Introduction to MCNP

Pavel Hejzlar

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Overview

- 48000 lines of Fortran and 1000 lines of C code (500 person-years)
- Continuously evolving, by LLNL (now version 5, we will use version 4c)
- Exact transport solution, but takes time
- Successfully parallelized, a factor of 100 speedup is possible

Manual

OAK RIDGE NATIONAL LABORATORY

managed by
UT-BATTELLE, LLC
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U.S. DEPARTMENT OF ENERGY

RSICC COMPUTER CODE COLLECTION

MCNP4C

Monte Carlo N-Particle Transport Code System

Contributed by:

Los Alamos National Laboratory
Los Alamos, New Mexico

RADIATION SAFETY INFORMATION COMPUTATIONAL CENTER

Input Deck

Title card

Three blocks (jungles of numbers):

```
Cell cards [block 1]

Surface cards [block 2]

Data cards (materials, physics) [block3]
```

Note that each part is separated by a single blank line.

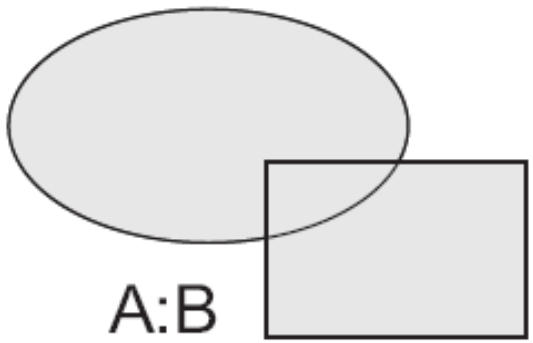
General Card Format

- First line of the input deck is title line
- 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 cont. of prev. line
  - blanks column 1-5 cont. of prev. line

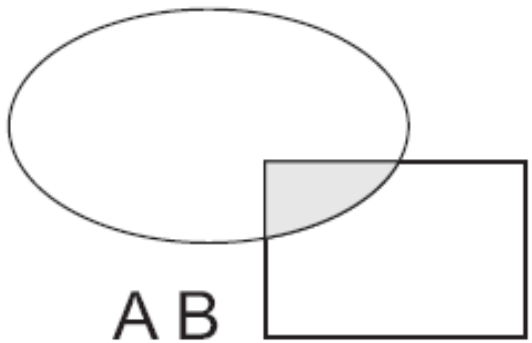
Geometry specification

- Problem treated in terms of regions or volumes (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)

Basic 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

* no entry if cell is a void
* positive entry = atom number density (atom/barn-cm)
* negative entry=mass density (gram/cc)

GEOM=listed of bounding surfaces

PARAMS=optional cell parameters

Basic Surface Card Format – Block 2

J A LIST

J=surface number, starting in columns 1-5

A=surface mnemonic

LIST=surface parameters

Example: a cylinder with a radius of 15 cm, extending with a z axis

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

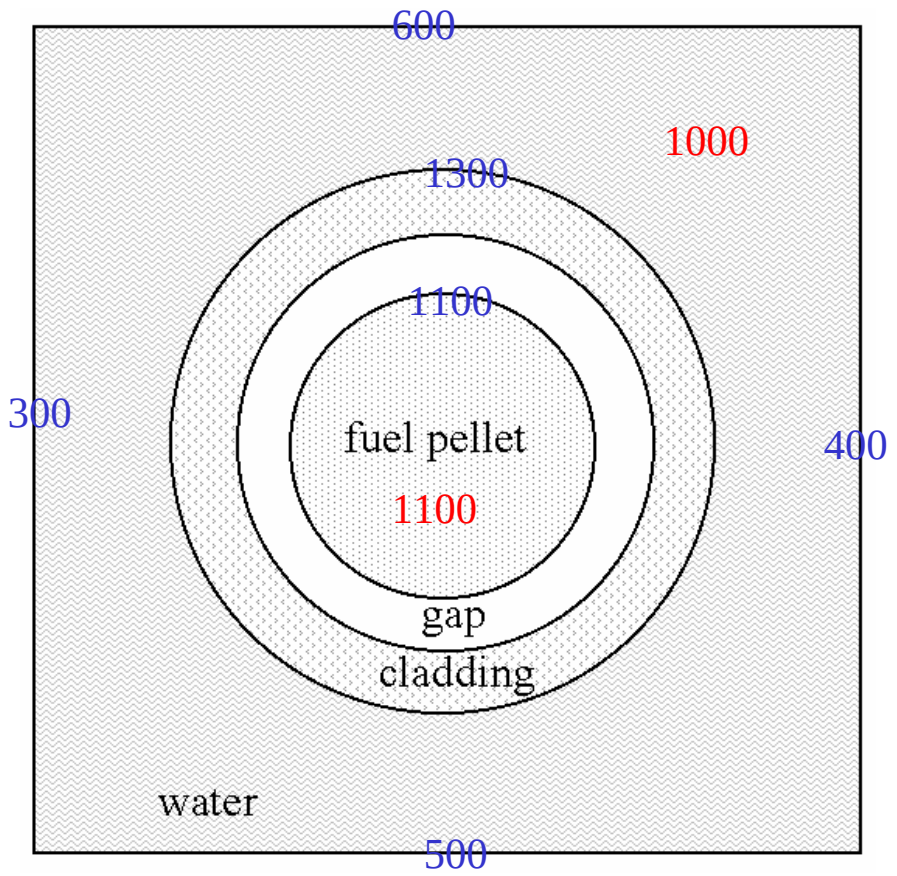
Key Surface Cards

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 Lattice

1100 11 -10.4 (-1100 100 -200) $ fuel pin definition

1000 10 7.06685e-2 (1300 500 -600 300 -400 100 -200) $coolant



Blue – surface #

Red – cell #

Data specifications – Block 3

Defines:

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

Materials specification

Defines:

- Material unique number
- The elemental (isotopic) composition
- Cross section compilation to be used

ZAID number = ZZZAAA (ZZZ=atomic #Z, AAA=mass #A)

```
c ---------------------------------------------------------
c WATER for neutron transport (by mass fraction)
c       (ignore H-2, H-3, O-17, and O-18)
c ---------------------------------------------------------
M1    1001.60c  -0.11190     $ H-1  and mass fraction
      8016.60c  -0.88810     $ O-16 and mass fraction
```

Cross section specification

- Cross section data tables
  - Section III of Chapter 2 of MCNP manual
- Comprehensive 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
- Watch out for temperatures
  - Xsections available mostly for 300K
  - Doppler broadening important – if library at given temperature not available, needs to be generated using NJOY

Tally specifications

- Surface current tally F1

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

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

  - Each time particle crosses a surface, it is added to tally
- Average surface flux tally, F2

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

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

Tally specifications

- Average cell flux tally, F4

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

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

F4 Tally example

F4:N *CELL#*

FC4:N YOUR COMMENTS HERE

E4:N 0.5E-6 20 $ ENERGY STRUCTURE

FM4:N *MULTIPLIERS*

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

Output tables available

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(α, β) nuclide assignment	198	WW from multigroup fluxes
110	First 50 starting histories	200*(b)*	WW generated windows

(d) = default, (b) = basic

MCNP statistics

- 1- relative error

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

  - Important but not sufficient information
- 2-figure of merit

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

FOM should remain constant after early cycles

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

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

  - VOV should be always less than 0.1 for all tallies

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, $\overline{x}$:

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/cm2/f-s-n
  - Reaction rates in n-barn/cm2/f-s-n
- f-s-n (fission source neutron) is directly proportional to power
- Normalization constant will be

$$(P*\nu)/(Q*k_{eff})$$

P=power (Watts)

ν =average number of neutrons per fission

$Q=200Mev*1.602x10^{-13}$ [J/MeV]

k_{eff}=eigenvalue= ν *(f-loss to fission)/f-src

Running MCNP

- Located on MIGHTYALPHA
- Command
  - mcnp4c3 inp=input.in out=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) $ Unit Cell Water
       imp:n=1 imp:p=1 tmp=5.0246e-8
 1100  11 -10.4     (-1100 100 -200)                  $ fuel pin
       imp:n=1 imp:p=1 tmp=7.7553e-8
 1200  12 1.00000e-4 (1100 -1200 100 -200)             $ Gap
       imp:n=1 imp:p=1 tmp=2.53e-8
 1300  13 4.34418e-2 (1200 -1300 100 -200)             $ Clad
       imp:n=1 imp:p=1 tmp=5.3512e-8
 9999  0            (-100:200:-300:400:-500:600)      $ External Void
       imp:n=0 imp:p=0 tmp=2.53e-8
c
c      BLANK LINE MUST FOLLOW
```

MCNP input file for lab 04 (Cont.)

```
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
```

MCNP input file for lab 04 (Cont.)

```
c          DATA
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 (Cont.)

```
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   1500    1.01   5   150
prdmp   150 150 150
print
```