

NJOY user group Meeting

OECD NEA Data Bank

21 November 2008

## SUMMARY

### 1. Welcome, Introduction of Participants

The meeting was chaired by Skip Kahler, manager of NJOY, who welcomed participants.

The meeting was attended by 22 participants from 8 countries, most of them expert users of NJOY.

### 2. S. Kahler: The NJOY Nuclear Data Processing System

NJOY-2008 will be released towards the end of 2008 to the Radiation Safety Information Computational Center (RSICC) and will be released through RSICC to the Data Bank.

This new version will contain a series of additional updates compared to the current version including as appropriate those proposed by users and documented at the NEA Data Bank Web site <http://www.nea.fr/html/dbprog/njoy-links.html>. Details are provided in the full presentation.

The new version will come with a new manual. One specific module will contain all physical constants following the CODATA 2002 standard. The "Issue Tracker" may be reactivated with the new release.

The QA procedure to validate changes includes full reprocessing of all recently released evaluated nuclear data files with not too strict a tolerance. Through a DIFF program the processed files are compared with those of runs made before applying the changes and the effect of changes are checked throughout and analysed.

The NJOY99 will be maintained for another year, allowing users to cross check the performance of the two codes. Later NJOY99 maintenance will be discontinued.

The new features of plotting covariance data, making the graphs better legible and by removing redundant graphs were presented. Now also angular and energy distribution uncertainties are plotted. The PLOTR module will provide enhanced flexibility for data display.

Future developments will include

- continuous evolution of covariance formats and processing
- a possible CINDER module for Residual Nuclide Production/Decay
- calculation of elastic scattering angular distributions from resolved resonance parameters
- Additional NJOY training and other upgrades on Web pages

If funding is made available the code management would agree to introduce specific requests by users.

### **3. A. Trkov: Co-ordination of updates within Europe**

A mechanism was introduced (<http://www.nea.fr/html/dbprog/njoy-links.html>) to help users and make a traceable set of patches available. This allows inspection of processing problems found by others while official NJOY updates are released with lower frequency than problems are identified. This sharing of possible solutions to problems found reduces duplication in searching for solutions and removes contradictory results during inter-laboratory comparisons of results. The updates reported represent an interim solution until the official updates are released. This provides a reference set of updates for data processing available to everyone so that traceability of processed data would be achieved, and helps the authors to implement the updates more quickly.

Concerning covariance data processing it was observed that an enormous progress was made in correcting the processing modules which have now stabilised. Wishes for extensions include the option of allowing user defined font sizes for improved readability and for publication and the need of adding one more decimal digit in the output of the BOXER format. It was noted that weight option 19 in ERRORR generates internal energy grids contradicting with GROUPE.

Other wishes expressed include displaying MF34 average cosines and plotting of MF10, and the extension of the manual describing PURR.

The manual will be in LaTeX, but a Web-based version allowing easy navigation might be posted on the Web.

Because of the free format for statements in NJOY-2008 a new version of the UPD will be released handling this format change.

The issue was raised, whether it will be possible to provide a beta-version of NJOY-2008 to a selected number of experienced users that would test the code, but not use it for applications or publications. Such a possibility will be investigated. The Data Bank would distribute such a version on special authorisation and on condition it respects export-control and licensing rules.

S. Kahler expressed appreciation for this mechanism being in place, as it has facilitated access to qualified and validated changes proposed by users outside the USA. This co-operation and work of A. Trkov is an important contribution to improving the code.

### **4. Experience and Feedback from Users on NJOY99**

- **C.J. Dean, R. Perry: Normalisation of Interpolated Secondary Energy Distributions for Thermal Scattering**

This presentation addressed a problem relative to interpolation of secondary energy distributions generated on an incident energy grid, in which the scatter matrix does not add to the cross section. Improvements to this had been introduced by MacFarlane for important peaks. But this method was adapted so that the integral of the distribution at interpolation points is preserved.

The changes solving this problem (id. UPWE6) have been made available and are now posted in [upnea040 up259 recommended updates to NJOY99.259](#) (20 November 2008) on the NEA Webpage.

- **M. Cornock: The Effect of Interpolation Scheme Choice on Critical Assembly Flux Spectra**

This presentation addressed problems found during analysis of flux spectra: a large increase in low energy flux spectra was observed. It was found (C. Dean) that this was the effect of interpolating linearly rather than using unit base. The presentation shows the effect due to this on several benchmarks.

The following discussion concentrated on whether NJOY should correct during processing obvious evaluation deficiencies (e.g. interpolation of emission spectra). The obvious action would be to correct evaluations, but this process is slow as it requires a new release. It is suggested that in obvious cases NJOY could take smart corrective actions, once the files are corrected this action is not activated. In particular this could be introduced for the INT=2 (linear) → INT=22 (unit base) interpolation law. But first, CSEWG should adopt this change for the manual: a formal request in this sense should be made. This feature has already been introduced in ACER.

## **5. Experience in Processing Covariance Data**

In absence of participants from JAEA, E. Sartori made a brief presentation of papers made available relative to the ERRORF module.

**ERRORF** is a brother code with the ERRORJ code. This code has the function to generate the group structure covariances of shielding factors (f-tables) from ENDF format covariance files. The user can evaluate the error of the Doppler reactivity by multiplying the covariances with the f-factor sensitivity coefficients which can be obtained the SAGEP-FR system. The papers made available are:

- N. Otuka, A. Zukeran, H. Takano, G. Chiba and M. Ishikawa: Covariance Analyses of Self-Shielding Factor and Its Temperature Gradient for Uranium-238 Neutron Capture Reaction
- N. Otuka, A. Zukeran, H. Takano, G. Chiba, M. Ishikawa: ERRORF - A code to Calculate Covariance of Self-shielding Factor and its Temperature gradient, JAEA-Data/Code 2008-012, June 2008.

ERRORJ is now fully integrated into NJOY: should ERRORF also be integrated into it?

S. Kahler stated that this is indeed very interesting work. Also it is programmed like in NJOY. While in the present scheme NJOY is used as a module, if integrated into NJOY, ERRORF should become a module of NJOY, thus some adaptation may be needed.

Participants have expressed interest in an integration of such a module into NJOY. This issue is of relevance to other NEA activities involving propagation of uncertainties from basic data to integral physics parameters.

The issue about the "zero-sum rule" for the covariances of emitted spectra (MF35) was discussed. The question was whether NJOY should renormalise the covariance matrices before (and after) processing, because this is important for the correct estimate of the uncertainties. The impact of the normalisation of the fission spectrum on the uncertainties in the multiplication factor was presented at the Conference in Port Jefferson, June 2008.

Testing for negative eigenvalues of covariance matrices was also mentioned. Logically, this should be part of the ENDF Utility Codes, but in many cases it would be simply a duplication a big chunk of the coding from NJOY. The problem is that the format allows several overlapping representations of the

covariance matrices, what requires processing to obtain a full matrix on a union grid, which can then be tested.

In both of the above cases it would be convenient if NJOY could do the checking at least as an option.

## **6. Discussion on Future Developments and Wish-list of Users, Need for NJOY User training**

Miscellaneous items were discussed under this topic

### ***S( $\alpha,\beta$ ) for very low temperatures***

M. Mattes confirmed that there were no outstanding problems for very low temperature processing, only when mixing together materials with different scattering properties care must be taken to do it right.

### ***Are there remaining problems for special purpose files or applications?***

Staff at CERN claims that there are problems with processing data with outgoing charged particles (spectra) for some nuclides. Specific information was not provided. It was recommended that those who have found such problems report for which nuclides and evaluations and provide the input file (and corresponding output) in order to facilitate the diagnostics as to whether it is a problem in the evaluation or in NJOY.

No outstanding problems with processing delayed neutron data were reported.

### ***Further processing of NJOY output files***

ACE files: interpolation for different temperatures:

New ACE files are provided with 5-6 temperatures (e.g. ENDF/B-VII) and the MAKSF module contains the DOPPLER module taking care of temperature interpolations. An alternative module for interpolation is "SIGACE, Code for Doppler broadening of ACE-formatted files" available from IAEA NDS and the NEA Data Bank. <http://www.nea.fr/abs/html/iaea1416.html>

TRANSX-2005 Fortran-90/95 - MATXS files: further processing into application libraries.

The new features are a capability to generate multi-group Monte Carlo data files for MCNP and changes to link with the PARTISN  $S_N$  code from Los Alamos, was presented at previous NJOY user group meetings. Considerable effort was invested by R.W. MacFarlane on this new module, but the release was delayed, due to other priorities. The plan is to release it after the release of NJOY-2008.

### ***Further developments***

#### **S.P. Simakov, A.Yu. Konobeyev, U. Fischer: Assessment of survived radiation defects by a modified version of NJOY**

This presentation was made at the previous NJOY user group meeting. Such issues are very important for plant lifetime extensions (M. Pescarini).

Incident neutrons produce Primary Knock on Atoms (PKA) in materials which propagate in media and produce a thermal spike. survived point defects and clusters contribute to radiation induced microstructural evolutions, damage accumulation and eventually make rise to the mechanical property changes. The HEATR module had to be modified to account for survived defects during processing of the evaluated data .

B. Becker from FZK agreed to discuss the release of the required changes with S. Simakov for submission to NJOY.

#### **D. Rochman: Processing MF-32 and the scattering radius with ERRORJ**

This presentation was discussed again at the NJOY user group meeting.

ERRORJ does not treat  $R'$  (scattering radius), consequently the  $(n,el)$  and  $(n,tot)$  uncertainties in the thermal range are underestimated. G. Chiba has recently produced a changed ERRORJ version so that it can process  $R'$ . However this requires a small format modification. The expansion of format to include this modification requires discussion and approval by CSEWG. As the latest meeting was held recently, this can be implemented only as of the next meeting. However, discussions will take place in order to achieve a timely update.

#### ***Training***

NJOY tutorials were presented at different recent ANS meetings. They were rather successful. It was recommended by participants that such tutorials or trainings be part of Summer Schools organised regularly (A. Koning, A. Plompen).

In general, the on-line version “A technical Tour to Nuclear Data” and in particular “[Learn About the NJOY Nuclear Data Processing System](#)” are considered to be very important educational tools. However these are not complete and a more comprehensive edition would be welcome. This is of particular importance for beginners in the field. Cross-section data are considered by many as ‘given’ an exact translation from the Latin “data”. It is important that data users are educated on data limitations: there is a lack of understanding by many on what data entail.

#### ***Other Issues***

JAEA has provided the full set of updates they have applied to NJOY99.90 for processing JENDL-3.2 and JENDL-3.3. Both S. Kahler and A. Trkov, agreed to verify whether these changes were introduced in later updates of NJOY99.