development at ORNL, and to support current and future radiation transport analysis needs for licensing applications.

The structure of AMPX-2000 is modular. The code system contains a set of 18 computational physics modules and 61 utility modules. Conversion of modules to FORTRAN 90/95 has

commenced. Detailed capabilities are described in the paper presented. In addition to multi-group libraries, continuous energy libraries are produced now. AMPX-2000 contains several interfaces to NJOY. The following physics modules are included:

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|---|---|
| POLIDENT | Resonance Reconstruction |
| BROADEN | Doppler Broadening |
| Y12 | Interaction & Yield Processing & Thermal Processing |
| PRUDE, TABU, FABULOUS | Unresolved Processing |
| PURM | Probability Table Generation, |
| X10, PMC, NITAWL- III | Multi-group Averaging |
| BONAMI, NITAWL- III, CENTRM | Resonance Processing |
| KRYSTAL | Multi-pole Parameters |
| PUFF- III | Uncertainty Data Processing |
| GINSENG | Generate S( $\alpha$,$\beta$) Data for Free Gas Model |

AMPX-2000 is more than just a system to generate processed cross sections. AMPX-2000 includes modules that perform resonance self-shielding and radiation transport calculations all integrated into a single system. This modular system makes it easy to import and use additional codes. For example, NJOY has been used in AMPX-2000 execution sequences without having to modify a single line of either AMPX-2000 or NJOY.

The testing phase includes among others the processing of more than 300 ENDF/B-VI evaluations and generation of prototypic data for the SCALE/CENTRM sequence. A draft for the user documentation has been circulated for internal review at ORNL and is near completion.

Future Plans include maintenance support for AMPX-2000, processing international files in ENDF-6 format (e.g. JEFF-3, JENDL-3, BROND-2, CENDL-2), energy deposition or radiation damage capability, and generation of production multigroup libraries (neutrons or coupled neutron/gamma) for distribution. A task has been initiated to examine the possibility of providing a method for generating cross section files for MCNP. This has already been done for point data with the MAKPEN module. The new task will look at the other capabilities provided by the ACER module of NJOY.

## Conclusions / Summary

The Workshop addressed current and future work on NJOY and the characteristics of the next version NJOY-2001, that is tentatively scheduled for release in autumn of 2001. Interaction between author and users allowed identifying some issues that need to be addressed. The NJOY modules are now rather stable, especially those carrying standard processing tasks. Recently introduced changes address mainly problems with new features used in data recently produced, such as cross-sections in the intermediate energy range (E>20 MeV) and for photo-nuclear reactions. Further changes and expansions will be made as needs arise, be it for new applications or new data types made available.

R.E. MacFarlane commented that the contributions and feedback received from the NJOY users is beneficial to maintain the quality, applicability and cover testing for a wide range of applications, which the author alone could not accomplish himself. The methods of SQA are now considered appropriate for the requirements of the users.

Independent developments and contributions to this field of expertise were presented, especially as concerns CALENDF and AMPX. This allows cross checking of methods and to building confidence in the codes and methods used.