XSMCNP Primer

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Version 1.5

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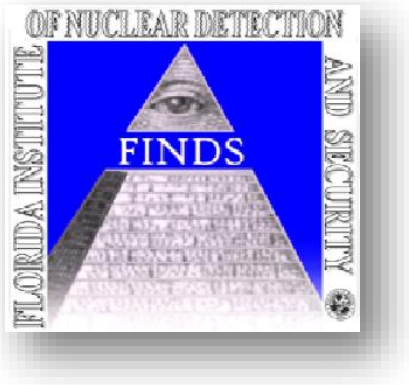

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Objective:

The purpose of this primer is to provide step-by-step instructions on the use of XSMCNP in order for the user to take PENTRAN cross section input files and transform them into a form that is readable by MCNP. This primer will include a sample input for the ZIPPY example reactor. This primer will focus the use of XSMCNP primarily on the Windows OS.

Getting Started

If the user has the xsmcnp.f90 source code it can be compiled using the g95 compiler which can be found at http://www.g95.org/ . Place the xsmcnp.f90 file into your …/g95/bin folder as shown below.

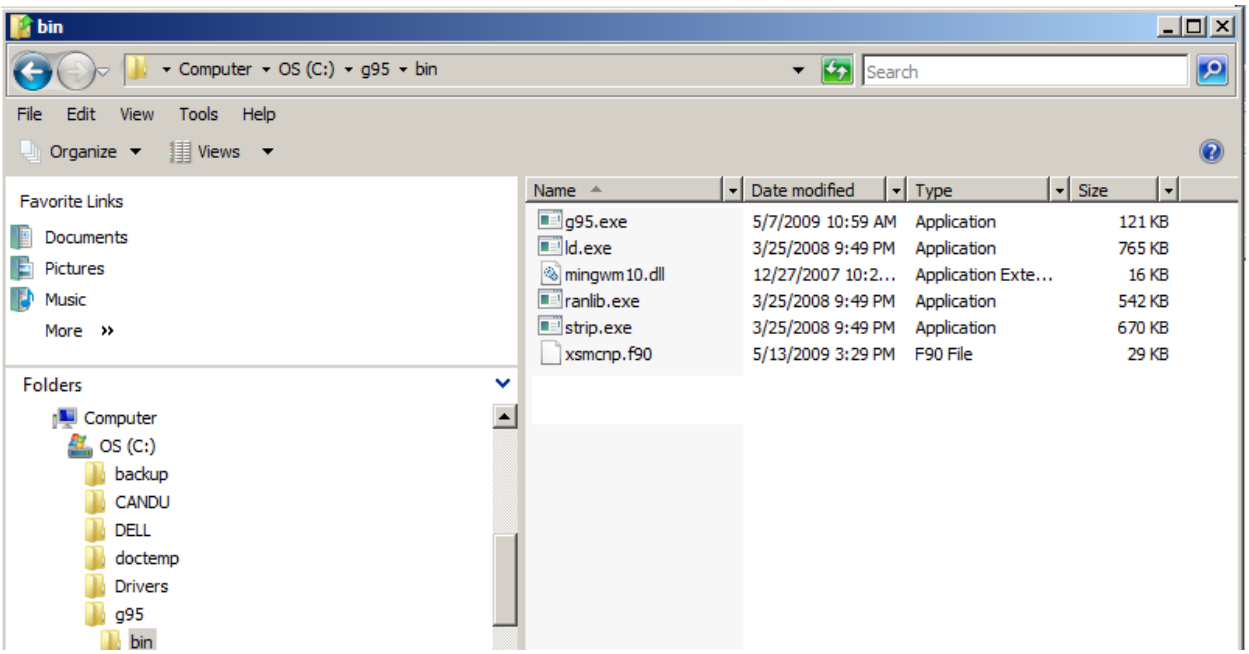


Figure 1: g95 directory with xsmcnp.f90 source code.

At this point proceed to the Windows command prompt and direct yourself to ../g95/bin/ to compile the source code. The user can compile the source by typing in the command prompt "**g95 –o xsmcnp xsmcnp.f90**" and pressing enter. This command is shown in detail in Figure 2 below. Once g95 compiles the source code the user will see several files in the ../g95/bin directory. The user can ignore a.out, ar.exe, as.exe, mlineparse.mod, mpoly.mod, and mxslib.mod. The latter three files are files automatically generated by g95. The primary executable of interest will be xsmcnp.exe. Create a working directory for XSMCNP either on the desktop or somewhere easily accessible. Move the xsmcnp.exe binary executable to this directory for future use. When using XSMCNP the user will primarily be working in the XSMCNP directory and the MCNP directory.

```
C:\g95\bin> g95 –o xsmcnp xsmcnp.f90
```

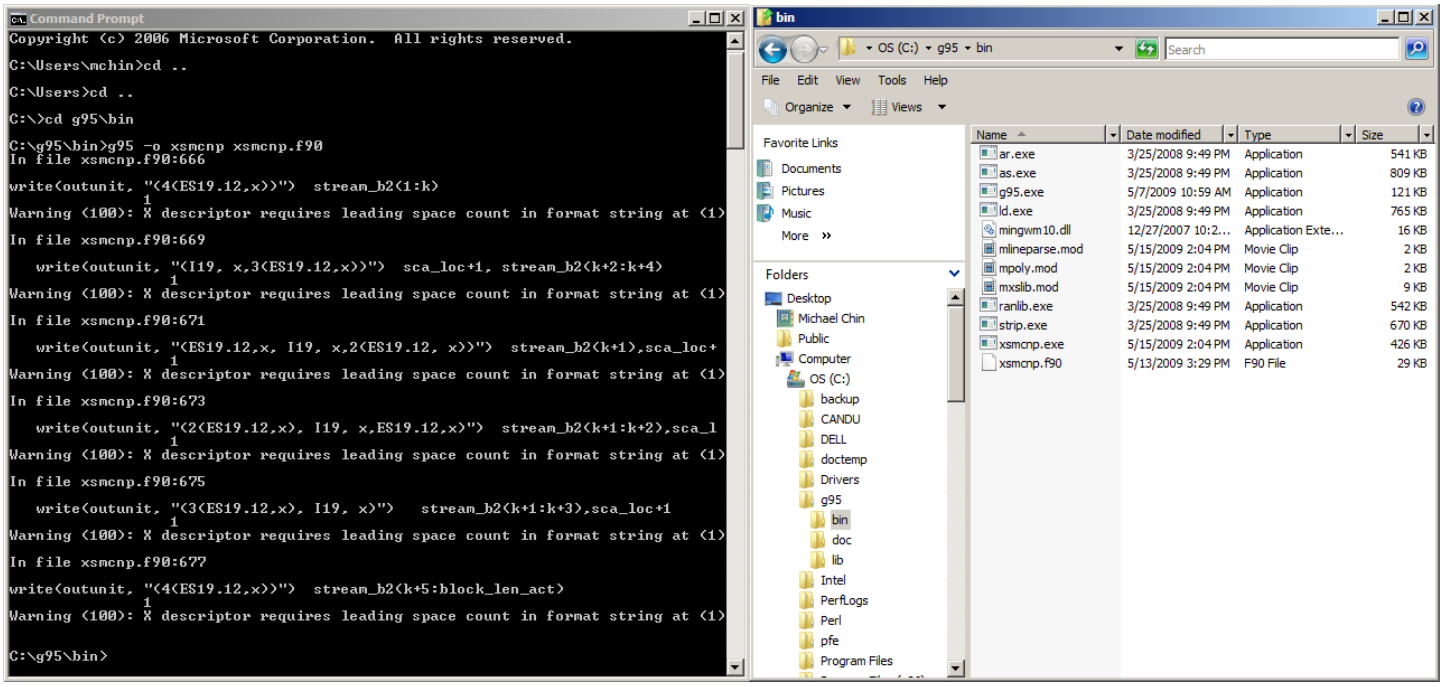
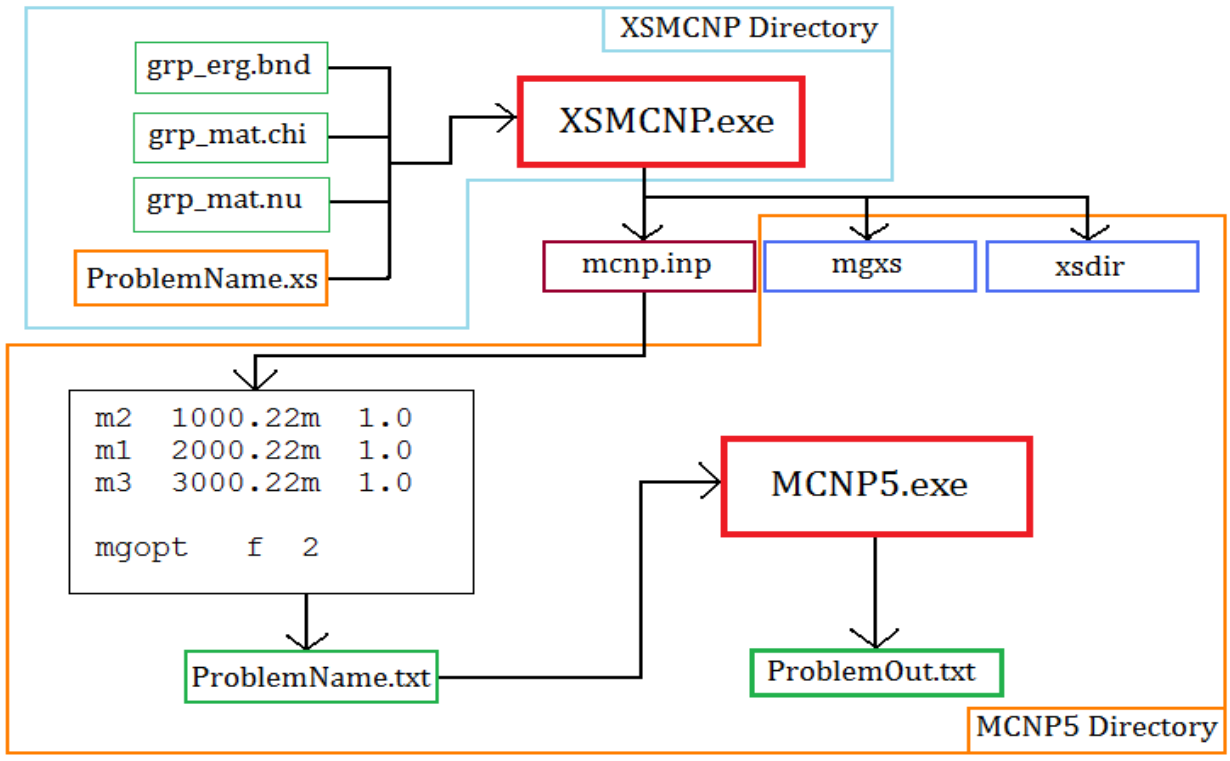


Figure 2: Compilation of xsmcnp.f90 source code using the "g95 –o xsmcnp xsmcnp.f90" command.

Needed files for the XSMCNP directory:

- xsmcnp.exe
- grp_mat.chi (Optional but highly recommended)
- grp_mat.nu (Optional but highly recommended)
- grp_erg.bnd (Optional but highly recommended)
- Cross section input file .xs from PENTRAN (in this example we will be using zippy.xs)

XSMCNP Flowchart



ZIPPY Reactor Example

The ZIPPY two-group reactor is a uranium dioxide fueled reactor with boron carbide control rods with water as a moderator. The light pink in the diagram below is the fuel region while the bulk of the green around the fuel is the moderator. The three light green blocks within the fuel can either be the boron carbide control rods or moderator. The ZIPPY reactor simulation typically includes group 2 → 1 down scattering only. By default the material indexes are 1 for fuel, 2 for moderator, and 3 for control rods.

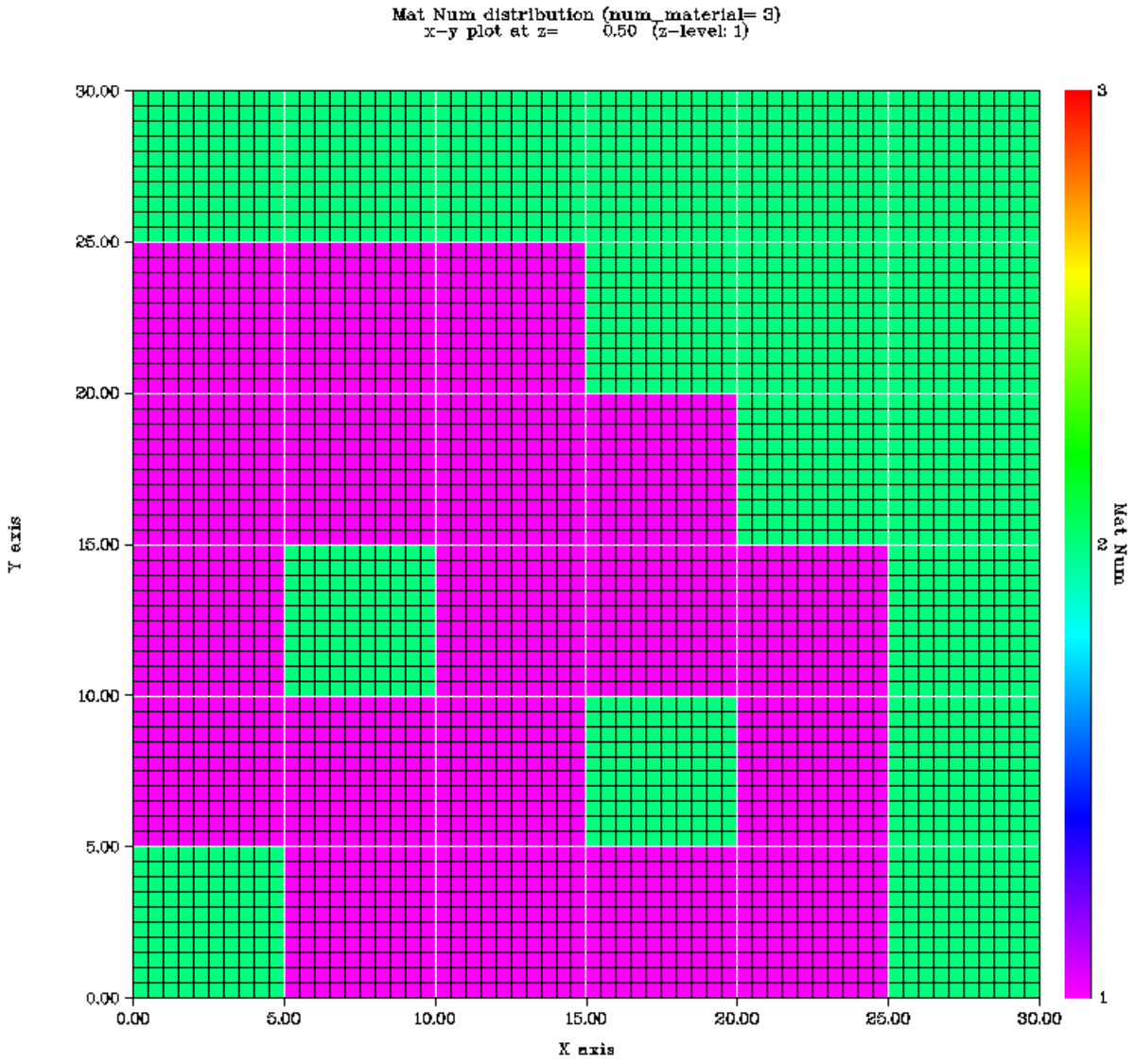


Figure 3: Material indices for the ZIPPY reactor. Light pink indicates fuel. Light green indicates moderator. If control rods were included in this diagram they would show up as red blocks where the light green moderator would be in between the fuel region.

The format for the grp_mat files are dependent on material and the file suffixes describe the problem. For example, grp_mat.chi describes the average fission spectrum Chi (χ) while grp_mat.nu describes the average fission neutron yield Nu (ν). Another file, grp_erg.bnd describes the upper energy bounds for the problem, starting with group 1. These three files may be supplied by the user in order for XSMCNP but are optional. The templates for the two grp_mat files are shown below.

grp_mat.XXX

Group 1 Group 2 … Group G // This is the general format for the optional input files, the group is not stated

```
Material  1 Material 1  …   Material 1
Material 2  Material 2  …   Material 2
     .            .       ..       …
     .            .         ..     …
     .            .           ..   …
Material n  Material n       Material n
```

For the ZIPPY reactor the specifications for chi and nu are given below.

grp_mat.chi

```
0.95 0.05
0 0
0 0
```

grp_mat.nu

```
2.440 2.436
0 0
0 0
```

Upper energy boundaries can be found in the file grp_erg.bnd and are specified in terms of increasing energy, in MeV. That is, the lowest group is listed first (group 1) and ends with the highest energy group. An example is shown below.

grp_erg.bnd

```
1.86 5 10
```

A sample cross section file for the ZIPPY reactor from PENTRAN is given below.

```
UO2  siga        sigf             sigt             sigss
1.0888E-02       8.84E-03         3.46E-01         3.12E-01         0.00E+00
1.37E-01         2.25E-01         1.49E+00         1.36E+00         2.31E-02
H2O siga         sigf             sigt             sigss
8.35E-04         0.0000           3.54E-01         3.14E-01         0.00E+00
2.85E-02         0.0000           2.06E+00         2.03E+00         3.83E-02
B4C siga         sigf             sigt             sigss
2.000E-04        0.000E+00        3.492E-01        3.100E-01        0.000E+00
8.000E-01        0.000E+00        1.000E+00        2.000E-01        3.900E-02
```

Running XSMCNP - Windows

Once all files are within the XSMCNP directory the user can run the XSMCNP executable. The user will see the following command prompt:

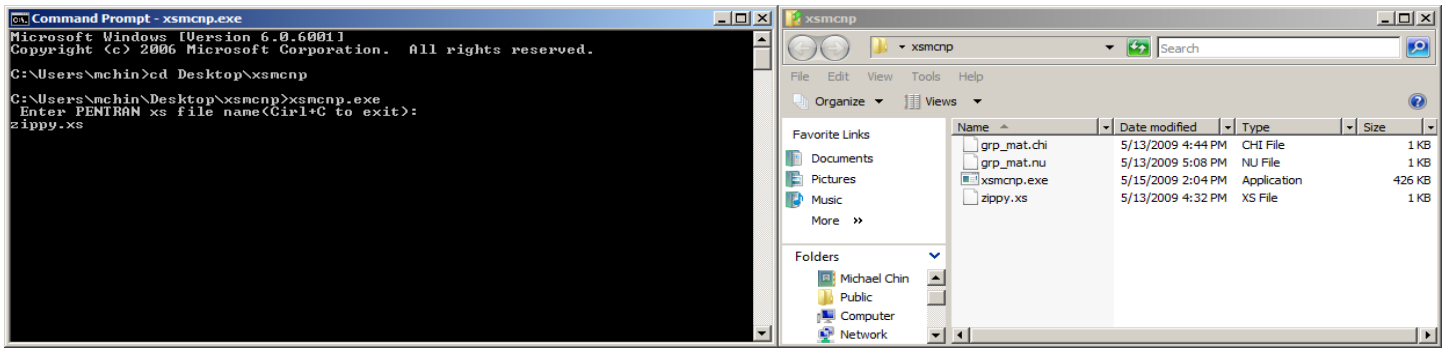


Figure 4: Starting XSMCNP.

Type in the cross section (make sure the cross section file is within the XSMCNP folder). After this XSMCNP will prompt whether the cross sections come from a gamma library (CEPXS) or a neutron library (ENDF-B). Enter 2 for photons, 1 for neutrons.

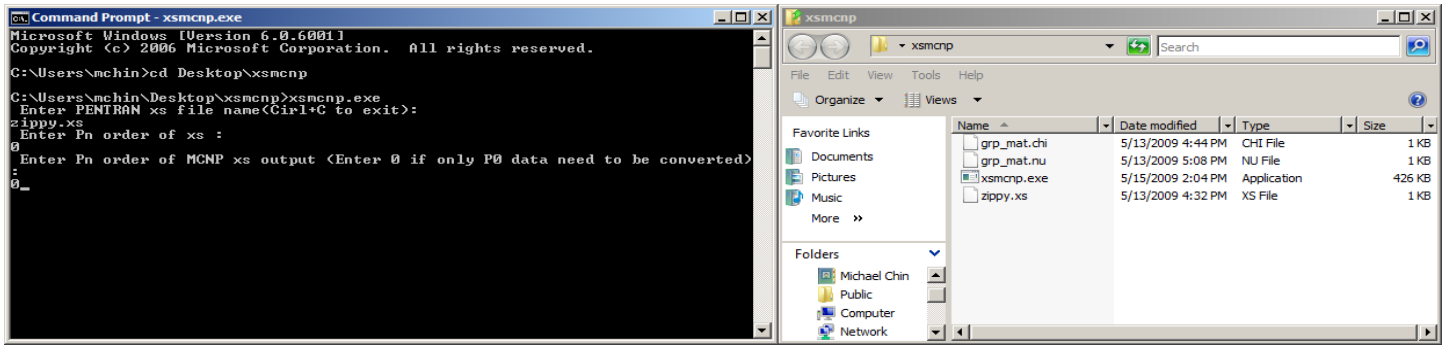


Figure 5: Inserting Legendre Pn cross section order.

At this point XSMCNP will prompt the user for the Legendre Pn order of the cross sections. In PENTRAN this refers to the variable legoxs and can be found in further detail in the Block III input section of the PENTRAN manual (Page 107). For the ZIPPY reactor the Pn order for both the cross sections as well as the MCNP cross section output are both zero.

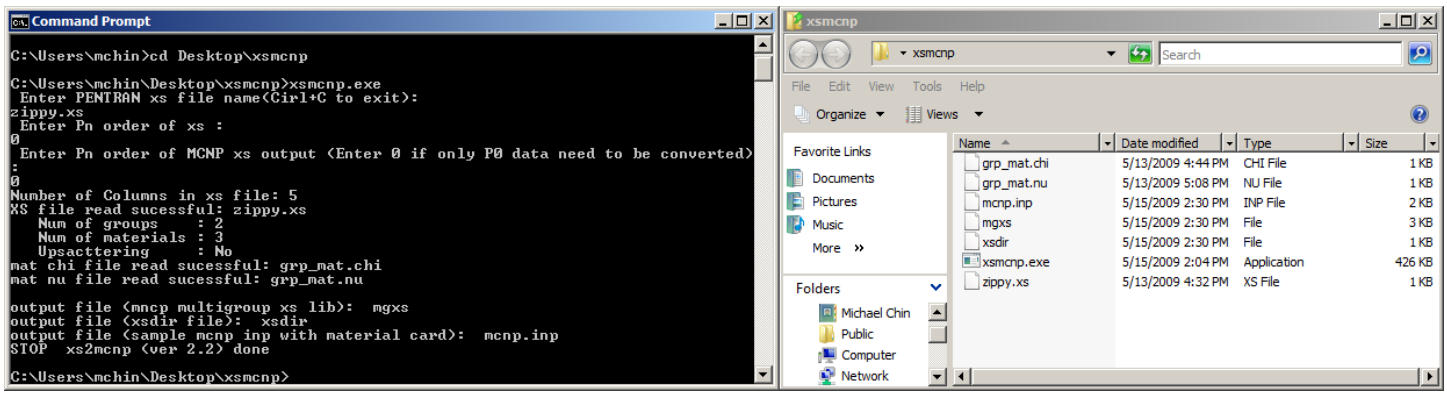


Figure 6: Successful run of XSMCNP.

Once this is done, XSMCNP will create three files: mcnp.inp, mgxs, and xsdir. The file mcnp.inp describes the multigroup input deck and contains cell, surface, and material cards. The file mgxs is the multigroup cross section input deck for use in MCNP. Mgxs is the equivalent of the PENTRAN input cross section file but for MCNP. The file xsdir contains atomic weight ratios and uses data from the mgxs file in order to complete the material data information.

Running XSMCNP - Linux

XSMCNP is run the same way as on Windows, however there are several differences that are worth mentioning. In Linux all files are case-sensitive. In addition, a dos2unix must be performed on all files to eliminate formatting differences between Windows and Linux. Also, if for whatever reason MCNP complains that the cross section file is missing, it is important to add DATAPATH=/$Path to Data/ to the first line of the xsdir file where the path to the data refers to the mgxs cross section file.

Running MCNP

Files to be placed in the MCNP working directory:

- mgxs
- xsdir
- MCNP input file (for the ZIPPY example the user can use zippy.txt

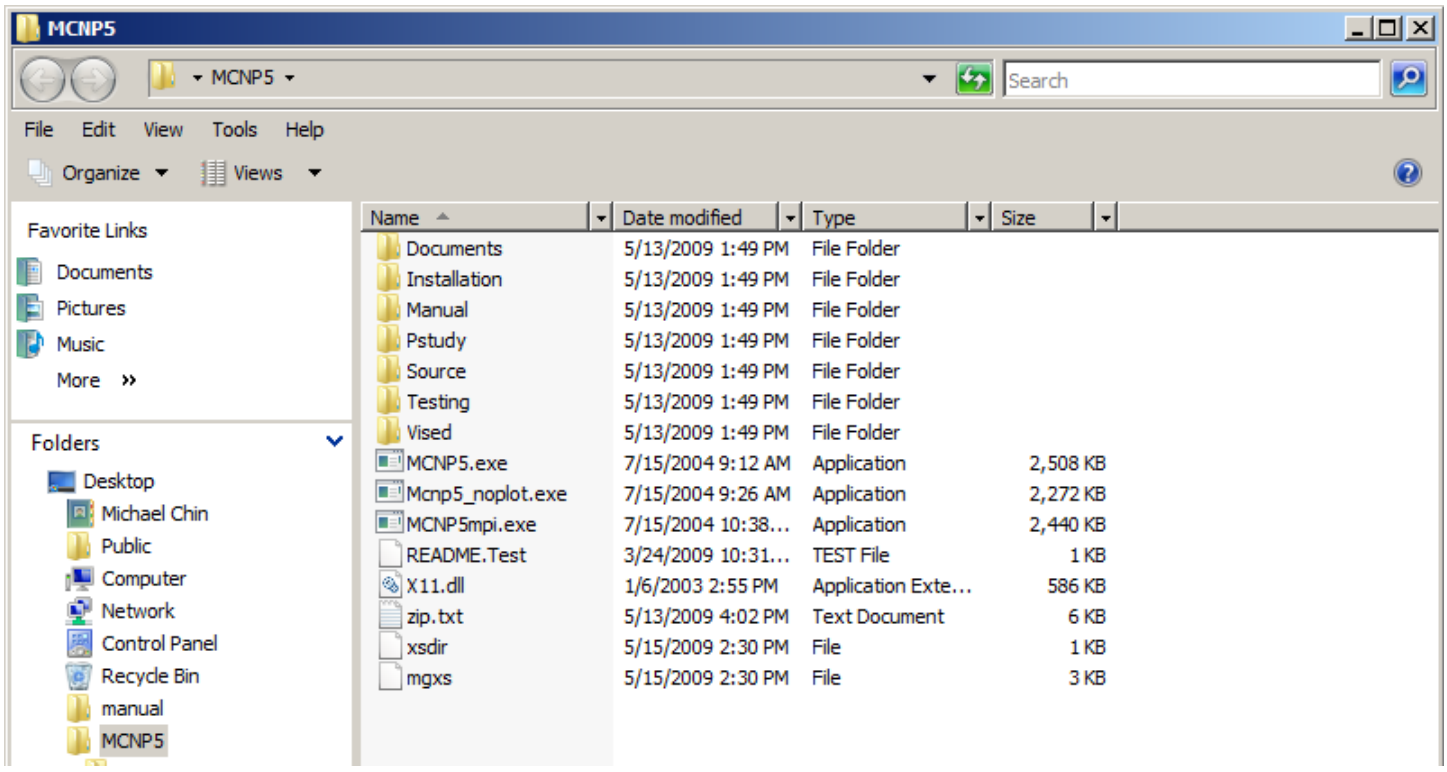


Figure 7: MCNP5 working directory with xsdir and mgxs multigroup cross section files.

Detailed information about the contents of each of these files can be found in the Appendix. At this point it is necessary for the user to copy over the files mgxs, and xsdir into the MCNP working directory. These files will be self referenced when the MCNP does a multigroup analysis on the input file. In order to have MCNP recognize multiple energy groups,

the new material information from mcnp.inp and xsdir must be referenced correctly in the MCNP input file. To do this, the user needs to include the updated information from mcnp.inp shown below into the MCNP input file in place of existing material cards.

```
m1  1000.22m  1.0
m2  2000.22m  1.0
m3  3000.22m  1.0
```

In addition another command option is needed for MCNP to recognize that a multigroup calculation needs to be done. This should be added near the end of the file. The MCNP mgopt card (Multigroup Adjoint Transport OPTion) has two required parameters, MCAL and IGM. MCAL has two possible options, F for forwards and A for adjoint problems and is problem dependent. IGM references the total number of energy groups detailed in the problem. For the ZIPPY example, we reference in the mgopt card and specify it as a forwards problem with 2 energy groups.

```
mgopt  f 2
```

Once this is set up the user is ready to run MCNP. The command to start the multigroup MCNP is the same as when running MCNP normally.

```
C:\Users\mchin\Desktop\MCNP5>mcnp5 i=zippy.txt o=zout.txt
```

The output of this run is shown below in Figure 8.

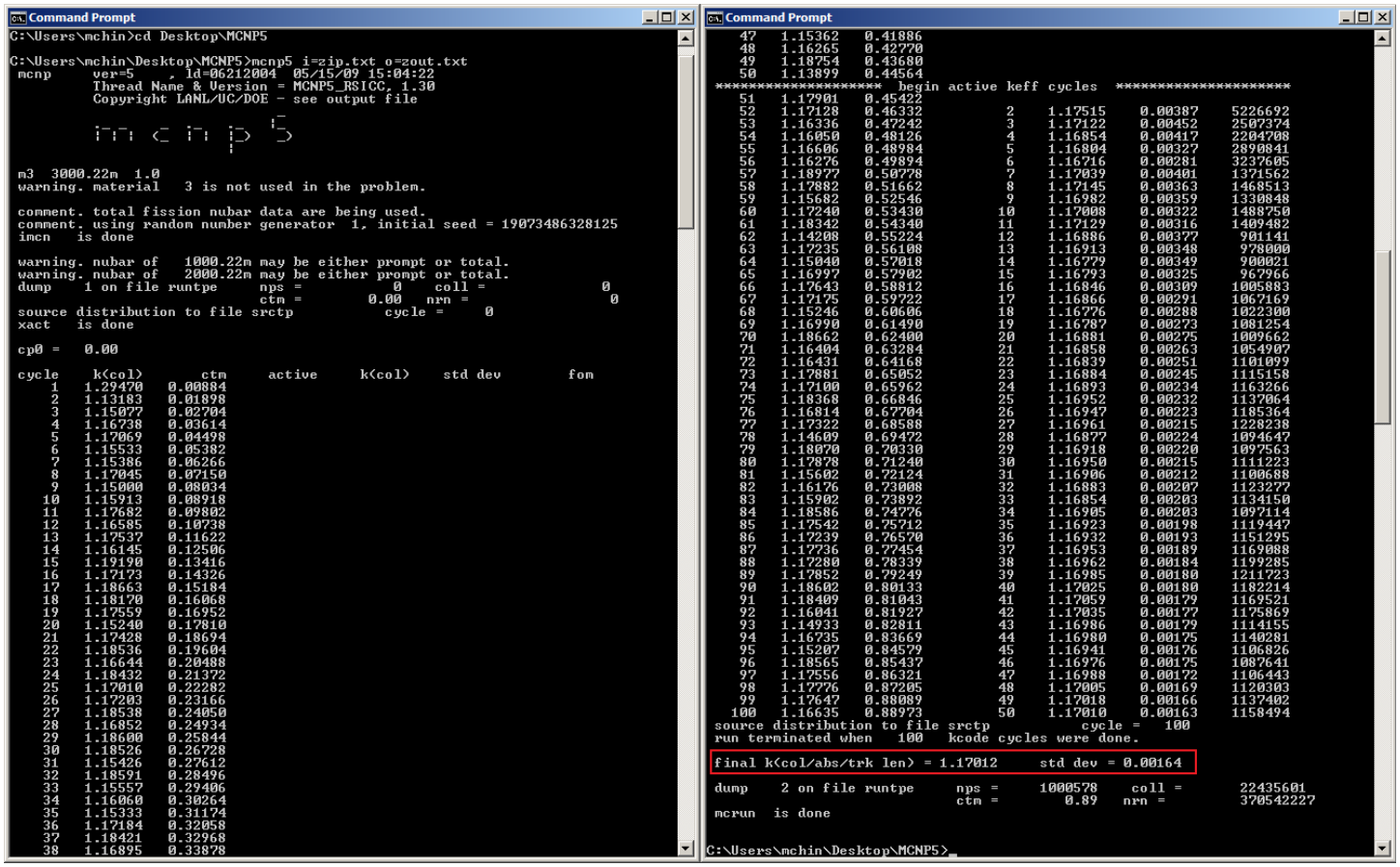


Figure 8: Sample run of ZIPPY reactor, all control rods out. Final result from MCNP indicates a k_{eff} of 1.17012 and a standard deviation 0.00164 with a kcode NSRCK (source histories per cycle) of 10000.

The transport corrected k effective for the ZIPPY reactor for all rods out is approximately 1.171 with inner and outer tolerances of $1x10^{-3}$ and $2x10^{-5}$ respectively. The results show that the MCNP multigroup cross section is within close agreement at 1.17012 with a standard deviation of 0.00164.

Appendix

These files are automatically created when XSMCNP runs. A sample output for zippy.xs is shown below.

mcnp.inp

```
title: sample multigroup input deck with mcard
c generated by xs2mcnp, a code to convert PENTRAN xs (row format P0 only) to MCNP mg format
c group structure, fission chi and nu can be defined by optional input files of xs2mcnp
c group upper boundary defined in a file named : grp_erg.bnd (note: group 1 first)
c fission chi can be defined in a file named : grp_mat.chi note: chi(num_grp, num_mat)
c fission nu can be defined in a file named : grp_mat.nu note: nu(num_grp, num_mat)
c group structure by default is 0.001MeV 1.0 2.0 3.0 ...
c chi by default is 1.0 for the first group, all other groups are zeros
c nu by default is 2.40 if nu_sigmaf (second column) in pentran xs not equal zero
c
c  cell cards
c  set cell density to 1.0, to make micro = macro xs
1    1   1.0  -1   imp:n=1
2      0       1   imp:n=0

c  surface cards
1  rpp  -1.0  1.0  -1.0  1.0  -1.0  1.0

c  source defination
c  point source at (0 0 0) in the first group
sdef erg= 1.50000E+00
c  material cards
m1  1000.22m  1.0
m2  2000.22m  1.0
m3  3000.22m  1.0
c
c  tally cards
f4:n 1
e0     1.000E+00  2.000E+00
c  NOTE: MCNP energy bin from lower energy to higher, so the first bin is the last group
nps  1e3
mgopt   f  2
```

The entries marked in red in the mcnp.inp file need to be inserted into the MCNP input deck shown at the bottom of this appendix. In addition, the cell card density needs to be changed to 1 in the MCNP input deck.

mgxs

```
  1000.22m    2.000000  0.00000E+00   05/14/2009




     19     1000        0        0        2        2        2        0
      0        1        0        1        0        0        0        0
      1        5        7        9       11       13        0        0
      0        0        0        0       15        0        0        0
      0        0        0        0        0        0        0        0
      0        0        0        0        0        0        0        0
1.5000000000000E+00  5.0000000000000E-01  1.0000000000000E+00  1.0000000000000E+00
3.4599998593330E-01  1.4900000095370E+00  3.6229507531970E-03  9.2364527285100E-02
2.4400000572200E+00  2.4360001087190E+00  9.4999998807910E-01  5.0000000745060E-02
1.0888000018890E-02  1.3699999451640E-01                   16  3.1200000643730E-01
2.3099999874830E-02  0.0000000000000E+00  1.3600000143050E+00
 2000.22m    4.000000  0.00000E+00   05/14/2009




     13     2000        0        0        2        2        2        0
      0        1        0        1        0        0        0        0
      1        5        0        0        0        7        0        0
      0        0        0        0        9        0        0        0
      0        0        0        0        0        0        0        0
      0        0        0        0        0        0        0        0
1.5000000000000E+00  5.0000000000000E-01  1.0000000000000E+00  1.0000000000000E+00
3.5400000214580E-01  2.0599999427800E+00  8.3500001346690E-04  2.8500000014900E-02
                10  3.1400001049040E-01  3.8300000131130E-02  0.0000000000000E+00
2.0299999713900E+00
 3000.22m    6.000000  0.00000E+00   05/14/2009




     13     3000        0        0        2        2        2        0
      0        1        0        1        0        0        0        0
      1        5        0        0        0        7        0        0
      0        0        0        0        9        0        0        0
      0        0        0        0        0        0        0        0
      0        0        0        0        0        0        0        0
1.5000000000000E+00  5.0000000000000E-01  1.0000000000000E+00  1.0000000000000E+00
3.4920001029970E-01  1.0000000000000E+00  1.9999999494760E-04  8.0000001192090E-01
                10  3.1000000238420E-01  3.9000000804660E-02  0.0000000000000E+00
2.0000000298020E-01
```

Notice that nubar data (red) is found along the two left hand columns while chi data (blue) is found on the right two hand columns. Top section is fuel, followed by moderator and control rod. Notice that nubar and chi only exist for the fuel, having that information in the moderator and control rods will be unphysical.

xsdir

```
ATOMIC WEIGHT RATIOS
1000   2.000000
2000   4.000000
3000   6.000000
DIRECTORY
1000.22m    2.000000 mgxs 0 1 1 19 0 0   0.00
2000.22m    4.000000 mgxs 0 1 18 13 0 0   0.00
3000.22m    6.000000 mgxs 0 1 34 13 0 0   0.00
```

Sample MCNP Input deck (Quarter core ZIPPY)

```
ZIPPY Quarter Core Reactor
    1     1      1 -20 15 -2 1 8 -9
    2     2      1 -20 15 2 -9 -3 8
    3     2      1 -20 15 3 -9 -4 8
    4     2      1 -20 15 4 -9 -5 8
    5     2      1 -20 15 5 -9 -6 8
    6     1      1 -20 15 6 -9 -7 8
    7     2      1 -20 15 1 -10 -2 9
    8     2      1 -20 15 2 -10 -3 9
    9     2      1 -20 15 3 -10 -4 9
   10     1      1 -20 15 4 -10 -5 9
   11     2      1 -20 15 5 -10 -6 9
   12     1      1 -20 15 6 -10 -7 9
   13     2      1 -20 15 1 -11 -2 10
   14     1      1 -20 15 2 -11 -3 10
   15     2      1 -20 15 3 -11 -4 10
   16     2      1 -20 15 4 -11 -5 10
   17     2      1 -20 15 5 -11 -6 10
   18     1      1 -20 15 6 -11 -7 10
   19     2      1 -20 15 1 -12 -2 11
   20     2      1 15 2 11 -12 -20 -3
   21     2      1 -20 15 3 -12 11 -4
   22     2      1 -20 15 4 -12 -5 11
   23     1      1 -20 15 5 -12 -6 11
   24     1      1 -20 15 6 -12 -7 11
   25     2      1 -20 15 1 12 -2 -13
   26     2      1 -20 15 2 -13 -3 12
   27     2      1 -20 15 3 -13 -4 12
   28     1      1 -20 15 4 -13 -5 12
   29     1      1 -20 15 5 -13 -6 12
   30     1      1 -20 15 6 -13 -7 12
   31     1      1 -20 15 1 -14 -2 13
   32     1      1 -20 15 2 -14 -3 13
   33     1      1 -20 15 3 -14 -4 13
   34     1      1 -20 15 4 -14 -5 13
   35     1      1 -20 15 5 -14 -6 13
   36     1      1 -20 15 6 -14 -7 13
   37     0         -1 :-8 :14 :7 :20 :-15

   *1        px 0
    2        px 5
    3        px 10
    4        px 15
    5        px 20
```

```
    6        px 25
   7        px 30
   *8        pz 0
    9        pz 5
   10        pz 10
   11        pz 15
   12        pz 20
   13        pz 25
   14        pz 30
   *15        py -1
   *20        py 1

mode  n
kcode 10000 1.000000 50 100
ksrc  6.250000 0.000000 1.250000
      6.250000 0.000000 3.750000
      7.500000 0.000000 2.500000
      8.750000 0.000000 1.250000
      8.750000 0.000000 3.750000
      11.250000 0.000000 1.250000
      11.250000 0.000000 3.750000
      12.500000 0.000000 2.500000
      13.750000 0.000000 1.250000
      13.750000 0.000000 3.750000
      16.250000 0.000000 1.250000
      16.250000 0.000000 3.750000
      17.500000 0.000000 2.500000
      18.750000 0.000000 1.250000
      18.750000 0.000000 3.750000
      21.250000 0.000000 1.250000
      21.250000 0.000000 3.750000
      22.500000 0.000000 2.500000
      23.750000 0.000000 1.250000
      23.750000 0.000000 3.750000
      1.250000 0.000000 6.250000
      1.250000 0.000000 8.750000
      2.500000 0.000000 7.500000
      3.750000 0.000000 6.250000
      3.750000 0.000000 8.750000
      6.250000 0.000000 6.250000
      6.250000 0.000000 8.750000
      7.500000 0.000000 7.500000
      8.750000 0.000000 6.250000
      8.750000 0.000000 8.750000
      11.250000 0.000000 6.250000
      11.250000 0.000000 8.750000
      12.500000 0.000000 7.500000
      13.750000 0.000000 6.250000
      13.750000 0.000000 8.750000
      21.250000 0.000000 6.250000
      21.250000 0.000000 8.750000
      22.500000 0.000000 7.500000
      23.750000 0.000000 6.250000
      23.750000 0.000000 8.750000
      1.250000 0.000000 11.250000
      1.250000 0.000000 13.750000
      2.500000 0.000000 12.500000
      3.750000 0.000000 11.250000
      3.750000 0.000000 13.750000
```

```
      11.250000 0.000000 11.250000
      11.250000 0.000000 13.750000
      12.500000 0.000000 12.500000
      13.750000 0.000000 11.250000
      13.750000 0.000000 13.750000
      16.250000 0.000000 11.250000
      16.250000 0.000000 13.750000
      17.500000 0.000000 12.500000
      18.750000 0.000000 11.250000
      18.750000 0.000000 13.750000
      21.250000 0.000000 11.250000
      21.250000 0.000000 13.750000
      22.500000 0.000000 12.500000
      23.750000 0.000000 11.250000
      23.750000 0.000000 13.750000
      1.250000 0.000000 16.250000
      1.250000 0.000000 18.750000
      2.500000 0.000000 17.500000
      3.750000 0.000000 16.250000
      3.750000 0.000000 18.750000
      6.250000 0.000000 16.250000
      6.250000 0.000000 18.750000
      7.500000 0.000000 17.500000
      8.750000 0.000000 16.250000
      8.750000 0.000000 18.750000
      11.250000 0.000000 16.250000
      11.250000 0.000000 18.750000
      12.500000 0.000000 17.500000
      13.750000 0.000000 16.250000
      13.750000 0.000000 18.750000
      16.250000 0.000000 16.250000
      16.250000 0.000000 18.750000
      17.500000 0.000000 17.500000
      18.750000 0.000000 16.250000
      18.750000 0.000000 18.750000
      1.250000 0.000000 21.250000
      1.250000 0.000000 23.750000
      2.500000 0.000000 22.500000
      3.750000 0.000000 21.250000
      3.750000 0.000000 23.750000
      6.250000 0.000000 21.250000
      6.250000 0.000000 23.750000
      7.500000 0.000000 22.500000
      8.750000 0.000000 21.250000
      8.750000 0.000000 23.750000
      11.250000 0.000000 21.250000
      11.250000 0.000000 23.750000
      12.500000 0.000000 22.500000
      13.750000 0.000000 21.250000
      13.750000 0.000000 23.750000
c m1    1001.      -0.111894  $MAT
c      8016.      -0.888106
c m2    92235.         -0.04  $MAT
c       92238.         -0.96
c m3    5010.      -0.782626  $MAT
c       6000.      -0.217374
m2  1000.22m  1.0
m1  2000.22m  1.0
m3  3000.22m  1.0
```

```
imp:n             1 35r                    0  $ 1, 37
mgopt   f  2
print
```