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THE SIGACE PACKAGE FOR GENERATING HIGH TEMPERATURE ACE FILES – USER MANUAL

prepared by

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**The SIGACE package for
Generating High Temperature Neutron Source Reactions
ACE files – USER MANUAL**

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Introduction:

A code package named SIGACE has been developed as a tool for MCNP users within the scope of a research contract awarded by the Nuclear Data Section of the International Atomic Energy Agency (IAEA) (Ref: 302-F4-IND-11566 B5-IND-29641). A new recipe has been evolved for generating high temperature ACE files for use with the MCNP code. Under this scheme the low temperature ACE file is first converted to ENDF formatted file using ACELST code and then Doppler broadened, essentially limited to the data in the resolved resonance region, to any desired higher temperature using SIGMA1. The SIGACE code then generates a high temperature ACE file for use with the MCNP code. A thinning routine has also been introduced in the SIGACE code for reducing the size of the ACE files. The SIGACE code which has been tested with several FENDL/MC files is available, free of cost, upon request, from the Nuclear Data Section of the IAEA.

This brief write-up provides instructions for the installation of the package and a help manual to the users of the SIGACE package. All users are encouraged to send their feedback and suggestions to the IAEA Nuclear Data Section (A. Trkov).

Instructions for installing the SIGACE package on Windows operating system of your computer:

1. Please copy the executable file **ACEDOP.EXE**, **Install.bat** and **Readme.doc** on your hard disk.
2. Execute the **Install.bat** batch script either by double clicking on the file icon from windows folder or by executing the file from the DOS prompt.
3. The file should self-extract to generate a folder '**ACEDOP**' in the present working directory.
4. Under the folder '**ACEDOP**' you should see the following folders
 - a. **Bin** (Compiled source code)
 - b. **Flib** (Source code)
 - c. **Test** (Five test cases)
 - i. **1** (Test run for ^{239}Pu)
 - ii. **2** (Test run for ^{27}Al)
 - iii. **3** (Test run for ^{54}Fe)
 - iv. **4** (Test run for ^{28}Si)
 - v. **5** (Test run for ^{208}Pb)
 - d. **PLOT** (COMPLOT - EVALPLOT)
 - e. **Docs** (Documentation, progress reports and publications)
 - f. Apart from these folders you should see five batch files to run the five test cases.

Package Contents:

Brief description of the folder and its contents

1. The folder '**Flib**' contains the source code of the ACELST, SIGMA1 and SIGACE code.
2. The folder '**bin**' contains the executable of ACELST, SIGACE and SIGMA1 codes.
3. The folder COMPLOT - EVALPLOT contains the executable of COMPLOT and EVALPLOT. This is included for the sake of completeness and to display the output of the test runs.
4. '**Test**' folder has **1, 2, 3, 4 and 5** as the sub-folder that contains the test input files.

To run the test cases execute the **test1.bat** file under the folder '**ACEDOP**'. This should run the complete package and generate output that can be viewed through COMPLOT.

Steps involved in the execution of SIGACE:

The following sequence is followed for Doppler Broadening of the ACE file.

1. The ACELST code is first used to convert the ACE file into ENDF file.
2. The SIGMA1 module of the PERPRO code system is used for Doppler broadening of the ENDF file.
3. The SIGACE code is then used to generate the Doppler Broadened ACE file.
4. **OPTIONAL:** The Doppler Broadened ACE file can then again be converted to ENDF file and graphically plotted using EVALPLOT and compared with other ENDF file using COMPLIT routines of the PREPRO code system for validation purposes.

The sequence of execution for the 4 steps mentioned above is the following:

```
acelst < inp-acelst
sigma1
sigace < inp
acelst < inp2-acelst (Optional)
```

There are 3 different input decks “inp-acelst”, “inp” and “inp2-acelst” that are to be prepared by the user.

Preparation of Input Files:

Apart for the test cases if the user wishes to process ACE files then user should copy the ACE file to desired folder and prepare the 3 input files mentioned above for execution. Step by step descriptions of these 3 input files and code execution are presented below.

Sample input file for Test Run of 239-Pu.

Input file #1 : *inp-acelst*. This deck consisting of 3 cards is the input file for the code ACELST, which converts the given ACE file into an ENDF/B formatted file.

```
Card 1:   The name of the ACE file (Input)
Card 2:   Second entry is the LOG file for the ACELST code
          (Output)
Card 3:   Third entry is the name of the ENDF file (Output)
```

A sample input file „inp-acelst“ is presented below:

```
pu239.ace
ACELST.LOG
endf.dat
```

Input file #2 : “SIGMA1.INP”. This is the input file for the SIGMA1 module of the PREPRO code system used for Doppler Broadening of the ENDF file. We currently use the latest available version of the SIGMA1 code.

```
0          2 2.99998+02 1.00000-10          1
endf.dat
sigma1.out
1          9999
(BLANK CARD TERMINATES MAT RANGE REQUESTS)
0.00000+ 0 1.00000-02
(BLANK CARD TERMINATES FILE 3 ERROR LAW)
0.00000+ 0 5.00000-04
1.00000+ 0 5.00000-04
2.00000+ 0 5.00000-03
2.00000+ 7 5.00000-03
```

```

                                (BLANK CARD TERMINATES FILE 3 ERROR LAW)
0.000000+ 0 1.000000-04
                                (BLANK CARD TERMINATES FILE 3 ERROR LAW)

```

```

====(this line and below is not read)=====
      0      2 1.20000+06 1.00000-10      1
tape.135.RECENT
tape.135.SIGMA1

```

Please refer to the PERPRO code system manual [D.E. Cullen, "PREPRO 2002: 2002 ENDF/B Pre-processing Codes", International Atomic Energy Agency, Vienna, Austria, Report IAEA-NDS-39, Rev. 11, Feb. 5, 2002] for further details.

Input file #3 : „inp“. This is the input file for the SIGACE code.

This deck consisting of 5 cards is the input file for the code SIGACE, which converts the output of SIGMA1 into ACE file.

```

Card 1:   The file name of the original ACE file (Input)
Card 2:   The file Name of the Doppler broadened ENDF file (Input)
Card 3:   The file name of the Doppler broadened ACE file (Output)
Card 4:   Material ID flag to be appended for the XSDIR file
Card 5:   (optional) Thinning tolerance in percentage for
           generation of new ace file

```

A sample input file is give below:

```

pu239.ace
sigma1.out
ace.out
99c
1.0

```

Input file #4 : inp2-ancelst (OPTIONAL)

This step is OPTIONAL. The high temperature ACE file created by the SIGACE approach can be converted to an ENDF file and the so created file can then be graphically visualized using the EVALPLOT code of the PREPRO code system, inter-compared with other ENDF file using COMPTOT routines of the PREPRO code system. The input decks for EVALPLOT and COMPTOT are not shown in order to save space as the user can refer to the manual of the PREPRO code system.

This deck consisting of 3 cards is the input file for the code ACELST, which converts the high temperature ACE file into an ENDF/B formatted file.

```

Card 1:   The name of the high temperature ACE file (Input)
Card 2:   Second entry is the LOG file for the ACELST code (Output)
Card 3:   Third entry is the name of the ENDF file (Output)
           Corresponding to the high temperature

```

```

ace.out
ACELST.LOG
endf-1.dat

```

Output displayed on the screen:

The output displayed on the screen for the test problem 1 is as follows:

```

D:\ACEDOP>cd TEST\1

```

D:\ACEDOP\TEST\1>testrun1.bat

D:\ACEDOP\TEST\1>rename inp-ac~1 inp-ancelst

D:\ACEDOP\TEST\1>rename inp2-a~1 inp2-ancelst

D:\ACEDOP\TEST\1>..\..\bin\ancelst 0<inp-ancelst

ACELST - List contents of an ACE-lib

=====

Default source filename : lib.ace
Enter new name to redefine :
Default output filename : ACELST.LOG
Enter new name to redefine :
Enter filename to convert to ENDF-6 :
Formatting of MF6 not coded for MT 16 Law 44
Formatting of MF6 not coded for MT 17 Law 44
Formatting of MF6 not coded for MT 37 Law 44
Formatting of MF6 not coded for MT 91 Law 44

D:\ACEDOP\TEST\1>..\..\bin\sigma1

Doppler Broaden ENDF/B Cross Sections (SIGMA1 2000-1)

Retrieval Criteria----- MAT
Monitor Mode----- On
Temperature----- 299.998000 KELVIN
Minimum Cross Section----- 1.00000-10
Negative Cross Section----- Make = 0 (No Negative Output)

ENDF/B Input and Output Data Filenames

endf.dat

sigma1.out

Requested MAT Ranges

Minimum Maximum

1 9999

Allowable Uncertainty

Energy Uncertainty per-cent

0.0 1.000000-2 1.0000

ENDF/B Tape Label

Converted from Ace file: endf.dat 6000

Projectile	MAT	MT	ENDF/B	Kelvin	Q-Value	Points	Points
Material			Format	In	eV	In	Out
n 94-Pu-239	9437	1	VI	2.999980+2	0.0	65035	65035
n 94-Pu-239	9437	2	VI	2.999980+2	0.0	65035	65035
n 94-Pu-239	9437	16	VI	2.999980+2	-5.646700+6	124	124
n 94-Pu-239	9437	17	VI	2.999980+2	-1.264800+7	59	59
n 94-Pu-239	9437	18	VI	2.999980+2	1.999200+8	65035	65035
n 94-Pu-239	9437	37	VI	2.999980+2	-1.850830+7	10	10
n 94-Pu-239	9437	51	VI	2.999980+2	-7.861000+3	399	399
n 94-Pu-239	9437	52	VI	2.999980+2	-5.727600+4	339	339
n 94-Pu-239	9437	53	VI	2.999980+2	-7.570600+4	332	332
n 94-Pu-239	9437	54	VI	2.999980+2	-1.637600+5	314	314
n 94-Pu-239	9437	55	VI	2.999980+2	-1.940000+5	310	310
n 94-Pu-239	9437	56	VI	2.999980+2	-2.855000+5	296	296
n 94-Pu-239	9437	57	VI	2.999980+2	-3.170000+5	292	292

n	94-Pu-239	9437	58	VI	2.999980+2	-3.301000+5	287	287
n	94-Pu-239	9437	59	VI	2.999980+2	-3.600000+5	283	283
n	94-Pu-239	9437	60	VI	2.999980+2	-3.874000+5	278	278
n	94-Pu-239	9437	61	VI	2.999980+2	-3.916000+5	275	275
n	94-Pu-239	9437	62	VI	2.999980+2	-4.280000+5	270	270
n	94-Pu-239	9437	63	VI	2.999980+2	-4.350000+5	269	269
n	94-Pu-239	9437	64	VI	2.999980+2	-4.520000+5	266	266
n	94-Pu-239	9437	65	VI	2.999980+2	-4.620000+5	264	264
n	94-Pu-239	9437	66	VI	2.999980+2	-4.698000+5	262	262
n	94-Pu-239	9437	67	VI	2.999980+2	-4.820000+5	258	258
n	94-Pu-239	9437	68	VI	2.999980+2	-4.880000+5	257	257
n	94-Pu-239	9437	69	VI	2.999980+2	-4.921000+5	256	256
n	94-Pu-239	9437	70	VI	2.999980+2	-5.055000+5	253	253
n	94-Pu-239	9437	71	VI	2.999980+2	-5.118000+5	252	252
n	94-Pu-239	9437	72	VI	2.999980+2	-5.380000+5	248	248
n	94-Pu-239	9437	73	VI	2.999980+2	-5.561000+5	246	246
n	94-Pu-239	9437	74	VI	2.999980+2	-5.650000+5	242	242
n	94-Pu-239	9437	75	VI	2.999980+2	-5.830000+5	239	239
n	94-Pu-239	9437	76	VI	2.999980+2	-6.200000+5	236	236
n	94-Pu-239	9437	77	VI	2.999980+2	-6.340000+5	235	235
n	94-Pu-239	9437	78	VI	2.999980+2	-9.390000+5	212	212
n	94-Pu-239	9437	79	VI	2.999980+2	-1.001000+6	207	207
n	94-Pu-239	9437	80	VI	2.999980+2	-1.135000+6	200	200
n	94-Pu-239	9437	81	VI	2.999980+2	-1.282000+6	194	194
n	94-Pu-239	9437	91	VI	2.999980+2	-6.340000+5	235	235
n	94-Pu-239	9437	102	VI	2.999980+2	6.533700+6	65035	65035
n	94-Pu-239	9437	4	VI	2.999980+2	0.0	399	399

--

No Unresolved Region MAT Totals 269238 269238

--

==Total Execution Time 2.48 Seconds

==

--

Tape Totals 269238 269238

--

==Total Execution Time 2.48 Seconds

==

D:\ACEDOP\TEST\1>..\..\bin\sigace 0<inp

=====

SIGACE

=====

Default source filename : ACE.INP

Enter new name to redefine :

=====

ACE INPUT FILE : pu239.ace

=====

Default Doppler broad-nd ENDF filename SIGMA1.OUT

Enter new name to redefine

=====

DOPPLER BROADENED ENDF FILE : sigma1.out

=====

Default high temperature ACE filename ACE.OUT

=====

OUPUT ACE FILE : ace.out

=====

```

Default ZAID flag           : 00c
Enter the XXC as in ZAID.XXC for ACE
Example 92235.23c if you enter 23c
=====
ZAID.XXC                     : 99c
=====
Default Thinning Tolerance   : 0.000
Enter the thinning tolerance for ACE
Example 0.1 represents 0.1% thinning
=====
THINNING TOLERANCE           : 1.000
=====
THE REACTIONS ARE
  1) 16    2) 17    3) 18    4) 37
  5) 51    6) 52    7) 53    8) 54
  9) 55   10) 56   11) 57   12) 58
 13) 59   14) 60   15) 61   16) 62
 17) 63   18) 64   19) 65   20) 66
 21) 67   22) 68   23) 69   24) 70
 25) 71   26) 72   27) 73   28) 74
 29) 75   30) 76   31) 77   32) 78
 33) 79   34) 80   35) 81   36) 91
 37) 102   38) 4
DOPPLER BROADENED ENDF FILE sigma1.out
MAT ID = 9437
THE FOLLOWING FILES ARE PRESENT FOR THIS ISOTOPE
1                                     GENERAL INFORMATION
3                                     REACTION CROSS SECTIONS
4                                     ANGULAR DISTRIBUTION FOR EMITTED PARTICLES
END OF TAPE

ZA = 94239

                                END OF FILE 1

NO RESONANCE PARAMETERS ARE GIVEN EXCEPT THE
SCATTERING RADIUS (AP). IT IS ONLY FOR THE CONVENIENCE
OF THE USER AND HAS NO CONTRIBUTION TO THE SCATTERING
CROSS SECTION REPRESENTED IN FILE 3.

***** NO MF=2 FOUND *****
1  MT = 1    MAT ID IS 9437
2  MT = 2    MAT ID IS 9437
3  MT = 16   MAT ID IS 9437
4  MT = 17   MAT ID IS 9437
5  MT = 18   MAT ID IS 9437
6  MT = 37   MAT ID IS 9437
7  MT = 51   MAT ID IS 9437
8  MT = 52   MAT ID IS 9437
9  MT = 53   MAT ID IS 9437
10 MT = 54   MAT ID IS 9437
11 MT = 55   MAT ID IS 9437
12 MT = 56   MAT ID IS 9437
13 MT = 57   MAT ID IS 9437
14 MT = 58   MAT ID IS 9437
15 MT = 59   MAT ID IS 9437
16 MT = 60   MAT ID IS 9437
17 MT = 61   MAT ID IS 9437
18 MT = 62   MAT ID IS 9437
19 MT = 63   MAT ID IS 9437
20 MT = 64   MAT ID IS 9437
21 MT = 65   MAT ID IS 9437
22 MT = 66   MAT ID IS 9437
23 MT = 67   MAT ID IS 9437
24 MT = 68   MAT ID IS 9437
25 MT = 69   MAT ID IS 9437
26 MT = 70   MAT ID IS 9437

```



```

27 MT = 71 MAT ID IS 9437
28 MT = 72 MAT ID IS 9437
29 MT = 73 MAT ID IS 9437
30 MT = 74 MAT ID IS 9437
31 MT = 75 MAT ID IS 9437
32 MT = 76 MAT ID IS 9437
33 MT = 77 MAT ID IS 9437
34 MT = 78 MAT ID IS 9437
35 MT = 79 MAT ID IS 9437
36 MT = 80 MAT ID IS 9437
37 MT = 81 MAT ID IS 9437
38 MT = 91 MAT ID IS 9437
39 MT = 102 MAT ID IS 9437
40 MT = 4 MAT ID IS 9437

```

END OF FILE 3

UNIONIZING GRID

+++++

MT

+++++

2

16

17

18

37

51

52

53

54

55

56

57

58

59

60

61

62

63

64

65

66

67

68

69

70

71

72

73

74

75

76

77

78

79

80

81

91

102

4

Thinning Tolerance = 1.0000000000000000 %

MAT	MT	Points In	Points Out

94239.99c	1	65035	9791
94239.99c	Tot. Abs.	65035	21560

94239.99c	2	65035	6181
94239.99c	Avg.Heat.Num.	65035	65035
94239.99c	16	124	23
94239.99c	17	59	12
94239.99c	18	65035	12765
94239.99c	37	10	5
94239.99c	51	399	25
94239.99c	52	339	20
94239.99c	53	332	25
94239.99c	54	314	21
94239.99c	55	310	22
94239.99c	56	296	37
94239.99c	57	292	34
94239.99c	58	287	34
94239.99c	59	283	43
94239.99c	60	278	35
94239.99c	61	275	33
94239.99c	62	270	33
94239.99c	63	269	35
94239.99c	64	266	32
94239.99c	65	264	34
94239.99c	66	262	38
94239.99c	67	258	33
94239.99c	68	257	42
94239.99c	69	256	37
94239.99c	70	253	31
94239.99c	71	252	34
94239.99c	72	248	35
94239.99c	73	246	27
94239.99c	74	242	32
94239.99c	75	239	33
94239.99c	76	236	30
94239.99c	77	235	31
94239.99c	78	212	20
94239.99c	79	207	14
94239.99c	80	200	19
94239.99c	81	194	14
94239.99c	91	235	36
94239.99c	102	65035	21560
94239.99c	4	399	35

 THE NAME OF THE OUTPUT FILE ace.out

D:\ACEDOP\TEST\1>..\..\bin\acelst 0<inp2-acelst
 ACELST - List contents of an ACE-lib
 =====

Default source filename : lib.ace
 Enter new name to redefine :
 Default output filename : ACELST.LOG
 Enter new name to redefine :
 Enter filename to convert to ENDF-6 :
 Formatting of MF6 not coded for MT 16 Law 44
 Formatting of MF6 not coded for MT 17 Law 44
 Formatting of MF6 not coded for MT 37 Law 44
 Formatting of MF6 not coded for MT 91 Law 44

D:\ACEDOP\TEST\1>copy complot.inp ..\..\plot\
 1 file(s) copied.
 D:\ACEDOP\TEST\1>cd ..\..\plot

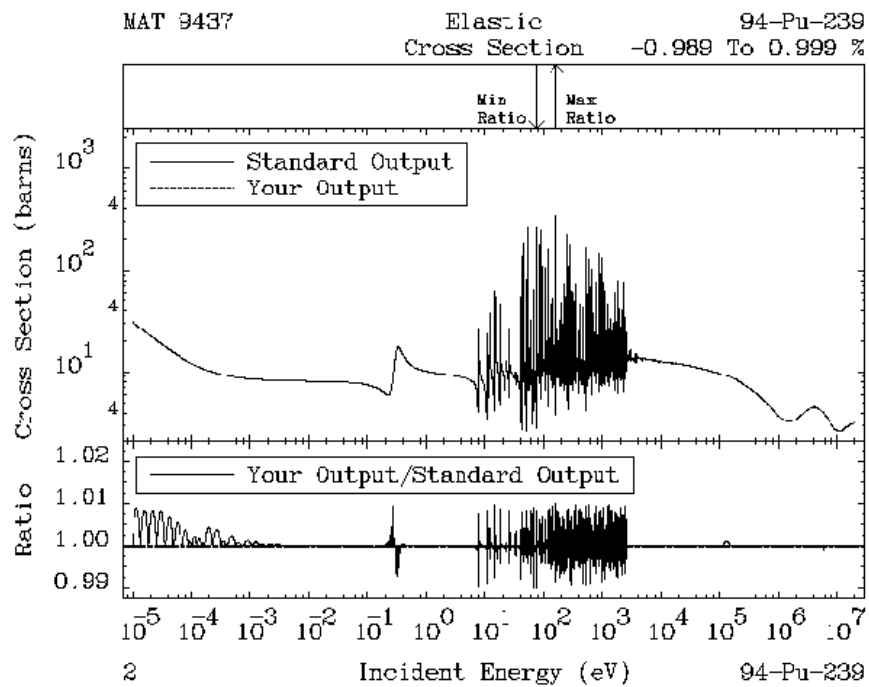
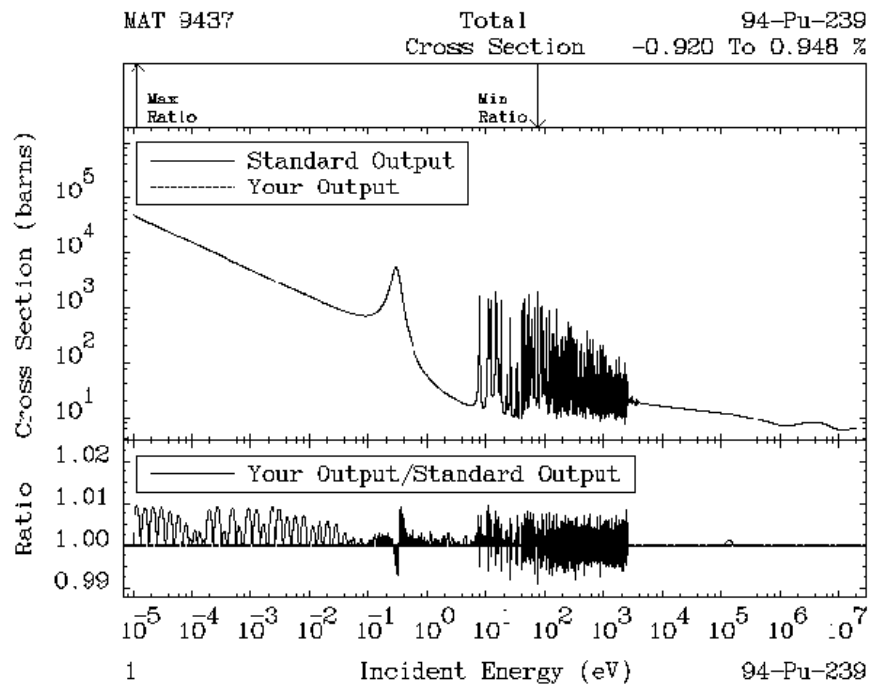
D:\ACEDOP\PLOT>complot

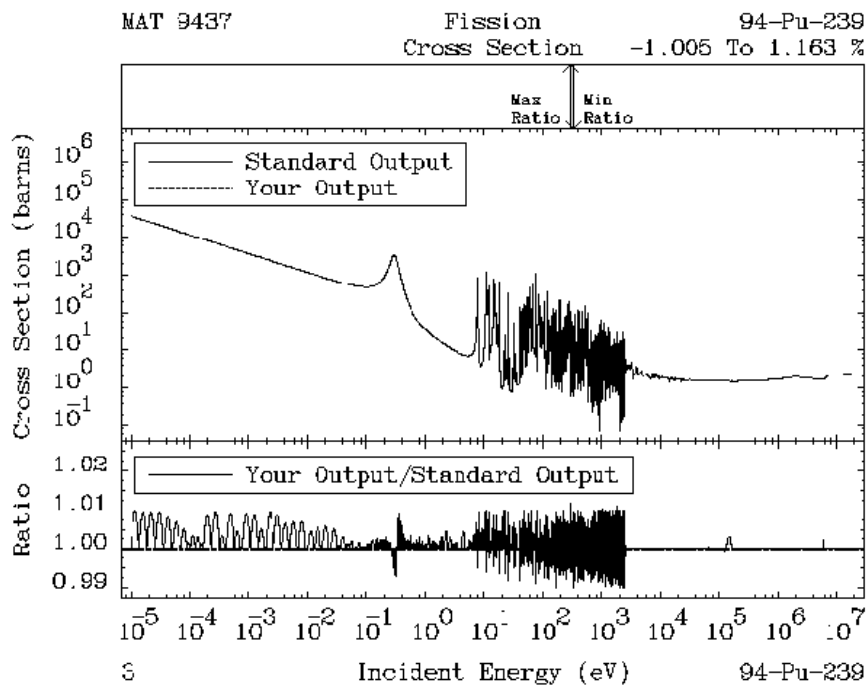
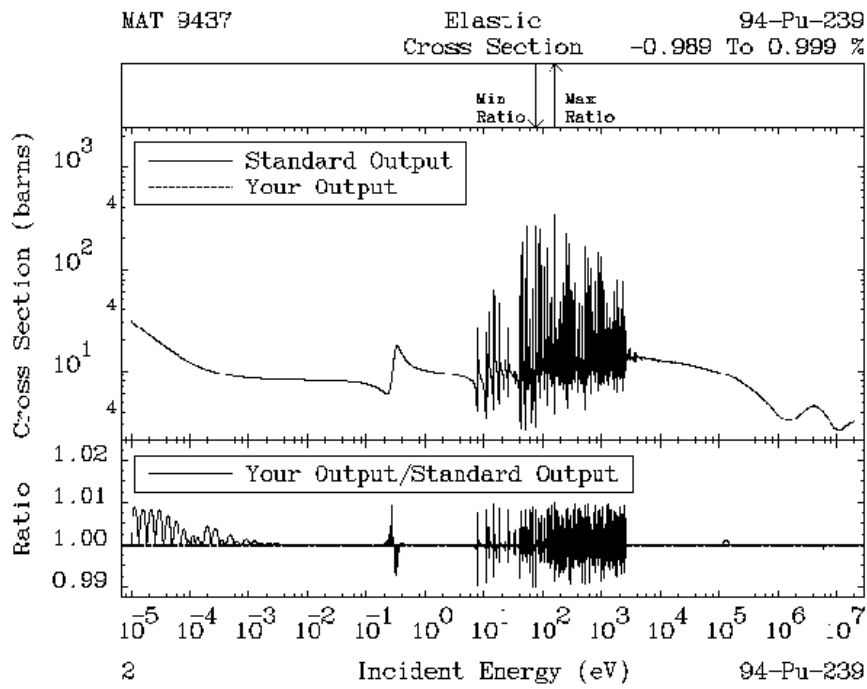
D:\ACEDOP\PLOT>cd ..

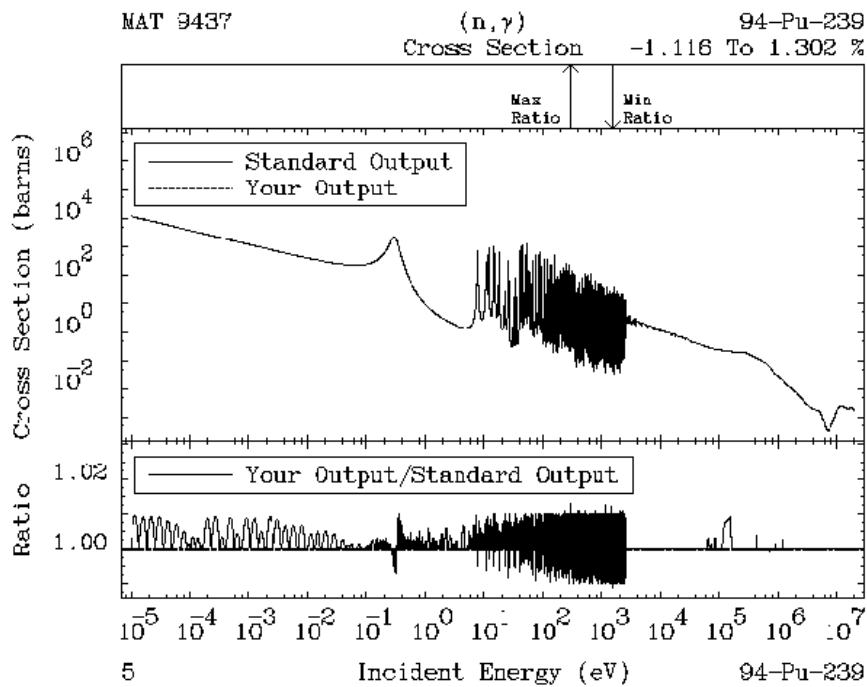
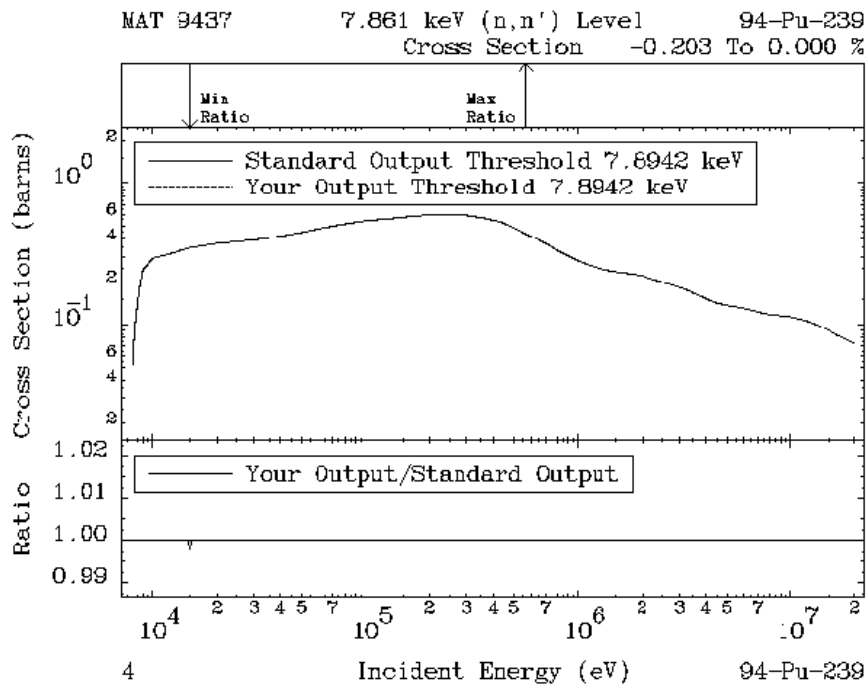
.....END OF SCREEN OUTPUT.....

Output of COMPLIT Run

The output of the COMPLIT program of the PREPRO code system generated on the screen by comparing the original ACE file (i.e., generated by using the NJOY code system) high temperature and the Doppler Broadened ACE file (i.e., generated using the SIGACE package) is provided below as illustration of the verification procedure.







The graphical intercomparison presented above for ^{239}Pu validates the SIGACE approach. Note that the SIGACE approach is not applicable by design in the unresolved resonance region. A number of actinides FENDL/E nuclides and light elements have also been successfully tested [1-3] by extensive graphical inter-comparison as in the above illustration.

It may be noted [1-3] that the SIGACE code and the recipe for generating ACE files at higher temperatures has been applied to the SEFOR fast reactor benchmark problem (Sodium cooled fast reactor benchmark described in ENDF-202/BNL-19302, 1974 document). The calculated Doppler Coefficient is in good agreement with the experimental value. A similar calculation using ACE files generated directly with the NJOY system also agrees with our SIGACE computed results. The SIGACE code and the recipe is further applied to study the numerical benchmark configuration of selected idealized PWR pin cell configurations with five different fuel enrichments as reported by Mosteller and Eisenhart. More details are available in [1-3] for the interested user.

The SIGACE package is meant to satisfy the needs of the users of the MCNP package who prefer to have a simple recipe to get ACE files at higher temperatures instead of becoming a specialist to perform direct nuclear data processing starting from the evaluated nuclear data file. Both the NJOY code and the MCNP package have been evolving. The present software of the SIGACE package has been tested with 2001 versions of the NJOY and the MCNP code systems as was available [2].

All users are encouraged to send their feedback and suggestions to the IAEA Nuclear Data Section (A. Trkov): Nuclear Data Section, International Atomic Energy Agency, A-1400 Vienna, Austria. Email: A.Trkov@iaea.org

References:

1. Amit Raj Sharma, S. Chaturvedi, D. Chandra, S. Ganesan and P.K. Kaw, "Final Report on Integral validation and Use of Improved Nuclear data in Fusion Blanket Studies" Progress Report for the Period 1 March to 28 February 2002, Submitted to the IAEA.
2. S. Ganesan, A. R. Sharma and A. Trkov, Summary Report of a Consultants Meeting (25 November to 6 December 2002), to modify the dedicated code SIGACE for operational use with the PCs and any FENDL-ace file, plus systematic verification of FENDL-ace files according to IAEA-NDS procedures, IAEA Dec. 2002.
3. Amit R. Sharma, S. Ganesan and A. Trkov, "SIGACE Code for Generating High Temperature ACE Files; Validation and Benchmarking," paper presented at the International Conference on Nuclear Data for Science and Technology, "ND2004", 26 September to 1 October 2004. Santa Fe, New Mexico, USA proceedings in press.