GRUCON-2018: Extension for ENDF/B-VIII Evaluated Data Processing. Preparing of Particle Production Cross Sections. Doppler Smoothing of Angular Parameters.

Statements of work:

- Extend standard data structures of GRUCON package to include tabulated form of Fission Energy Release (F.E.R.) and incident-energy dependent probabilities P(ν) for fission neutrons
- Provide possibility of inclusion gamma and gas production data to the ACE file for Monte Carlo calculations
- Develop modules needed for Doppler broadening of angular distribution moments reconstructed y from resonance parameters
- Perform verification the GRUCON extended possibilities of data processing by comparison with NJOY-2016 and PREPRO-2017 processing codes
- Validate ACE files prepared by updated version of GRUCON.

1. Extensions in GRUCON Standard Data Structures

The ENDF-6 format extensions for the ENDF/B-VIII evaluated data library [1] have been taken into account by
- Inclusion to the *EF* data structure the tabulated form of F.E.R.
- Inclusion to the *AE* data structure the probabilities and spectra for fission neutrons and gammas from MF=6/MT=18 (options JPX=1, JPX=2)

Description of the new data structures is given in the Appendix I. The corresponding changes are performed in the ENDF (input and output options), ACE (output data in the ACE format) and TABLE (output data in form of annotated tables) modules of GRUCON.

2. The PROD module for Gammas and Particles Production Cross Section Calculations

The PROD module has been revised to include particles production in breakup reactions, described implicitly, by LR flag.

The ACE module (ACE file preparation) is updated to include
- cross sections with MT=203 – 207 (gas production) to the ACE table 7.SIG
- complete set of ACE tables with gamma production data:
  12.GPD, 13.MTRP, 14.LSIGP, 15.SIGP,
  16.LANDP, 17.ANDP, 18.LDLWP, 19.DLWP, 20.YP

3. Doppler Smoothing of Legendre Polynomial Coefficients

To take into account temperature dependency of elastic cross section on angular distributions, the smoothing procedure of Legendre Polynomial coefficients restored from resonance parameters is implemented. This procedure is based on usage of the SXTXS Doppler broadening module, developed for cross sections. The calculation is performed in three steps:

- Legendre polynomial coefficients a_l (represented in *A* structure), reconstructed from resonance parameters by Blatt-Biedenharn formulae, are processed by AXXS module. This module multiplies elastic cross sections, obtained from the same resonance parameters at zero temperature, by factor a_l and converts obtained cross section moments to the *S* representation;
- obtained cross section moments are broaden by the SXTXS module for given temperature, and then
- are processed by SXXA module, that divide moments by corresponding cross section values and reconstructs *A* structure with smoothed a_l coefficients.

To implement this calculation scheme, the AXXS module has been updated and a new one for *S* to *A* conversion – the SXXA module - has been included to the package. To optimize energy grids in the *S* and *A* structures, the S/E-S and A/E-A thinning modules can be used for intermediate data. The SXXA module has also option of joining the reconstructed a_l with other angular distribution parameters, to get data in all energy range.

Below are the sample of input deck for reconstruction and smoothing of angular distribution parameters with generation of the ENDF MF4 file and results of comparison of cross sections and Legendre polynomial coefficients for elastic scattering of neutron on W-186 target nuclei are given at Fig.2 for all RR energy range (left column) and in 7.4-7.5 keV energy interval (right column).

```
! Reconstruction and Doppler Smoothing of Legendre Polynomial Coefficients
,,,init,1,0,10000k
,,,init,2,0,20000k
,,,init,3,0,20000k
,in                 ! read local parameters
,in,1,endf          ! read control parameters
,in,2,rxtxs         !
,in,3,sxcxs         !
,in,4,sxexs         !
,in,5,sxlxa         !
,in,6,axxs          !
,in,7,sxtxs         !
,in,8,sxxa          !
,in,9,axexa         !
,in,10,endf         !
,1,20,data          ! read *r* and *a* from mf2 and mf4 endf files
20,2,32,s,2         ! calculate cross sections
32,3,33,s,3         ! join cross sections
33,4,21,s           ! thin energy grid
20,2&-10,32,s       ! calculate collision function
32,5&20,33,a        ! prepare angular distribution parameters
33,6&21,32,s        ! convert *a* to *s* structure
32,4,33,s           ! thin energy grid points in *s* structure
33,7,32,s           ! smooth by doppler broaden of cross section
32,8&20,33,a        ! convert *s* to *a* structure
33,9,32,a           ! thin energy grid points in *a* structure
32,10               ! write ENDF MF4 file
,,,end
!--------------------------------------------------
!    local parameters
*mt:2,
*de:1.e-5,20.e6,
*nt:1,
*tem:293.6,
*eps:0.001
!--------------------------------------------------
!    control parameters
*endf:ntape=20,nmat=0,nmf=2,nmt=1,mf=2,4,*mt
*r/t-s:nfor=0,nt=1,*de,*eps,tem=0.
*s/c-s:ncom=0,ns=1,*mt,*de,*eps
*s/e-s:*eps
*s/l-a:nl=0,ns=1,*mt,*de,*eps
*a/-s:*eps
*s/t-s:*nt,*de,*eps,*tem
*s/-a:*eps
*a/e-a:*eps
*endf:ntape=21,nmat=0,nmf=1,nmt=0,mf=4
```

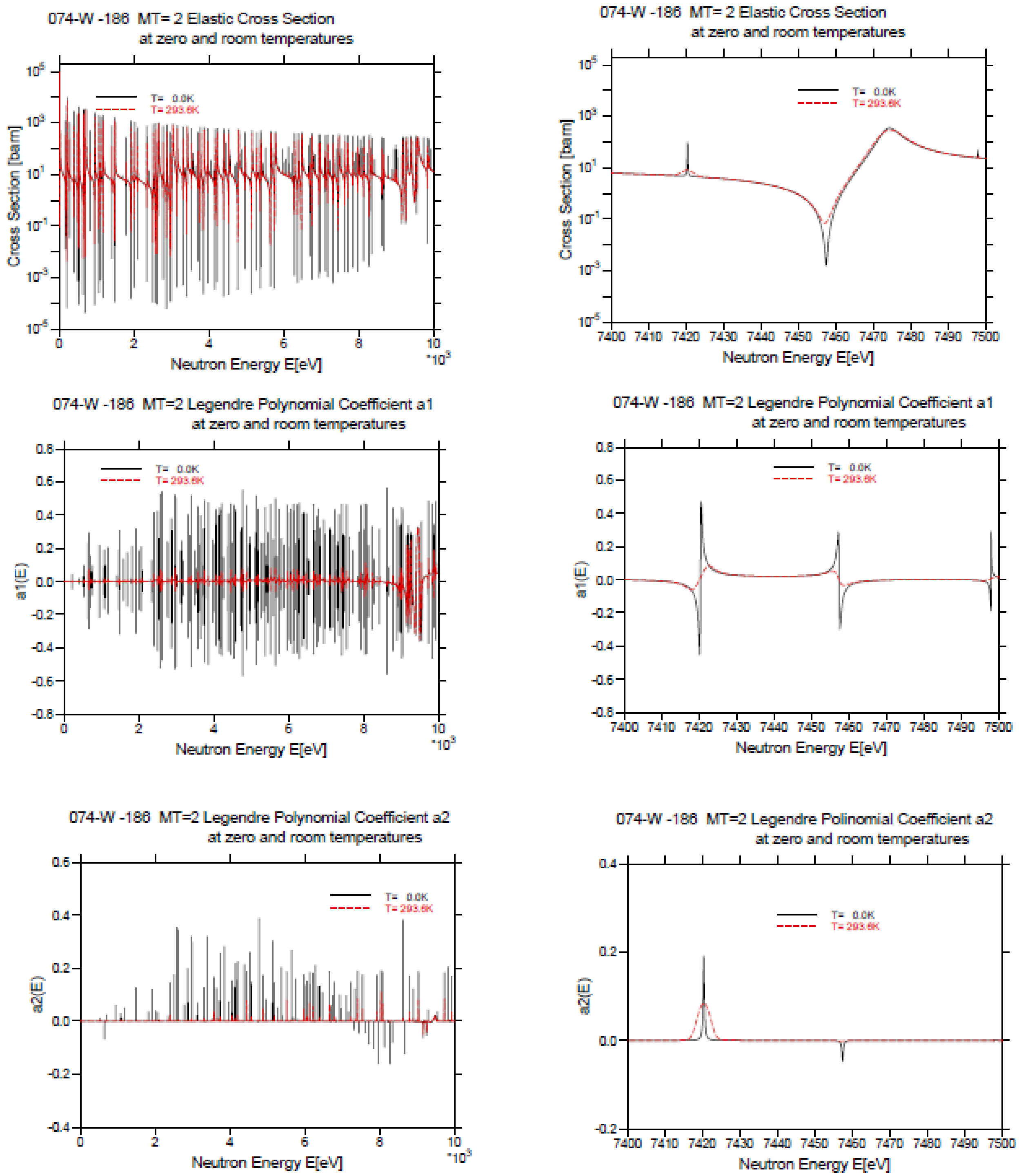

Fig.2 Cross-sections and angular distribution parameters for neutron elastic scattering on W-186, for zero temperature and at T=293.6K, after Doppler smoothing.

4. Integral Verification Calculations

The Doppler broadening of angular distributions, reconstructed from resonance parameters has been
implemented by including to the AXXS module additional function, allowing to convert *A* structure (angular distribution parameters) to *S* structure with Legendre coefficients, multiplied on elastic cross sections. It gives possibility to use the SXTXS module and obtain angular moments for any required temperature. An additional - the SXXA module has been developed and included to the package, to make invert conversion and prepare structure *A*, joined with the rest of angular distribution parameters outside RRR. So, probably, the problem of preparing the angular distributions from resonance parameters is closed.

Some peculiarities has been found in the ENDF/B-VIII.0 evaluation (for example, usage of URR without RRR). They have been taken into account by tuning the corresponding modules.

Functionality of the new package has been checked by running the GRUCON-2018 package on the ENDF/B-VIII.0 data files with input task for preparing of the ACE files.

The most part of runs was successful, with a few exceptions:
- Dy159 has been stopped due to loop
- Es-252 stopes with diagnostics of wrong interpolation.

So, the ACE library contains presently 555 materials for room temperature T=293.6K

Some ACE thermal scattering data files, needed for integral tests, has been prepared also though the GRUCON package:
H in H2O, D in D2O, H in CH2, Be metallic, Be in BeO, C in graphite (10% porous), C in graphite (30% porous),

The comparison with cross sections, obtained by grucon-2018.6 and njoy-2016 code, reveals essential discrepancies only in gas productions cross sections for light nuclides: He-3, Li-6, Li-7, Be-7, B10.

References

1. Cross Section Evaluation Working Group, "**ENDF-6 Formats Manual, Data Formats and Procedures for the Evaluated Nuclear Data File ENDF/B-VI, ENDF/B-VII and ENDF/B-VIII**", BNL-2032018-2018-INRE, Brookhaven National Laboratory, edited by A. Trkov, M.W. Herman and D.A. Brown with contributions from N. Holden and G. Hedstrom (February 1, 2018)
2. A. Kahler, J.L. Conlin, A.P. McCartney, **NJOY2016**
   Los Alamos National Laboratory, Los Alamos, NM, USA,
   [Online] Available at https://njoy.github.io/NJOY2016/
3. D.E. Cullen **PREPRO 2017 home page**
   International Atomic Energy Agency, Vienna, Austria (2017)
   [Online] Available at https://www-nds.iaea.org/public/endf/prepro/
4. D.E.Cullen **PLOTTAB** – Plot continues and/or Discrete Data, Version 2014-1,
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5. International Handbook of Evaluated Criticality Safety Benchmark Experiments, NEA/NSC/DOC(95)/03, OECD NEA, Paris, France (2015)

Appendix I. GRUCON Data Structures, changed for including the ENDF/B-VIII extensions

***EF* - Components of Energy Release Due to Fission**	
LMF	Class identifier of the ENDF original data (MF)
LMT	Data type identifier (MT in the ENDF format)
LFC	Representation Flag: 0/1 = polynomial/tabular
NEFC	Number of components (LFC=1) or 0 (LFC=0)
NPLY	Order of the polynomial expansion
MNFC(NEFC)	Number of energy points for each component (NEFC>0)
MLDRV(NEFC)	List of flags LDRV=1 - derived data, = 2- primary evaluation (NEFC>0)
MKINT(NEFC)	Interpolation law (NEFC>0)
MINT(*)	Interpolation table (NEFC>0)
EL	Lower limit of the energy range (eV)
EH	Upper limit of the energy range (eV)
EPS	Relative processing uncertainty (zero for evaluated data)
AW	Mass of the target nucleus (C^{12})
TAB(*)	Table of energy release components: ET - sum of the partial energies EFR - kinetic energy of the fission products ENP - kinetic energy of the prompt fission neutron END - kinetic energy of the delayed fission neutrons EGP - total energy released by the emission of prompt γ rays EGD - total energy released by the emission of delayed γ rays EB - total energy released by delayed β's ENU - energy carried away by neutrinos ER - total energy less the energy of the neutrinos

Appendix 2. Criticality Calculation Results

Benchmark	Experiment		NJOY		GRUCON		G/N-1
heu-met-fast-001	**1.00000**	100	1.00016	8	1.00002	8	-14
heu-met-fast-002	**1.00000**	300	0.99961	17	0.99971	12	10
heu-met-fast-003_ni	**1.00000**	500	0.99944	8	0.99949	12	5
heu-met-fast-003_u1	**1.00000**	500	0.99275	12	0.99315	11	40
heu-met-fast-003_u2	**1.00000**	500	0.99224	11	0.99247	11	23
heu-met-fast-003_u3	**1.00000**	500	0.99701	11	0.99729	12	28
heu-met-fast-003_u4	**1.00000**	300	0.99488	12	0.99509	12	21
heu-met-fast-003_u5	**1.00000**	300	0.99918	12	0.99945	12	27
heu-met-fast-003_u6	**1.00000**	300	0.99965	12	0.99971	12	6
heu-met-fast-003_u7	**1.00000**	300	1.00050	12	1.00050	12	0
heu-met-fast-028	**1.00000**	300	1.00085	4	1.00109	12	24

Benchmark	Experiment		NJOY		GRUCON		G/N-1
heu-sol-therm-009_1	**0.99900**	430	1.00134	14	1.00158	18	24
heu-sol-therm-009_2	**1.00000**	390	1.00214	15	1.00223	40	9
heu-sol-therm-009_3	**1.00000**	360	1.00208	16	1.00247	19	39
heu-sol-therm-009_4	**0.99860**	350	0.99738	14	0.99727	20	-11
heu-sol-therm-010_1	**1.00000**	290	1.00257	13	1.00268	16	11
heu-sol-therm-011_1	**1.00000**	230	1.00541	14	1.00605	15	64
heu-sol-therm-011_2	**1.00000**	230	1.00135	15	1.00173	15	38
heu-sol-therm-012	**0.99990**	580	1.00102	10	1.00036	20	-66
heu-sol-therm-013_1	**1.00120**	260	0.99819	8	0.99833	20	14
heu-sol-therm-013_2	**1.00070**	360	0.99755	9	0.99772	11	17
heu-sol-therm-013_3	**1.00090**	360	0.99421	10	0.99440	12	19
heu-sol-therm-013_4	**1.00030**	360	0.99590	10	0.99612	12	22

Benchmark	Experiment		NJOY		GRUCON		G/N-1
pu-met-fast-001	**1.00000**	110	0.99985	6	0.99988	11	3
pu-met-fast-002	**1.00000**	200	1.00144	6	1.00146	11	2
pu-met-fast-006	**1.00000**	300	0.99962	8	0.99974	13	12
pu-met-fast-009	**1.00000**	270	0.99945	13	0.99947	11	2
pu-met-fast-010	**1.00000**	180	0.99775	9	0.99794	11	19
pu-met-fast-011	**1.00000**	100	1.00070	10	1.00085	14	15
pu-met-fast-023	**1.00000**	220	0.99927	9	0.99828	11	-99
pu-met-fast-024	**1.00000**	220	1.00133	9	1.00092	12	-41
pu-met-fast-031	**1.00000**	210	1.00513	14	1.00442	13	-71

Benchmark	Experiment		NJOY		GRUCON		G/N-1
pu-sol-therm-006_1	**1.00000**	350	0.99422	28	0.99461	20	39
pu-sol-therm-006_2	**1.00000**	350	0.99571	31	0.99578	20	7
pu-sol-therm-006_3	**1.00000**	350	0.99550	28	0.99540	14	-10
pu-sol-therm-009_2a	**1.00000**	330	1.01387	7	1.01356	13	-31
pu-sol-therm-011_16_5	**1.00000**	520	0.99987	12	1.00054	17	67
pu-sol-therm-011_18_1	**1.00000**	520	0.98762	11	0.98834	27	73
pu-sol-therm-011_18_6	**1.00000**	520	0.99359	12	0.99417	15	58

Benchmark	Experiment		NJOY		GRUCON		G/N-1
ieu-met-fast-007d	**1.00450**	70	1.00442	7	1.00369	10	-73
ieu-met-fast-007s	**1.00490**	80	1.00419	8	1.00379	10	-40

Benchmark	Experiment		NJOY		GRUCON		G/N-1
mix-met-fast-001	**1.00000**	160	0.99936	9	0.99957	11	21

Benchmark	Experiment		NJOY		GRUCON		G/N-1
u233-met-fast-001	**1.00000**	100	1.00026	6	1.00052	10	26
u233-met-fast-002_1	**1.00000**	100	1.00148	11	1.00003	11	-145
u233-met-fast-002_2	**1.00000**	100	1.00015	10	1.00167	11	152
u233-met-fast-003_1	**1.00000**	100	0.99868	10	0.99963	11	95
u233-met-fast-003_2	**1.00000**	100	0.99823	12	1.00021	11	198
u233-met-fast-006	**1.00000**	140	0.99998	17	1.00037	12	39