

HOW TO CUSTOMIZE *NJOY* TO PC?

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My first PC:

PC486/33MHz, 8Mbyte RAM, 100Mbyte hard disk

Today:

PC586/100MHz, 32Mbyte RAM, 500Mbyte hard disk

Software:

**DOS 6.22, WINDOWS 3.1, MULTIEDIT text editor, Lahey
5.1 compiler, INTERNET access.**

Possibility offered by the NJOY design:

**modules can be used as separate programmes - interfaced by
standardized files.**

Consequently, the simplest way to get a PC version for NJOY:

**Modules are transformed to separate programs whose work is
controlled by DOS batch**

**This can be accomplished in various ways, one of which is
described below.**

**We obtain new ENDF files through INTERNET from the
DATA CENTERS, so each isotope will be in separate file and
this occurred to be convenient for handling and storing them in
PC.**

Storing files in NJOY binary format is advantageous as far as NJOY calculations and space saving are concerned - however, to have simply a look into them requires an excess MODER run.

Processing is facilitated by a convention concerning the data file names:

For name (7 characters):

first two characters is the chemical symbol of the nuclide, if this is only one character, then the 2nd character is an '_', third character is the last figure of the rounded atomic weight, the 4-7 character is the MAT number (according to the ENDF convention), instead of lacking figures also '_' is to be used. The resulting file of GROUPT calculation has an eight-th character which is used to distinguish the different group constant calculation.

e.g. U_89237, PU99437, O_6_825, U_89237r etc.

For extension (3 characters):

1st character:

- 'e' evaluated data file,
- 'p' point-wise cross-section,
- 'g' group constants.

2nd character

in the case of point-wise cross-sections:

- 'd' 0 Kelvin data (RECONR output),
- 't' Doppler broadened data (BROADR output),
- 'u' unresolved, self-shielded cross-sections (UNRESR

output).

'h' file with thermal scattering cross-sections

in the case of group-constants:

- 'n' neutron data,

'g' γ data
3rd character
'b' blocked-binary format
'd' BCD format

e.g. U_89237.pdb unbroadened point-wise data in binary format

Evaluated data files (extension: 'evb') and the RECONR output (extension: 'pdb') are stored in one directory which I called 'dl'.

When running an NJOY module then the *data file name* is passed either as command line argument or through an input file separately from other control input; extensions are assigned by modules

Thus, from the control input
unit numbers
and MAT
are omitted.

For instance, if our task is to generate a group constant library with given temperatures, dilutions and group structures then first we create a task directory where the control input files for modules BROADR, UNRESR and GROUPR are placed. When starting the batch, the data file name is to be specified. The GROUPR requires this file with extension 'pub' which is the output of module UNRESR. If no such file then the batch will branch to UNRESR. This requires file with 'ptb' i.e. the output of BROADR. If no such file then we go to BROADR. This requires file with 'pdb'. If no such file in 'dl' then the RECONR should be invoked. RECONR uses file with extension 'evb'. If no such file the error message follows. This approach is convenient when e.g. constants for the same temperature and dilution but for different group structures are to be generated.

A slightly different customization is that when the data file names are read from a file. Such file can be easily made by means of the DOS command dir *.evb. By this way all nuclei in one directory can be processed by a module at one hit. (Once, I had to calculate (n,γ) cross-sections for 140 nuclei)

This work has been accomplished for our actual needs and therefore the required modifications, up to now, have been done not for all NJOY modules.

Modified modules are:

**RECONR, BROADR, UNRESR, HEATR, THERMR,
GROUPE, GAMINR, MODER, ACER, MIXR**

I tried NJOY94 on PC as it is. It runs. Exe file is somewhat larger than 9Mbyte. Some minor corrections have been required:

**in PLOTIT (module COVR): in format comma required
in PRESS (module COVR): Hollerith changed to character
in the main routine: nsyse=6.**

**GENERAL INTERFACE SUBROUTINE TO GROUP
CONSTANTS FILES AND A SPACE SPARING
STORAGE METHOD FOR GROUP CONSTANTS**

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Revision of AEKI group constant system:
3 years programme (1995-1997) funded by Comittee for
Technical Development of Hungary

Evaluated data to be used: ENDF/B-VI
Basic software tool: NJOY system
(Earlier FEDGROUP was used but its updating would
require too much effort)

Up to now accomplished:

Basic library:

Group averaged constants, group transfer matrices in
epithermal and thermal region and from epithermal to
thermal energy points. In thermal region the constants are
point-wise for a given energy grid rather than group-
averaged.

35 epithermal groups + 35 thermal energy points

Resonance library:

PEACO library (51832 groups)

Resonance self-shielded constants for such groups of the
above group system, where this effect is significant

Fission product library:

absorption cross-sections: 35 epithermal groups + 35 thermal groups, for 140 fission products.

Fission yields and decay constant library: out of NJOY scope (TIBSO was used)

For the above enlisted tasks:

MODER, RECONR, BROADR, UNRESR, GROUPR and THERMR

NJOY modules have been required

Planned for the next year:

Heat generation constants for coupled reactor kinetics (HEATR module will be needed)

ORIGEN type library for VVER reactors and revision of yields and decay constants using the newest ENDF/B-VI data.

The above tasks required some modifications in GROUPR beside those ones done for PC customization.

(point-wise cross-section for a specified energy grid, a slight modification in slowing down parameters)

Other developments:

Compilation of any group constant library from the standard GROUPR output files requires sometimes a cumbersome rearrangement of calculated constants.

Therefore, we have created a subroutine named 'aekigr' for retrieving any specified constant set from the standard GROUPR output files. This subroutine in one 'call' retrieves a given type of constants for a given nuclide for all groups, σ_0 and temperature values. For handling the GROUPR output files it uses the corresponding auxiliary routines of NJOY system.

aekigr(fmat,mf,mt,il,ig2,w,lfr)

fmat - the name of file with 'gnb' extension(8 characters)

w(lfr) - field containing the retrieved group constants, group boundaries, σ_0 and so on.

The redundancy in GROUPR standard output is inconvenient when the number of groups is large and it has some other disadvantages, too.

Therefore, an alternative way of storing group constants has been developed.

This is the

BINDIR library = binary direct access file + index file
Very effective tool for group constant library compilation

Construction:

Each group constant set is represented by two records on the index file:

1. record

fmat	8 characters, name of the group constant file (without "gnb" extension)
awr	mass of the isotope (in neutron mass unit)
nsig0	number of σ_0 values
lz	pointer for the σ_0 vector
ngn	number of neutron groups
lng	pointer for neutron group boundaries
ngg	number of gamma groups
lgg	pointer for gamma group boundaries
ntemp	number of temperature values
ltp	pointer for temperature values

2. rekord

mf	file number
mt	section number
il	legendre component
ig2	0 scattering matrix 1 group flux 2 group cross-section
ldat	pointer of group constant vector

A pointer points to a place on the binary file which is a direct access file with recl=4000bytes.

The form of a group constant record:

((sig(ig,iz,it),ig=1,ngn),iz=1,nsig0),it=1,ntemp)

The form of a matrix record:

(rgroup,(rigup,riglo,((tsig(jg,iz,ig,it),jg=igup,iglo),iz=1,nsig0),ig=1,igroup),
it=1,ntemp)

where

igroup=nint(rgroup), the lowest energy group, where the constant is not 0, and

iglo=nint(riglo)=ngn-ig2lo+1

igup=nint(rigup)=ngn-ig2lo-ng2+3

lower and upper boundaries of inscattering group, respectively.

This form is the same as it is retrieved by **aekigr**.

For BINDIR libraries a program package is developed:

GROLIB - adds group constant sets from GROUPR output to
BINDIR file; if the latter does not exist then it is created.

INTLIB - retrieves and interpolates group constants.

BINCNT - lists of the content of a BINDIR library

UNILIB - merges BINDIR libraries.

And, of course, each target library is compiled by own
program constructed from standard retrieval routines.

**(future: group constant data base and utilization of
professional data base management tools??!!)**