22.251 LAB Exercise 4
PWR Fuel Unit Cell Analysis with MCNP4C

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MCNP Overview

- 48000 lines of Fortran and 1000 lines of C code
- 500 person-years
- Continuously evolving, developed by LANL
- Most current version MCNP5
  - we will use version MCNP4c
- Exact solution of transport equation by simulation of large number of individual particles histories
- Takes time to get accurate results
- Easy to run on many CPUs
  - a factor of 100 speedup is possible

Input file structure

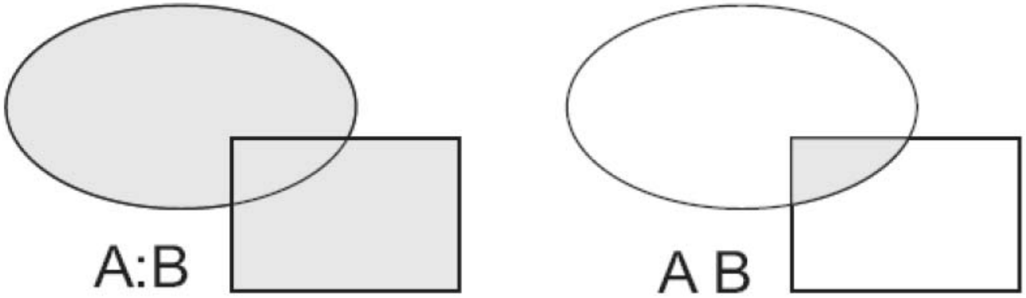
- Title card
- Three blocks:
  - Cell cards [block 1]
  - Surface cards [block 2]
  - Data cards (materials, physics) [block3]
- Each block is separated by a single blank line

General Card Format

- First line of the input deck is a title
- Input lines can not exceed 80 columns
- Insensitive to capital/small letters
- Special characters:
  - C in column 1-5 denotes a comment
  - $ after input data denotes a comment
  - & after input data continuation of previous line
  - Blanks in column 1-5 continuation of previous line

Geometry specification

- Modeled system is represented by a collection of regions (or cells) bounded by surfaces
- Cells are defined by intersections, unions and complements of regions
  - Union (A or B)
  - Intersection (A and B)



(A : B) is all space outside union A and B (complement)

Cell Card Format: Block 1

- ***J M D GEOM PARAMS***
  - J = cell number, starting in columns 1-5
  - M = material number (0 if cell is void)
  - D = cell material density
    - positive = atom number density (atom/barn-cm)
    - negative = mass density (gram/cc)
  - GEOM listed of bounding surfaces
  - PARAMS optional cell parameters

Surface Card Format: Block 2

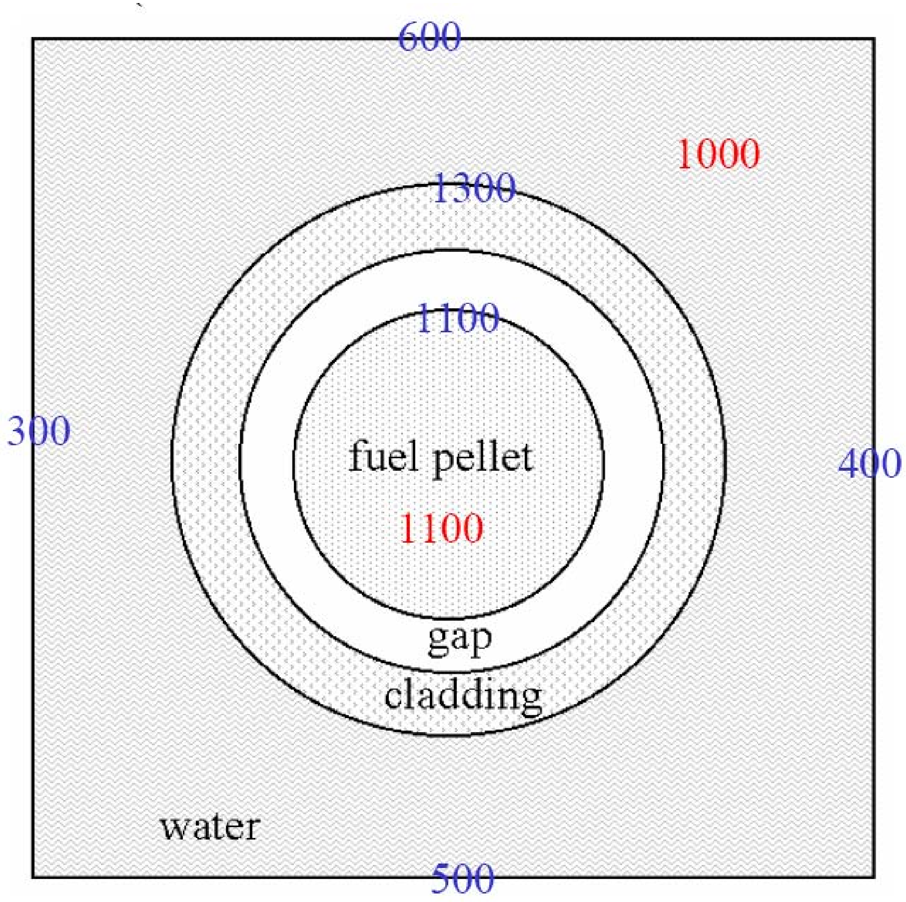
- ***J A LIST***
  - J = surface number, starting in columns 1-5
  - A = surface mnemonic
  - LIST = surface parameters
- Example:
  - cylinder with r = 15 cm, extending along z axis

```
1 cz 15      $ cylinder of radius 15 cm
```

Mnemonic	Type	Description	Equation	Card Entries
P	plane	general	$Ax + By + Cz - D = 0$	$A\ B\ C\ D$
PX		normal to x-axis	$x - D = 0$	D
PY		normal to y-axis	$y - D = 0$	D
PZ		normal to z-axis	$z - D = 0$	D
SO	sphere	centered at origin	$x^2 + y^2 + z^2 - R^2 = 0$	R
S		general	$(x-\bar{x})^2+(y-\bar{y})^2+(z-\bar{z})^2-R^2=0$	$\bar{x}\ \bar{y}\ \bar{z}\ R$
SX		centered on x-axis	$(x - \bar{x})^2 + y^2 + z^2 - R^2 = 0$	$\bar{x}\ R$
SY		centered on y-axis	$x^2 + (y - \bar{y})^2 + z^2 - R^2 = 0$	$\bar{y}\ R$
SZ		centered on z-axis	$x^2 + y^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{z}\ R$
C/X	cylinder	parallel to x-axis	$(y - \bar{y})^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{y}\ \bar{z}\ R$
C/Y		parallel to y-axis	$(x - \bar{x})^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{x}\ \bar{z}\ R$
C/Z		parallel to z-axis	$(x - \bar{x})^2 + (y - \bar{y})^2 - R^2 = 0$	$\bar{x}\ \bar{y}\ R$
CX		on x-axis	$y^2 + z^2 - R^2 = 0$	R
CY		on y-axis	$x^2 + z^2 - R^2 = 0$	R
CZ		on z-axis	$x^2 + y^2 - R^2 = 0$	R

PWR Unit Cell

```
1100 11 -10.4      (-1100 100 -200)                    $ fuel
1100 10 7.06685e-2 (1300 500 -600 300 -400 100 -200) $ coolant
```



Blue – surface #

Red – cell #

Data specifications: Block 3

- Type of particles
- Problem materials
- Specification of sources
- How results scored (tallies)
- Level of details for physics of particle interactions
- Cross section libraries
- …. and much more

Materials specification

- Material unique number
- Elemental (isotopic) composition
- Cross section compilation to be used
- ID number = ZZZAAA

```
m11   8016.50c 4.64149E-02
     92234.86c 8.49269E-06
     92235.54c 1.05705E-03
     92238.86c 2.21413E-02
```

Cross section library specification

- Cross section data tables
  - Section III of Chapter 2 of MCNP manual
  - List of cross sections – Appendix G, Table G2
- Sometimes available for elements
  - 24000.60c – natural chromium
- Sometimes natural elements need to be put together from isotopes
- The physics of XS temperature dependence
  - only partially treated by MCNP
  - XS available mostly for 300K
  - Scattering is treated but not $S(\alpha,\beta)$
  - Absorption Doppler effect – XS lib should be generated for each temperature

Tally specifications

- Surface current tally, F1
  - Each time particle crosses a surface, it is added to the tally
- Average surface flux tally, F2
- Average cell flux tally, F4

$$\mathrm{F1} = \int_A dA \int_E dE \int_{4\pi} d\Omega \, \mathbf{n}\bullet\mathbf{J}(\mathbf{r}_s, E, \boldsymbol{\Omega})$$

$$\mathrm{F2} = \frac{1}{A} \int_A dA \int_E dE \int_{4\pi} d\Omega \, \Phi(\mathbf{r}_s, E, \boldsymbol{\Omega})$$

$$\mathrm{F4} = \frac{1}{V} \int_V dV \int_E dE \int_{4\pi} d\Omega \, \Phi(\mathbf{r}, E, \boldsymbol{\Omega})$$

F4 Tally example

```
 F4:N CELL#
FC4:N YOUR COMMENTS HERE
 E4:N 0.5E-6 20         $ ENERGY STRUCTURE
FM4:N 1.0 1000 (-6)     $ MULTIPLIERS
```

$$C\int \varphi(E) R_m(E)\,dE$$

−1 total cross section without thermal
−2 absorption cross section
−3 elastic cross section without thermal
−4 average heating number (MeV/collision)
−5 gamma-ray production cross section, barns
−6 total fission cross section
−7 fission ν
−8 fission Q (MeV/fission)

MCNP output tables

- Input listing
- Summary of particle loss/creation
- Summary of kcode (neutron criticality)
- Tallies and tally fluctuation charts
- Output controlled by print command
  - `print            $ produce everything`
  - `print 110        $ print basic + table 110`
  - `print -110       $ All tables except 110`

Summary of output tables

Table No.	Table Description	Table No.	Table Description
10	Source information	120	Importance function analysis
20	Weight windows information	126	Cell particle activity
30	Tally descriptions	128 *(b)*	Universe map
35	Coincident detectors	130	Particle weight balances
40	Material compositions	140	Neutron/photon nuclide activity
50	Cell vols & masses; surface areas	150	DXTRAN diagnostics
60 *(b)*	Cell importances	160 *(d)*	TFC bin tally analysis
62 *(b)*	Forced coll.; expon. transform	161 *(d)*	$p(x)$ tally PDF plot
70	Surface coefficients	162 *(d)*	Cumulative $p(x)$ plot
72 *(b)*	Cell temperatures	170	Source frequency; surface source
85	Electron range & straggling	175	Estimated k_{eff} by cycle
90	KCODE source data	178	Estimated k_{eff} by batch size
98	Physics const.& compile options	180	WWG bookkeeping summary
100 *(b)*	Cross section tables	190 *(b)*	WWG summary
102	$S(\alpha, \beta)$ nuclide assignment	198	WW from multigroup fluxes
110	First 50 starting histories	200 *(b)*	WW generated windows

(d) = default, (b) = basic

MCNP statistics

- Relative error
  - Important but not sufficient information

Range of R	Quality of Tally
> 0.5	Meaningless
0.2 to 0.5	Factor of a few
< 0.1	Reliable (except for point/ring detectors)
< 0.05	Reliable even for point/ring detectors

- Figure of Merit
  - should remain constant after early cycles

$$\mathrm{FOM} = \frac{1}{R^2 T},$$

T-run time

MCNP statistics

- Variance of variance (VOV)
  - R indicates precision of the tally mean
  - VOV indicates how accurate is the estimate of R
  - Hence relative variance of R calculated
  - VOV should be always less than 0.1 for all tallies

$$\mathrm{VOV} = \frac{S^2(S_{\overline{x}}^2)}{S_{\overline{x}}^2} = \frac{\sum_{i=1}^{N}(x_i - \overline{x})^4}{\left[\sum_{i=1}^{N}(x_i - \overline{x})^2\right]^2} - \frac{1}{N}.$$

Example of tally fluctuation chart

	tally 4					tally 14				
nps	mean	error	vov	slope	fom	mean	error	vov	slope	fom
16000	2.5565E-19	0.1546	0.0460	0.0	13	1.6147E-20	0.1550	0.0990	0.0	13
32000	2.6267E-19	0.1057	0.0219	0.0	14	1.5614E-20	0.1098	0.0404	0.0	13
48000	2.9321E-19	0.0822	0.0129	10.0	15	1.5964E-20	0.0868	0.0228	0.0	13
64000	2.9096E-19	0.0725	0.0108	10.0	14	1.6062E-20	0.0760	0.0189	0.0	13
80000	2.9088E-19	0.0655	0.0086	10.0	14	1.6037E-20	0.0687	0.0161	4.9	13
96000	2.9487E-19	0.0595	0.0072	10.0	14	1.5578E-20	0.0631	0.0130	2.7	13
112000	2.9758E-19	0.0545	0.0061	10.0	15	1.5749E-20	0.0571	0.0105	3.0	13
128000	3.0167E-19	0.0509	0.0052	10.0	15	1.5970E-20	0.0528	0.0086	2.7	14
144000	3.0142E-19	0.0483	0.0050	10.0	14	1.5824E-20	0.0496	0.0075	2.7	14
160000	3.0284E-19	0.0461	0.0046	10.0	14	1.6205E-20	0.0465	0.0064	2.8	14
176000	3.0391E-19	0.0443	0.0042	10.0	14	1.6276E-20	0.0441	0.0056	3.2	14
192000	3.0143E-19	0.0427	0.0040	10.0	14	1.6351E-20	0.0420	0.0050	3.5	14
200000	3.0080E-19	0.0420	0.0040	10.0	14	1.6317E-20	0.0410	0.0048	3.9	14

Ten statistical tally tests

Tally Mean, x:

1. The mean must exhibit, for the last half of the problem, only random fluctuations as N increases. No up or down trends must be exhibited.

Relative Error, R:

2. R must be less than 0.1 (0.05 for point/ring detectors).
3. R must decrease monotonically with N for the last half of the problem.
4. R must decrease as $1/\sqrt{N}$ for the last half of the problem.

Variance of the Variance, VOV:

5. The magnitude of the VOV must be less than 0.1 for all types of tallies.
6. VOV must decrease monotonically for the last half of the problem.
7. VOV must decrease as $1/N$ for the last half of the problem.

Figure of Merit, FOM:

8. FOM must remain statistically constant for the last half of the problem.
9. FOM must exhibit no monotonic up or down trends in the last half of the problem.

Tally PDF, $f(x)$:

10. The SLOPE determined from the 201 largest scoring events must be greater than 3.

Tally Normalization

- Tallied results
  - Flux in units of n/cm^2/f-s-n
  - Reaction rates in n-barn/cm^2/f-s-n
  - f-s-n(fission source neutron) is directly proportional to power
- Normalization constant will be
  - FMF = $(P \times \nu)/(Q \times k_{eff})$
- P = power (Watts)
- ν = average number of neutrons per fission
- Q = 200Mev $\times$ 1.602 $\times$ 10^{-13} [J/MeV]
- k_{eff} = eigenvalue = $\nu \times$ (f-loss to fission)/f-src

Running MCNP

- Located on MIGHTYALPHA
- Command
  - `mcnp4c3 i=input.in o=outp.out`
  - `outp.out – output file`
- Other outputs
  - `runtpe` – binary restart file
  - `mctal` – separate tally file
- File name must be less than 8 characters

MCNP input file for Lab 04

```
REPRESENTATIVE PWR UNIT CELL (4.5 w/o UO2 FUEL) -for solution
c
c CELL DEFINITIONS
c
1000 10 7.06685e-2 (1300 500 -600 300 -400 100 -200) imp:n=1 tmp=5.0246e-8 $ Water
1100 11 -10.4      (-1100 100 -200)                  imp:n=1 tmp=7.7553e-8 $ fuel pin
1200 12 1.00000e-4 (1100 -1200 100 -200)             imp:n=1 tmp=2.53e-8   $ Gap
1300 13 4.34418e-2 (1200 -1300 100 -200)             imp:n=1 tmp=5.3512e-8 $ Clad
9999  0            (-100:200:-300:400:-500:600)      imp:n=0 tmp=2.53e-8   $ External Void
c
c BLANK LINE MUST FOLLOW

c SURFACE DEFINITIONS
c
*100 pz -2.00   $ bottom of active core
*200 pz  2.00   $ top of active core
*300 px -0.63   $ low-x edge of unit cell
*400 px  0.63   $ high-x edge of unit cell
*500 py -0.63   $ low-y edge of unit cell
*600 py  0.63   $ high-y edge of unit cell
1100 cz  0.4096 $ Fuel Pin
1200 cz  0.4178 $ Gap
1300 cz  0.4750 $ Clad
c
c BLANK LINE MUST FOLLOW
```

MCNP input file for Lab 04

```
c DATA
c
c H2O
m10 8016.50c 1.0 1001.50c 2.0
mt10 lwtr.04t
c
c 4.5 w/o UO2
m11   8016.50c 4.64149E-02
     92234.86c 8.49269E-06
     92235.54c 1.05705E-03
     92238.86c 2.21413E-02
c Helium
m12 2004.50c 1.0
c Zircaloy-4
m13 40000.60c 1.0
c
ksrc 0.0 0.0 -1.0
     0.0 0.0  0.0
     0.0 0.0  1.0
```

MCNP input file for Lab 04

```
c
c tally materials
m1000 92235.54c 1.0
m1001 92238.86c 1.0
c
c Reaction Rates
fc4 reaction rates
f4:n 1100
sd4  2.10829
e4   0.625E-6 20.0 T
fm4 (1.0 1000 (-6))(1.0 1001 (102))
c
c
mode n
kcode 5000 1.0 5 150
prdmp 150 150 150
print
```