

OECD/NEA Data Bank

NJOY USER GROUP MEETING

NJOY: a comprehensive nuclear data processing computer code system for producing pointwise and multigroup neutron, photon, and charged particle cross sections from ENDF format evaluated nuclear data

12 April 1999

NEA, Issy les Moulineaux

Summary**1. Welcome, Introduction of Participants**

The NJOY User Group Meeting was attended by 31 participants from 12 countries and 20 organisations. The List of participants is provided as Annex 1.

2. R.E. MacFarlane: NJOY in 1999

Bob MacFarlane presented recent developments of the NJOY evaluated nuclear data processing system including

- Reproducibility of results across different platforms (7 digits issue, literal constants, portable constants, rounding off, significance for differences, standardised constants - showing finally the small differences that are left, mostly in the last digit of small numbers not affecting results in real applications).
- Changes applied in the methods and options in NJOY97, in particular the issues of the displacement damage problem)
- NJOY99 was then introduced, in which a general cleanup has been undertaken aiming at improved portability and Fortran90 compatibility. In addition a large number of changes affect the charged particle and photonuclear capabilities for MCNPX, the introduction of cumulative angular distributions and Law 61 for non-Kalbach CM distributions, particle production, charged particle elastic scattering, heating in all-particle transport, processing of activation file.

3. Brief Presentations by Users

Processing of Unresolved Resonances

Broeders asked about catching unphysical f-factors. MacFarlane replied that negative values could normally be avoided by not going too low in σ_0 . Perhaps there should be an alarm message to alert the user. Trkov reported on "anomalous self-shielding factors of U-235 from ENDF/B-VI in the unresolved resonance range". Selfshielding factors slightly larger than 1 have been observed. This might be due to considerable overlap of the resonances and the fact that single Level B-W is used. A multilevel approach would be better - it is a problem in part due to evaluation. The use of ladders would remove the problem (See PURR and CALENDF). Hwang from ANL seems to have solved the problem in the UNRESW module that is however not in the public domain.

Ribon and Nouri pointed out an ambiguity in dealing with average neutron width in the unresolved resonance energy range. When there are 2 neutron channels, the neutron width found in evaluations is generally half of the right value, however, this is in agreement with processing codes which multiply this value by 2. As a short-term action it is decided to accept this anomaly, and therefore modify evaluations that are per se correct (such as Rh-103 of JEF-2.2). In the long run, it is proposed to change the definitions in ENDF-102 (formats and procedures) to use the physically correct representation, to modify processing codes and adjust the evaluations to match.

Activation Processing

Koning asked about the status of activation processing. MacFarlane described an activation patch for GROUPT that makes it easier to process the ENDF-style version of EAF, but that has not been put into the general release as yet. Sublet presented EAF-99 in ENDF-6 Format: format issues and SYMPAL, NJOY processing. MacFarlane pointed out that some of these problems could be solved by using MF3 x MF9 for the low-threshold reactions like capture. Sublet and Koning would like this activation patch issued within a few months, and said it could wait for NJOY99.

PKA Spectra Processing

Fischer presented a paper by P. Vladimirov: Using NJOY for PKA Spectra Calculations. The data flow for damage calculations under neutron irradiation particularly useful for light nuclei has been presented. Some of the problems encountered had been reported to MacFarlane and have been corrected. A few more issues need to be resolved such as the reason for a jump in the PKA spectrum for Li-6 when refining the energy groups and the handling of multiple subsections for separate recoils. Pescarini noted that PKA spectra are useful also for computing of DPA for mixtures such as SS.

4. Future Evolution of NJOY

Standard NJOY Versions

The NJOY version to be used for JEFF-3 processing was discussed. It could be

- a) NJOY 97.62 as already released
- b) NJOY 97.95 + a few more patches, which will be issued by RSICC soon, or
- c) NJOY 99, which will be available to NEA in a few months.

It was noted that c) has few advantages over b) for reactor applications. It was suggested that a) be adopted, with users being able to make specific patches from later versions when needed for special problems.

Pending Patches to NJOY 97.95

- a) Fix infinite loop in *getwtf* for some machines
- b) Fix bias in *sigfig* for 32-bit machines
- c) Fix some typos that affect HEATR output.

Other Suggestions

Add the XMAS-172 group structure. Sartori will send it to MacFarlane. Broeders asked for generalised comment cards to be re-enabled in the NJOY input, and suggested a method using a pre-processor. He also suggested putting the scratch files in the user area to avoid using up *temp* area for other users on the machine. In addition, he suggested separating ACER from NJOY as an independent program. MacFarlane did not seem to like that idea. Pelloni wanted more weight functions without fusion peaks for reactor work. Finally it was suggested that a cut-off energy to allow high energy evaluations to be processed up to only 20 MeV would be useful. The issue of introducing gamma-DPA cross section generation based on the algorithms developed by Baumann (WEC-SRL) in HEATR was raised by Pescarini. This may be introduced in a later release. Kodeli had prepared and sent to MacFarlane a patch concerning MF 34 (SAD:

covariances for angular distributions of secondary particles) processing with NJOY. MacFarlane has not yet had the time to review the proposal, therefore this option will be introduced in a future release.

List of Papers distributed

1. Proposed Agenda and items for Discussion
2. Tentative list of Participants
3. NJOY/MACFARLANE-27 R.E. MacFarlane: NJOY in 1999, 6 April 1999
4. NJOY/RIBON-01 P. Ribon, A. Nouri: ENDF-B6 Format and Processing Codes -The Average Neutron Width for 2 Degrees of Freedom, April 1999 JEFDOC-788
5. NJOY/VLADIMIROV-01 P.V. Vladimirov: Using NJOY for PKA Spectra Calculations, April 1999
6. NJOY/TRKOV-10 A. Trkov: On an Anomalous Self-Shielding Factors of U-235 ENDF/B-VI in the Unresolved Resonance Range, 12 April 1999
7. J.CH. Sublet: EAF-99 in ENDF-6 Format: format issues and SYMPAL, NJOY Processing, EFF-DOC-677

Annex 1

OECD Nuclear Energy Agency

NJOY User Group Meeting

12 April 1999

Issy-les-Moulineaux

List of Participants

BELGIUM

DE RAEDT, Charles
Project Leader
SCK CEN Nuclear Research Centre
Boeretang, 200
2400 Mol
Tel: +32 14 33 22 71
Fax: +32 14 32 15 29
Eml: cdraedt@esckcen.be

CZECH REPUBLIC

ZALESKY, Karel
Nuclear Research Institute Rez plc
CZ 250 68 Rez near Prague
Tel: +420 2 6617 2388
Fax: +420 2 2094 0156
Eml: zal@nri.cz

FRANCE

COSTE, Mireille
CEA/DRN/DMT
SERMA/LENR
CEA Saclay
91191 Gif sur Yvette Cedex
Tel: +33 (0)1 69 08 44 40
Fax: +33 (0)1 69 08 94 90
Eml: mireille.coste@cea.fr

DOS SANTOS UZARRALDE, Pierre
C.d'Et. de Bruyeres-le-Chatel
CEA/B3/DPTA/PN
B.P. 12
F-91680 BRUYERES-LE-CHATEL
Tel: +33 1 69 26 57 66
Fax: +33 1 69 26 70 63
Eml: dossanro@bruyeres.cea.fr

HEBERT, Alain
CEA Saclay
DRN/DMT/SERMA/LENR
Bat. 470
F-91191 GIF SUR YVETTE CEDEX
Tel: +33 (0)1 69 08 27 44
Fax: +33 (0)1 69 08 23 81
Eml: alain.hebert@cea.fr

MOUNIER, Claude
CEA Saclay
DMT/SERMA/LENR
Batiment 470
F-91131 GIF-SUR-YVETTE CEDEX
Tel: +33 (1) 69 08 95 11
Fax: +33 (1) 69 08 94 90
Eml: claudemounier@cea.fr

RAEPSAET, Caroline
CEN Saclay
DMT/SERMA/LEPP
Bat. 470
F-91191 GIF-SUR-YVETTE CEDEX
Tel: +33 (1) 6908 5687
Fax: +33 (1) 6908 4572
Eml: caroline.raepsaet@cea.fr

RIBON, Pierre
57E, Les Monts Lories
91440 BURES-SUR-YVETTE

Tel: +33 1 69 07 58 44
Fax:
Eml: ribon@nea.fr

GERMANY

BROEDERS, Cornelius H. M.
Inst. fuer Neutronenphysik
und Reaktortechnik
Forschungszentrum Karlsruhe
Postfach 3640
D-76021 KARLSRUHE

Tel: +49 (7247) 82 24 84
Fax: +49 (7247) 82 38 24
Eml: cornelis.broeders@inr.fzk.de

FISCHER, Ulrich
Forschungsz. Karlsruhe
Institut fuer Kern
und Energietechnik (IKE)
P.O. box 3640
D-76021 KARLSRUHE

Tel: +49 (7247) 82 3407
Fax: +49 (7247) 82 4837
Eml: ulrich.fischer@inr.fzk.de

MATTES, Margarete
Universitaet Stuttgart
Institut fuer Kernenergetik
und Energiesysteme
Postfach 801140
D-70550 STUTTGART

Tel: +49 (711) 685 2136
Fax: +49 (711) 685 2010
Eml: mattes@ike.uni-stuttgart.de

ITALY

BUCCAFURNI, Aldo
ANPA/NUC-TECN
Via Vitaliano Brancati, 48
I-00144 ROMA

Tel: +39 6 500 72 130
Fax: +39 6 500 72 044
Eml: aldo@anpa.it

MENAPACE, Enzo
E.N.E.A.
Applied Physics Division
Via Don G. Fiammelli 2
I-40128 BOLOGNA

Tel: +39 (51) 60 98 239
Fax: +39 (51) 60 98 359
Eml: menapace@bologna.enea.it

ORSI, Roberto
ENEA - Centro Ricerche
'E. Clementel'
Via Martiri di Montesole, 4
I-40129

Tel: +39 (51) 6098174
Fax: +39 (51) 6098705
Eml: orsi@nudace.arcoveggio.enea.it

PESCARINI, Massimo
ENEA - Centro Ricerche
'E. Clementel'
Via Martiri di Montesole, 4
I-40129 BOLOGNA

Tel: +39 (051) 6098233
Fax: +39 (051) 6098705
Eml: pescarini@nudace.arcoveggio.enea.it

JAPAN

KONNO, Chikara
Fusion Neutronics Source (FNS)
JAERI
Tokai-mura, Naka-gun
Ibaraki-ken 319-11

Tel: +81 (292) 82 6016
Fax: +81 (292) 82 5709
Eml: konno@fnshp.tokai.jaeri.go.jp

- present address: FZ Karlsruhe

KONNO, Chikara
Forschungsz. Karlsruhe
Institut fuer Kern
und Energietechnik (IKE)
P.O. box 3640
D-76021 KARLSRUHE

Tel: +49 (7247) 82 3494
Fax: +49 (7247) 82 4837
Eml: konno@inrfusion.fzk.de

NETHERLANDS

DE LEEGE, Piet F.A.
Delft University of Techn.
Interfaculty Reactor Inst.
Reactor Physics Dept.
Mekelweg 15
2629 JB DELFT

Tel: +31 (15) 278 66 18
Fax: +31 (15) 278 64 22
Eml: leege@iri.tudelft.nl

KONING, Arjan
Nuclear Analysis Group
B.U. Nuclear Energy
NRG
Postbus 25
NL-1755 ZG PETTEN

Tel: +31 (224) 56 4051
Fax: +31 (224) 56 4480
Eml: koning@nrg-nl.com

SLOVENIA

KODELI, Ivan
Institut Josef Stefan
Jamova 39
1000 Ljubljana

Tel: +386 (61) 188 5412
Fax: +386 (61) 161 2335
Eml: ivan.kodeli@ijs.si

TRKOV, Andrej
Jozef Stefan Institut
Jamova 39
1000 LJUBLJANA

Tel: +386 (61) 1885 324
Fax: +386 (61) 1612 335
Eml: andrej.trkov@ijs.si

SPAIN

RUGAMA, Yolanda
Universidad Politecnica de Valencia
Departamento Ingenieria Quimica
y Nuclear
Camino del Vera sn
46022 VALENCIA

Tel: +34 96 3879631
Fax:
Eml: yrugama@iqn.upv.es

SWITZERLAND

PELLONI, Sandro
Paul Scherrer Institut
CH-5232 VILLIGEN PSI

Tel: +41 (56) 310 20 75
Fax: +41 (56) 310 44 12
Eml: sandro.pelloni@psi.ch

UNITED KINGDOM

DEAN, Christopher John
Performance Safety Services
Dept., Rm. 347, Bldg. A32
Asset Management Services Grp
AEA Technology Winfrith
DORCHESTER, Dorset DT2 8DH

Tel: +44 1305 20 2357
Fax: +44 1305 20 2746
Eml: christopher.dean@aeat.co.uk

MILLS, Robert W.
British Nuclear Fuels plc
Lab 48/B229
Sellafield Site

Tel: +44(19467) 74682
Fax: +44(19467) 76984
Eml: rwm3@bnfl.com

Cumbria CA20 1PG

SUBLET, J.-Ch.
UKAEA Government Division Fusion
D3 Culham
ABINGDON
Oxfordshire OX14 3DB

Tel: +44 (1235) 463492
Fax: +44 (1235) 463435
Eml: j-ch.sublet@ukaea.org.uk

UNITED STATES OF AMERICA

MACFARLANE, Robert E.
MS B243
Los Alamos National
Laboratory
LOS ALAMOS, NM 87545

Tel: +1 (505) 667 7742
Fax: +1 (505) 667 9671 OR 1754
Eml: ryxm@lanl.gov

International Organisations

KELLETT, Mark A.
NEA Data Bank
OECD
Le Seine Saint Germain
12 Bld. des Iles
92130 Issy-les-Moulineaux

Tel: +33 1 4524 1085
Fax: +33 1 4524 1110
Eml: kellett@nea.fr

MANSOUR, Sophie
Agence de l'OCDE Pour L'Energie Nucleaire
Le Seine St-Germain
12, Blvd des Iles
92130 Issy-les-Moulineaux

Tel: +33 1 4524 1035
Fax: +33 1 4524 1110
Eml: mansour@nea.fr

NA, Byung Chan
OECD Nuclear Energy Agency
Data Bank
12 boulevard des Iles
92130 Issy les Moulineaux

Tel: +33 1 4524 1091
Fax: +33 1 4524 1110
Eml: na@nea.fr

NOURI, Ali
OECD Nuclear Energy Agency
Le Seine St-Germain
12, Boulevard des Iles
92130 Issy-les-Moulineaux

Tel: +33 (0)1 45 24 10 84
Fax: +33 (0)1 45 24 10 11
Eml: nour@nea.fr

SARTORI, Enrico
OECD/NEA Data Bank
Le Seine-Saint Germain
12 boulevard des Iles
F-92130 ISSY-LES-MOULINEAUX

Tel: +33 (0)1 45 24 10 72
Fax: +33 (0)1 45 24 11 10
Eml: sartori@nea.fr