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Verification of GRUCON Modules and Calculation Procedures for ACE File Generating

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CONTENT

1. Comments to the 1st stage of the ACE Verification Project (U-235 and U-238 without probability tables)
2. Processing of Photon and Particle Production Data in the GRUCON Package. Inter-comparison of Production Cross Sections
3. New functionality of GRUCON package
4. Processing of Generalized Nuclear Data Structures in the GRUCON package

1. Comments to the 1st stage of the ACE verification project (U-235 and U-238 without probability tables)

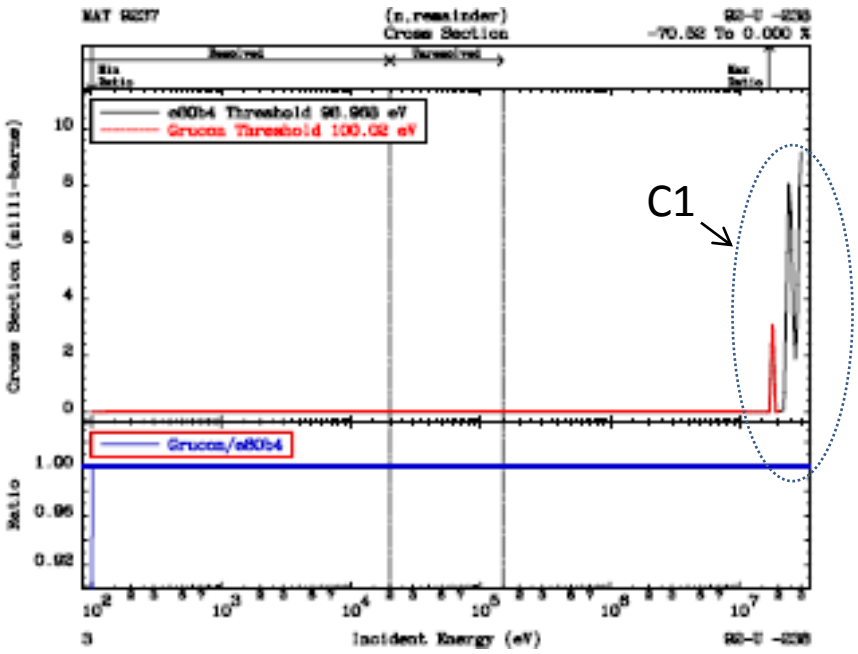
(A) Neutron Cross Sections
(B) Energy-Angular Distributions
(C) Integral Testing

https://www-nds.iaea.org/ACE_verification/

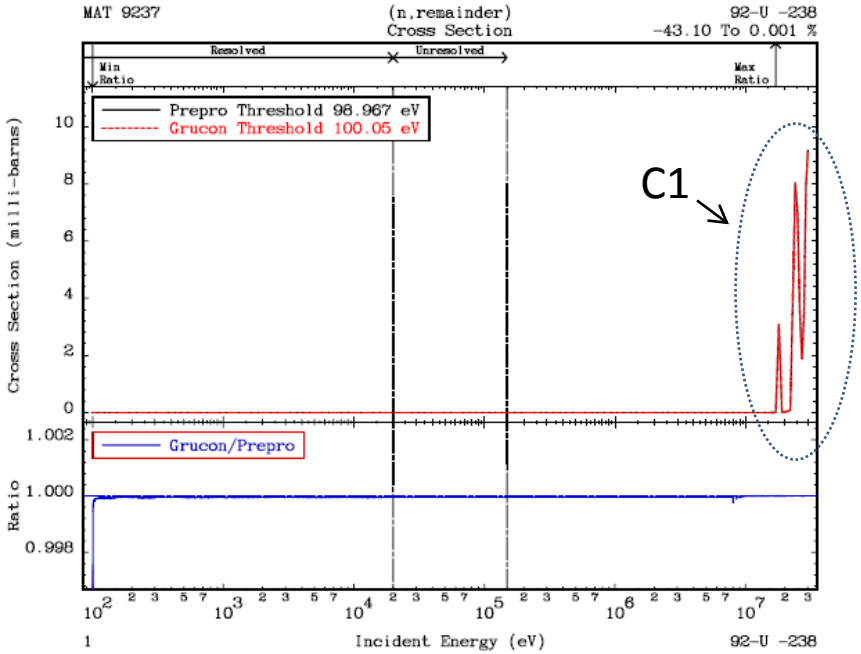
(A) U-238 MT = 5 (sum of all reactions not given explicitly in another MT's)

Neutron energy upper limits En = 20MeV and En =30MeV

Grucon vs. Reference (e80b4)



Grucon corrected vs. Prepro

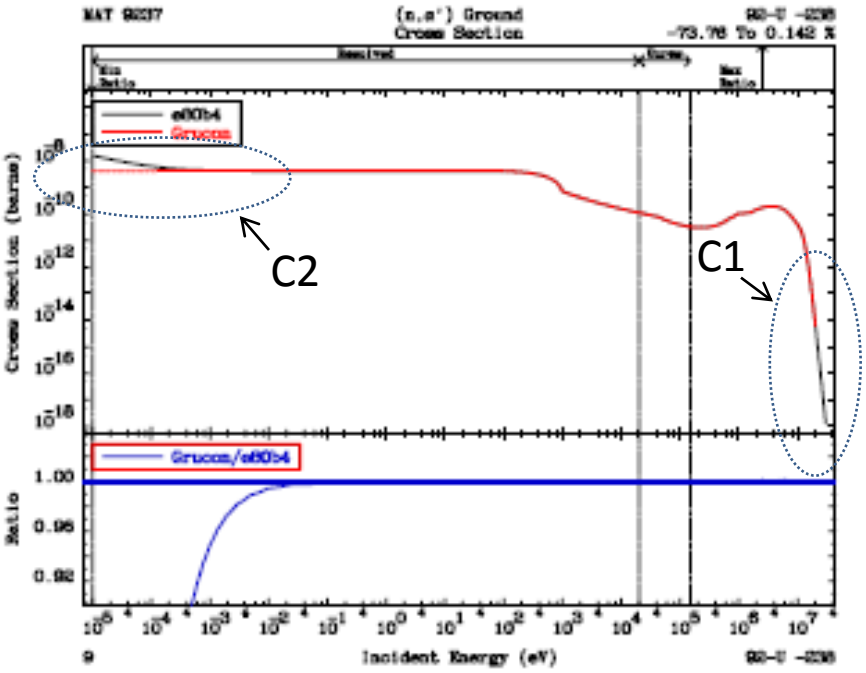


<u>Correction 1</u>. Upper limit of neutron energy range in GRUCON input deck is changed from 20 MeV to value defined in file (30 MeV)

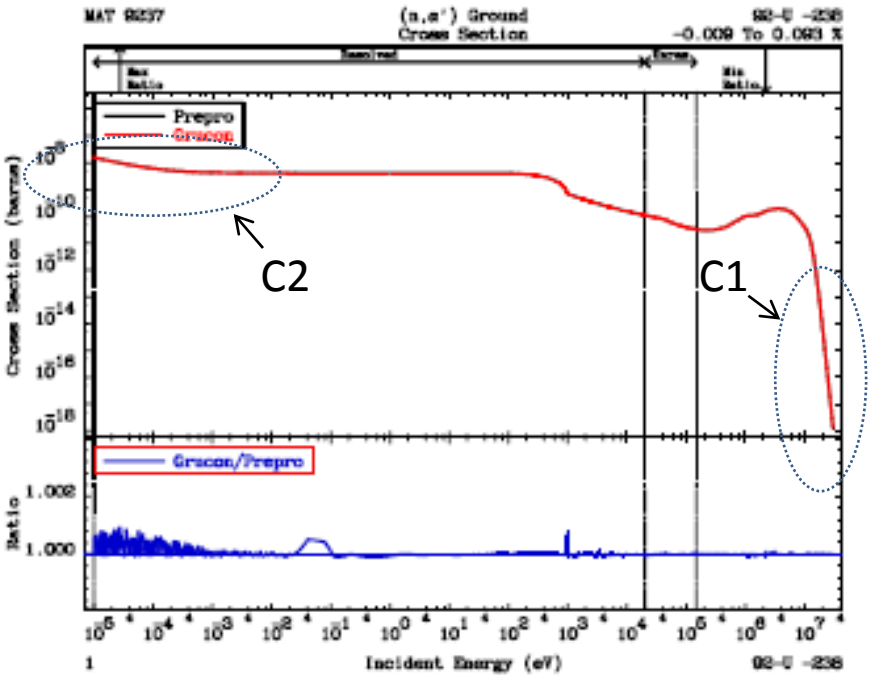
(A) U238: MT = 800 (n,α_0) reaction

Temperatures T=0. K and T=293.6K

Grucon vs. Reference (e80b4)



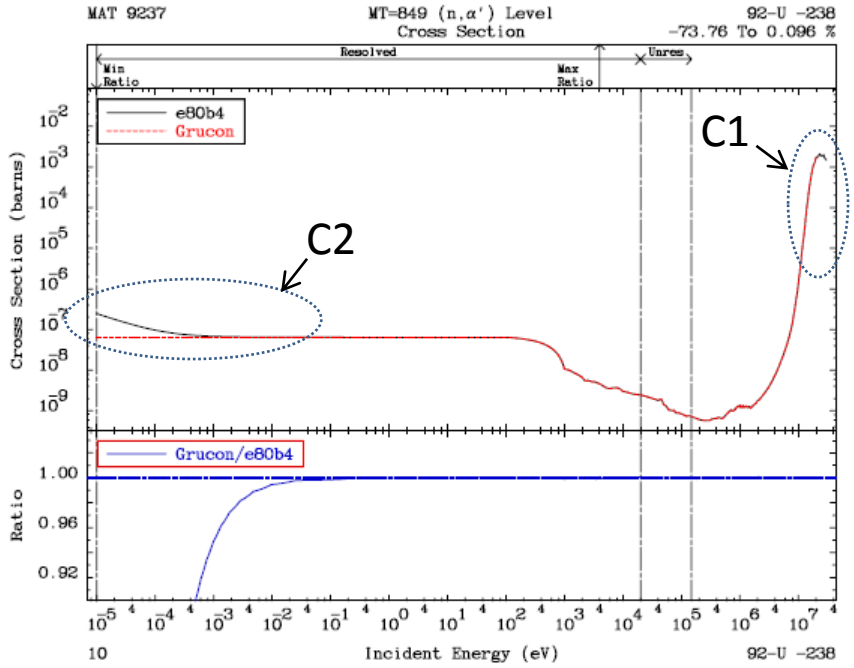
Grucon corrected vs. Prepro



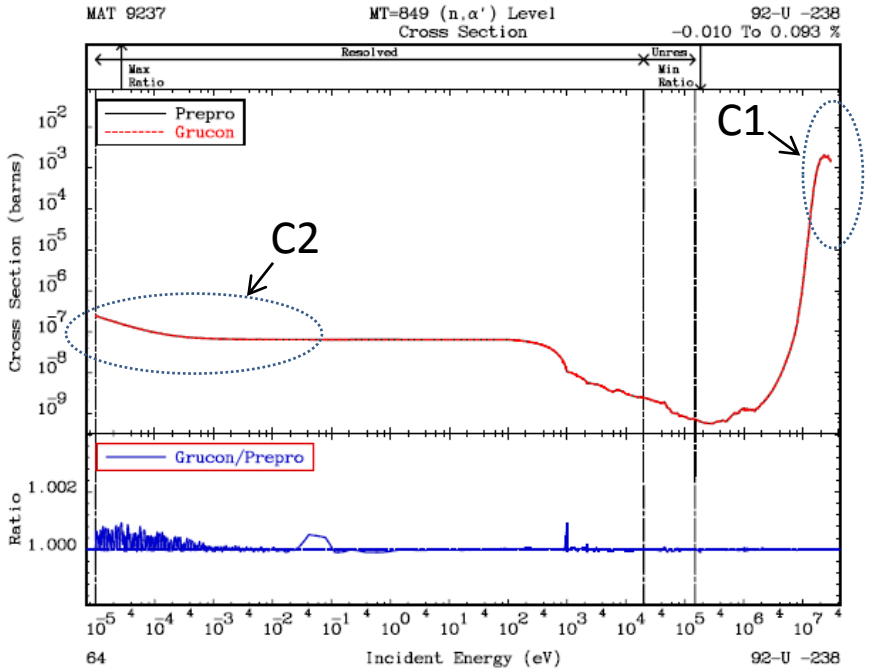
<u>Correction 2</u>. Doppler broadening is applied to all cross sections (in previous calculation procedure it was performed for cross sections reconstructed from resonance parameters only)

(A) MT = 849 (n,α_{contin}) reaction

Grucon vs. Reference (e80b4)

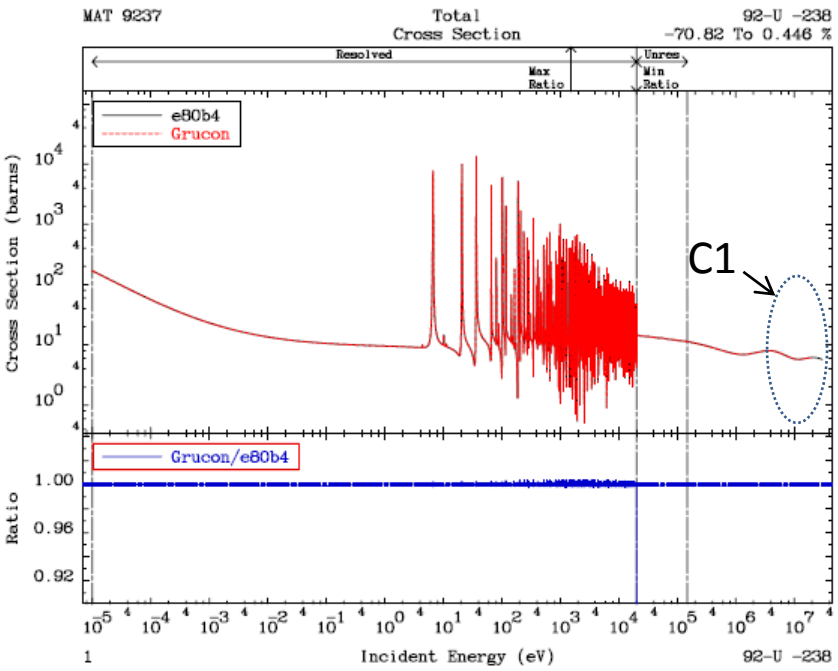


Grucon corrected vs. Prepro

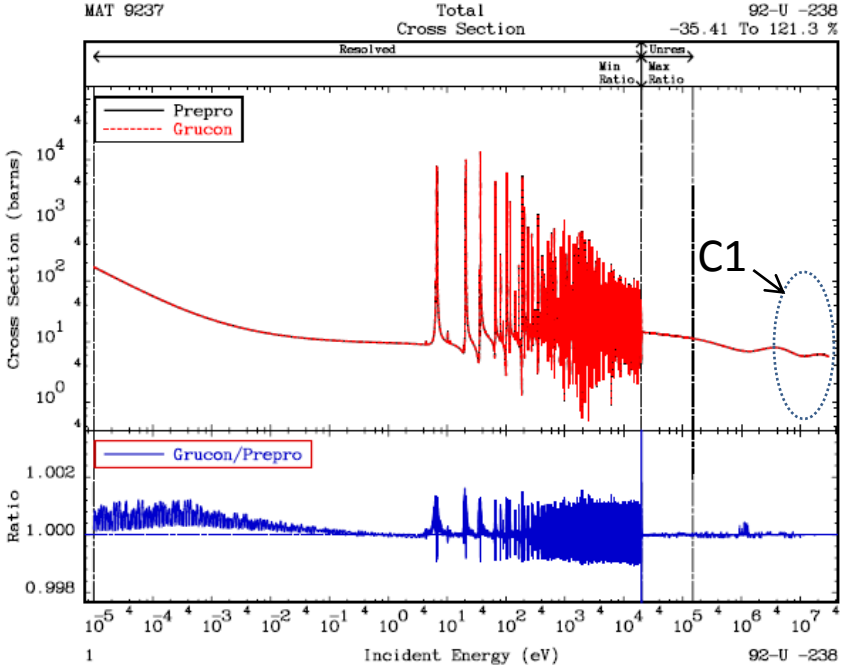


(A) MT=1 Total cross section

Grucon vs. Reference (e80b4)

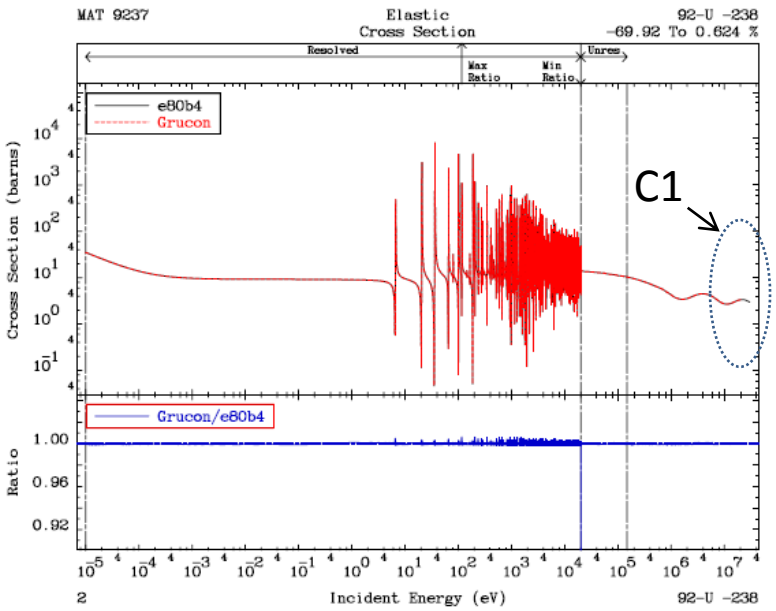


Grucon corrected vs. Prepro

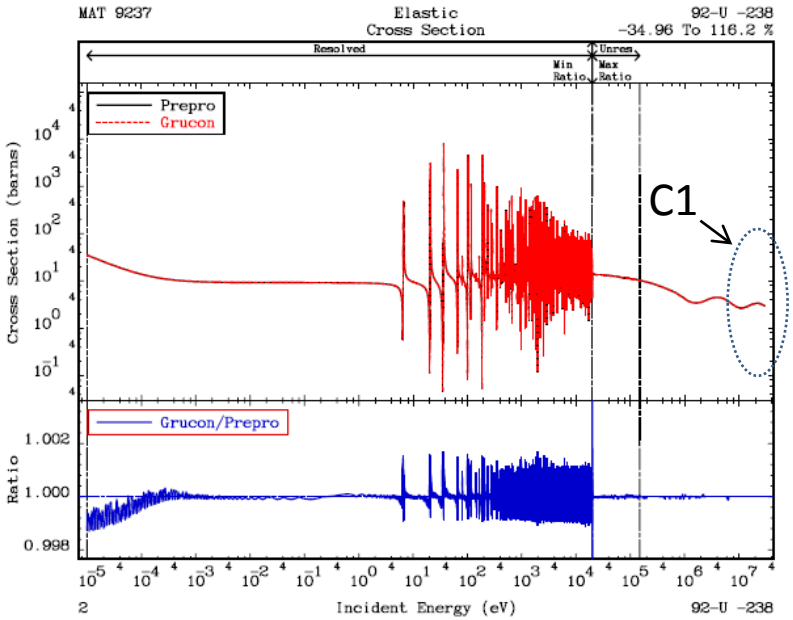


(A) MT=2 Elastic scattering

Grucon vs. Reference (e80b4)

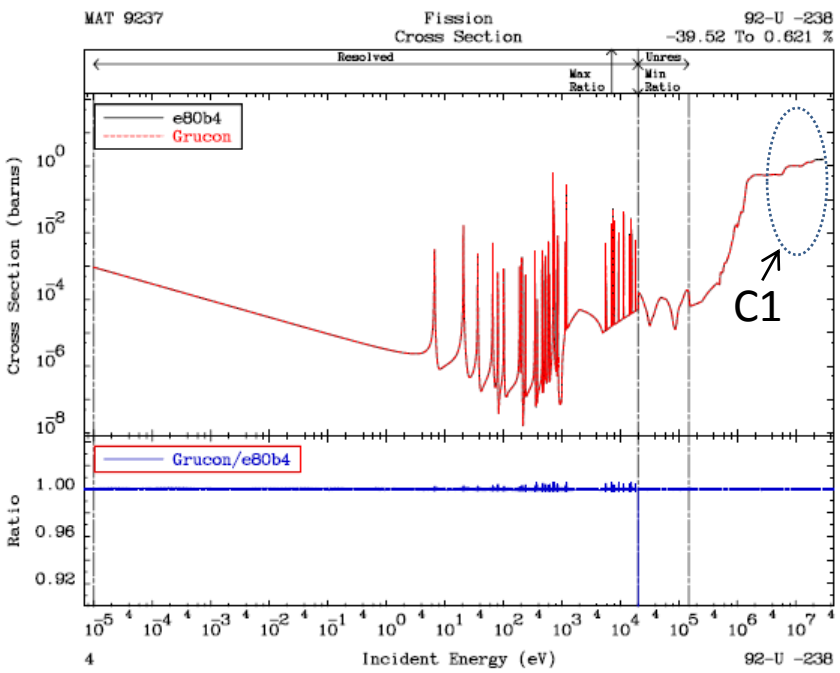


Grucon corrected vs. Prepro

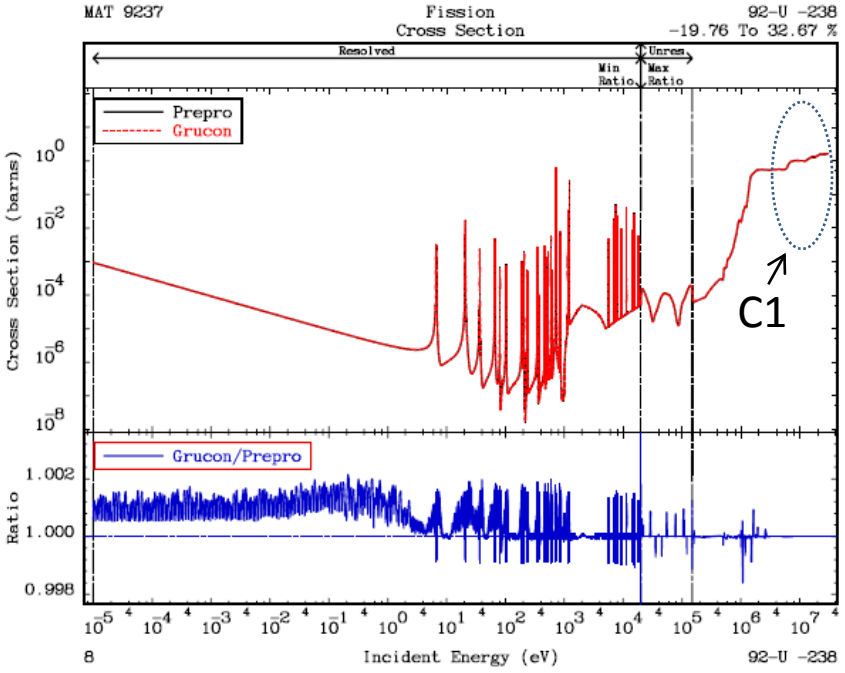


(A) MT=18 Fission

Grucon vs. Reference (e80b4)

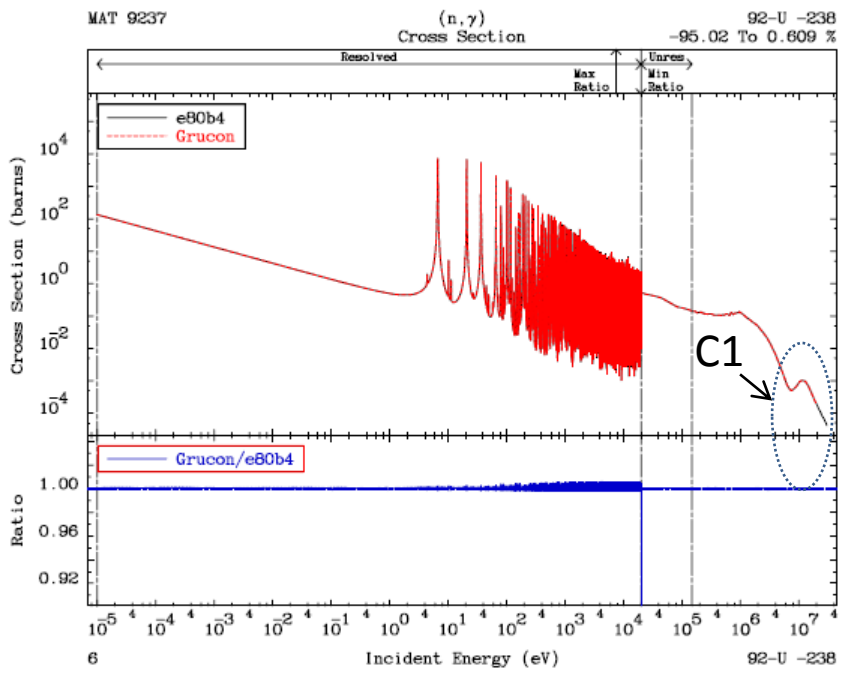


Grucon corrected vs. Prepro

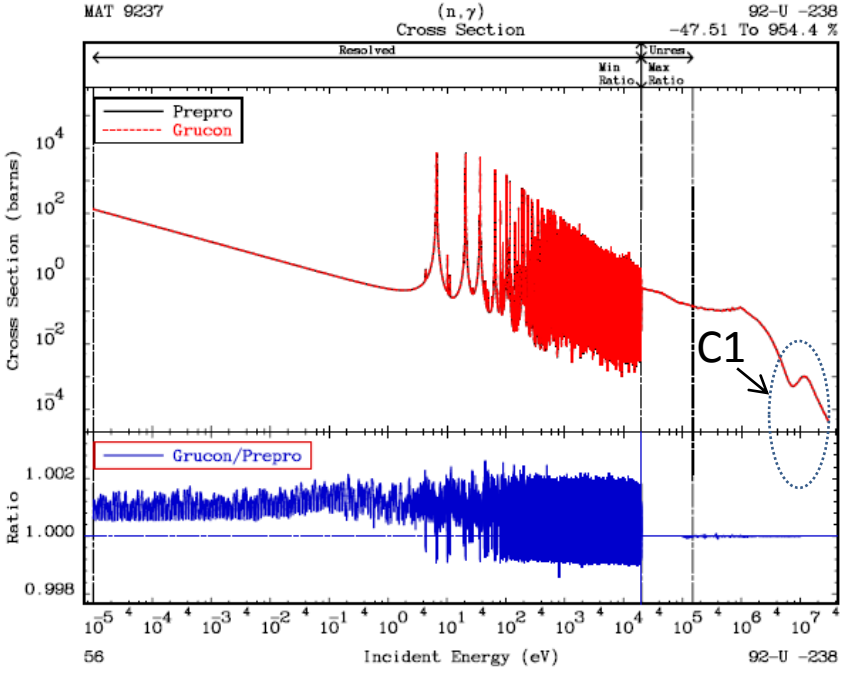


(A) MT=102 Radiative capture

Grucon vs. Reference (e80b4)

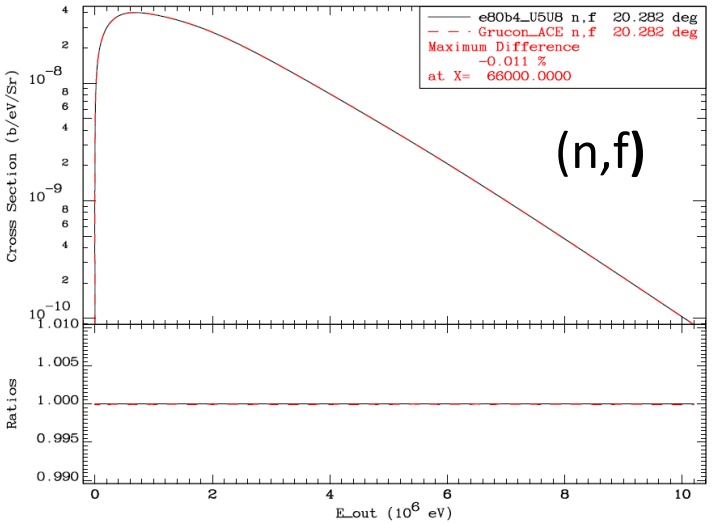


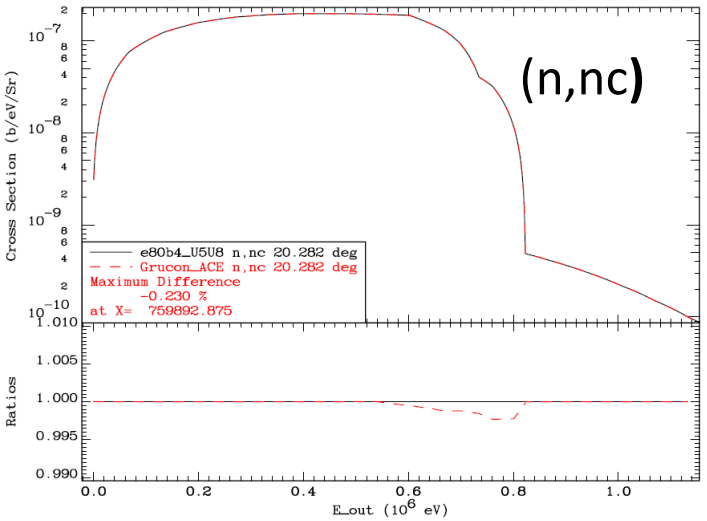
Grucon corrected vs. Prepro

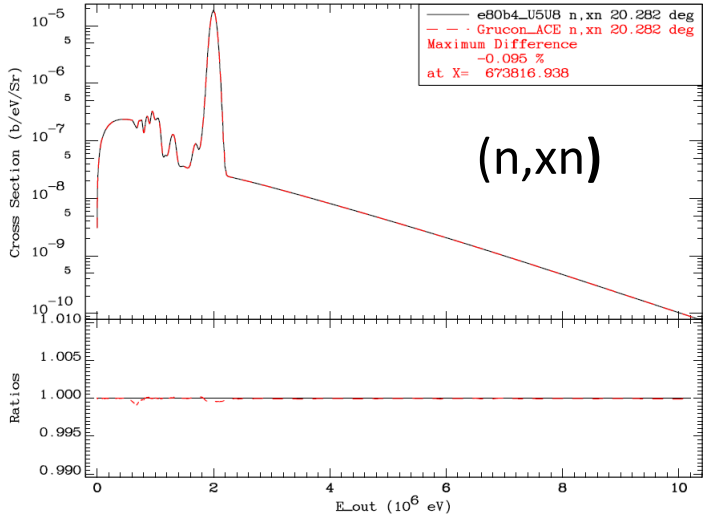


(B) Double-differential cross sections

ENDF/B-VIII-beta4 92-U-238 E_in=2 MeV θ=20.282 deg

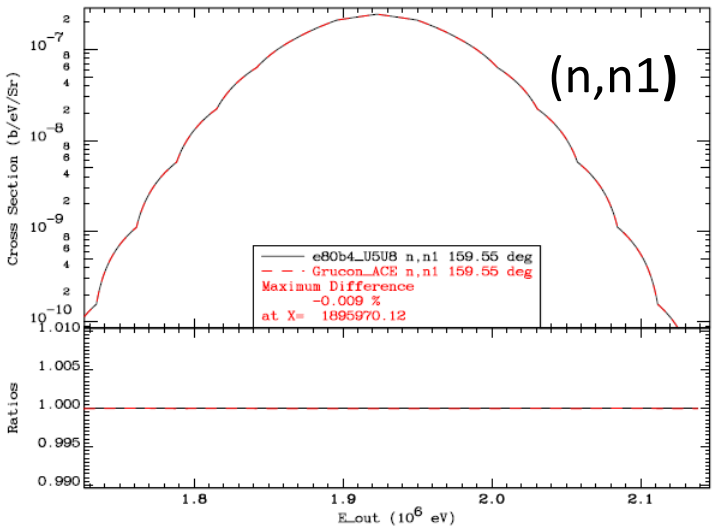


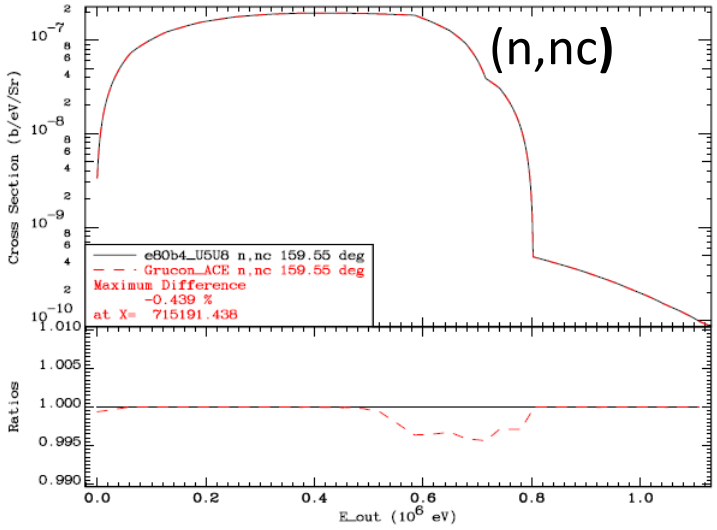


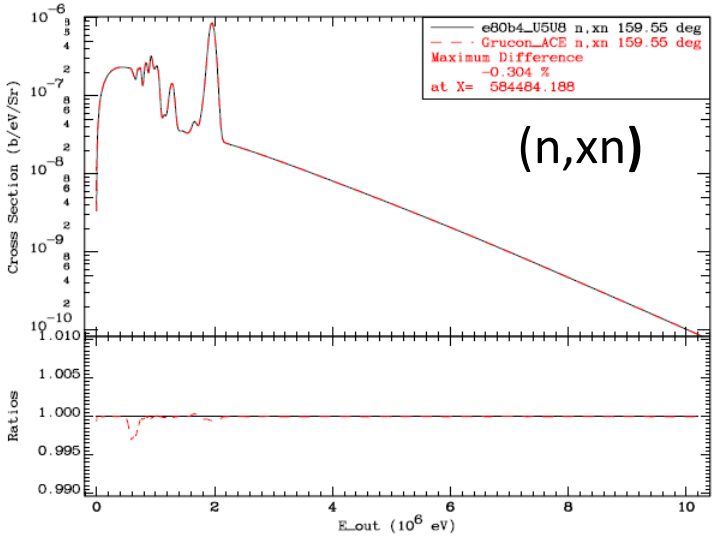


(B) Double-differential cross sections

ENDF/B-VIII-beta4 92-U-238 E_in=2 MeV θ=159.55 deg







(C) AVP Stage 1. Integral testing. List of benchmarks

Criticality Benchmarks

	ICSBEP Label	Short name	Common name	Comment
1	HEU-MET-FAST-001	hmf001	Godiva	
2	HEU-MET-FAST-002	hmf002-002	Topsy-002	
3	HEU-MET-FAST-003	hmf003-001	Topsy-U_2.0in	Uranium reflector
4	HEU-MET-FAST-003	hmf003-002	Topsy-U_3.0in	Uranium reflector (*)
5	HEU-MET-FAST-003	hmf003-003	Topsy-U_4.0in	Uranium reflector
6	HEU-MET-FAST-003	hmf003-010	Topsy-W_4.5in	Tungsten reflector (*)
7	HEU-MET-FAST-003	hmf003-011	Topsy-W_6.5in	Tungsten reflector (*)
8	HEU-MET-FAST-014	hmf014	VNIIEF-CTF-DU	
9	HEU-MET-FAST-032	hmf032-001	COMET-TU1_3.93in	
10	HEU-MET-FAST-032	hmf032-002	COMET-TU1_3.52in	(*)
11	HEU-MET-FAST-032	hmf032-003	COMET-TU1_1.742in	(*)
12	HEU-MET-FAST-032	hmf032-004	COMET-TU1-0.683in	
13	IEU-COMP-FAST-004	icf004	ZPR-3/12	
14	IEU-MET-FAST-007	imf007s	Big_Ten (simplified)	
15	IEU-MET-FAST-007	imf007d	Big _Ten (detailed)	Big_Ten (*)
16	IEU-MET-FAST-010	imf010	ZPR-6/9(U9)	
17	IEU-MET-FAST-012	imf012	ZPR-3/41	
18	IEU-MET-FAST-013	imf013	ZPR-9/1	Reference for tungsten reflector
19	IEU-MET-FAST-014	imf014-002	ZPR-9/2	Tungsten reflector (*)
20	IEU-MET-FAST-022	imf022-001	FR0_3X-S	
21	IEU-MET-FAST-022	imf022-002	FR0_5-S	
22	IEU-MET-FAST-022	imf022-003	FR0_6A-S	
23	IEU-MET-FAST-022	imf022-004	FR0_7-S	
24	IEU-MET-FAST-022	imf022-005	FR0_8-S	
25	IEU-MET-FAST-022	imf022-006	FR0_9-S	
26	IEU-MET-FAST-022	imf022-007	FR0_10-S	
27	MIX-MISC-FAST-001	mif001-001	BFS-35-1	
28	MIX-MISC-FAST-001	mif001-002	BFS-35-2	
29	MIX-MISC-FAST-001	mif001-003	BFS-35-3	
30	MIX-MISC-FAST-001	mif001-009	BFS-31-4	
31	MIX-MISC-FAST-001	mif001-010	BFS-31-5	
32	MIX-MISC-FAST-001	mif001-011	BFS-42	

(C) ACE library content

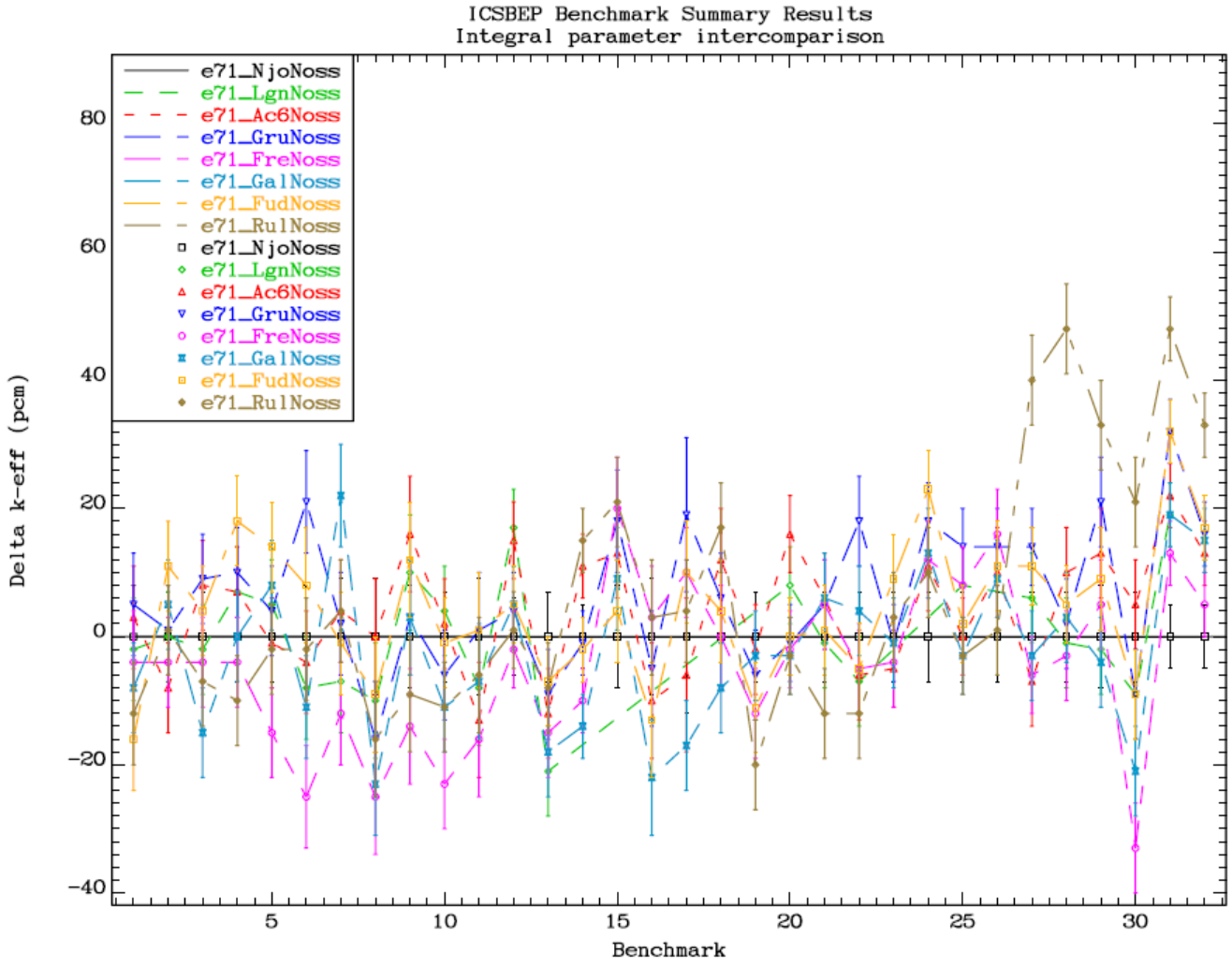
Isotopes

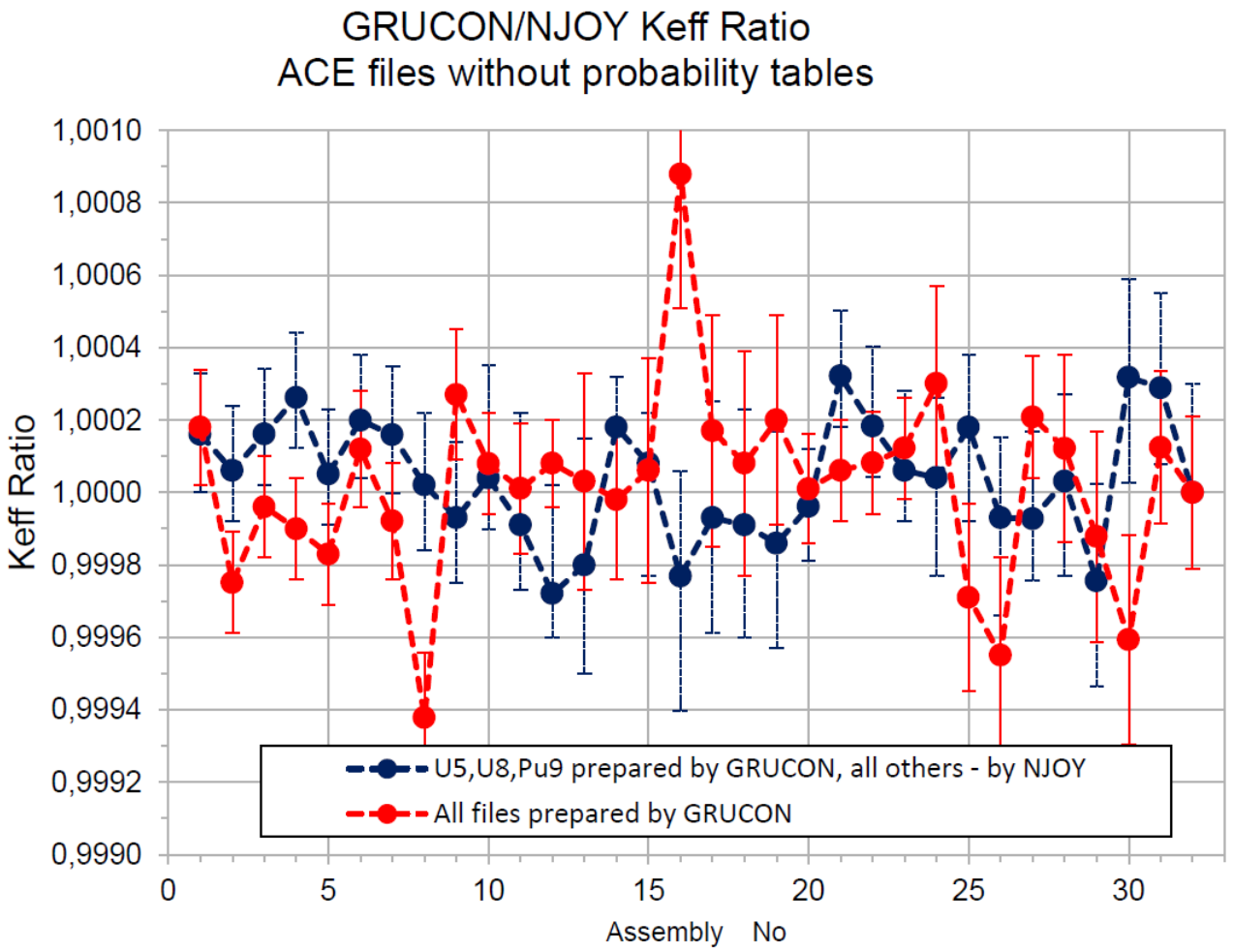
001H_001	001H_002					
003Li006						
005B_010						
006C_000	006C_012	006C_013				
007N_014						
008O_016						
009F_019						
012Mg024	012Mg025	012Mg026				
013Al027						
014Si028	014Si029	014Si030				
015P_031						
017Cl035	017Cl037					
021Sc045						
022Ti046	022Ti047	022Ti048	022Ti049	022Ti050		
024Cr050	024Cr052	024Cr053	024Cr054			
025Mn055						
026Fe054	026Fe056	026Fe057	026Fe058			
027Co059						
028Ni058	028Ni060	028Ni061	028Ni062	028Ni064		
029Cu063	029Cu065					
031Ga069	031Ga071					
041Nb093						
042Mo092	042Mo094	042Mo095	042Mo096	042Mo097	042Mo098	042Mo100
047Ag107	047Ag109					
049In115						
074W_180	074W_182	074W_183	074W_184	074W_184		
079Au197						
092U_233	092U_234	092U_235	092U_236	092U_238		
093Np237						
094Pu239	094Pu240	094Pu241				
095Am241						

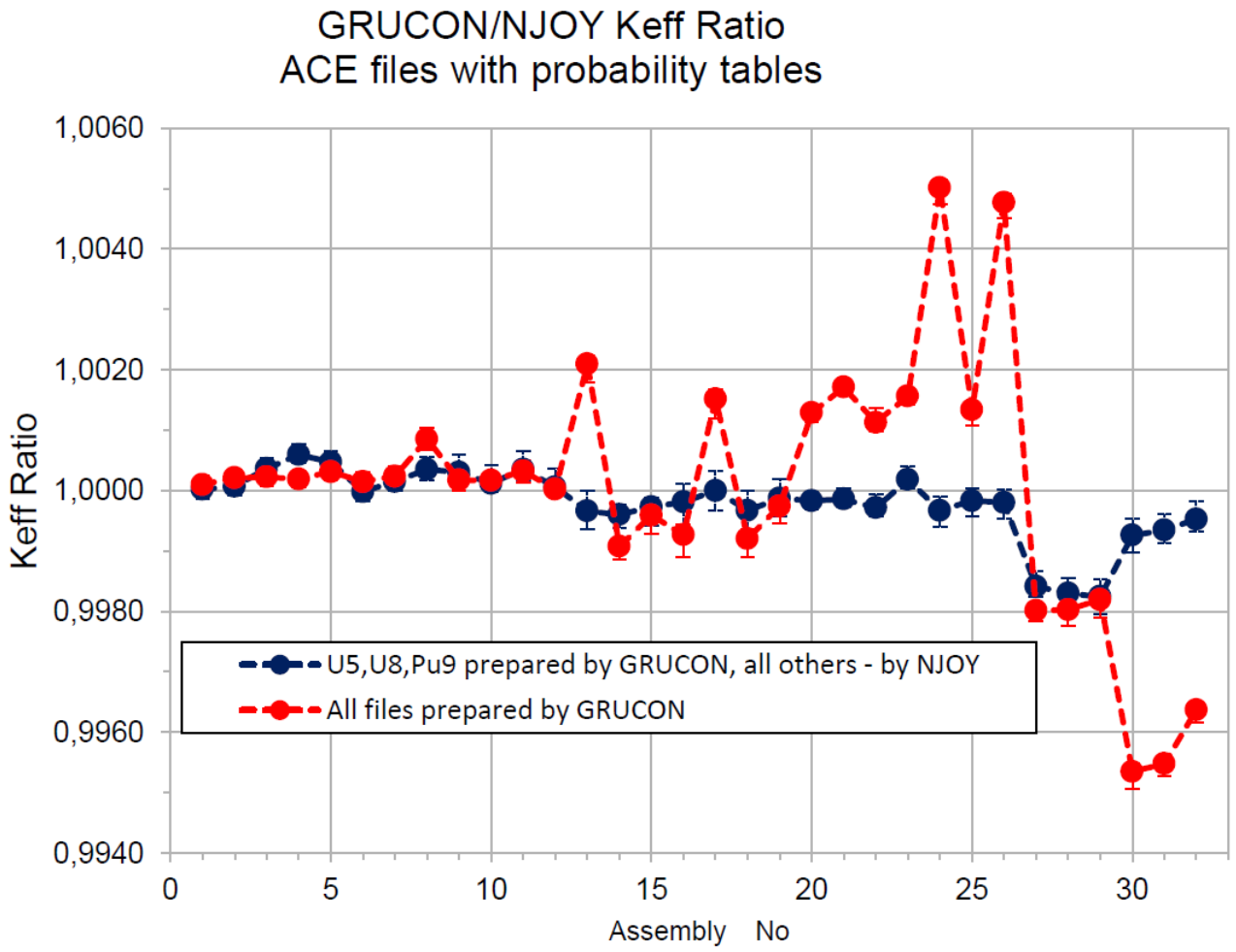
Bound Nuclides

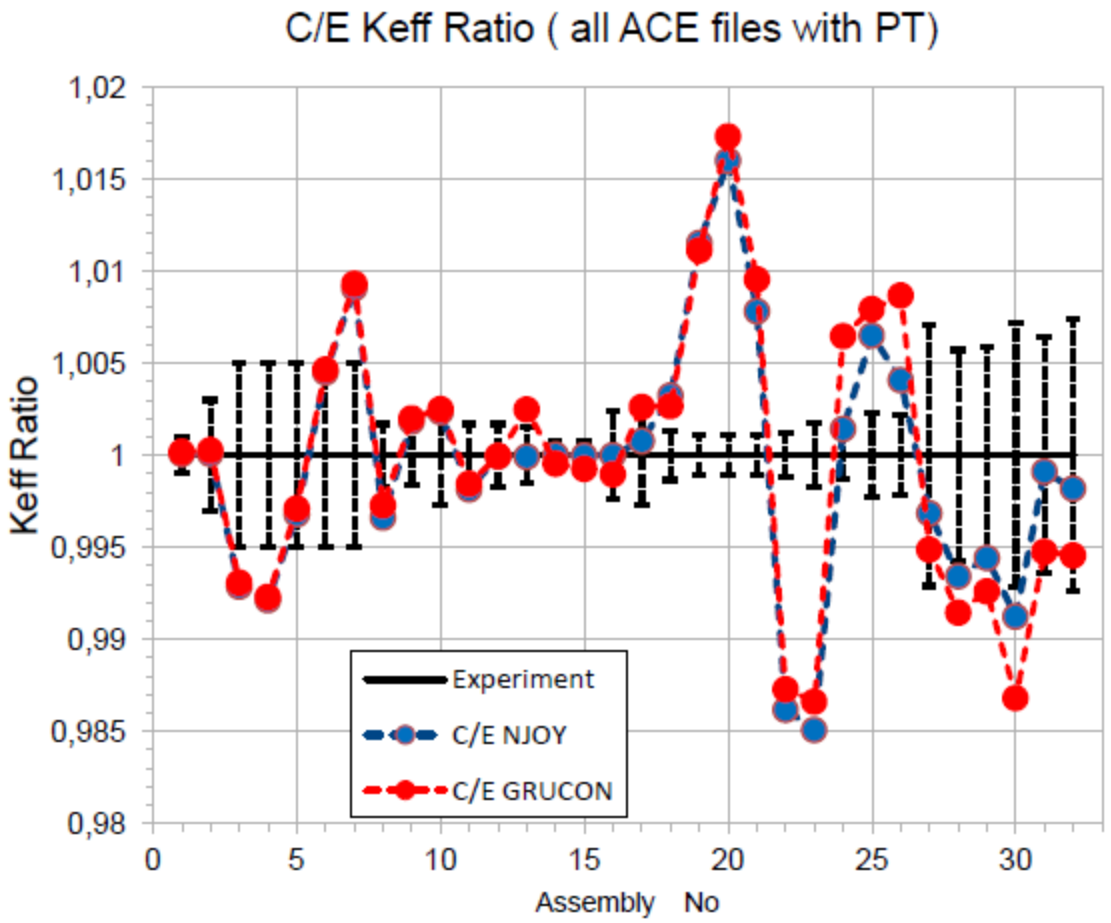
H_CH2

AVP Stage 1. ACE files without PT (NoSS)
Keff GRUCON/Reference inter-comparison




GRUCON/NJOY Keff Ratio
ACE files without probability tables
Keff Ratio
1,0010
1,0008
1,0006
1,0004
1,0002
1,0000
0,9998
0,9996
0,9994
0,9992
0,9990
0
5
10
15
20
25
30
Assembly No
U5,U8,Pu9 prepared by GRUCON, all others - by NJOY
All files prepared by GRUCON


GRUCON/NJOY Keff Ratio
ACE files with probability tables
Keff Ratio
1,0060
1,0040
1,0020
1,0000
0,9980
0,9960
0,9940
0
5
10
15
20
25
30
Assembly No
U5,U8,Pu9 prepared by GRUCON, all others - by NJOY
All files prepared by GRUCON


C/E Keff Ratio (all ACE files with PT)
Keff Ratio
1,02
1,015
1,01
1,005
1
0,995
0,99
0,985
0,98
0
5
10
15
20
25
30
Assembly No
Experiment
C/E NJOY
C/E GRUCON

2. Processing of Photon and Particle Production Data in the GRUCON Package. Inter-comparison of Production Cross Sections

(A) GRUCON/PROD and GRUCON/ACE modules
(B) Gas Production Cross Sections
(C) Photon Production Cross Sections

2. Processing of Photon and Particle Production Data in the GRUCON Package. Inter-comparison of Production Cross Sections

(A) GRUCON/PROD and GRUCON/ACE modules
(B) Gas Production Cross Sections
(C) Photon Production Cross Sections

(A) The PROD and ACE Modules of GRUCON package

The **GRUCON/PROD** module is designed to prepare production cross sections **MT=202-207** from **MF=2,3** and **MF=6, 12, 13** data files, taking into account the **LR** flags from **MF=3** file, describing breakup reactions. These cross sections can be used by the **GRUCON/ACE** module for preparing **ACE** tables:

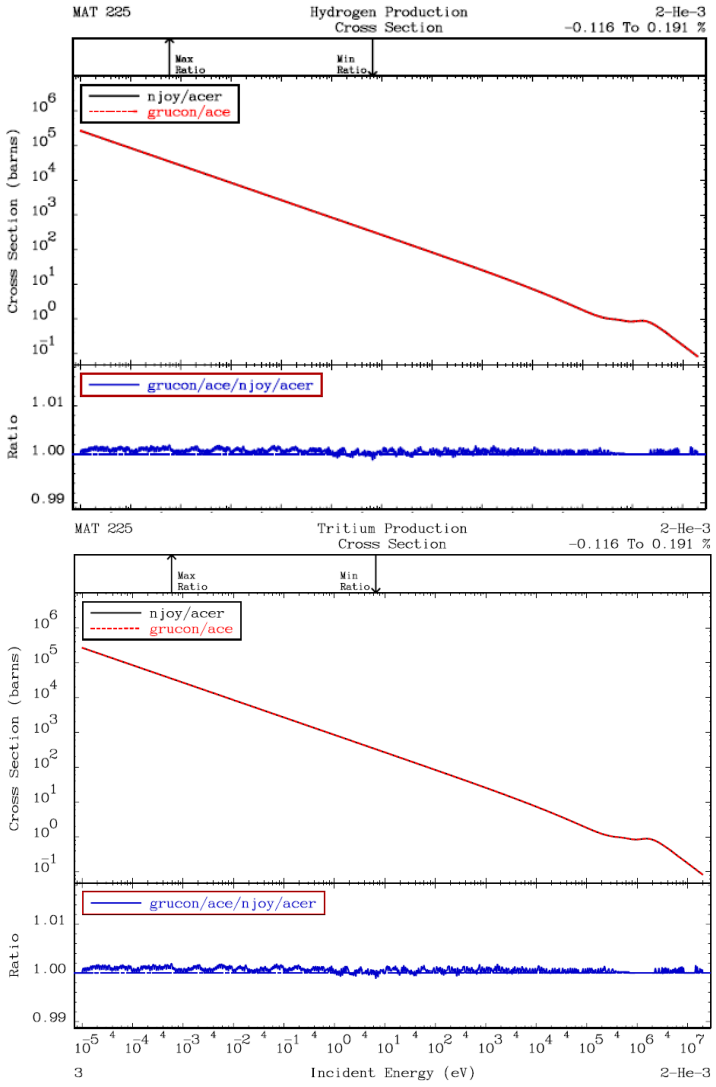
7.SIG - gas production cross-sections with MT=203 – 207
12.GPD - total photon production cross section MT=202

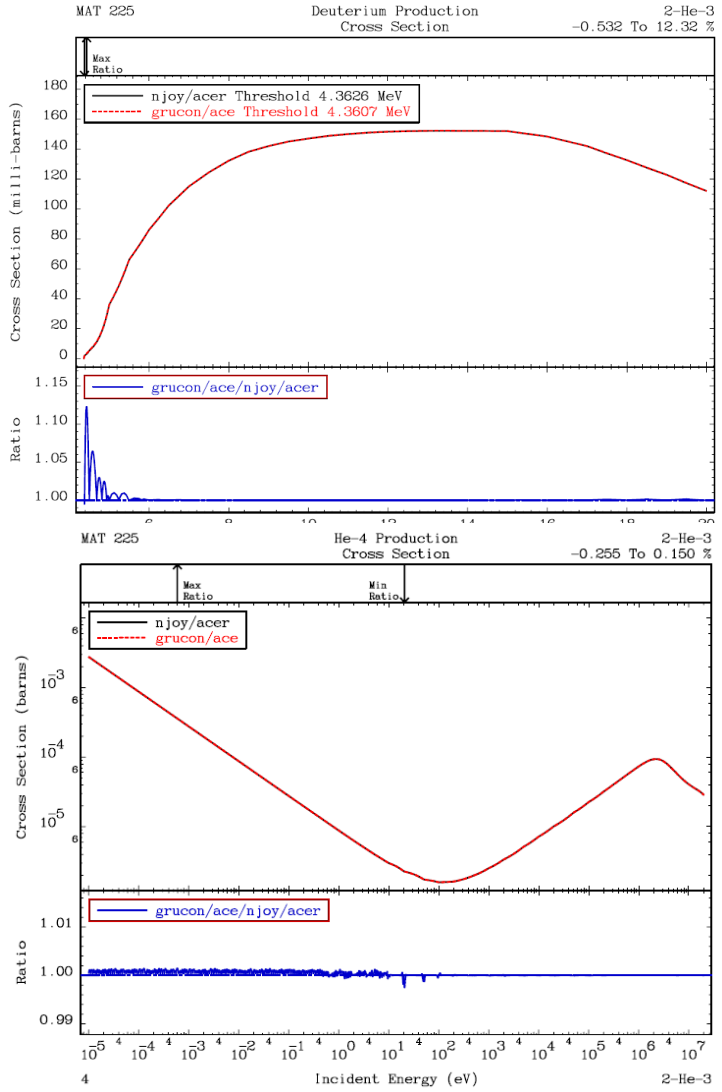
The **GRUCON/ACE** module is extended to supply complete set of **ACE** tables with photon production date, namely:

13.MTRP - partial photon-production reaction types MT
14.LSIGP - partial photon-production cross section locators
15.SIGP - partial photon production cross sections
16.LANDP - photon-production angular distribution locators
17.ANDP - photon-production angular distributions
18.LDLWP - photon-production energy distribution locators
19.DLWP - photon-production energy distributions
20.YP - neutron MT needed as photon-production yield multipliers

(B) He-3: Gas Production Cross Sections. GRUCON/ACE & NJOY/ACER comparison

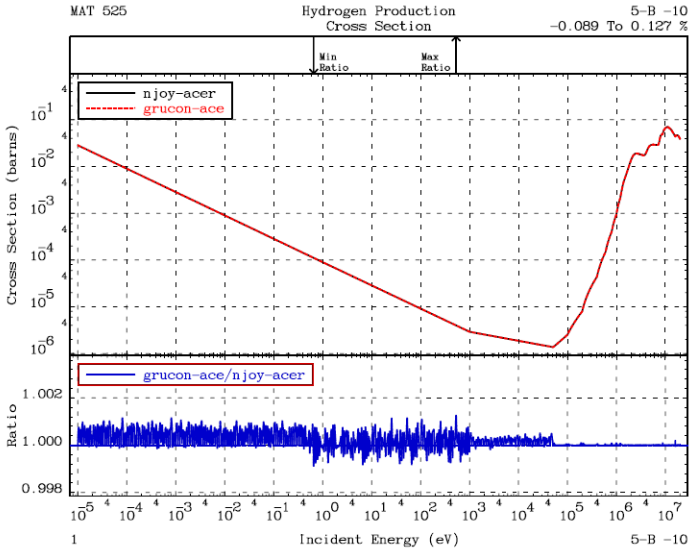
(residual nuclides are taken into account)

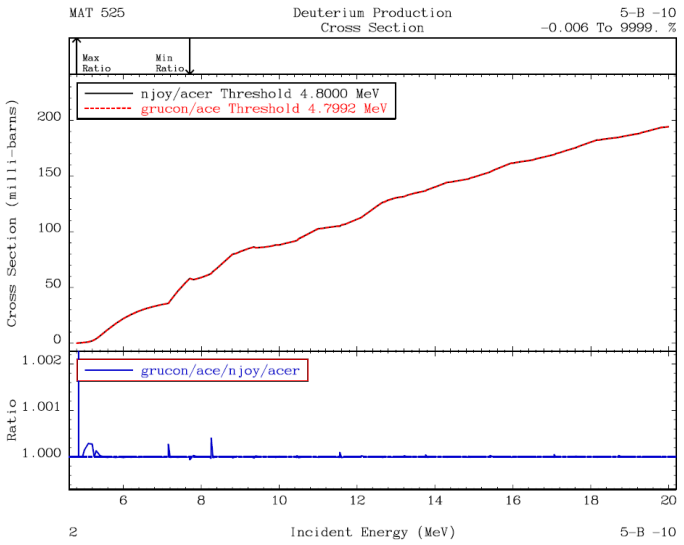


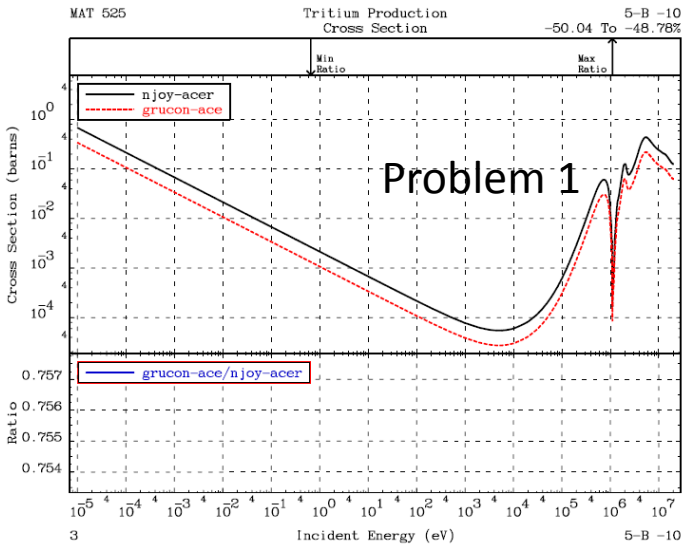


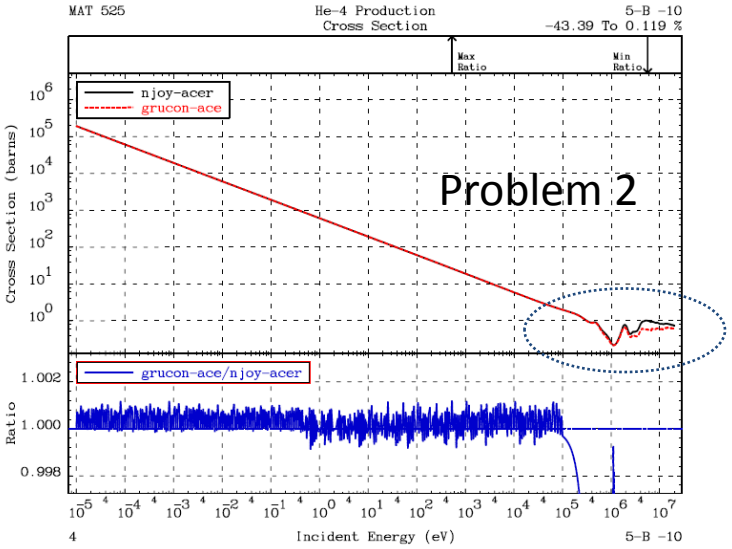
(B) B-10: Gas Production Cross Sections. GRUCON/ACE & NJOY/ACER comparison

(break-up reactions are taken into account)

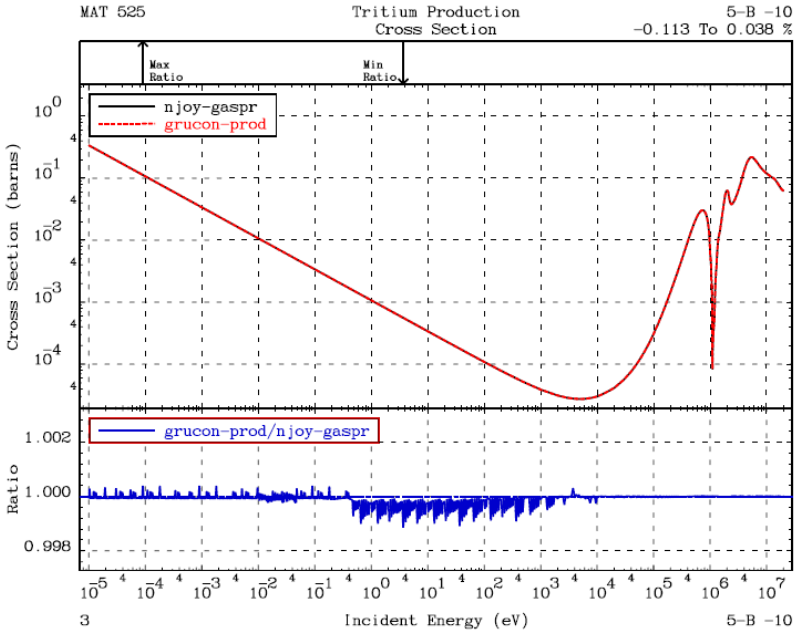


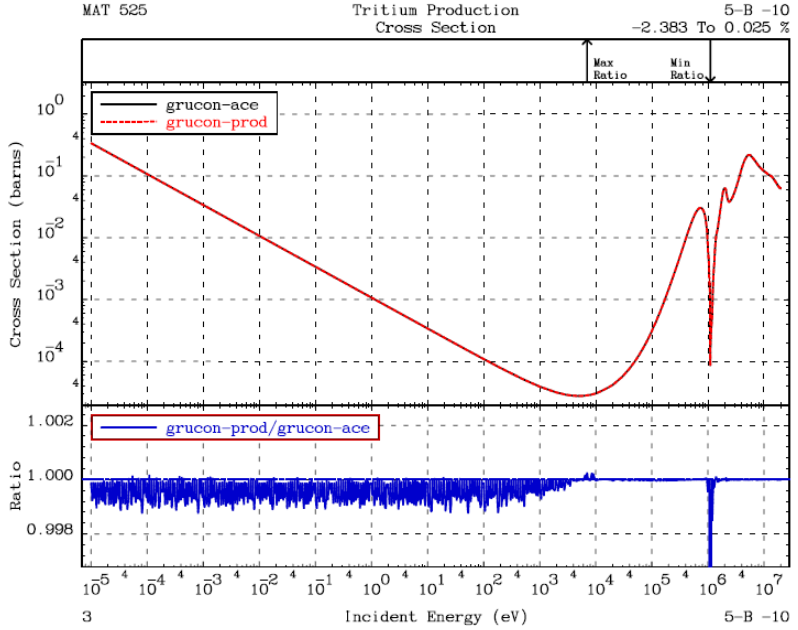


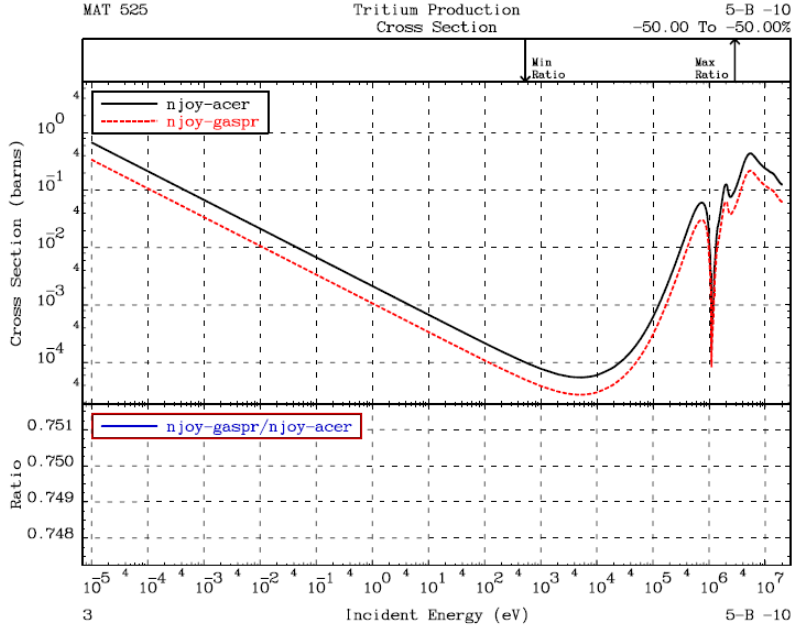




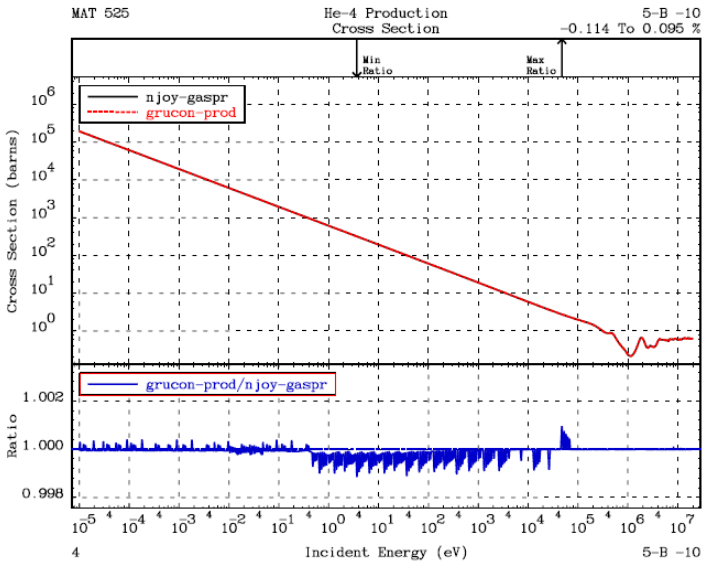
B-10: Problem 1. Tritium production.

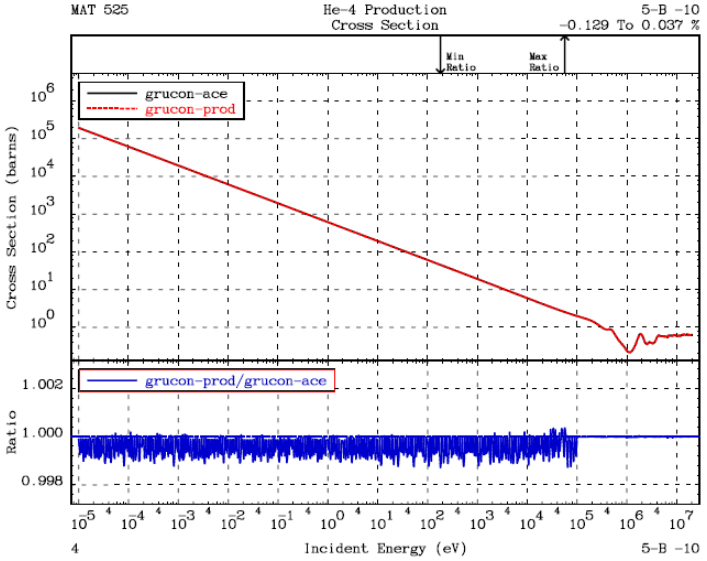


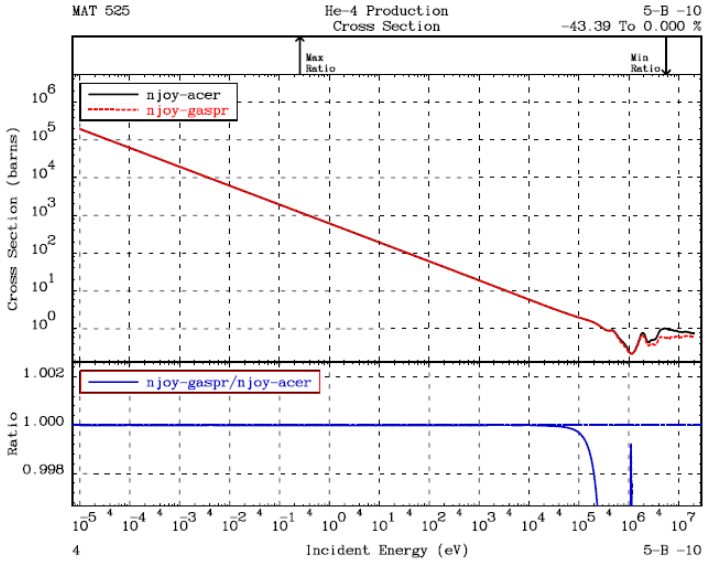




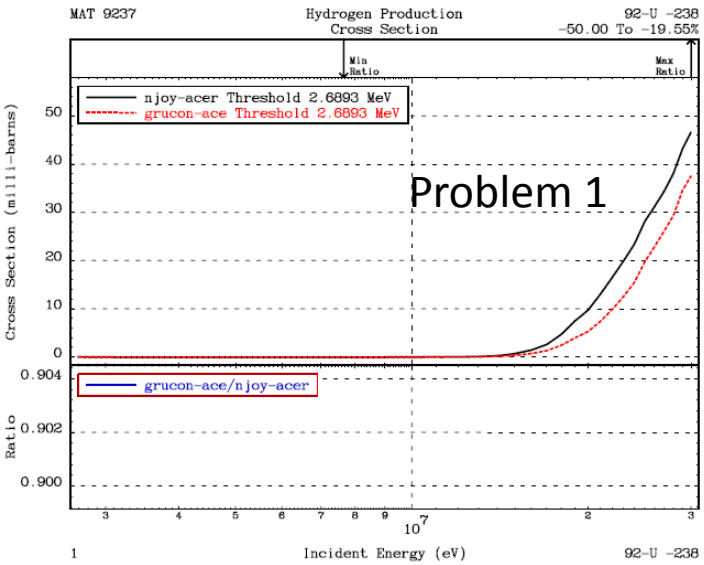
B-10: Problem 2. He-4 production.

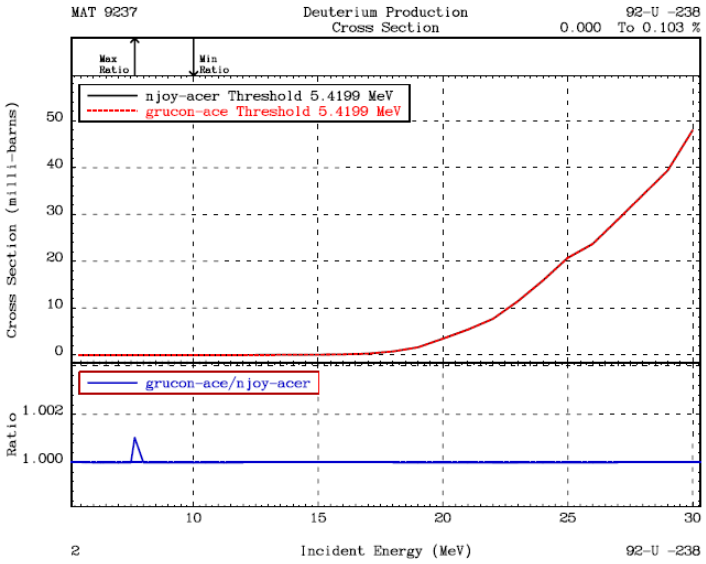


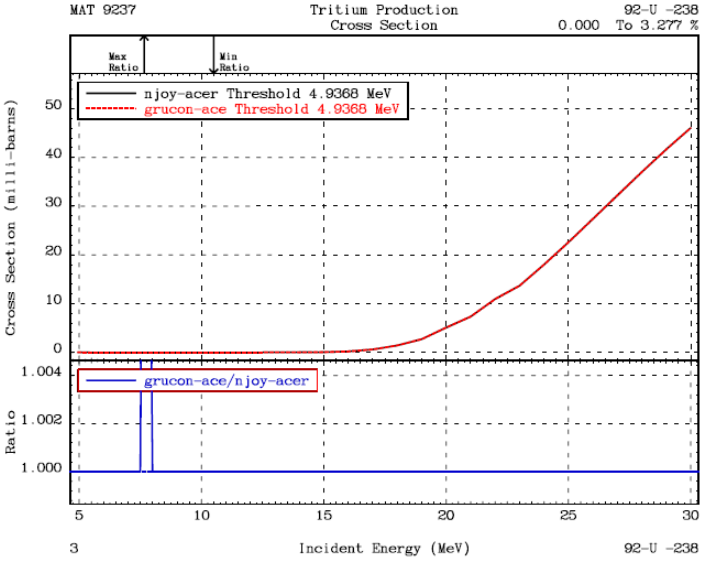


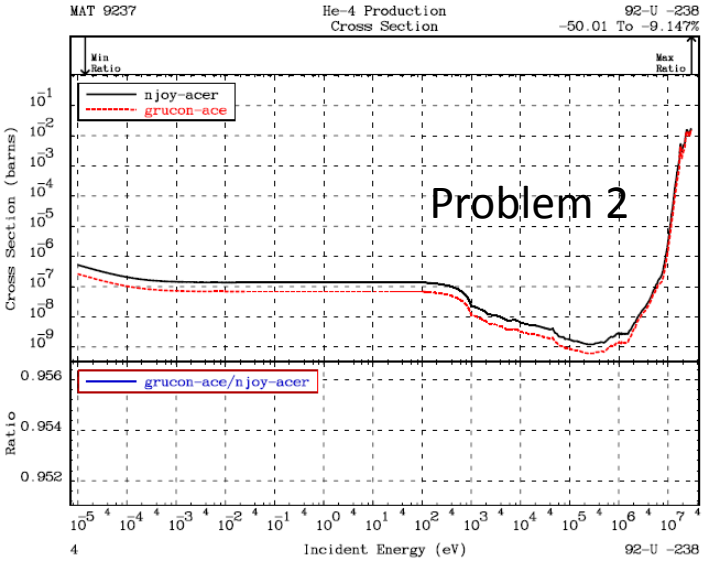


(B) U-238: Gas Production Cross Sections. GRUCON/ACE & NJOY/ACER comparison

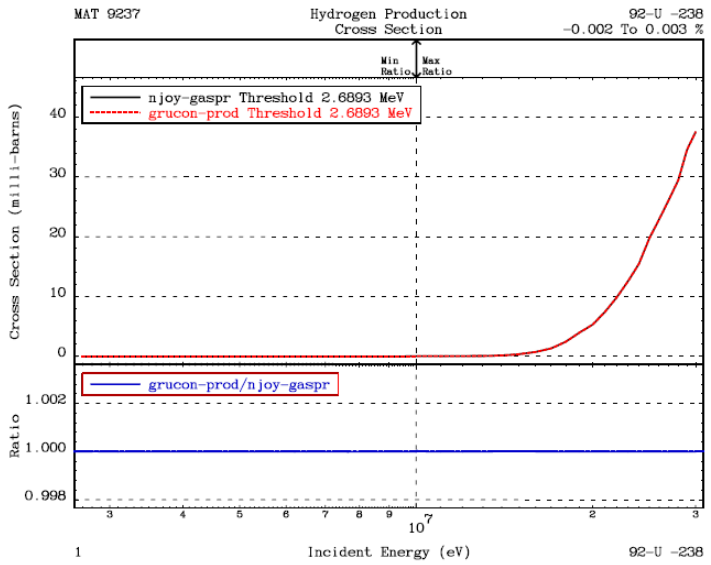


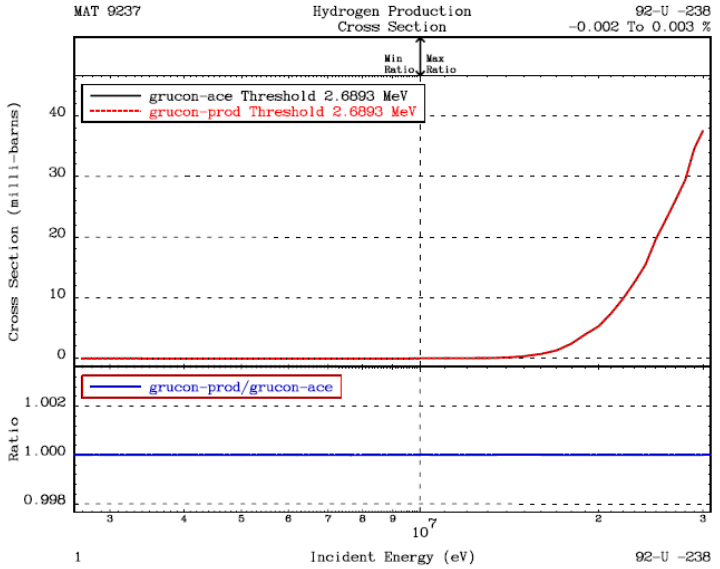


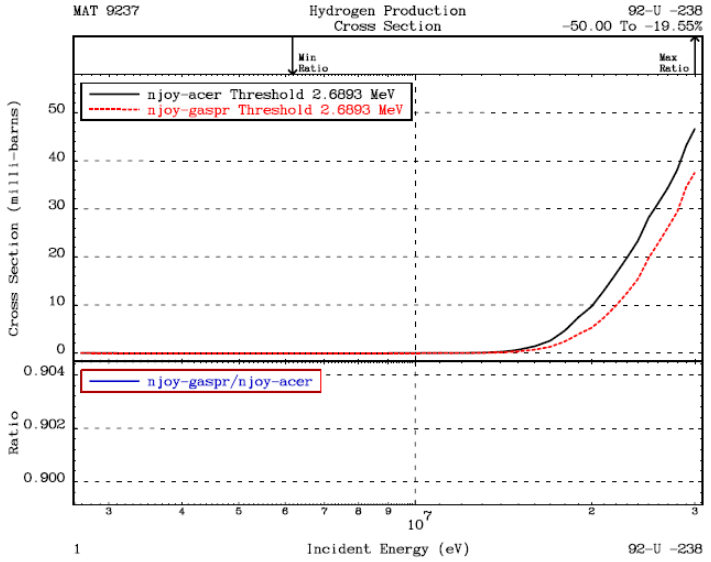




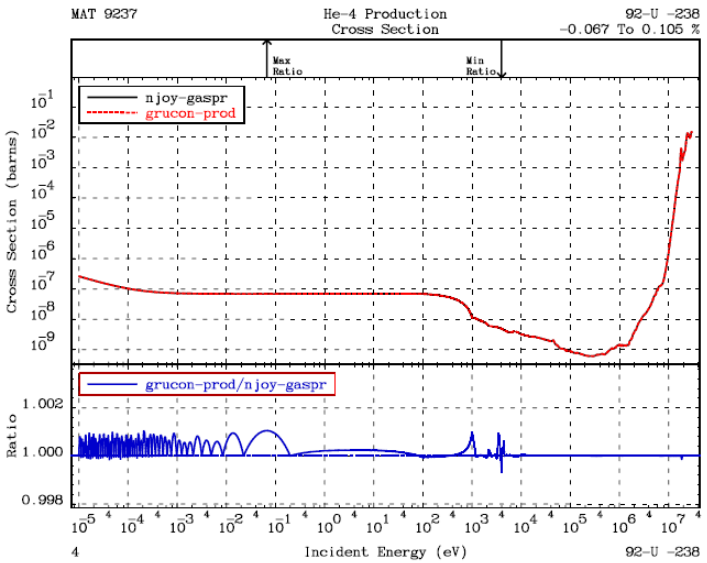
U-238: Problem 1. Hydrogen production.

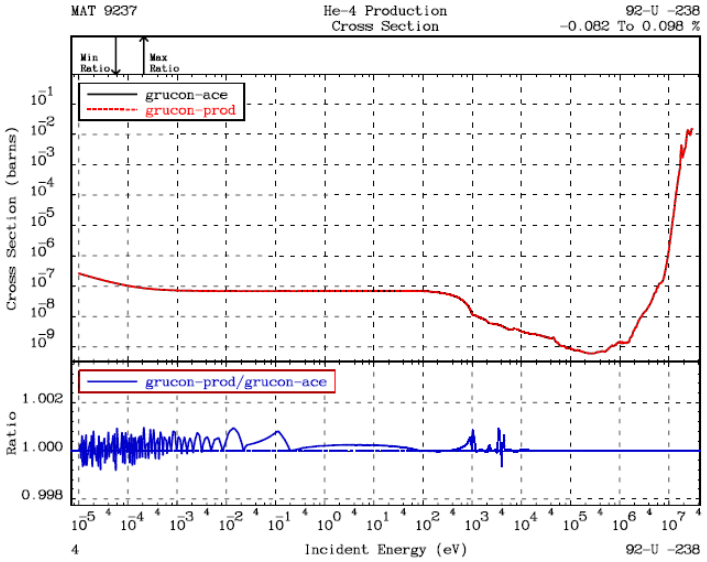


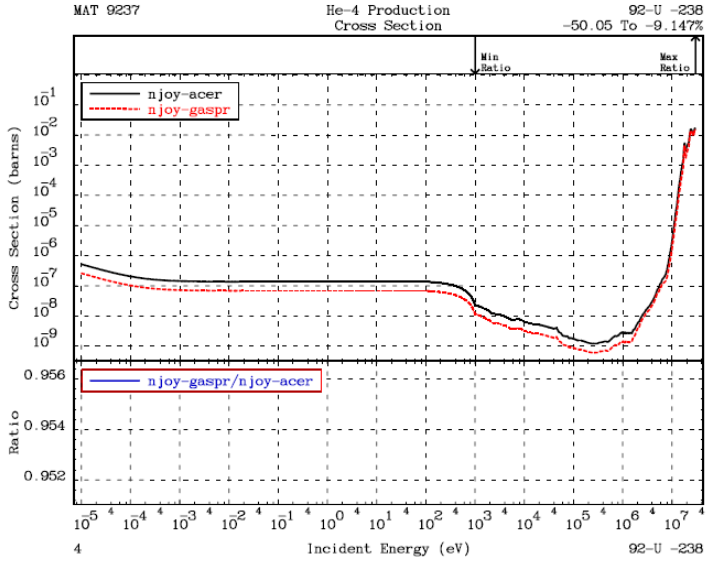




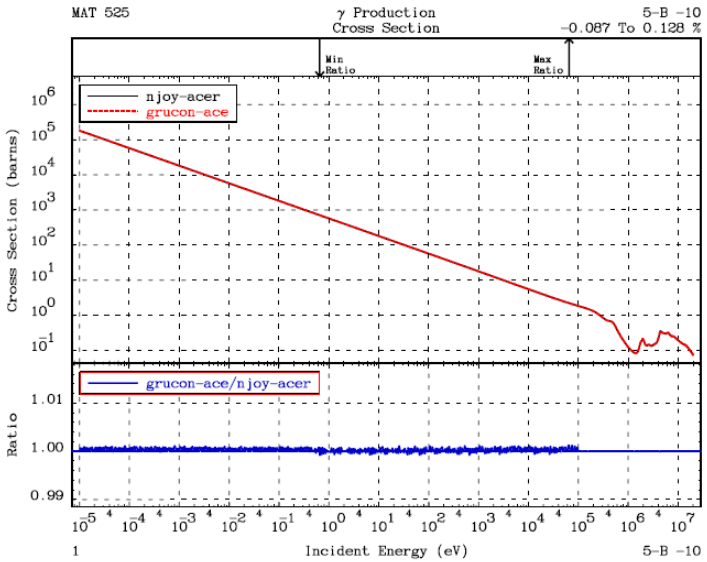
U-238: Problem 2. He-4 production.

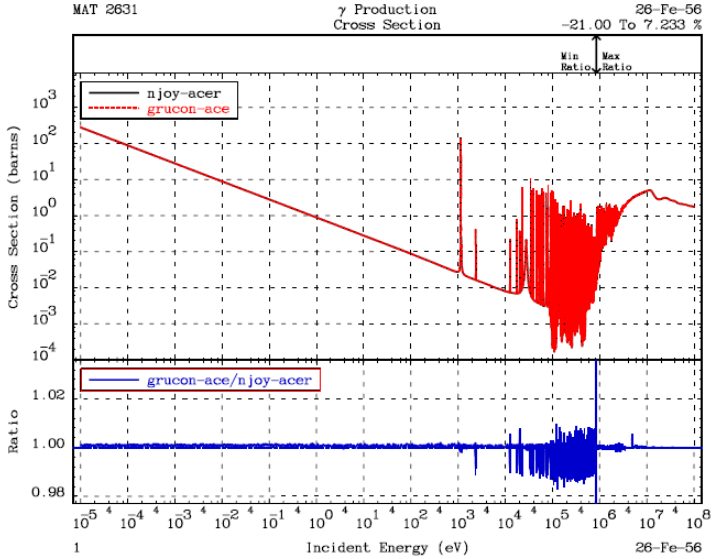


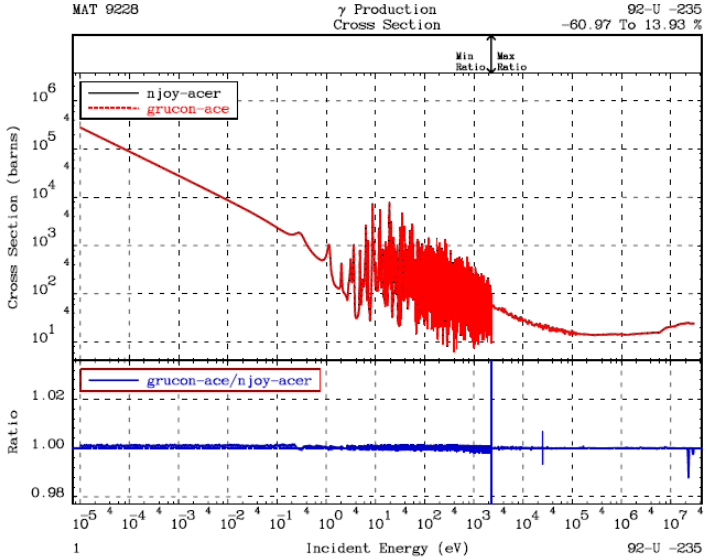


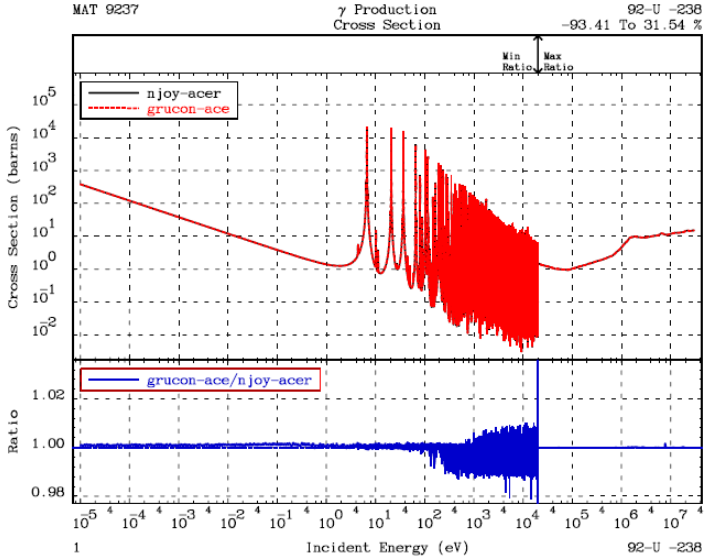


(C) Photon Production Cross Sections









3. New functionality of the GRUCON package

(A) Revision of GRUCON Standard Data Structures to include ENDF-6 for ENDF/B-VIII Format Extensions

(B) Doppler smoothing of Legendre Polynomial Coefficients reconstructed from Resolved Resonance Parameters

(A) Revision of GRUCON Standard Data Structures

The ENDF-6 format extensions for the ENDF/B-VIII evaluated data library 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)

Corresponding updates has been performed in the modules of GRUCON:

- ENDF (input and output options)
- TABLE (output data in form of annotated tables)
- ACE (output data in the ACE format) and

Question: how to include these new data representations in the ACE file?

(B) Doppler smoothing of Legendre Polynomial Coefficients reconstructed from Resolved Resonance Parameters

Computing procedure for Doppler smoothing of angular parameters obtained by Blatt-Biedenharn formulae at zero temperature, based on the GRUCON/SXTXS module for Doppler broadening of cross-sections, is implemented. It was required to extend the functionality of existing AXXS module and to add two new modules: SXXA and AXEXA.

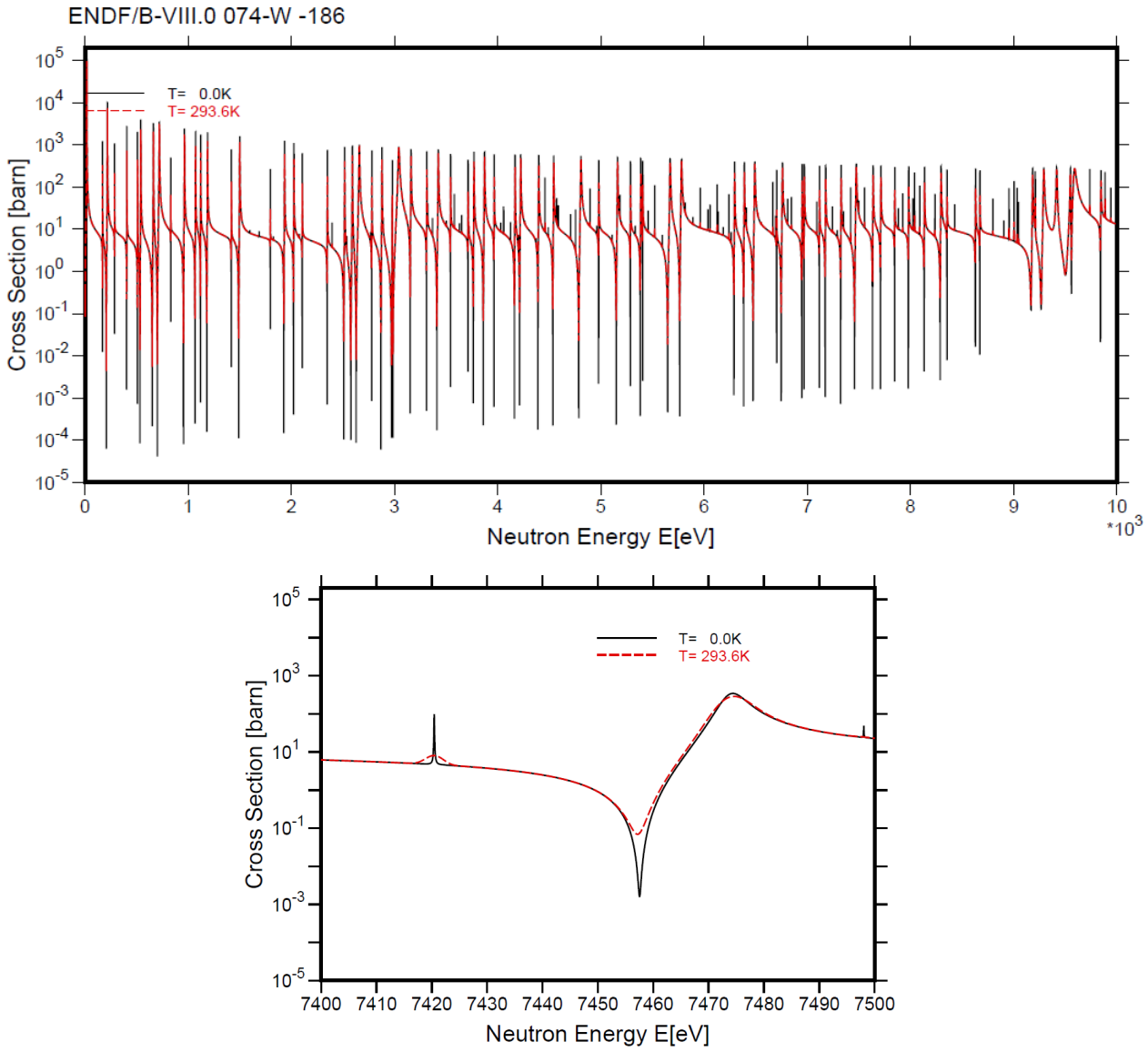
AXXS module multiplies elastic cross sections, obtained from the same resonance parameters at zero temperature, by factor α_l and converts obtained scattering cross section moments to the *S* representation;

SXTXS performs Doppler broadening of cross section angular moments;

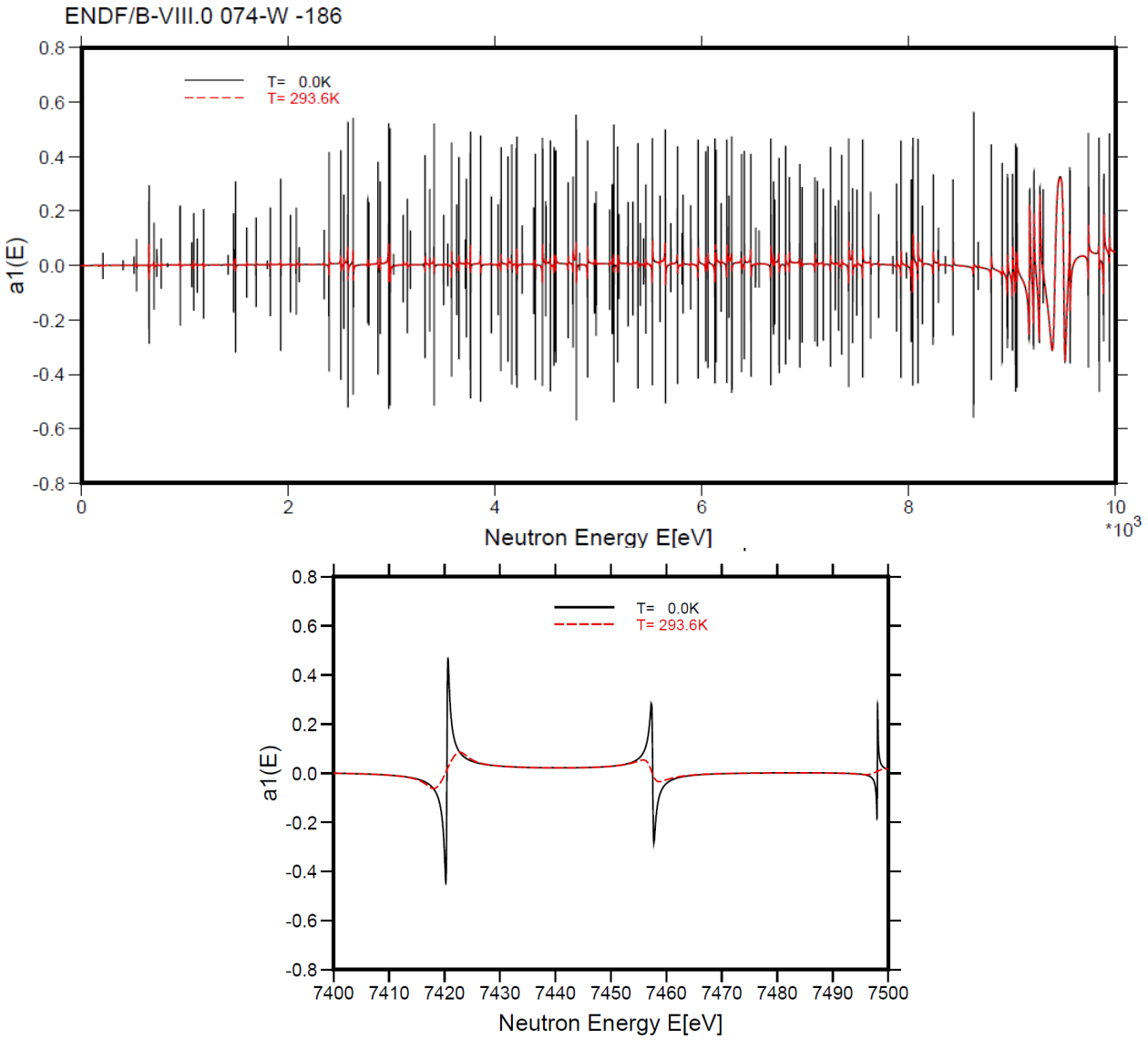
SXXA reconstructs the Legendre polynomial coefficients, dividing smoothed cross section angular moments by corresponding Doppler broadened cross section, and

AXEXA thins energy grid by removing excessive points with given interpolation tolerance parameter.

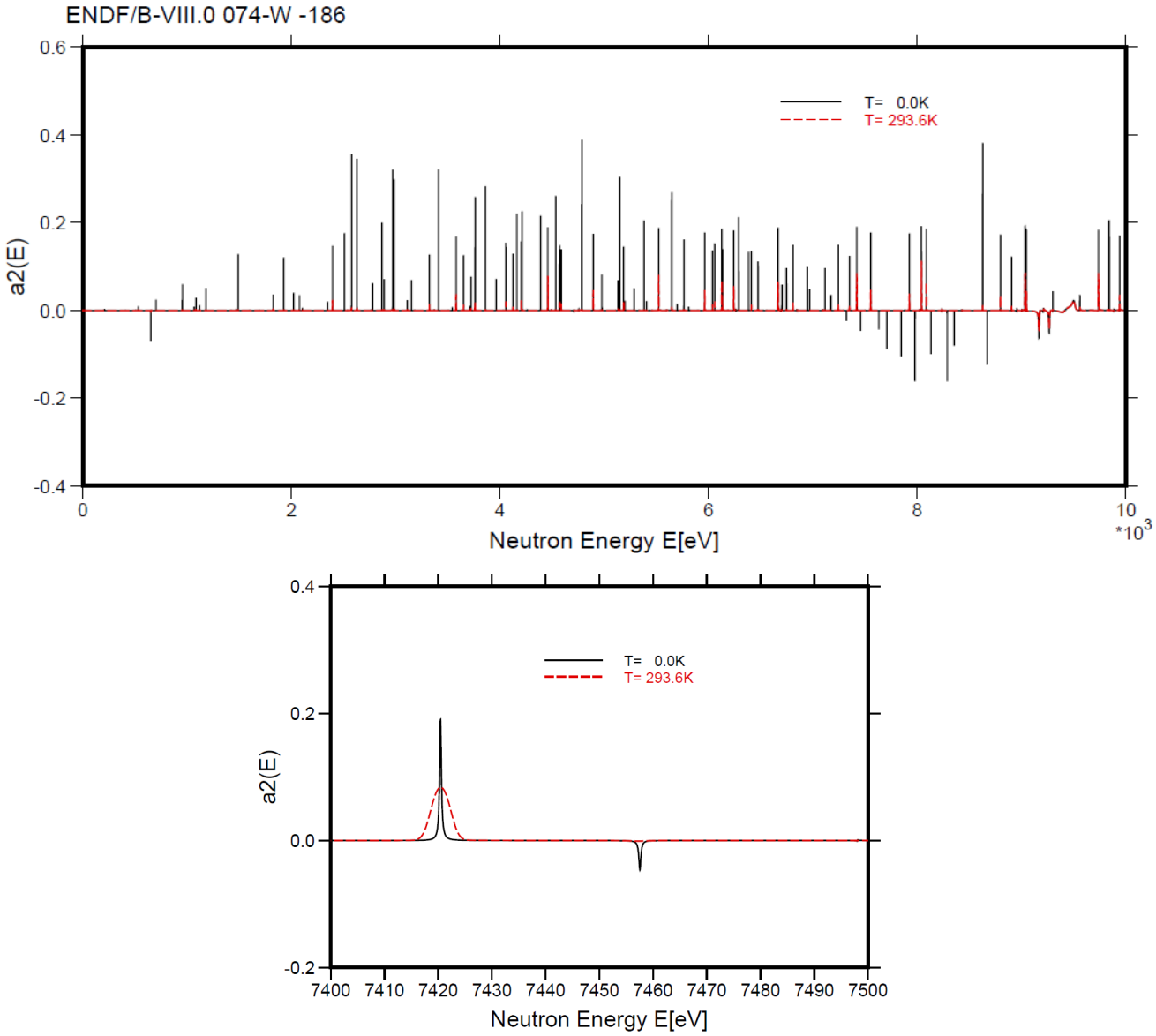
(B) W-186 elastic cross section at T=0K and T=293.6K



(B) W-186 a1(E) Polynomial Coefficient at T=0K and T=293.6K



(B) W-186 a2(E) Polynomial Coefficient at T=0K and T=293.6K



Processing of the Generalized Nuclear Data Structures in the GRUCON package.

(A) GNDS module of GRUCON
(B) Access Functions for Handling GNDS file
(C) Testing of Access Functions
(D) Status and Plans

(A) GNDS Module of GRUCON

GRUCON/GNDS module is assigned for converting data in XML format from GNDS files to GRUCON Standard Structures.

Control parameters:
NTAPE = input tape number
NGS = number of standard structures
NMT = number of reaction types
LGS = list of standard structures (in GRUCON nomenclature)
MT = list of reaction types (in ENDF nomenclature)

Example: reading GNDS file named as TAPE20 и preparing *S* structures (GRUCON system number = 2) for reactions MT=2, 18, 102 (elastic, fission, radiative capture)

*GNDS: NTAPE=30, NGS=1,NMT=3, LGS=2, MT=2,18,102

(B) Access Functions for Handling GNDS File

Subroutine SET_STRUCTURE (hteg)

Function: increase structure level and define position of structure with name **hteg**: **ilevel=ilevel+1, iline, ipos, kline, kpos**

Subroutine UNSET_STRUCTURE

Function: decrease structure level: **ilevel=ilevel-1**, restore position of structure on this level: **iline, ipos,kline,kpos**

Subroutine SET_LINE(jline)

Function: set **iline=jline** and read XML line with serial number **iline**

Logical Function FOUND_TEG(hteg)

Function: find teg position **iline, ipos** starting from the current position, in current structure; return **.TRUE.**, if teg is found, otherwise return **.FALSE.** and restore starting position

Function IGET_PAR ('ipar_name=')

Function RGET_PAR ('rpar_name=')

Function HGET_PAR('hpar_name=', lpar)

Function: find and return parameter value of integer, real or character type

Subroutine GET_VALUES (lval,val)

Function: find <value> teg and read array **val(lval)**

Subroutine GET_DATA (lrow,lcol,dat)

Function: find <data> teg and read array **dat(lcol,lrow)**

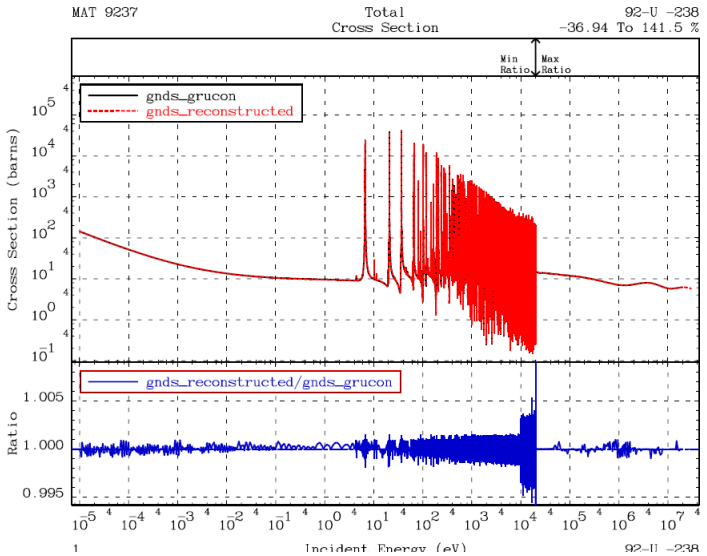
(B) Example: Define number of energy points in reconstructed cross sections

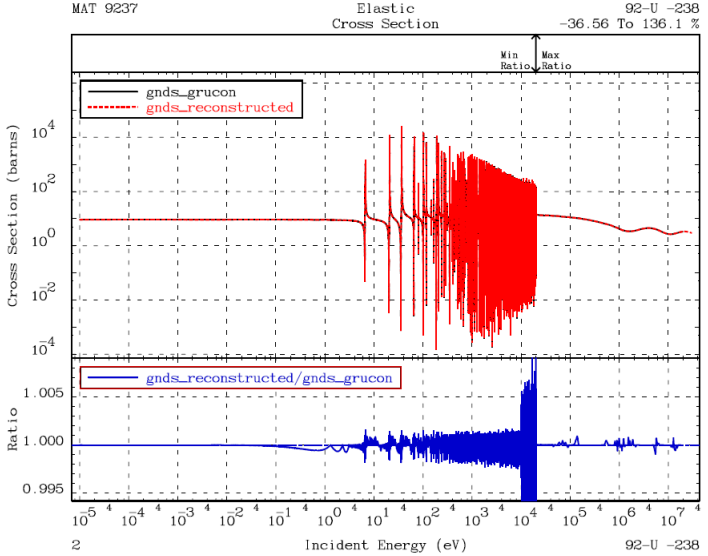
```
subroutine example
common/bteg/ilevel,iline,kline,ipos,kpos
logical :: FOUND_TEG
character(64) hpar,HGET_PAR
dimension :: val(1500000)
external SET_STRUCTURE,UNSET_STRUCTURE,FOUND_TEG,IGET_PAR,HGET_PAR
ilevel=0
iline=0
call SET_STRUCTURE('<reactionSuite')
hpar=HGET_PAR('target=',1)
write(*,*) 'target=',hpar(1:1)
call SET_STRUCTURE('<reactions')
do while (FOUND_TEG('<reaction_'))
      mt = IGET_PAR('ENDF_MT=')
      call SET_STRUCTURE('<crossSection')
      do while(FOUND_TEG('<XYs1d'))
           call SET_STRUCTURE('<XYs1d')
           hpar=HGET_PAR('label=',1)
           call GET_VALUES(nval,val)
           if (hpar(1:1) == 'recon' ) write (*,*) 'mt=',mt,'ne=',nval/2
           call UNSET STRUCTURE ! <XYs1d
      end do
      call UNSET_STRUCTURE  ! <crossSection
end do
call UNSET_STRUCTURE ! <reactions
Call UNSET_STRUCTURE ! <reactionSuite
end subroutine example
```

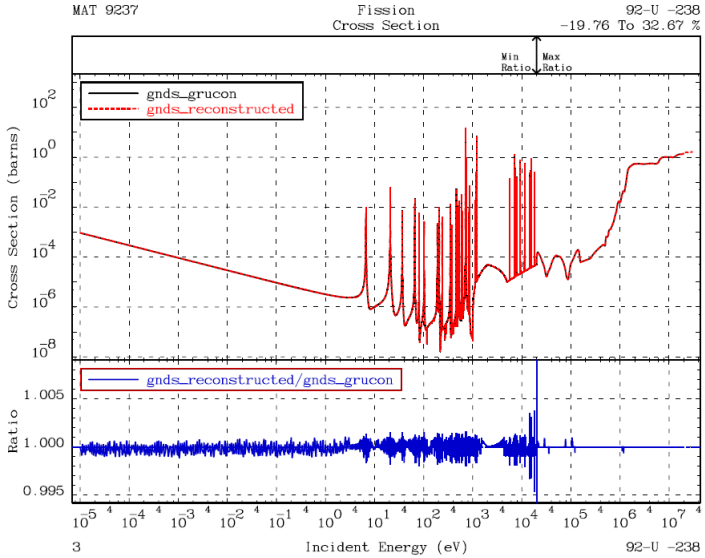
```
target=U238
mt =                2  ne =              376774
mt =               18  ne =               24206
mt =              102  ne =             1004638
```

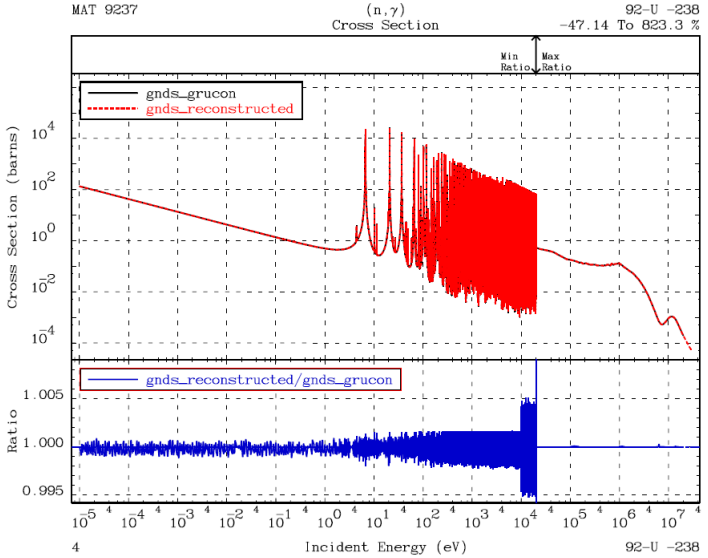
(C) Testing of GNDS Access Functions.

GNDS / U-238 : Comparison of cross sections with label="recon" with cross sections reconstructed by GRUCON from resonance parameters

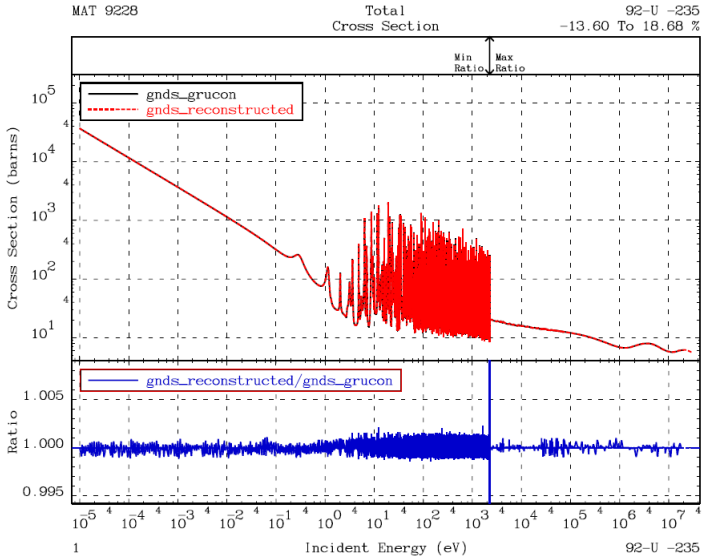


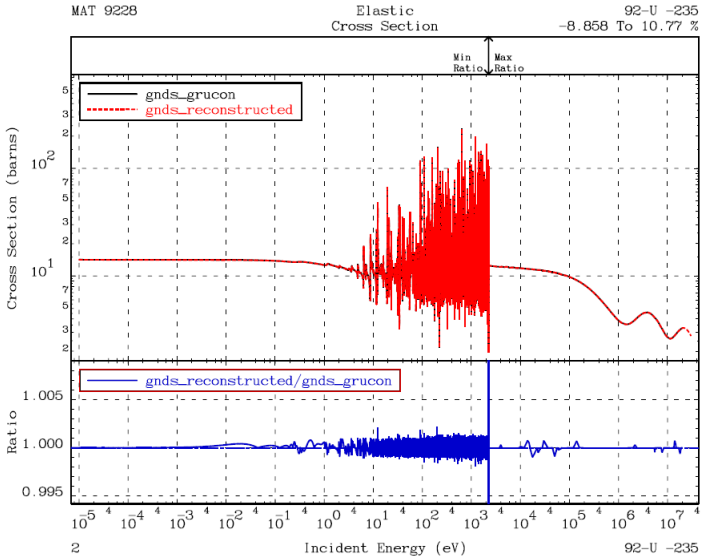


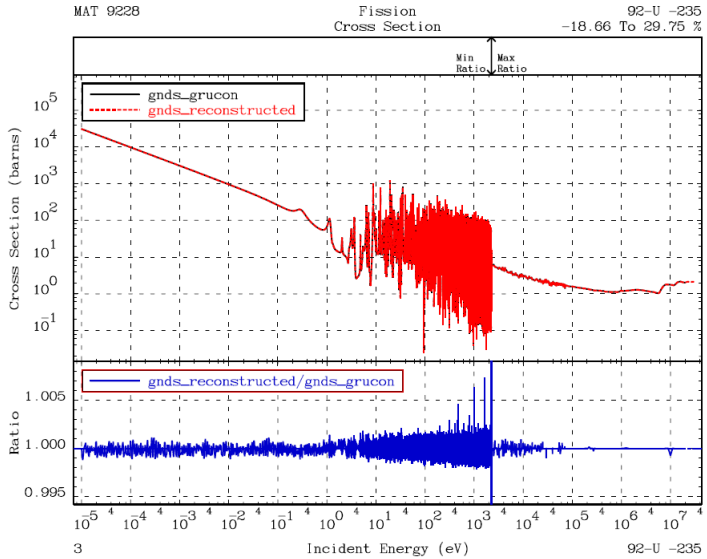


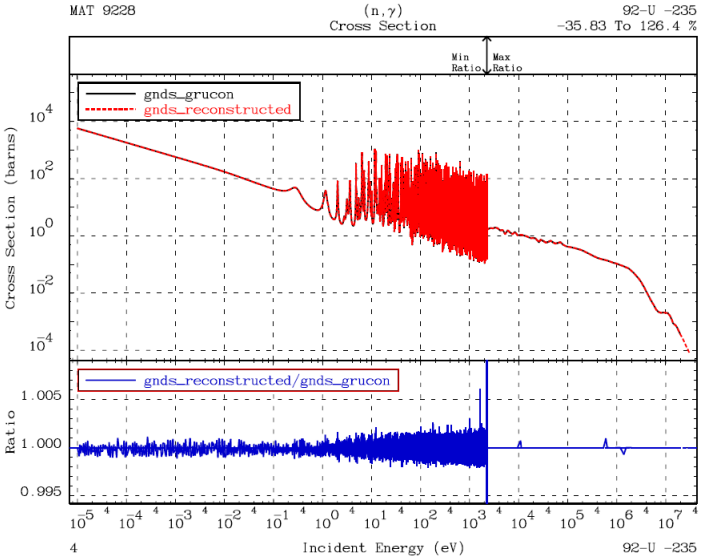


GNDS / U-235 : Comparison of cross sections included to the GNDS file (recon) and reconstructed by GRUCON









(D) Status and Plans

The two GRUCON data structures can be prepared now from the GNDS file:
S point-wise cross sections and yields
R resolved resonance parameters

To prepare of complete ACE file, it is necessary to add:
NU number of fission neutrons
U average resonance parameters
A angular distributions
E energy distributions
AE energy-angular distributions
GP photon production data

Farther development of GRUCON will be in direction of providing set of data from GNDS files needed for preparing complete ACE file

SUMMARY

Comparison of the cross sections, prepared on the 1-st Stage of the ACE Verification Project, revealed discrepancies that do not affect the results of integral testing (the upper energy range is limited to 20 MeV, the Doppler effect in $^{238}U(n, \alpha)$ reaction is missed). These inconsistences has been eliminated by correcting the calculation task.

Comparison of the double differential cross-sections obtained from the ACE file does not reveal any significant differences in the data.

Comparison of Keff calculations performed for 32 critical assemblies on the ACE libraries, prepared completely by GRUCON and NJOY (rather than partially, by replacing U-235, U-238 and Pu-239, according to AVP, Stage 1), revealed essential increasing of discrepancies (up to 0.5%) for assemblies with a large number of isotopes. The reason is to be clarified.

Further development of the package is planned to provide:

- calculation of the energy release cross sections,
- preparation of ACE files for photo-atomic interactions,
- generation of ACE files from the GNDS library.

Thank You for Attention!