New Features and Functions of the GRUCON Processing Code Package, version 2021.

1. Extension of the GRUCON Standard Data Structures (SDS) Set

The set of the GRUCON SDS is extended by inclusion Atomic Relaxation Data *AR* to include to the ACE file with photo-atomic Interaction cross sections the fluorescence data. The *AR* structure contains:

LMF	Class identifier of the ENDF original data (MF)
LMT	Reaction type identifier (MT in the ENDF format)
NSS	Number of subshells
LTR	Total number of transitions
NTR(NSS)	Number of transitions from subshell
MELN(NSS)	Number of electron in subshell when neutral
MSUBI(NSS)	Subshell designator
MSUBJ(NSS)	Secondary subshell designator
MSUBK(NSS)	Tertiary subshell designator
EL	Lower limit of the energy range (eV)
EH	Upper limit of the energy range (eV)
EPS	Relative processing uncertainty (zero for evaluated data)
ZA	Material charge parameter
AW	Material mass parameter (C^{12})
EBI(NSS)	Binding energy for subshell (eV)
ETR(LTR)	Energy of transition (eV)
FTR(LTR)	Fractional probability of transition

2. Functionality Extensions in the Existing Modules

The **ACE** module has been extended to provide processing the Photo-Atomic (MF23, MF26, MF27) and Atomic Relaxation (MF28) data files from the NSUB3 and NSUB6 ENDF sub-libraries correspondingly, and prepare ACE formatted files for Monte-Carlo calculations. The needed function is set up by flag NTYP:
NTYP=1 - fast neutron and gamma production data,
NTYP=2 - thermal neutron scattering data,
NTYP=4 - photo-atomic and atomic relaxation data (new).

The **ENDF** input module was revised to take into account possibility of including to the ENDF-6 format a new mixed (coherent and incoherent) elastic scattering data to support advanced moderator development [1].

Other useful function, added to this module, is possibility to check input ENDF files on the matter of consistency and correspondence to rules, adopted in the ENDF-6 format. Output information appears as a "warning", allowing to decide, is it possible to continue or is necessary to stop processing and made necessary corrections.

The **SXAXS** module was simplified for usage by including default lists of partial cross sections that forms needed redundant cross section. For example, to prepare total inelastic, instead of

*s/a-s: nop=1, mti=4,-91, mto=4, lop=1

now is enough to write:

*s/a-s: nop=1,mti=0, mto=4, lop=0

The list of redundant cross sections, which can be prepared in this way, is given below (according to ENDF-6 definitions [2]):

MTO	Description	Σ (MTI)
1	total	2,4-5,11,16-17,22-27,41-42,44-45, 152-154, 156-181, 183-190,194-196,198-200
4	total inelastic	50-91
16	(n,2n)	875-891
18	fission	19-21,38
27	absorption	18,101
101	disappearance	102-117,155,182,191-193,197
103	(n,p)	600-649
104	(n,d)	650-699
105	(n,t)	700-749
106	(n,he3)	755-799
107	(n,alpha)	800-849

There are also two special MT's, unassigned in the ENDF manual, that used for preparing of some group data libraries (BNAB, TEMBR):

13	Sum of all (n,xn) cross sections, except elastic
14	Sum of all (n,xn) cross sections, except elastic, multiplied on neutron yields

One of the function of the SXAXS module is preparing the cross sections, that are used as background under reconstruction cross sections from resonance parameters in the resolved and/or unresolved resonance energy ranges. To define the list of reactions, represented by the resonance parameters, the control parameters can be used with command option &N to point the address the position of structures *R*,*RM*,*U* with resonance parameters in the library through number N of catalog string, in which they are registered. It can be done, for example, by commands:

```
,in,1,endf     ! read control parameters for the ENDF input module
,in,2,sxixs    ! read control parameters for the SXIXS module
,in,3,sxcxs    ! read control parameters for the SXCXS module
,in,4 sxaxs    ! read control parameters for the SXAXS module
……..
,1,20,data       ! read the ENDF file
20,2,21,s        ! linearize cross sections
21,3,22,s        ! join all cross sections in one table
22,4&20,23,s ! prepare background cross sections
…….
```

In this case, the control parameters for the SXAXS module can be:
S/A-S: nop=0

Cross sections, reconstructed by RXTXS and UXDXS module in the resolved and unresolved resonance ranges (if exist), should be joint by SXCXS module with obtained background cross sections.

The **EXTRA** module is revised to include similar possibility to form the list of resonance cross sections implicitly, by means of command option &N. The presence of this options gave a signal, that in the list of reactions should be added MT's, taken from the structures *R*,*RM* and *U*. The sign of parameter N is used to

N > 0 - extract all cross sections with MT's, given in the *R*,*RM*,*U* structures
N < 0 - extract all cross sections except that of given in the *R*,*RM*,*U* structures.

The **PN/D-PC** module for computing matrices of subgroup correlation under collision in the resolved resonance range has now additional possibility to take into account energy distribution of scattered neutrons. Connection with these data is provided by the &N command parameter, where N is number of catalogue line with address of needed data. Such data may be table of mu-bar data in the *S* structure, obtained preliminary from *A* structure by the AXXS module or *D* energy angle distributions of scattered neutrons. These distributions can be obtained with THXXDS or SXTXDS modules in free-gas or resonance scattering approaches. The calculation is controlled by parameter NMOD

with values:
Energy distribution type
NMOD=0 - equally-likely energy distribution in all energy range (no correlation)
NMOD=1 - constant in the interval of maximal loss of energy
NMOD=2 - constant in the interval of average logarithmic loss of energy
NMOD=3 - detail distribution in *S* or *D* structures, pointed in the command option.

3. Functional Modules added to the GRUCON package

Some of the group libraries (CCCC, TEMBR) require special group characteristics, such as group average neutron energy, group average neutron inverse velocity etc. To prepare such values, a service module, named as INXXS is added to the package. The needed values
are represented in form of *S* structure, with identification numbers MAT, MZA borrowed for other data, prescribed by command option &N. Now are available three types of special values, namely:

MT	Description
257	neutron energy (to calculate average energy in groups)
258	neutron lethargy (to calculate average lethargy in groups)
259	Neutron inverse velocity (sec/m)

Another feature of common group libraries is the wise usage of isotope natural mixtures. To ensure the completeness of the set of functional modules, a module for matrix convolution – the **MXCXM** module - has been developed and added to the package. The input data for this module are the group transition matrices *M* for separate isotopes, depending on the temperatures and dilution cross sections. The result is group transition matrix for mixture (natural) of isotopes. The convolution of matrices is performed by algorithm of iteration on dilution cross section. The same algorithm has been implemented to the **FXCXF** module for convolution cross section moments and preparing self-shielding factors, in addition to previous two, based on the *Padé-I* and *Padé-II* approximations. The GRUCON procedure for preparing total set of group data is in the **Attachmen**t. The procedure is assigned to convolution 4 isotopes (the lead isotopes
are used as a sample) to the natural mixture from point-wise (in energy ranges with overlapping detail cross sections) and group-wise (in the unresolved energy range) cross section and matrices. The tapes with input data can be prepared by procedure Test20 (see GRUCON Manual 2021). The tapes 21-24 are with endf data (resonance parameters are

needed to
define type of convolution: point-wise or group-wise),tapes 31-34 contain cross sections without resonance structure, tapes 41-44 contain cross section moments (for shielding)< tapes 51-54 – group transition matrices.

4. Verification activity.

In frame of ACE File Verification Project initiated by the NDS IAEA and coordinated by A.Trkov , the ACE files for nuclide bounded in H_H2O, D_D2O, Be_met, Be_BeO, C_gph, H_ZrH and Zr_ZrH has been obtained by GRUCON and compared with NJOY. The integral testing of these files has been performed in Keff calculations for benchmarks from ICSBEP [3]. More complete information can be found on the website [4].

References

1. M.L.Zerkle, Mixed Elastic Scattering Format Proposal, CSEWG – Format&Processing Commettee, November 30,2020
2. Edited by A.Trkov,M.Herman,D.A.Brown, ENDF-6 Formats Manual, http://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf
3. Sinitsa V.V., Listov A.S.,Zhukov V.A., Capabilities of the GRUCON code package in the TSL data processing, available at https://www-nds.iaea.org/index-meeting-crp/TM-NDP-2021/doc/Sinitsa_TM_NDP_2021.pdf
4. https://www-nds.iaea.org/index-meeting-crp/TM-NDP-2021/

Attachment. GRUCON Procedure for Preparing Group Cross Section and Matrices for Natural Mixtures of Isotopes.

```
! mixing of isotopes
 ,in              ! enter local parameters
 ,in,1,read       ! enter control parameters
 ,in,2,read       !
 ,in,3,read       ! enter control parameters
 ,in,4,read       !
 ,in,5,extra      !
  in,5,extra      !
 ,in,7,axxs       !
 ,in,8,s/c-s      !
 ,in,9,s/a-s      !
 ,in,10,exttem     !
 ,in,11,sxexs     !
 ,in,12,s/c-s     !
 ,in,13,sxaxs     !
 ,in,14,sxaxs     !
 ,in,15,sxgxf     !
 ,in,16,fxxs      !
 ,in,17,sxaxs     !
 ,in,18,sxgxf     !
 ,in,19,redef     !
 ,in,20,fxcxf     !
 ,in,21,fxcxf     !
 ,in,22,mxcxm     !
 ,in,23,gendf     !
 ,1,30,data       ! read resonance parameters
 ,2,31,s          ! read cross sections
 ,3,32,f          ! read moments
 ,4,33,m          ! read matrices
 31,5,52,s,2      ! extract mt=1,2,102-117
 52,8,53,s,3      ! join
 53,9,52,s        ! prepare mt=101
```

```
 31,6,34,s     ! extract all except 1,2,102,-117
 34,10,35,s      ! extract T300
 35,11,36,s     ! thin grid points
 36,8,37,s      ! join
 52,10,53,s      ! extract mt1,2,101 t=300
 30,7,53        ! add mt 251,252
 53,8,38,s      ! join
 38,13,39,s     ! prepare product mt2*(mt252,252)
 37,14,39       ! prepar and add mt13,14
 39,12,53,s     ! summarize with ro
 53,15,40,f     ! integrate in groups
 40,16,41,s     ! convert f to s
 41,17,42,s     ! devide mt251,252 by mt2,prepare mt13,15
 32,19,43,f     ! redefine mt102 to mt101
 52,18&-30,44,f  ! prepare moments outside the urr
 43,20&30,44     ! collapce moments in the urr
 44,21,45,f     ! join moments
 33,22,45       ! join matrices and add to f
 42,cp,45       ! add cross sections
 45,23,,ENDFB8_0 !
 ,,,end
! --------------------------------------
!    local parameters
*de:1.e-5,20.e6,
*nmat:4,
*lmat:8225,8231,8234,8237,
*ro:0.014,0.241,0.221,0.524,
*ngn:30,
*egn:1.e-4,0.2154434,0.4641589,1.0,2.154434,4.641589,
     10.0,21.54434,46.41589,100.,215.4434,464.1589,
     1.e3,2.154434e3,4.641589e3,1.E4,2.154434e4,4.641589e4,
     1.E5,2.e5,4.e5,8.e5,1.4e6,2.5e6,4.e6,6.5e6,10.5e6,
     13.9818e6,15.0196e6,17.3318e6,20.e6,
*iwn:4,
*nsigz:26,
*sigz:1.e-3,0.1,0.215,0.465,1.,2.15,4.65,
      1.e1,2.15e1,4.65e1,1.e2,2.15e2,4.65e2,
      1.e3,2.15e3,4.65e3,1.e4,2.15e4,4.65e4,
      1.e5,2.15e5,4.65e5,1.e6,2.15e6,4.65e6,1.e7,
*eps:0.001
```

```
! ----------------------------------------
!    control parameters
*read:ntape=-21,
*read:ntape=-22,
*read:ntape=-23,
*read:ntape=-24
*read:ntape=-31,
*read:ntape=-32,
*read:ntape=-33,
*read:ntape=-34
*read:ntape=-41,
*read:ntape=-42,
*read:ntape=-43,
*read:ntape=-44
*read:ntape=-51,
*read:ntape=-52,
*read:ntape=-53,
*read:ntape=-54
*extra:kdat=2,nmod=3,nr=3,lr=1,2,102,-117
*extra:kdat=2,nmod=3,nr=-3,lr=1,2,102,-117
*a/-s:*eps
*s/c-s:nmat=0,ns=0,*de,*eps
*s/a-s:nop=3,
       lsi=1,2,102,-117,
       lso=0,0,101,
       lop=0,0,1
*exttem:ntem=-1,ktem=1
*s/e-s:*eps
*s/c-s:*nmat,ns=0,*lmat,*de,*eps,*ro
*s/a-s:nop=7,
       lsi=1,2,101,2,251,2,252,
       lso=0,0,0,251,251,252,252,
       lop=0,0,0,1,3,1,3
*s/a-s:nop=2,
       lsi=0,0,
       lso=13,14,
```

```
       lop=0,0
*s/g-f:nfun=1,*ngn,nig=1,*iwn,nr=0,nsigz=0,nl=0,nh=0,
       nng=1,nsg=1,nmg=1,*eps,
wn=0.1,0.025,2.5e6,1.4e6,
       *egn
*f/-s:nr=0,km=0,kt=1,kp=0
*s/a-s:nop=10,
       lsi=1,2,13,14,13,101,251,2,252,2,
       lso=0,0,13,15,15,0,251,251,252,252,
       lop=0,0,1,1,4,0,1,4,1,4
*s/g-f:nfun=1,*ngn,nig=1,*iwn,nr=0,*nsigz,nl=-2,nh=0,
       nng=1,nsg=1,nmg=1,*eps,*sigz,
        wn=0.1,0.025,2.5e6,1.4e6,
       *egn
*redef:ntyp=3,nmt=1,mti=102,mto=101
*f/c-f:nreg=210,*nmat,nmt=0,*nsigz,nl=-2,nh=0,*lmat,
       *de,*eps,tr=0.,*sigz,*ro
*f/c-f:nreg=0,nmat=0,ns=0,nz=0,nl=-2,nh=0,
       *de,*eps,tr=0.
*mxcxm:*nmat,nmt=0,*lmat,*eps,*ro
*gendf:ntape=60,nmat=0,ntem=0,nf=0,nmt=0
```