

Status of NJOY91 at Winfrith

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INTRODUCTION

This paper describes the current status of the NJOY91 (1) processing code system at Winfrith. At the NJOY Users Meeting at the OECD in June 1994, NJOY91.91 was officially recommended. A beta-release version of NJOY91.91 was made available to users at Winfrith in June 1994 and called NJOY91.91w24 (2) to indicate the 24 local enhancements which had to be made, NJOY89.62w (3)(4) remained the recommended version. In August 1994, a problem with the beta-release version of NJOY91.91 was encountered which had to be resolved before NJOY91.91 could be officially recommended for use at Winfrith. This paper describes the problem and its solution. It also discusses some views on implementation and verification plans for future releases of the code.

PROBLEM DESCRIPTION

The beta-release version of NJOY91.91w was used for a project whose aim was to recommend an improved method of representing U238 unresolved resonance data in libraries used in the shielding and criticality Monte-Carlo codes MONK(5) and MCBEND(6). One of the requirements for the proposed improved method was the production of ultra-fine group cross-sections (12630 groups). A local post-processing module, MOULD, was extended to include the new method and additional consistency checks. One of these consistency checks was to confirm that the partial cross-sections summed to the total in all groups. The processed JEF2.2 U238 evaluation contained groups, in the energy range above the threshold of the unresolved region, which did not compare to a specified tolerance.

Winfrith test case 17 processes JEF2.2 U238 cross-sections into 172 energy groups, the "XMAS" scheme, for inclusion in a WIMS format library(7). Results from NJOY91.91w24 also showed inconsistencies at the threshold of the unresolved resonance region which were not present in NJOY89.62w results. It was thus decided to investigate the problem further using this test case.

INVESTIGATION OF PROBLEM

Test case 17 was run using both NJOY89.62w and NJOY91.91w24 and the PENDF files kept so that point data could be compared. The total group cross-sections on the output files were compared and differences were found in the groups around 10 keV, the threshold of the unresolved energy region. The partial cross-sections in the NJOY91.91w24 output did not sum to the total cross-section. The PENDF files from BROADR were then compared using COMPLIT (see Figure 1) and the difference at 10 keV was shown. The point data, for the total reaction (MT=1), around this energy range were examined and it was noted that the RECONR PENDF produced by NJOY91.91w24 contained no cross-section value at 10 KeV, the threshold of the unresolved region. It contained a value of ~5.5 at 9.999999 keV and a value of ~15 at 1.000001 keV, spanning the threshold energy. The NJOY89.62w PENDF contained a value of ~15 at 10 keV. The BROADR PENDF produced by NJOY91.91w24 contained two points at 10 keV with the same cross-section of ~6.5. The next point on the file was a value of ~15. at 11.43 keV. The BROADR PENDF produced by NJOY89.62w also contained two points at 10 keV with values of ~5.6 and 15.5. The next point on the file was a value of ~15 at 11.43 keV.

The point data for partial reactions compared within an acceptable tolerance and appeared to be correct, i.e for capture the broadened cross-section values at 10 keV were ~5.5 and 0.7 and the elastic cross-section values were ~0.14 and ~14.7. Summing these values (fission is insignificant at this energy) gave a total cross-section of ~5.6 and ~15.4, consistent with the NJOY89 values. Thus, the BROADR PENDF file produced by NJOY91.91w24 was inconsistent and gave incorrect total cross-section values in the range 10 keV to 11.43 keV (see Figure 2).

Before detailed investigations of the coding was initiated, Enrico Sartori of the OECD Data Bank was contacted to ascertain the current status of the code and ensure the problem had not

already been encountered and a correction recommended. We were informed that additional modifications (up92 - up115) had been made by the code author since the official release of NJOY91.91. These modifications had not been formally released but unofficial versions were available direct from Los Alamos. These were obtained via the gateway machine at Harwell. Appendix 2 gives brief details of the 115 updates as supplied by the code author.

A preliminary version of NJOY incorporating these updates and Winfrith local modifications was installed at Winfrith. Test case 17 was rerun with this version and correct group cross-sections were obtained. The RECONR PENDF was examined and found to include two values at 10.0 keV, ~5.6 and ~15.5. The BROADR PENDF contained the following values: 11.345 at 9.9978 keV, 15.468 at 10.0 keV and 15.221 at 11.43 keV.

The table below summarises the point cross-sections on the PENDFs output from test case 17 at the join of the resolved and unresolved energy region.

Table 1 : Total Point Cross-sections

Code Version	Reaction/ Energy	RECONR				
		9.999999+3	1.000000+4	1.000000+4	1.000001+4	1.143000+4
NJOY89.62w	Total	5.497	15.468	-	15.468	
NJOY91.91w24	Total	5.497	-	-	15.468	
		BROADR				
NJOY89.62w	Total	5.527	5.588	15.47	-	15.22
	Elastic	0.134	0.136	14.75	-	14.54
	Capture	5.393	5.452	0.719	-	0.681
NJOY91.91w24	Total	5.500	6.488	6.488 *	-	15.22
	Elastic	0.136	0.138	14.75	-	14.54
	Capture	5.393	5.452	0.719	-	0.681
NJOY91.91w25	Total	11.34 [#]	-	15.47	-	15.22
	Elastic	10.73 [#]	-	14.75	-	14.54
	Capture	0.614 [#]	-	0.719	-	0.681

* value is wrong, # at energy 9.99978+3.

The group cross-sections at the threshold of the unresolved region are given in the table below for the different versions of the NJOY program.:

Table 2 : Group Averaged Total Cross-sections

Group (Energy Range)		128	129	130
Code Version	Reaction	9.1188 - 11.138 keV	11.138 - 15.034 keV	15.034 - 16.616 keV
NJOY89.62w	Total	14.59	15.00	14.66
	Elastic	13.92	14.35	14.06
	Capture	0.6638	0.6466	0.5929
NJOY91.91w24	Total	11.64 *	14.92	14.66
	Elastic	13.92	14.35	14.06
	Capture	0.6640	0.6466	0.5929
NJOY91.115	Total	14.59	15.00	14.66
	Elastic	13.92	14.35	14.06
	Capture	0.6638	0.6466	0.5929
NJOY91.91w25	Total	14.59	15.00	14.66
	Elastic	13.92	14.35	14.06
	Capture	0.6638	0.6466	0.5929

The results from the revised NJOY91.91 now agree with those from NJOY89.62w and NJOY91.115.

RECOMMENDED VERSION

As NJOY91.115 had not been officially released it was decided that only the correction to RECONR (up92 as of Feb 94) would be extracted from the new update file and applied at Winfrith as a local update to NJOY91.91. Thus a new version of NJOY91.91 has been created at Winfrith, NJOY91.91w25, and the verification tests rerun.

The version of NJOY91.115 will be used for test purposes only until it is officially released through RSIC.

The current recommended version of NJOY at Winfrith is NJOY91.91 with local modifications to include additions and corrections. These modifications include a private version of WIMSR. We hope to include the standard version of WIMSR next year. At that time we will incorporate appropriate comments from others. We are particularly grateful to Andrez Trekov for his comments.

AVAILABILITY

The NJOY91.91w25 executable program is stored in the standard code area and is available as
`/eagle2/jeflib/codes/njoy91/fort/xnjoy91.91w25`

All README files for NJOY refer to this as the recommended version. The macro "njoy" has been updated to link to this code. The macro "getnjoy" will now obtain source coding for the NJOY91.91w25 code.

The beta release version, NJOY91.115w, and the old NJOY89.62w code are available from the author on request.

DOCUMENTATION

New documentation for NJOY91 has been produced at Los Alamos in postscript form. The documentation has not yet been officially released but copies of the files have been transferred via the gateway machine to a SUN workstation at Winfrith. These postscript files are stored in the standard code area in the directory

`/eagle2/jeflib/codes/njoy91/DOC`

with a separate file for each NJOY module. This documentation is subject to update by Los Alamos so the current version should be obtained from that source until published.

FUTURE DEVELOPMENTS

The status and developments to NJOY as defined by the code author are given in this section. NJOY 91.114 was frozen by Los Alamos on 29 October 1994 and NJOY 94.0 was established on the same day. NJOY 94.0 uses the same structure as 91, except that it has Postscript plotting, LEAPR, a new version of PURR, and ACE consistency checks installed. Both 91.114 and 94.0

will be sent to RSIC soon. NJOY 95 is still under development. It is based on NJOY 94, but it uses the new module structure. It also will have extensive on-line help capabilities. It will run on IBMPC and PowerMac, in addition to the normal unix and VMS versions.

VERIFICATION TESTS

The NJOY test cases in use at present involve the use of a combination of modules, i.e. test case 1 uses MODER, RECONR, BROADR, HEATR, THERMR and GROUPT. When significant differences are found between output listings they usually appear in the group averaging or post processing modules. However, these differences are generally caused by changes to the PENDF files which are produced by the modules which reconstruct the point files. Tracing the origin of any differences can be a time consuming and difficult task. If test cases were available for individual modules, with output listings and input and output PENDF files provided, the installation of new versions of NJOY would be a much simpler exercise. The PENDF files could be compared using the COMLOT program and any significant differences would be flagged. Further investigations involving just the module concerned could then be instigated. Testing of other modules would be unaffected as all input files would be independent.

The use of graphical comparisons for module output files also gives a clear view of the importance of any significant differences. It would also be possible for the code author to issue these graphical comparisons between different NJOY versions with each new release of the code, giving reasons for any significant change.

CONCLUSIONS

- NJOY91.91 is recommended to users at Winfrith
- NJOY91.115 beta release available on request
- preliminary documentation for all modules is available
- improved testing procedure recommended

References

- 1 R E MACFARLANE and D W MUIR
The NJOY Nuclear Data Processing System, Version 91
August 25, 1994
To Be Published
- 2 C R EATON, C J DEAN
Modifications to NJOY91.91 Made at Winfrith
May 1994
- 3 C R EATON, R J PERRY, C J DEAN.
Modifications to NJOY89.62 Made at Winfrith.
LWPC/P(91)38
- 4 R E MACFARLANE
Introducing NJOY89.
Page 7 etc. of Proceedings of the Seminar on NJOY and THEMIS.
Saclay, 20-21 June 1989.
- 5 The ANSWERS Software Package MONK. A Monte Carlo Program for
Nuclear Criticality Safety Analyses. User Guide for Version 7A.
ANSWERS/MONK(94)3
- 6 The ANSWERS Software Package MCBEND. A Monte Carlo Program for
Nuclear Shielding Safety Analyses. User Guide for Version 9A.
ANSWERS/MMCBEND(94)3
- 7 R J PERRY, C J DEAN
WIMS DATA LIBRARY
AEA-RS 1254 Revision 1
October 1994

Figure 1. Graphical Comparison of BROADR PENDs for JEFF.2 U238 Produced by NJOY89.62w and NJOY91.91w24

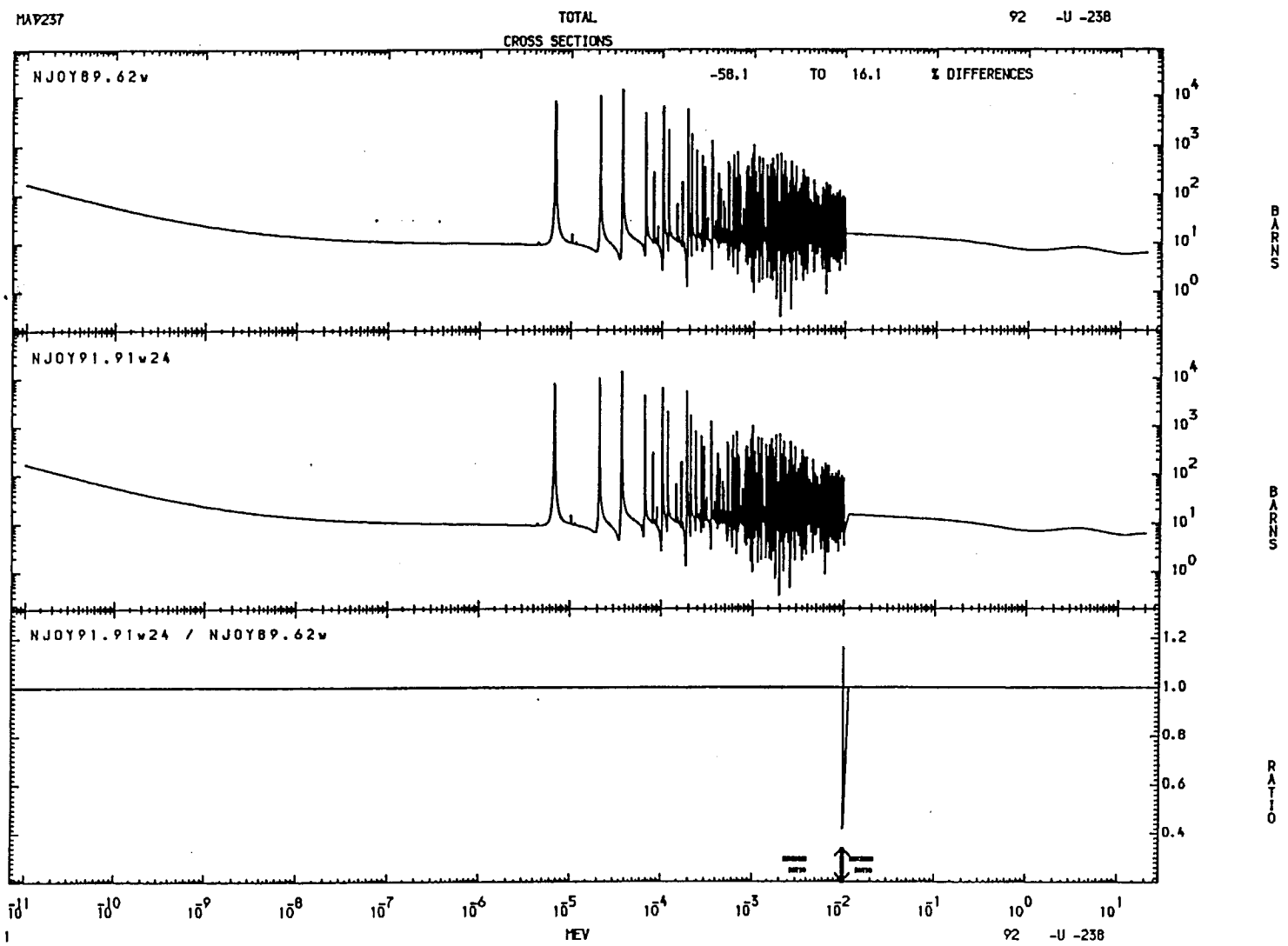
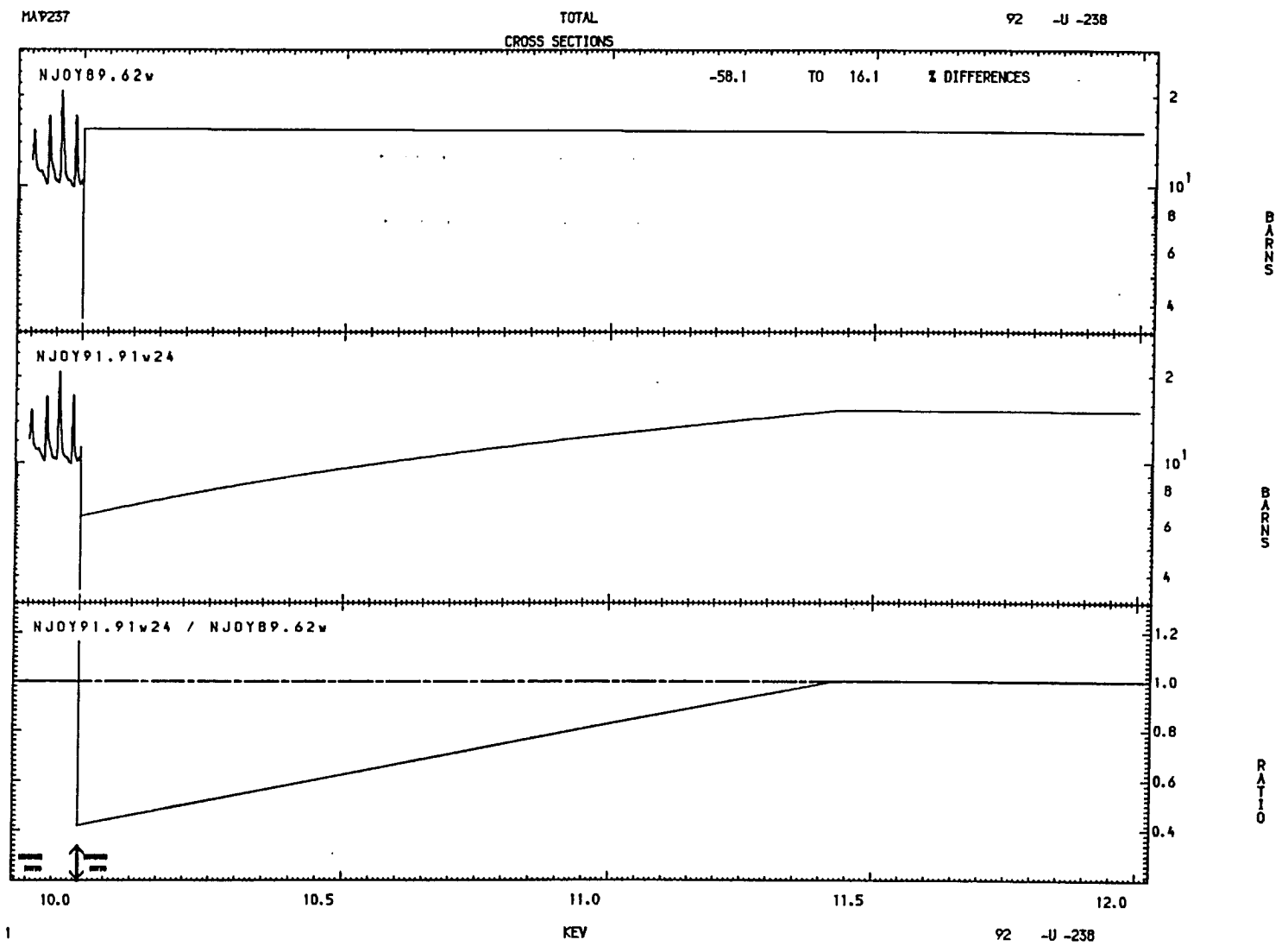


Figure 2. Graphical Comparison of BROADR PENDF for JEFF2.2 U238 at the Threshold of the Unresolved Resonance Region



Appendix 1 Description of Updates (README115)

NJOY 91.115 ----- 31 Oct 1994

This is NJOY91.115. The preceeding README91 file is repeated with some changes below. Comments on the differences between 91.91 and 91.115 have been added. A new test problem (in8) has been added to test some ENDF-6 features, including Reich-Moore resonance reconstruction, energy-angle matrices in GROUPT, and energy-angle distributions in ACER. This test problem uses ENDF/B-VI Ni-64.

The 91.115 release is basically configured for unix. The test problem input files are unix shell scripts, and the test problem results are from runs on a Cray Y-MP8/4-64 running UNICOS.

This is the 1991 release of the NJOY Nuclear Data Processing System. It includes many bug fixes, major improvements in several modules (especially matxsr and acer), and some new capabilities (see resxsr, wimsr, mixr, and purr). The capabilities for processing ENDF-6 files are almost complete. To help the user, the following sections start with specific key phrases; use your editor to search for the desired topics.

<< major changes from NJOY 89 >>
<< changes made between 91.0 and 91.38 >>
<< changes made between 91.39 and 91.91 >>
<< changes made between 91.91 and 91.115 >>
<< status of endf-6 capability >>
<< distribution files >>
<< version control with upd >>
<< changes made to UPD for 91.38 >>
<< installation on UNICOS machines at Los Alamos >>
<< installation on UNICOS machines at NERSC or SDSC >>
<< preparing a Sun version >>
<< preparing a VAX version >>
<< preparing an IBM mainframe version >>
<< running NJOY at NERSC >>

<< major changes from NJOY 89 >>

1. Truncation of real numbers into integers was changed uniformly to use the FORTRAN NINT(X) function. This helps to make the code more portable because "i=a" varies between machines.
2. The ACER module was almost completely rewritten to improve portability, clean it up, and add new features. This allowed the very long ACEOUT routine to be broken up into shorter parts. The way integer and real ACE values are stored in memory and written out to Type 1, Type 2, or Type 3 files was completely reworked. Caution: ACER input has changed.
3. A capability to generate ACE dosimetry libraries was added to ACER.
4. A start was made on a section to generate ACE photoatomic cross sections from the ENDF/B-VI photoatomic sublibrary. The new coding produces all the cross section and form factor tables, but it doesn't produce the fluorescence data. The new data files have new information on subshell cross sections, and it may be possible to improve the methods used in MCNP. This is under investigation.

5. ACER can now convert the "type" of an ACE library (for example, ASCII Type 1 libraries to binary Type 2 libraries), and it can edit some of the parameters in an existing library (in particular, the ZAID value and the information string).
6. Coding was added in several modules to take advantage of some secondary-energy spectra where the shape is independent of energy at low incident neutron energies. Examples are fission neutron production and capture gamma production. GROUPT determines the energy where significant energy-dependence starts. Below that energy, it computes the normalized spectrum only once. It then computes a production cross section for the incident energy groups. For fission, these numbers are just chi and nu*sigf. Above the break energy, GROUPT computes a group-to-group matrix as usual. This trick significantly reduces the size of the GENDF file for group structures with many thermal groups.

The output modules DTFR, CCCCR, POWR, and WIMSR use the spectrum and production records from the GENDF tape plus the records for the partial group-to-group matrix to reconstruct the proper data for their formats. The output files and listings are the same as for previous versions.

MATXSR was modified to have a new general matrix format that includes places for the constant spectrum and its production cross section. This reduces the size of MATXS files that have many thermal groups. Caution: NJOY 91 MATXS files are not compatible with previous versions, and any codes that read MATXS files (such as TRANSX) will have to be fixed!

7. The MATXSR module and the MATXS format have been modified to change the order of "data type" and "material". The new version first loops on material, and then on data type. This makes it much easier to write utility codes that insert new materials in a MATXS library, or codes that extract materials from a library. This latter option can be used to make a small library for a group of TRANSX runs, thereby making the runs much faster. Caution: The MATXSR input has been changed. Caution: new MATXS files are not compatible with the old files. The codes that use MATXS data will have to be fixed.
8. A new MIXR module has been added. It can make a new ENDF or PENDF tape where the sections of File 3 are weighted sums of the sections of File 3 from several input tapes. This is useful for making elemental cross sections for plotting. MIXR does not make a complete elemental ENDF tape.
9. A new WIMSR module has been added to make cross sections libraries for the WIMS-D and WIMS-E reactor codes. This version is still rough in several ways, but it has been installed to provide a common basis for an ultimate WIMS capability. Please use it with caution and send in your suggestions for improvements.
10. The PURR code, which has been around for several years, has been installed in this version. PURR generates unresolved-region probability tables for the MCNP code. This module also has some problems, and the UR capability for MCNP has not been released in final form. Expect some changes in both PURR and ACER to finish a complete Monte Carlo unresolved capability.
11. The system I/O units have been changed to allow for a special error unit as found on unix systems. In addition, a whole new system has been introduced for both fatal error and warning messages (see the subroutines ERROR and MESS). This has allowed many format statements to be removed.

12. An attempt was made to remove most non-ANSI constructs. The following exceptions remain: lower case characters, variable-format write commands, and equivalencing of arrays in subroutines to arrays in named common.

<< changes made between 91.0 and 91.38 >>

These changes are summarized by giving an annotated list of the comment cards from UP38.

```
*ident up1
*/ heatr -- 21 mar 91 -- allow for more mf6 reactions.
*/                               also, isotropy message should not be
*/                               printed if mf6 is present.

*ident up2
*/ reconr -- 26 mar 91 -- simplify mlbw and make sure that
*/                               duplicate j values are treated correctly.
*/ reconr -- 26 mar 91 -- install dunford's patch to treat
*/                               duplicate j values for reich-moore.
```

This change is important for getting the correct value of the potential scattering cross sections for a few ENDF/B-VI isotopes.

```
*ident up3
*/ plotr -- 4 apr 91 -- use more points when plotting
*/                               3-d energy distributions.
*/ plotr -- 4 apr 91 -- last point in 3d ang plot missing
*/ plotr -- 4 apr 91 -- add 3d ang dist truncation message
*/ plotr -- 4 apr 91 -- protect storage for 3d energy plots
*/ plotr -- 4 apr 91 -- echo input to output
*/                               to help in finding input errors

*ident up4
*/ heatr -- 8 apr 91 -- fix interpolation range problem in sixbar

*ident up5
*/ mixr -- 16 apr 91 -- fix bad error message
*/ mixr -- 16 apr 91 -- fix interpolation problem

*ident up6
*/ moder -- 19 apr 91 -- allow file 40 to be processed

*ident up7
*/ reconr -- 19 apr 91 -- add a grid point for low-energy
*/                               resonance evaluations (protects
*/                               reconstruction stack from overflow)
*/ reconr -- 18 apr 91 -- fix some problems with
*/                               discontinuities and thresholds

*ident up8
*/ matxsr -- 24 apr 91 -- fix length of file id block
*/ matxsr -- 24 apr 91 -- increase container size
*/ matxsr -- 24 apr 91 -- fix indexing in indexm
*/                               change to 80-column format
*/ matxsr -- 24 apr 91 -- allow for more reactions
*/ matxsr -- 29 apr 91 -- fix paging errors.
*/                               keep last block smaller than maxw.

*ident up9
*/ resxsr -- 18 jun 91 -- fix material control and blocking

*ident up10
*/ gaminr -- 11 jul 91 -- nint ngg and fix eq in gpanel
```

*ident up11
*/ groupr -- 11 jul 91 -- add vitamin-j photon group structure

*ident up12
*/ njoy -- 17 jul 91 -- fix jump back from resxsr

*ident up13
*/ groupr -- 18 jul 91 -- add more t-dep weight functions

These options allow the Maxwellian part of the weighting function to change with the temperature of the material.

*ident up14
*/ unresr -- 29 sep 91 -- increase to 10 temps and 10 sigzeros
*/ update card count in directory (raepsaet, cea-dmt)

*ident up15
*/ reconr -- 3 dec 91 -- fix channel radius (rowlands and eaton).
*/ fix enode name for reserv, etc. (panini).

This change is important to get the correct results for ENDF/B-VI evaluations of iron, nickel, chrome. The effect shows up in the cross section value at the center of a resonance.

*ident up16
*/ wimsr -- 3 dec 91 -- fix name for reserv, etc. (panini)

Also see up34 for more important wimsr changes.

*ident up17
*/ groupr -- 3 dec 91 -- fix type of id in call to reserv
*/ groupr -- 16 dec 91 -- fix allocation for sed (laughton, aecl)
*/ groupr -- 16 dec 91 -- fix print of mfd=5/mtd=18 (laughton, aecl)
*/ groupr -- 16 dec 91 -- extend lower limit for tabulated secondary
*/ distributions to 1e-5 and upper limit to
*/ 50e6 as is done for analytic sections.
*/ noticed by laughton, aecl.

*ident up18
*/ njoy -- 3 dec 91 -- pad string parameter with spaces for
*/ better comparisons on vax (gauld, whiteshell)

This one is needed on short-word machines when matching the names used in the dynamic storage system used throughout NJOY.

*ident up19
*/ matxsr -- 4 dec 91 -- fix hollerith word size and pointers

*ident up20
*/ moder -- 4 dec 91 -- fix gendf processing (dean, winfrith).
*/ moder -- 4 dec 91 -- fix file 34 processing (muir, iaea).

*ident up21
*/ heatr -- 4 dec 91 -- prevent div by zero in sed (decher, ce)

So far, this has only happed on Apollo machines.

*ident up22
*/ thermr -- 4 dec 91 -- set sabflg for sw machines (dean, aguilar)
*/ thermr -- 4 dec 91 -- fix tolerance on test for x(i)=0 (decher, ce).

*ident up23

```
*/ broadr -- 4 dec 91 -- don't thin lowest threshold (dean, winfrith).
*ident up24
*/ groupr -- 4 dec 91 -- impr. to flux calculator (winfrith, lanl, cea).
```

There are still some parts of these changes that have not been checked out. Please check them carefully before using them.

```
*ident up25
*/ acer -- 6 dec 91 -- misc acer fixes
*/   fix messages in etopl routines
*/   fix date in output file
*/   fix up case of no photon production
*/   fix up type 3 output and input
*/   fix up dosimetry output (vontobel, psi)
*/   fix one of the acer prompts (mattes)
*/   tighten up initial tolerance for integral thinning
*/   file 6 patches to topfil
*/   prevent writing of cont in conver if mf.gt.15 is present
*/   generalize transfer of mf6 photons to mf16
*/   define nin in gamout (vontobel)
*/   allow for larger nu tables (mattes)
*/   supress extra 1e-5 at start of table (mattes)
*/   move inactive message
*/   patches for file 6 in acelod
*/   vontobel fixes for mf16 photons
*/   allow for coupled energy-angle distributions (mattes)
*/   missing increments in law 1 section (mattes)
*/   add branch for mf16 data (mattes)
*/   fix typen to prevent two output lines for i=4 (vontobel)
*/   reintroduce lost lines (mattes)
*/   part of thermal inelastic missing (lazo)
*/   thermal zaid should be a name, not a number
*/   increase the size of the container arrays
*/   make sure mt600,etc are available for mf6 photons
*/   fix up reaction naming
```

```
*ident up26
*/ dtfr -- 9 dec 91 -- fix pointer for photon prod xsec
*/   fix reaction list for pointwise plotting
```

```
*ident up27
*/ matxsr -- 21 dec 91 -- allow bcd output, modify format.
*/   remove print and index in favor of bbc.
```

There is a small change in the input specifications that goes with this change. Test problem 3 is affected. The use of the BBC code to print and index matxs files is discussed in the TRANSX2 manual.

```
*ident up28
*/ reconr -- 6 mar 91 -- avoid the reserved name "save"
*/   fix the value of boltzmann's constant
```

```
*ident up29
*/ heatr -- 5 mar 92 -- avoid the reserved name "save"
```

```
*ident up30
*/ groupr -- 5 mar 92 -- fix format for message
*/ groupr -- 5 mar 92 -- avoid the variable name "save" (cea-dmt)
*/ groupr -- 5 mar 92 -- fix tabulated mf6 option (konieczny)
*/ groupr -- 5 mar 92 -- fix dimensions (raepsaet, cea-dmt)
*/ groupr -- 5 mar 92 -- supress excess upscatter messages
```

```
*ident up31
```

*/ gaminr -- 5 mar 92 -- include endf-6 gheat

This is important to get the correct photon heating factors.

*ident up32

*/ acer -- 10 mar 92 -- convert legendre law1 to kalbach form

This is an experimental approach that may allow all the ORNL evaluations from ENDF/B-VI without having to make such extensive changes in MCNP and in the ACE format.

*ident up33

*/ unresr -- 11 mar 91 -- fix multi-isotope case

*ident up34

*/ wimsr -- 11 mar 91 -- fix bugs (mann, hanford)

*/ wimsr -- 15 may 92 -- fix problems with fission matrix

The original version gave bad values for nu*sigf and chi.

*ident up35

*/ gaminr -- 16 apr 92 -- increase container array to allow p9

Needed for the FENDL library.

*ident up36

*/ matxsr -- 21 apr 92 -- make sure of word boundaries

Needed for 32-bit machines.

*ident up37

*/ groupr -- 22 apr 92 -- fix problem with vit-e temperature dependent weighting (sartori)

*ident up38

*/ reconr -- 15 may 92 -- fix problem with u.r. fission widths for jef (nordborg)

This problems showed up for a few JEF-2 isotopes like cm245 that specified energy-dependent fission widths that didn't really change with energy.

<< changes made between 91.38 and 91.91 >>

These changes are summarized by giving an annotated list of the comment cards from UP91.

*ident up39

*/ broadr -- 15 jun 92 -- fix problem at resolved range boundary

*ident up40

*/ acer -- 15 jun 92 -- be careful with ang. dist. loop

*/ acer -- 16 jun 92 -- be careful with partial fission reactions

*/ acer -- 17 jun 92 -- fix conversion of real to integer

*ident up41

*/ acer -- 13 jul 92 -- fix problem with law44 for photons

*/ acer -- 17 jul 92 -- fix mf6/mt51-90 problems

*/ acer -- 22 jul 92 -- fix problem with sorting of thresholds

*/ acer -- 23 jul 92 -- fix problem with the use of moreio

*/ acer -- 18 aug 92 -- be more careful with conv check

*/ acer -- 18 aug 92 -- add positive threshold test

*/ acer -- 18 aug 92 -- fix error in up25

*/ acer -- 18 aug 92 -- date should be right justified in field of 10

*/ dater now expects a character argument

The original installation of Kalbach systematics only included the leading term and only allowed for neutrons. The next three idents add the complete Kalbach formula to heatr, groupr, and acer.

*ident up42
*/ groupr -- 1 aug 92 -- extend kalbach option
*/ to higher energies and other particles

*ident up43
*/ heatr -- 1 aug 92 -- extend kalbach option
*/ to higher energies and other particles

*ident up44
*/ acer -- 1 aug 92 -- extend kalbach option
*/ to higher energies

*ident up45
*/ reconr -- 18 aug 92 -- fix duplicate e-sigma check

*ident up46
*/ groupr -- 19 aug 92 -- fix some c.p.-related labels

*ident up47
*/ acer -- 21 aug 92 -- fix type3 with no detailed g.p.
*/ acer -- 21 aug 92 -- fix type3 comment field
*/ acer -- 7 oct 92 -- fix problem with discrete photon law
*/ acer -- 7 oct 92 -- discontinuities were not being handled
*/ correctly for photon sections with nk=1
*/ acer -- 7 oct 92 -- move all thinning to unionx.
*/ don't remove discontinuities or thresholds.
*/ make sure there is a sharp break at
*/ discontinuities.
*/ acer -- 9 oct 92 -- provide messages for kalbach conversion.

The source code was run through the Cray UNICOS code CFLINT to find things that might cause trouble in compilation and execution. These include variables that might not be defined before use, unused variables, etc. We also paid closer attention to the warning and caution messages from CFT77. The following idents contain changes from this work; they should help improve portability and reliability.

We also started adding SAVE statements, but the code has only been run in static mode so far.

*ident up48
*/ njoy -- 24 nov 92 -- revise driver to avoid hollerith
*/ njoy -- 24 nov 92 -- add save statements

*ident up49
*/ broadr -- 24 nov 92 -- remove some cft77 caution messages

*ident up50
*/ unresr -- 24 nov 92 -- remove some cft77 caution messages
*/ and some things found by cflint

*ident up51
*/ heatr -- 24 nov 92 -- remove some cft77 caution messages
*/ heatr -- 11 mar 93 -- fix up some problems found by cflint

*ident up52
*/ thermr -- 24 nov 92 -- remove some cft77 caution messages

```

*/ thermr -- 11 mar 93 -- fix up problems found by cflint
*ident up53
*/ groupr -- 24 nov 92 -- remove some cft77 caution messages
*ident up54
*/ errorr -- 24 nov 92 -- remove some cft77 caution messages
*ident up55
*/ covr -- 24 nov 92 -- remove some cft77 caution messages
*ident up56
*/ matxsr -- 24 nov 92 -- fix missing path
*/ matxsr -- 11 mar 93 -- increase number of materials allowed
*/ matxsr -- 11 mar 93 -- fix some problems found by cflint
*ident up57
*/ moder -- 28 nov 92 -- don't compare
*/
*/      real variables containing hollerith
*/ moder -- 28 nov 92 -- remove previous change that
*/
*/      damages gendf fission matrices
*ident up58
*/ plotr -- 28 nov 92 -- fix error and cft77 cautions
*ident up59
*/ njoy -- 25 nov 92 -- make free recognize uppercase e
*/
*/      and ignore leading zero in exponents
*/ njoy -- 11 mar 93 -- fix up problems found by cflint
*/ njoy -- 1 apr 93 -- fix pointer problem in scana
*ident up60
*/ groupr -- 21 dec 92 -- fix problem with hnab that leads
*/
*/      to errors for e-dep watt spectrum.
*/ groupr 21 dec 92 -- remove some nuisance messages
*ident up61
*/ broadr -- 21 dec 92 -- fix problem in hnabb for sw mach.
*/ broadr -- 11 mar 93 -- fix up problems found by cflint
*/ broadr -- 15 mar 93 -- fix problem with restart

```

The following ident fixes up the previous problem with the ENDF/B-VI material F-19, which uses two subsection in File 6 for (n,2n), one for first neutron, and one for second neutron. The code now reads all File 6 data into memory rather than paging through, and more memory is required than for older versions.

```

*ident up62
*/ groupr -- 22 dec 92 -- fix groupr to handle multiple
*/
*/      emissions in file 6 (f-19).
*ident up63
*/ plotr -- 26 feb 93 -- add more 2-d and 3-d options for gendf data
*/ plotr -- 15 mar 93 -- move frame in window slightly

```

PLOTTR can now do overplots of pointwise and multigroup emission spectra for selected incident energies, and it can do 3-d perspective plots of multigroup P0 matrices.

```

*ident up64
*/ groupr -- 1 mar 93 -- fix error in up30
*/
*/      that causes bad mt50+n gamma yields

```

This error caused important problems with the photon production in the matxs files originally put up on NERSC

*/ acer -- 28 apr 93 -- fix polynomial nubar
*/ acer -- 28 apr 93 -- fix index for coherent elastic printing
*/ acer -- 28 apr 93 -- fix subsection pointer
*/ acer -- 28 apr 93 -- increase size of container array
*/ acer -- 29 apr 93 -- fix iz array for moderator components
*/ and fix variable-weighting flag
*/ acer -- 29 apr 93 -- xsdir cards need for digits for awr
*/ acer -- 29 apr 93 -- limit interpolation law to 1 or 2

*ident up76

*/ powr -- 29 apr 93 -- problem reported by helen connell, bnl

*ident up77

*/ thermr -- 29 jun 93 -- put limits on extrapolation.

Newer versions of THERMR attempt to use three-point interpolation on $S(\alpha, \beta)$ to get better results for the normal shapes. However, some evaluations have very jagged shapes, especially on the wings of the function, and the interpolation scheme breaks down. This patch prevents extrapolation to absurd values.

*ident up78

*/ acer -- 29 jun 93 -- eb should use channel energy.
*/ noticed by seamon (lanl).

See also up79 up80. Bob Seamon (LANL Group X-6) noticed that the implementation of Kalbach systematics in NJOY (HEATR, GROUPE, ACER) should be using the "channel energy" instead of the center-of-mass energy. This patch fixes that error.

*/ acer -- 29 jun 93 -- fix grid for generalized yields
*/ acer -- 29 jun 93 -- fix nk for mf5/6

*ident up79

*/ groupr -- 29 jun 93 -- eb should use channel energy

See related comment in up78.

*/ groupr -- 29 jun 93 -- make sure c.p. are identified.
*/ noticed by panini (enea bologna).

On some machines, it is necessary to take special care with the comparison of particle ID numbers.

*ident up80

*/ heatr -- 29 jun 93 -- eb should use channel energy

See related comment in up78.

*/ heatr -- 29 jun 93 -- use lin-lin on heat and damage.
*/ noticed by panini (enea bologna).

HEATR was choosing the incident-energy interpolation scheme for heat and damage inappropriately. It is most consistent to use linear interpolation for both. This fix makes the EBAR(E) values printed out on the listing look much more reasonable close to the thresholds.

*ident up81

*/ matxsr -- 30 jun 93 -- fix hollerith constant

*ident up82

*/ plotr -- 2 jul 93 -- fix s(a,b) plotting for +&- beta

This fix allows one to make good plots for liquid hydrogen and deuterium, which are not symmetrical for +&- beta.

```
*ident up83
*/ groupr -- 17 jul 93 -- fix constant gamma spectra to have
*/                                     correct normalization (graham robinson).
```

This error caused the constant spectra for gammas to be normalized wrong whenever there was a number in the low-energy group (which is most of the time!).

```
*/ groupr -- 17 jul 93 -- sw machines have trouble with
*/                                     cc very close to 1
```

```
*/ groupr -- 17 jul 93 -- give up using 201-220 for thermal
```

For ENF/B-IV, NJOY used the special MT numbers starting at 201 for thermal reactions. When ENDF/B-V was issued, these MT values were used for gas production reactions, and we moved the thermal range up to 221. It doesn't really seem necessary to leave this code in place any longer.

```
*/ groupr -- 17 jul 93 -- abandon stripping low-energy thermal
*/                                     groups to remove thermal range messages.
```

For years, GROUPE has issued strange messages about thermal range problems that I have never been able to explain to the users. They had to do with trying to get the maximum stripping of zeroes in the thermal matrices, but the overhead and confusion are just not worth the gain. We are giving up and accepting the fact that thermal matrices may have more low-energy zeroes than are absolutely necessary.

```
*ident up84
*/ reconr -- 17 jul 93 -- fix double counting of MT522 in MT501
*/                                     (zidi and ganesan, iaea)
*/ reconr -- 22 jul 93 -- fix pseudo threshold problem in cl
*/                                     and watch for initial discontinuities
```

These problems both result from the changes in the photoatomic data introduced to allow for subshell cross sections. We have fixed the code to treat MT522 as "redundant" if the subshell cross sections are found (that is, it is reconstructed as the sum of its parts, and it is not included in the total cross section). In addition, RECONR was not recognizing the discontinuities at the beginning of each subshell section. This has been fixed, and comparison plots by Ganesan show the RECONR results are consistent with the input ENDF file except that double energy points have been changed to steep slopes in the normal NJOY manner.

```
*ident up85
*/ acer -- 19 jul 93 -- fix tyr flag for mf6 data
*/ acer -- 22 jul 93 -- fix phase space problem
*/ acer -- 1 aug 93 -- tyr for f19 gets wrong sign
```

After these changes, ACER seems to be able to handle ENDF/B-VI OK.

```
*ident up86
*/ plotr -- 20 jul 93 -- repair errors for 3d ang. distributions.
*/ plotr -- 20 jul 93 -- fix input instructions
```

```
*ident up87
*/ errorr -- 5 april 93 -- spin covariances no longer permitted in vers. 6
*/ errorr -- 5 april 93 -- add message for illegal or misplaced ner value
*/ errorr -- 5 april 93 -- add message for missing u.r.r. capability
*/ errorr -- 5 april 93 -- fix typo in error message
*/ errorr -- 5 april 93 -- add message for missing sc. radius capability
```

*/ errorr -- 5 april 93 -- add message for missing "new mf32" capability
*/ errorr -- 5 april 93 -- fix screen print of group structure option

These are mostly minor changes. Some are intended to make ERRORR run smoothly with ENDF/B-VI; however, none of the new covariance features supported by the ENDF-6 format are supported by ERRORR as yet, except for LB=8.

*ident up88

*/ heatr -- 28 jul 93 -- fix up fission kerma factors.
*/ provide details and message for qdel.
*/ reduce q for excess in nubar.
*/ print yields with ebar.

Graham Robinson has pointed out that HEATR should be treating the fission Q value as a variable, because the increase in nubar with energy causes the mass of the residual fission fragments to decrease. There are other smaller effects affecting the fission product mass, and the neutrino emission is also slightly energy dependent. This problem is discussed in detail in another note "NJOY Treatment of Energy Release in Fission." More work is needed on this problem.

We also changed the listing to include energy-dependent particle yields. The EBAR values are now normalized to one particle consistently.

*/ heatr -- 28 jul 93 -- fix error in damage cutoff
*/ (noticed by bersillon)

This is an important problem first noticed by Olivier Bersillon. It causes the elastic component of damage to be too small below about 10 -- 100 keV (depending on material).

*ident up89

*/ matxsr -- 1 aug 93 -- fix awr values on matxs matc record

MATXSR was using the elemental mass extracted from the photoatomic file for every isotope of an element.

*ident up90

*/ groupr -- 4 aug 93 -- fix econst logic in getsed

The value of "econst" was being chosen incorrectly in some cases. This would sometimes result in a spectrum being given together with a complete matrix, and the spectrum would be incorrectly normalized.

*ident up91

*/ groupr -- 20 aug 93 -- fix problem with getsed for nktot.gt.1

We introduced a problem for sections of File 5 with more than one subsection in UP64 (there is no problem with the 6 subsections of the delayed neutron files). A list of materials affected by this problem will be found in the news message "Problem with NK in GETSED for NJOY 91.76."

*/ groupr -- 20 aug 93 -- fix problems with upscatter corr. in file 6

If GROUPE finds upscatter values in the computed scattering matrix, it attempts to remove them by putting them in the ingroup element. The code was putting them in the ingroup OK, but it wasn't zeroing them in the upscatter position. Small upscatter elements like these are normally due to interpolation, and they are not real upscatter.

The code prints an informative message if the upscatter is large. There are some cases in bismuth and lead of real positive Q neutron emission reactions. They lead to these messages, but the upscatter is not available in the final matrices.

This test is not made for analytic sections; therefore, the real upscatter in Am242m MT51... comes through in the matrices. The user should take care if these upscatter values might cause problems for later applications.

*/ groupr -- 20 aug 93 -- const. spectra not allowed with file 6.

This problem occurs if File 6 is used for MT18 or MT102 photon production. The only case in ENDF/B-VI is F-19.

*/ groupr -- 20 aug 93 -- fix elo for file 6, law 7

This error causes the n2n matrix to be omitted for Be-9.

<< changes made between 91.91 and 91.115 >>

These changes are summarized by giving an annotated list of the comment cards from UP91.

*ident up92

*/ reconr -- 10 jan 94 -- need more storage id's
*/ reconr -- 10 jan 94 -- initialize to zero before sum
*/ reconr -- 10 jan 94 -- fix typo in error message
*/ reconr -- 29 jan 94 -- allow for more ur sequences
*/ reconr -- 25 feb 94 -- fix loophole in threshold logic
*/
print all threshold changes

*ident up93

*/ broadr -- 31 jan 94 -- take care with threshold reactions

These changes are needed if broadening is extended to energies above the first few threshold reactions.

*/ broadr -- 19 jun 94 -- fix restart print

*ident up94

*/ unresr -- 5 jan 93 -- allow for more spin sequences (jendl monat)

*ident up95

*/ heatr -- 4 jan 94 -- allow for general file 5 contents

This patch allows for File 5 sections with more than one tabulated subsection or with tabulated subsections that appear before analytic subsections. The corresponding changes in GROUPE were made previously. More memory is required because of this change.

*/ heatr -- 5 jan 94 -- install more file 6 options

This allows for evaluations using tabulated angular distributions in File 6, and it also allows for the use of discrete lines in the CM (as in BROND H-2).

*/ heatr -- 15 jan 94 -- add sn120 as major isotope of sn

*/ heatr -- 1 jun 94 -- avoid fortran reserved name

*ident up96

*/ groupr -- 5 jan 94 -- install more file 6 options

This allows for evaluations using tabulated angular distributions in File 6, and it also allows for the use of discrete lines in the CM (as in BROND H-2).

```
*/ groupr -- 15 jan 94 -- add sn120 as major isotope for sn
*/ groupr -- 27 jan 94 -- more room for gamma lines
*/ groupr -- 31 jan 94 -- fix stounr error messages
*/ groupr -- 1 mar 94 -- fix problem with multiple sections in mf5
```

This fixes a small error in the previous File 5 patch.

*ident up97

Miscellaneous ERRORR changes.

*ident up98

```
*/ ccccr -- 16 feb 94 -- fix problems with delayed neutron file
```

*ident up99

```
*/ acer -- 31 dec 93 -- fix area for tabulated semilog distr.
*/ acer -- 31 dec 93 --allow for more mf12, mt>600 sections
*/ acer -- 15 jan 94 -- add sn120 as the major isotope of sn
*/ acer -- 27 jan 94 -- fix incorrect change of ref. frame for law 7
```

Law 7 must be in the lab frame.

```
*/ acer -- 1 feb 94 -- watch out for histogram case
*/ acer -- 17 feb 94 -- fix printing controls
*/ acer -- 3 mar 94 -- fix value of boltzmann constant
```

Previous versions used .0253 eV for 300 K. This patch makes the Boltzmann constant consistent with other modules.

```
*/ acer -- 3 mar 94 -- provide band error cutoff for thinning
*/ acer -- 21 mar 94 -- convert madland-nix lf=12 to ace law 4
```

MCNP does not have the logic to sample from the Madland-Nix fission spectrum. Therefore, we have provided logic to build a tabulated version of this law in ACER instead of changing MCNP and the ACE format to include a new law.

```
*/ acer -- 29 mar 94 -- fix problem with type 1 and type 3 in law 44
*/ acer -- 8 apr 94 -- make sure findf doesn't go to wrong temp
*/ acer -- 26 may 94 -- increase size of xss array
```

This changes allows for ACE files up to 600 000 words. Petten uses even more. If 600 000 is insufficient, your choices are to change the size again, or use thinning to reduce the size of the main energy grid.

```
*/ acer -- 26 may 94 -- remove hollerith from thrprt
```

Full use of character data is more portable.

```
*/ acer -- 26 may 94 -- misc acer fixes from ecn petten
```

We appreciate the help received from all the NJOY users. These changes from ECN Petten were very useful.

```
*/ increase jscr pointer
*/ correct typo in up32
*/ fix bad reaction namme
*/ integer declaration for 'fis'
*/ use real constant zero in call to getyl
*/ correct typo (2+i instead of 2*i)
*/ correct typo (41 instead of 21)
```

```

*/ delete two (twice given) statements
*/ correct error in up68 for aceprt
*/ correct treatment of iopp.eq.0 for gamsum
*/ make dimension of /astore/ consistent throughout acer
*/ fix index in acelod for generalized yields
*/ use generic names for easier transportability
*/ prevent division by zero in topfil

*/ acer -- 9 jun 94 -- fix normalization of law 4/44 disc. lines
*/ acer -- 21 jun 94 -- fix problem with gammas
*/ acer -- 9 jul 94 -- add gas production names

```

The previous version of acer did not include the names for gas production reactions, such as (n,xp) or (n,xt). This versions still ignores reactions with mt values in the range 201 through 207, thus making them unavailable for tallys. To change this, look at acer.3832.

```
*ident up100
```

```
*/ njoy -- 29 mar 94 -- upgrade the math functions e1 and gami
```

An error in one of these functions showed up in connection with the Madland-Nix fission spectrum, and we decided to upgrade all of them to publicly available coding.

```
*/ njoy -- 19jun94 -- avoid numerical problems
```

The Cray doesn't compute $\log(x/x1)$ correctly when $x.eq.x1!$ The quotient is one bit short, and the log is a small negative number.

```
*ident up101
```

```
*/ matxsr -- 25 apr 94 -- abandon the old thermal mt numbers
```

The original choice for thermal MT numbers in NJOY was 201 to 250. Later, CSEWG adopted numbers in the 200 range for gas production reactions, and NJOY started using 221 to 250. This patch makes the change permanent. We hope that it doesn't cause trouble for users with old data files.

```
*ident up102
```

```
*/ groupr -- 19 jun 94 -- fix error in up64 for thermal interpolation
```

This patch fixes an error made during the introduction of a new thermal interpolation scheme that interpolates along lines of constant energy transfer in an attempt to represent the peaks in the thermal excitation better. The symptom of the error was ragged results for the thermal flux above the thermal peak and violation of detail balance. It was reported by Petten, Stuttgart, and CE.

```
*/ groupr -- 9 jul 94 -- fix case of yy=0
```

```
*ident up103
```

```
*/ heatr -- 9 jul 94 -- fix case of yy=0
```

```
*/ heatr -- 9 jul 94 -- fix heatr for incomplete file 12 sections
```

There are several evaluations in endf-6 format that give file 6 subsections for neutrons and/or charged particles, but do not give a subsection for the recoil particles. There is also one case known where capture is given in file 6 with no recoil subsection provided. This patch takes care of these cases by computing new heating and damage values using the approximation that the heaviest emitted particle causes all the recoil. Any energy-balance errors are put

into the mt300-series heating values. The computed recoil is used for the mt443 kinematic value and the damage.

*ident up104

*/ acer -- 11 aug 94 -- use law7 instead of kalbach for mf6 law1 lang1

The MCNP Monte Carlo code cannot currently handle data that are given in File 6 using LAW=1, LANG=1 or 11--12 (Legendre data or tabulated data). This means that the important ORNL evaluations for F, Cr, Mn, Fe, Ni, Cu, and Pb cannot be used in their normal form. Our initial solution to this problem was to convert these materials to use Kalbach systematics in the CM frame, which is handled by MCNP. There are several problems with this, including violating the evaluator's intent and getting nonphysical results because of problems with the underlying distributions. This update provides a conversion to LAW=7, the lab angle-energy format used for Be-9 in ENDF/B-VI, which is also now available in MCNP. The distributions sampled in MCNP should be close to the evaluator's intent, and they should differ from the results that would be obtained by a direct use of LANG=1 only through the approximation introduced by selecting 10 angles for the angle-energy representation.

*/ acer -- 22 aug 94 -- add fixup for endf/b-vi f19

ENDF/B-VI F-19 is unique in that it represents the emission from (n,2n) reactions using two different subsections in File 6, namely, first neutron and second neutron. If the distribution is changed to LAW 7 for consistency with the current version of MCNP, two subsections cannot be used. This patch splits the two neutrons from MT16 into MT6 and MT46 as used in ENDF/B-V Be.

*/ acer -- 22 aug 94 -- allow for nr>1 in file 5 (jendl monat)

The ACE format used by MCNP only allows for a single interpolation law for secondary distributions, and the law should specify histogram or linear interpolation to help in preserving the area under the distribution during interpolation. Materials that violate these limitations are rare; if encountered, the outgoing particle distribution is linearized using adaptive reconstruction before being stored in ACE format.

*ident up105

*/ groupr -- 22 aug 94 -- try again on thermal interpolation

The fix given in up102 to an error made in up64 was observed to be incorrect by Uli Decher, ABB Combustion Engineering. It is fixed again in this update. The symptom was absurdly large emission cross sections for the lowest energy group.

*/ groupr -- 22 aug 94 -- make sure to mark the top of the group

See below.

*ident up106

*/ gaminr -- 22 aug 94 -- make sure to mark the top of the group

M. Mattes of U. Stuttgart observed that some photoatomic coherent and incoherent matrices showed upscatter for the VITAMIN-J 42-group structure. This turned out to be due to numerical problems when the upper group boundary was also a grid energy in the file. They were then different by one bit, and the code missed the top of the group. The false

upscatter was then filled in with whatever was in memory, which was sometimes the reaction cross section! This basically doubled the scattering cross sections for these groups. This patch was also made in groupr (see above). The problem is more serious for fine-group gamma structures, but all libraries of photoatomic data should be reprocessed.

*ident up107
*/ resxsr -- 29 aug 94 -- correction from m. mattes, u. stuttgart

*ident up108
*/ matxsr -- 29 aug 94 -- to handle gg when ng is missing (mattes)

*ident up109
*/ moder -- 29 oct 94 -- fix typo in moder (piet de leege)

*ident up110
*/ groupr -- 29 oct 94 -- allow more digits in flux messages (de leege)
*/ groupr -- 29 oct 94 -- fix grammar in comments (made in manual)

*ident up111
*/ broadr -- 29 oct 94 -- fix bad fortran (peter vertes, hungary)
*/ broadr -- 29 oct 94 -- fix grammar in comments (made in manual)

*ident up112
*/ thermr -- 29 oct 94 -- extend thermal energy range to 5.1 ev to
*/ accomodate bugle93 structure (white, rsic)
*/ thermr -- 29 oct 94 -- protect thermr against exp underflows

This prevents some unwanted underflow messages on machines that provide them, such as the Sun.

*ident up113
*/ njoy -- 29 oct 94 -- remove non-ansi variable format

Besides being a non-ANSI feature, variable formats are not allowed by the Lahey compiler used for our DOS version of NJOY.

*ident up114
*/ acer - 29 oct 94 -- fix problems in tabize found by kosako (sumitomo)

*ident up115
*/ heatr -- 31 oct 94 -- more fixes for missing recoil sections

The changes in up103 to handle MF6 evaluations with missing recoil subsections was failing for the explicit two-body recoil subsections in some of the ORNL evaluations. This has been fixed. The logic in hinit tries to identify reactions with missing recoil by subtracting the zap*yld values from ZA+1 and looking at the remainder. If there are errors in the ZAP values, this can lead to impossible recoil nuclei. The ZA values for these nuclei will show up in a message from heatr. The user will have to pay attention. A special check is provided for elements. For example, Ti-nat with AWR=22000 could use ZAP=22000 for its recoil without generating an additional recoil with a small or negative value of ZA.

<< status of endf-6 capability >>

NJOY 91.115 processes all of the ENDF-6-type evaluations that have been tried so far. The following list gives some of the known ENDF-6 problems.

1. RECONR won't process Generalized R-Matrix parameters or the energy-dependent scattering radius.
3. ACER can only handle evaluations in File 6 that use Legendre

coefficients by converting them to Kalbach or Law 7 format. The latter is the best representation.

4. PURR can't handle the LSSF "shelf-shielding factor" option for the unresolved range. Also, the connection between PURR and MCNP is not really developed in NJOY 91. This new module has been included to provide a basis for installing the full probability table capability in a future version.
5. Although not strictly an ENDF-6 format problem, the very large tabulations produced for the new U-235 and U-238 evaluations cannot be handled by ACER without unreasonably heavy thinning. A probability-table thinning approach is under development for the upper part of the resolved range for these materials.
6. GAMINR and ACER do not take advantage of the new photoelectric fluorescence information available in the LLNL/ENDF6 version of the photoatomic data sublibrary.
7. The H-2 evaluation from BROND2 cannot be used with the current version of MCNP, and therefore, it cannot be processed with ACER.

