Monte Carlo Theory & Practice (MCNP)

For Radiation Transport Solutions

Lecture 2

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Lecture 2 Summary

- Material Definitions
- Source
- Tallies

Mode – what is MCNP simulating?

MODE N *neutrons only*

MODE P *photons only*

MODE E *electrons only*

MODE N P *neutrons and photons [can have neutron-induced photons, (n,γ)]*

MODE P E *photons and electrons [photon-induced electrons, e.g. Compton scatter, pair production]*

MODE N P E *all three, including induced production*

Data Cards - Materials

Mm $ZAID_1$ $fraction_1$ $ZAID_2$ $fraction_2$ ....

m is a unique material number

ZAID is a code to represent the atoms of the material

ZAID = zaaa.nnX

z= atomic number (1 or 2 digits)

aaa=3 digit atomic weight (can use 000 for photons)

nn = a 2 digit number representing the nuclear data library

X = C for continuous energy data (usually recommended), D for discreet energy library, m for multigroup cross-sections, y for “dosimetry” data

$fraction_k$ is the atom fraction for the k^{th} listed atom

If *fraction* is negative, then it is interpreted as weight fraction

Source – SDEF Card

Can be very complex distributions in space, energy, angle and time.

Can have dependent distributions

Angle-dependent energy distributions

Spatially varying particle distributions

Volume sources, surface sources, line sources & point sources

SDEF Card

SDEF source variable = specification ....

Source variables are as listed below

Specification depends on variable, “=“ is optional

1. explicit value,
2. a distribution number prefixed by a D, or
3. the name of another variable prefixed by an F, followed by a distribution number prefixed by a D. Var = Dn means that the value of source variable var is sampled from distribution n. Var Fvar′ Dn means that var is sampled from distribution n that depends on the variable var′. Only one level of dependence is allowed. Each distribution may be used for only one source variable.

Three levels of source description:

1 Source variable has a single explicit value (e.g. ERG=14.0)

2 Source variable has a probabilistic distribution (e.g. DIR=D1)

This requires SI and SP cards to define the distribution

3 Source variable depends on selected value of another variable

Requires use of DS card e.g. DIR=D1 ERG=FDIR D2

SDEF Card

- Read source specification section of Chapter 3 of the manual
- A source particle needs to know
  - What it is (N, P or E)
  - Where it is (x, y, z and which cell) – don’t start exactly on a cell surface
  - Where it is going (u, v, w vectors)
  - What energy is has
  - What weight it has (usually 1.0)

SDEF Card Variables

Variable	Meaning	Default
CEL	Cell	Determined from XXX, YYY, ZZZ and possibly UUU, VVV, WWW
SUR	Surface	Zero (means cell source)
ERG	Energy (MeV)	14 MeV
TME	Time (shakes)	0

Variable	Meaning	Default
DIR	μ, the cosine of the angle between VEC and UUU, VVV, WWW (Azimuthal angle is always sampled uniformly in 0° to 360°)	Volume case: μ is sampled uniformly in –1 to 1 (isotropic) Surface case: *p(μ)* = 2μ in 0 to 1 (cosine distribution)
VEC	Reference vector for DIR	Volume case: required unless isotropic Surface case: vector normal to the surface with sign determined by NRM
NRM	Sign of the surface normal	+ 1
POS	Reference point for position sampling	0,0,0
RAD	Radial distance of the position from POS or AXS	0
EXT	Cell case: distance from POS along AXS Surface case: Cosine of angle from AXS	0
AXS	Reference vector for EXT and RAD	No direction
X	x-coordinate of position	No X
Y	y-coordinate of position	No Y
Z	z-coordinate of position	No Z
CCC	Cookie-cutter cell	No cookie-cutter cell
ARA	Area of surface (required only for direct contributions to point detectors from plane surface source.)	None
WGT	Particle weight	1
EFF	Rejection efficiency criterion for position sampling	.01
PAR	Particle type source will emit	1=neutron if MODE N or N P or N P E 2=photon if MODE P or P E 3=electron if MODE E
TR	Source particle transformation TR=n or distribution of transformations TR=Dn	None

SDEF Example 1

- Gamma line source, discreet energies, isotropic

```
SDEF PAR=P ERG=D1 POS=0 0 0  AXS=0 0 1 EXT=D2
SI1   L   0.662 1.173 1.333  $ Carefully chosen energies
SP1  D  0.5     0.8    0.8    $ Relative emission probability
C
SI2   H  -5.0  0.0  5.0   $ Range of line source in Z(cm)
SP2  D  0.0  0.5   1.0   $ Source strength varies along line
```

Remember that total source is 1.0 – whatever the sum of your relative source strengths

Source – SDEF Card examples

```
SDEF PAR=N ERG=3.2 CEL=4
```

Isotropic 3.2 MeV neutron point source uniformly distributed in cell 4

```
SDEF PAR=P ERG=D1 POS=1.0 1.0 0.0
```

Isotropic photon point source at (1,1,0). Energy distribution defined by D1 e.g.

```
SI1   H 0.01  0.5  1.0  2.0    $ Histogram bin upper boundaries
SP1   D 0.0   0.8  1.3  0.5    $ Prob. of bin selection
```

Note – these probabilities are re-normalised to 1.0

```
SI1   L 0.667   1.35    $ Discreet energy lines (MeV)
SP1   D 0.6     0.333  $ Probability of line selection
```

Source – Built-in Functions

SPn $-f$ a b

n = source distribution number

f = negative number selecting a built-in function e.g. fission source

a & b are parameters for the chosen distribution function

```
SDEF PAR=N ERG=D10 POS=1.0 1.0 0.0
```

Isotropic photon point source at (1,1,0). Energy distribution defined by D10 e.g.

```
SP10 -3 0.965 2.29
```

$\underline{f = -3}$ Watt fission energy spectrum: $p(E) = C \exp(-E/a) \sinh(bE)^{1/2}$.
Defaults: $a = 0.965$ MeV, $b = 2.29$ MeV^{-1}.
See Appendix H page H–3 for additional parameters appropriate to neutron-induced fission in various materials and for spontaneous fission.

Source Built-In Functions

Table 3.4: Built-In Functions for Source Probability and Bias Specification

Source Variable	Function No. and Input Parameters	Description
ERG	–2 *a*	Maxwell fission spectrum
ERG	–3 *a b*	Watt fission spectrum
ERG	–4 *a b*	Gaussian fusion spectrum
ERG	–5 *a*	Evaporation spectrum
ERG	–6 *a b*	Muir velocity Gaussian fusion spectrum
ERG	–7 *a b*	Spare
DIR, RAD, or EXT	–21 *a*	Power law $p(x) = c\|x\|^a$
DIR or EXT	–31 *a*	Exponential: $p(\mu) = ce^{a\mu}$
TME, X, Y, or Z	–41 *a b*	Gaussian distribution of time *t* or position coordinates *x*,*y*,*z*.

See p 3-64 of Manual (96)

Tallies – What do we want to know?

- Particle flux
  - At a surface, over a volume, at a point
- Dose rate
  - Usually derive from flux using a response function
  - Can be calculated explicitly by tracking the energy released as charged particles
- Reaction rate
  - Or interaction rate
  - Derived from flux using cross-section data

Tallies – what do we want to know?

- Everything? – Best to use a deterministic code
- Particle fluxes at specific points (Type 5)
- Fluxes averaged over regions of space (Type 4)
- Fluxes averaged over parts of surfaces (Type 2)
- Number of particles crossing a surface (Type 1)
- Usually we don't actually want flux
  - Dose rate
  - Reaction rate – e.g. fission, absorption, gamma production ….
  - Damage rate ….

Flux Averaged Over a Volume

- MCNP "Cell flux" – Type 4 – a scalar flux
- Can be calculated from "Track length" or "Collision Density" methods

$$\text{Flux } \phi = \int_V \int_t \int_E \phi(\vec{r}, E, t)\, dE\, dt\, \frac{dV}{V}$$

- Flux = particle density x speed

$$\phi(\vec{r}, E, t) = u\, N(\vec{r}, E, t)$$

$$u = ds/dt \quad \therefore \quad \phi\, dt = \phi\, ds/u = N\, ds$$

Flux averaged over a volume

- Scalar flux becomes

$$\phi = \int_V \int_t \int_E N(\vec{r}, E, t)\, ds\, dE\, \frac{dv}{V}$$

- N ds = track length density
- As a sum $\phi = \frac{1}{VN} \sum_i s_i$

- Can set limits on integrals to define energy or time bins

$$\int_{E_{k-1}}^{E_k} dE$$

Particle "Weight"

- Represent how much each particle contributes to the flux
- Introduced through the use of biased sampling
  - "Acceleration" methods depart from analogue Monte Carlo. There are many methods in MCNP
- Each particle, *i*, is assigned a "weight" W_i

$$\phi = \frac{1}{V N} \sum_i S_i W_i$$

Type 4 MCNP Format (cell flux)

Fn4:p C_1 C_2 …. C_i

n = any number from 0 to 99 (tally identifier)

p = particle type (P, N or E)

C_i = cell number(s) – may have several or just one

Use E card to define the energy bins (upper limits)

En4 E_1 E_2 E_3 ….. E_i

The flux averaged over the cell volume(s) – particles/cm^2

FC104 A tally comment (useful for interpreting output)

F104:N 5   6

E104 1.0e-6 1.0e-5 1.0e-4 0.001 0.01 0.1 1.0 10.0

Flux of neutrons averaged over each of cells 5 & 6 binned into energy decades (MeV)

Surface Flux – Type 2

- Special case of track-length cell flux
- Particles with weight W_i
- Crossing surface
- Area = A

$$\varnothing = \sum_i \frac{W_i}{A|\mu|} \cdot \frac{1}{N}$$

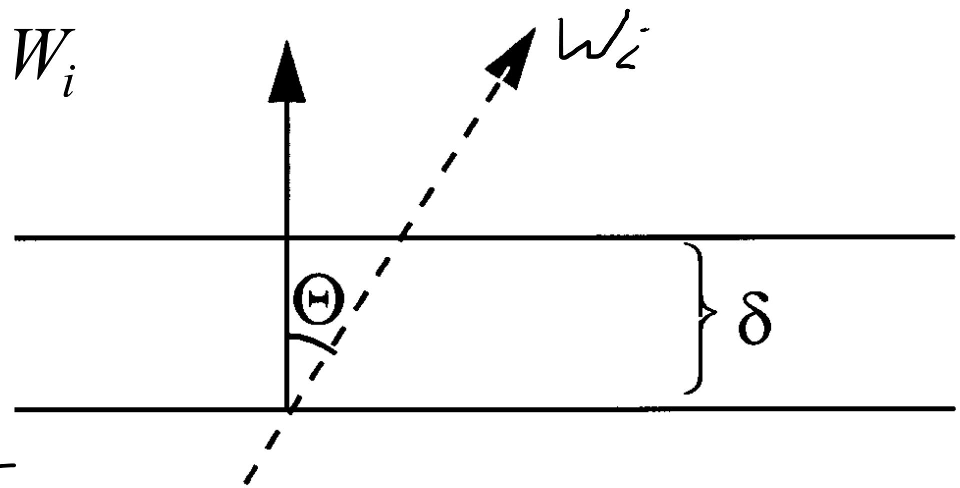

Figure 2-6.

$$F2 = \lim_{\delta \to 0} W T_l / V$$

$$= (W\delta / |cos\theta|)/(A\delta) = W/(A|\mu|)$$

Type 2 MCNP Format (surface flux)

`Fn2:p` S_1 S_2 …. S_i

n = any number from 0 to 99 (tally identifier)

p = particle type (P, N or E)

S_i = surface number(s) – may have several or just one

The flux averaged over the surface(s) – particles/cm^2

`FC212 A tally comment` (useful for interpreting output)

```
F212:P 5  123  10  T
E212  0.02 0.2 0.4 0.6 1.0
```

Flux of photons averaged over each of surfaces 5, 123 & 10

"T" means average flux over all three surfaces is calculated

Energy bins at 20keV, 200keV, 400keV, 600keV, 1MeV

Surface Current – Type 1

- A count of particle crossing the surface

$$\bar{J} = \sum_i w_i \cdot \frac{1}{N}$$

$$\bar{J} / \phi A = \bar{\mu}$$

A measure of how collimated a beam of particles is

For 100% collimated $\bar{\mu}$=1

Type 1 MCNP Format (surface current)

`Fn1:p` S_1 S_2 …. S_i

n = any number from 0 to 99 (tally identifier)

p = particle type (P, N or E)

S_i = surface number(s) – may have several or just one

Simply counts the particles crossing the surface(s)

```
FC11  Current of neutrons exiting the door
F11:N 3  5  10  T
```

Number of neutrons crossing surfaces 3, 5 & 10

“T” means total number over all three surfaces

Flux at a Point – Type 5

- How many particles pass through a point?

$$\phi(\vec{r}, E, t, \mu) = \sum_i \frac{w_i P(\mu) e^{-\lambda}}{N 2\pi R^2}$$

- R = distance from collision to detector
- λ = mean free paths between collision & detector
  - Integrated over all cells between the two points
- $P(\mu)$ = probability of particle scattering into angle of cosine μ

Type 5 MCNP Format (point detector)

Fn5:p x_1 y_1 z_1 $\pm R_{01}$ x_2 y_2 z_2 $\pm R_{02}$ …

n = any number from 0 to 99 (tally identifier)

p = particle type (P or N, but <u>not</u> E)

x_i y_i z_i = coordinates of point i – may have several or just one

R_{0i} = radius of sphere of exclusion

in cm if +ve, in mfp if –ve, can be 0 for a detector in a void

Used to limit high weight contributions from collisions near the detector.

Avoid putting detectors in materials, otherwise use R_0

Must only encompass one material

Tallies – Summary of Units

Type	Particles	Description	Fn Units	*Fn Units
F1	N P E	Surface current	Particles	MeV
F2	N P E	Surface flux	Particles/cm^2	MeV/cm^2
F4	N P E	Cell flux	Particles/cm^2	MeV/cm^2
F5	N P	Point detector	Particles/cm^2	MeV/cm^2
F6	N P E	Energy deposition average over cell	MeV/g	jerks/g
F7	N	Fission energy deposited over a cell	MeV/g	jerks/g
F8	P E or P,E	Energy distribution of pulses in a detector	Pulses	MeV
+F8	E	Charge deposition in a cell	Charge	n/a
1 MeV = 1.602191 x 10^{-22} jerks All tally types except 8 can be modified				

Summary

- More on tallies
- Source definition

Basic Flux Tally

$$\text{Flux } \phi = \int_V \int_t \int_E \phi(\vec{r}, E, t)\, dE\, dt \, \frac{dV}{V}$$

- Each particle, i, is assigned a "weight" W_i
- Track length S_i
- Volume of cell V
- N source particles

$$\phi = \frac{1}{V N} \sum_i s_i W_i$$

Variations on Tallies

Fn4 - cell flux (track length)

*Fn4 – **cell energy-weighted flux**

$$\text{Flux } \phi = \int_V \int_t \int_E E\,\phi(\vec{r}, E, t)\, dE\, dt\, \frac{dv}{V}$$

$$\phi = \frac{1}{VN} \sum_i E_i s_i w_i$$

Variations on Tallies

CFn - Cell flagging

F12:N 5 $ Flux of neutrons crossing surface 5

CF12 1 10 $ Separate tally for those passing through either cell 1 or cell 10

SFn - Surface flagging

F114:P 5 $ Flux of photons in cell 5

SF114 100 $ Separate tally for those which have crossed surface 100

Tally Segmentation

Can be used to subdivide cells or surfaces into sub-tallies

F2:N 1 $ neutron flux over surface 1

FS2 -3 $ Separate tally for those inside surface 3 and those outside

Variations on Tallies

- Tally Multipliers – Response functions
- Enable conversion from fluence to dose or anything

DEn $E_1\ E_2\ E_3\ .....\ E_k$

DFn $F_1\ F_2\ F_3\ .....\ F_k$

The values of *F* represent a pointwise function of energy (*E*). Logarithmic (default) or linear interpolation is used between these values. Use DEn LIN $E_1\ E_2\ E_3\ .....\ E_k$ for linear.

Can be used to calculate any required response function

e.g. dose rate, damage rate, reaction rate, etc.

If value of response function at energy *E* is *R(E)*, then

$$\phi = \frac{1}{VN} \sum_i s_i w_i R(E_i)$$

Table H.2
Photon Flux-to-Dose Rate Conversion Factors

ANSI/ANS–6.1.1–1977		ICRP-21	
Energy, E (MeV)	**DF(E) (rem/hr)/(p/cm^2-s)**	**Energy, E (MeV)**	**DF(E) (rem/hr)/(p/cm^2-s)**
0.01	3.96E–06	0.01	2.78E–06
0.03	5.82E–07	0.015	1.11E–06
0.05	2.90E–07	0.02	5.88E–07
0.07	2.58E–07	0.03	2.56E–07
0.1	2.83E–07	0.04	1.56E–07
0.15	3.79E–07	0.05	1.20E–07
0.2	5.01E–07	0.06	1.11E–07
0.25	6.31E–07	0.08	1.20E–07
0.3	7.59E–07	0.1	1.47E–07
0.35	8.78E–07	0.15	2.38E–07
0.4	9.85E–07	0.2	3.45E–07
0.45	1.08E–06	0.3	5.56E–07

Other Tally Multipliers

- Energy multiplier

EMn $M_1\ M_2\ M_3 \ldots\ldots M_k$

n = tally number

M_k = multiplier for the k^{th} energy bin

- Time bin multiplier *TMn*
- Cosine bin multiplier *CMn* (Type 1 only)

EM0, TM0 or CM0

  - Tally bin multiplier applies to all tallies unless specifically overridden by another EM, TM or CM card

General Tally Multiplier FM Card

- Can specify several multipliers for one tally
  - MCNP reports the results for each
  - i.e. the same tracks are weighted in different ways to achieve different results
  - E.g. to tally several reaction rates in the same cell

FMn (multiplier set 1) (multiplier set 2)

n = tally number

For each multiplier set

C m reaction list

C = multiplicative constant (e.g. atom density)

m = material number (defined on a *Mm* card)

reaction list = list of reaction numbers required

see Appendix G of manual e.g. 102 = (n,γ), 103 = (n,p), 19 = (n,f)

FM Example from Manual

Consider the following input cards.

```
F4:N      10
FM4       0.04786     999  102
M999      92238.13    1
```

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

The F4 neutron tally is the track length estimate of the average fluence in cell 10. Material 999 is ^{238}U with an atomic fraction of 100%.

$C = 0.04786$	normalization factor (such as atom/barn·cm)
$M = 999$	material number for ^{238}U as defined on the material card (with an atom density of 0.04786 atom/barn·cm)
$R_1 = 102$	ENDF reaction number for radiative capture cross-section (microscopic)

The average fluence is multiplied by the microscopic (n,γ) cross section of ^{238}U (with an atomic fraction of 1.0) and then by the constant 0.04786 (atom/barn·cm). Thus the tally 4 printout will indicate the number of ^{239}U atoms/cm^3 produced as a result of (n,γ) capture with ^{238}U.

- Cell 10 need not actually contain material 999
- You can pretend that it does