Monte Carlo Theory & Practice (MCNP)

For Radiation Transport Solutions

Lecture 1

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Course Summary

- Series of five lectures on Monte Carlo theory
  - Introduction - the basics – radiation transport, codes, applications
  - Random numbers – their generation and use
  - Collision modelling
  - Scoring
  - Statistics – interpreting the answers
  - Neutron interactions, Gamma interactions, Electrons?
    - Types on interaction, cross-sections, nuclear data
  - Acceleration
- Parallel MCNP workshops
  - Will therefore intersperse theory with MCNP tutorial
  - MCNP – its main capabilities
  - MCNP "Building Blocks"
    - Sources, tallies, nuclear data
    - Analogue calculations, "accelerated" calculations
    - Fixed source calculations, neutron multiplication, criticality

Boltzmann Transport Equation

$$\frac{1}{v}\frac{\partial \Phi}{\partial t} + \underline{\Omega} \cdot \underline{\nabla} \Phi + \Sigma_t . \Phi = \int_{4\pi} \int \Sigma_s (E' \rightarrow E, \Omega' \rightarrow \Omega) \Phi(E', \Omega') \, dE' \, d\Omega' + S^{+}$$

- Can you identify the terms?

Radiation Transport

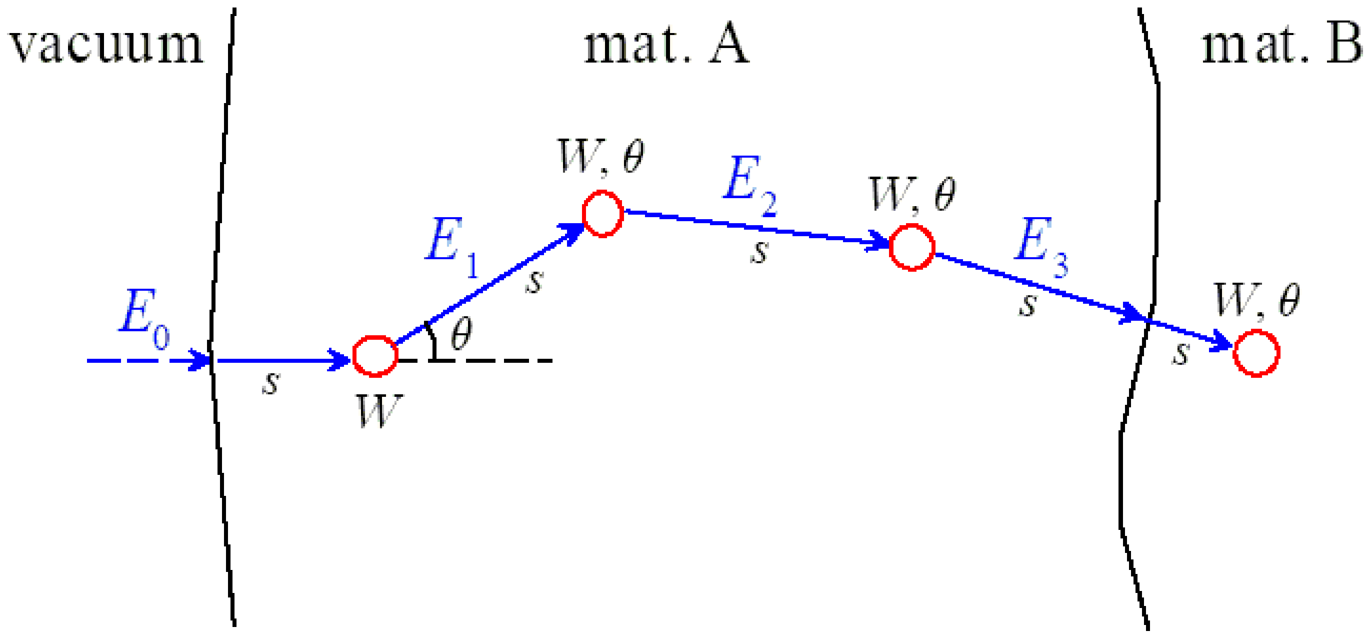
- Cannot usually be solved precisely – approximations required
  - Diffusion equation
  - Discreet ordinates
  - Spherical harmonics
- Why would we want to solve it?
  - Examples?

Monte Carlo - General

- But what if we think we know the physics of individual particle behaviour?
- We can model all the physical processes represented by the transport equation.
- Don’t need to introduce approximations to solve it

Particle Scattering

- All interaction events are simulated in chronological succession:



Monte Carlo - General

- Minimal approximations required
- Can define simple boundary conditions
- Can cope with voids
- But we do need to sample enough particles to
  - Produce good statistical accuracy in the region of interest
  - Make sure that all relevant regions of the problem are adequately sampled (space, energy, angle etc.), so that the simulation is representative of reality

Law of Large Numbers

- Theoretical basis of Monte Carlo
- The weighted average value of the function, $\bar{f}$

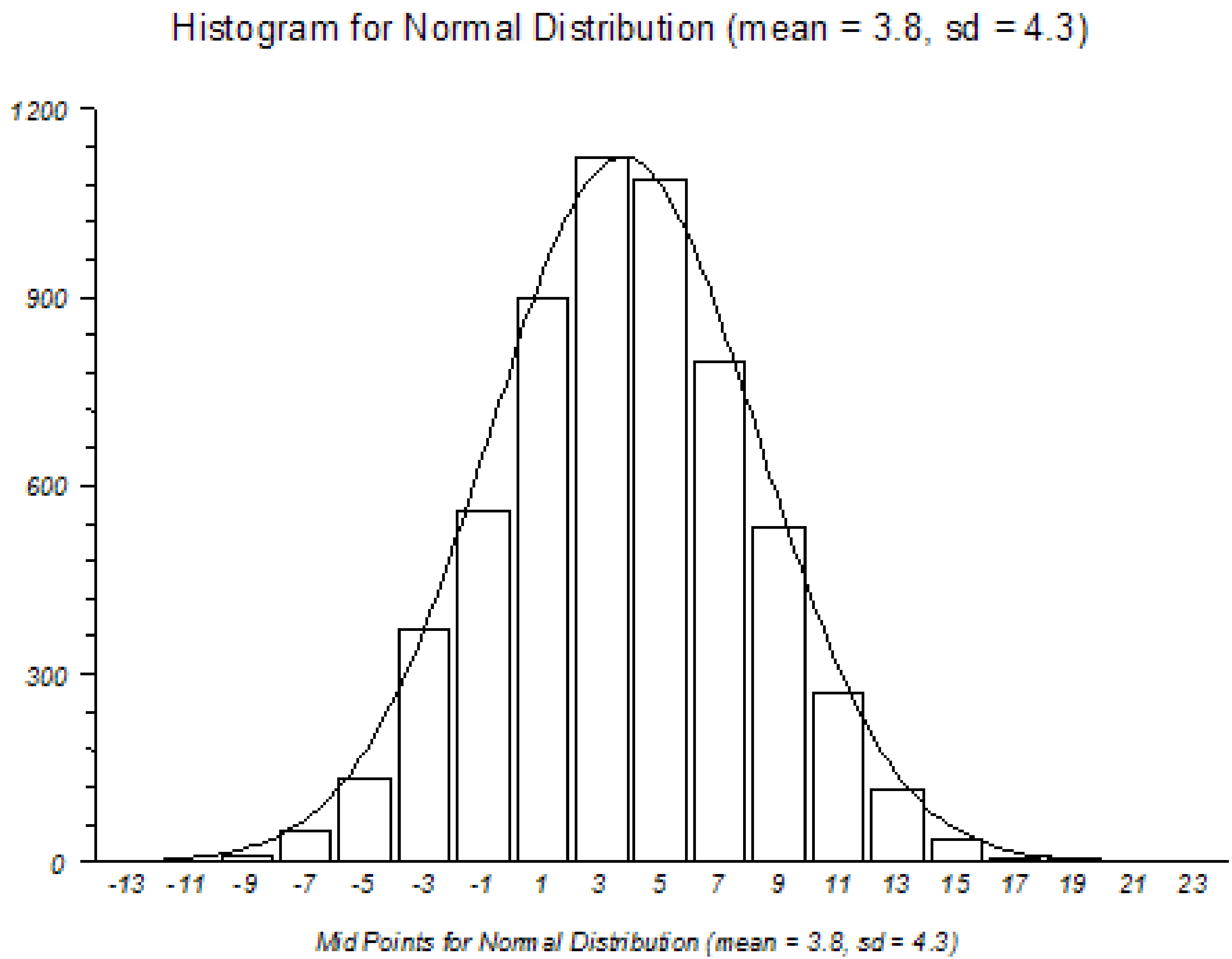
$$\bar{f} = \int_a^b f(x)\,p(x)\,dx = \lim_{N\to\infty} \frac{\sum_{i=1}^{N} f(x_i)}{N},$$

$$\text{where } x_i \text{ are chosen using } p(x)$$

- This relates the result of a <u>continuous</u> integration to the result of a <u>discrete</u> sampling.
- All MC comes down to this

Central limit theorem

- The sum of a sufficiently large number (N) of independent identically distributed random variables <u>eventually</u> becomes normally distributed as N tends to infinity
- This is useful for us because we can draw useful conclusions from the results from a large number of samples
  - (e.g., 68.7% within one standard deviation, etc.)
- But how large is large enough?


Histogram for Normal Distribution (mean = 3.8, sd = 4.3)
1200
900
600
300
0
-13
-11
-9
-7
-5
-3
-1
1
3
5
7
9
11
13
15
17
19
21
23
Mid Points for Normal Distribution (mean = 3.8, sd = 4.3)

Monte Carlo for Radiation Transport

- What particles can we model with Monte Carlo?
    - Just about anything that we think we understand the physics of
        - Photons (x-rays & gammas)
        - Neutrons (fast, epithermal & thermal)
        - Electrons
        - Positrons
        - Muons
        - Protons
        - Ions ...
    - Neutral or charged

Some Monte Carlo Codes

Code	n	γ	e^-	e^+	p^+	ions$^\pm$
MCNP	√	√	√	√	√	
MCBEND	√	√	√			
MONK	√					
TRIPOLI	√	√				
EGS5		√	√	√		
GEANT4	√	√	√	√	√	√
PENELOPE		√	√	√		
TRIM					√	√

Introduction to MCNP

MCNP – Main Capabilities

- Particles
  - Neutrons 10^{-5} eV – 20 MeV
  - Photons 1 keV – 100 GeV
  - Electrons 1keV – 1 GeV
- Full 3D geometry using standard surfaces
  - Repeated geometry features, lattices
- Highly flexible source definition
- Highly flexible scoring methods (tallies)
  - User-defined response functions (e.g. flux to dose)
  - Surface/cell flagging

MCNP – The Building Blocks

- Cell "Cards"
  - Define 3D regions of space
  - Material within each regions, including density
  - Other attributes can also be defined here (importance)
- Surface "Cards"
  - Define the surface used to form the cells
  - Various possibilities
    - Planes, spheres, cones, cylinders, ellipsoids (hyperboloids & parabolas), general quadratic, tori
    - Special attributed can be defined – reflecting or periodic
    - Can be transformed into different coordinate systems
- Data "Cards" – everything else
  - Source definitions, acceleration details, tally definitions, tally modifiers, nuclear data ….

MCNP – The Input File Structure

MESSAGE BLOCK (optional)

TITLE CARD – Text to give your model a title

CELL CARDS – define the cells

SURFACE CARDS – define the surfaces

DATA CARDS – define everything else

C   Comment cards – use anywhere

Card Format (horizontal)

- Limited to 80 characters (columns) per line
  - Continuation lines can be used (end line with " &")
- Alphabetic characters can be upper or lower case
- Cell, surface & data cards begin in 1st 5 columns
- "C " in 1st column, followed by a blank indicates that whole line is a comment
- "$" used to indicate the rest of the line is comment
- Entered in "blocks" – cell, surface, data cards
- Blank lines used a delimiters between blocks
- Integers must be used where an integer is expected
- Where floating point is expected, any format can be used
  - E.g. 10.0 can be written as "10" or "1.0E+01" or "10.000"

Surfaces - examples

Planes (unbounded)

1 PX 1.0 $ plane perpendicular to x-axis at x=1.0

2 PZ −10.2 $ plane perpendicular to z-axis at z=-10.2

6 P x1 y1 z1 x2 y2 z2 x3 y3 z3

plane passing through the 3 points with coordinates (x_1 y_1 z_1) etc.

Spheres (bounded)

10 SO 100.1 $ sphere centred on origin with radius 100.1

11 SY 10.0 3.0 $ sphere centred on (0,10,0) of radius 3.0

15 S 1.5 2 3 2.0 $ sphere centred on (1.5,2,3), radius=2.0

All dimensions are in cm

All parameter need to be separated by at least one space

Only use spaces, DO NOT USE TABS!

Beware of other invisible characters

Surfaces – more examples

Cylinders (unbounded)

1 CY 1.5 $ cylinder along y axis, radius=1.5

10 C/Z 3.0 5.5 2.4 $ cylinder parallel to z axis passing through (3.0,5.5, …), radius=2.4

Cones – on x axis (unbounded)

100 KX x t2 ±1 or K/X x y z t2 ±1

x defines vertex, t=tan(θ), ±1 (optional) defines direction of cone

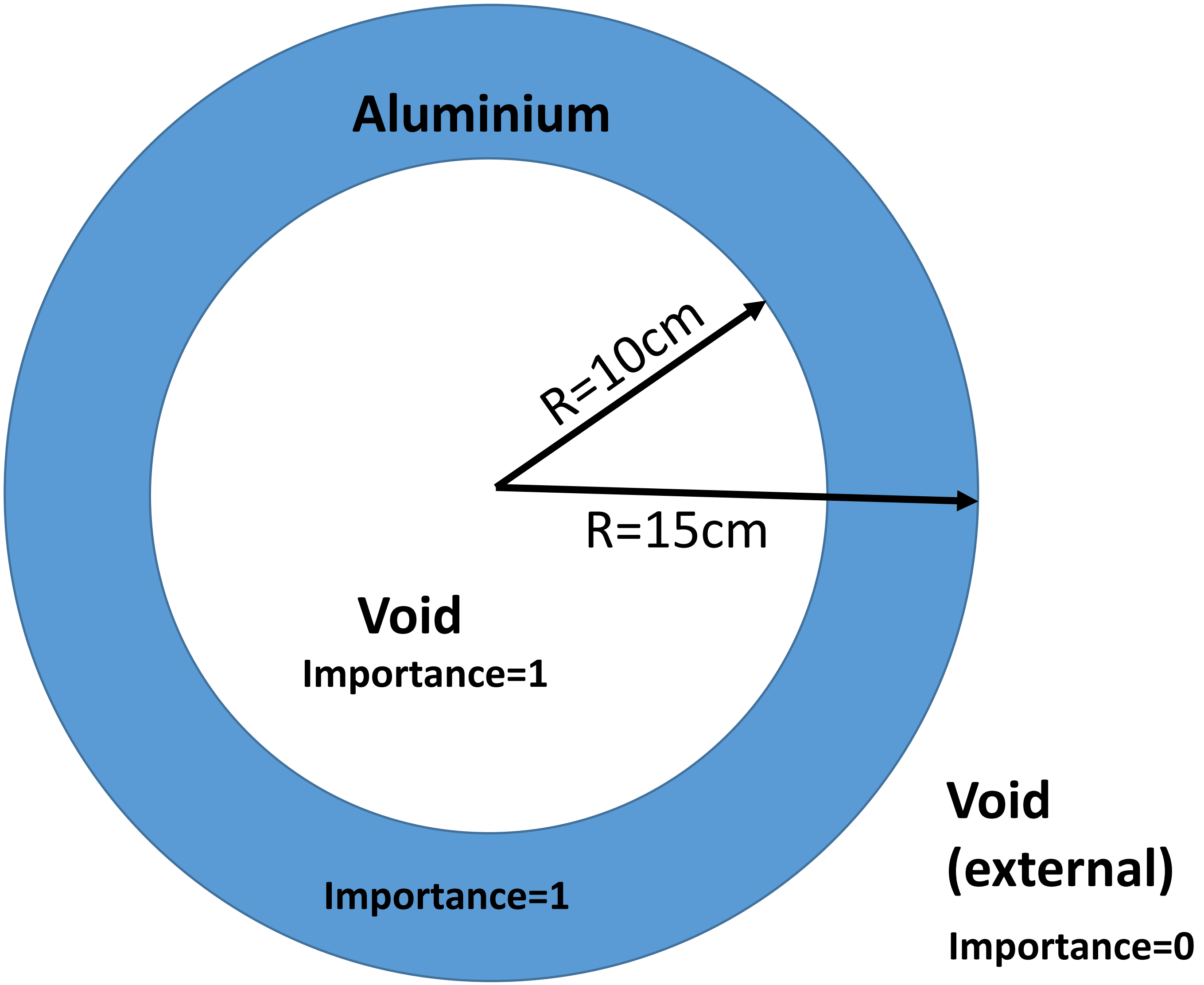
101 KX 3.5 0.25 +1 $cone with vertex at (3.5,0,0), $\theta=\tan^{-1}(0.5)$

102 K/Y 1.0 2.0 1.5 0.09

C double cone with vertex at (1,2,1.5), $\theta=\tan^{-1}(0.3)$

MCNP Geometry

- All space must be defined as something
  - Up to the boundary of your problem
- All cells must:
  - be either void or allocated to a defined material with a chosen density
  - be defined using pre-defined surfaces
    - Using surface numbers and a combination of union (:), intersection ( ) and complement (#) operators
  - have an “importance” for each particle type in the problem


Aluminium
R=10cm
R=15cm
Void
Importance=1
Importance=1
Void
(external)
Importance=0

A Simple Model of an Aluminium Shell Containing a Void

```
C Model created 6/2/16 by DA Allen, last modified 19/11/16
C  The Cell Cards
1    0   -1              $ Void cell inside surface 1
2    1   -2.7  1  -2     $ Shell of m1 outside 1, inside 2, ρ=2.7g/cc
3    0              2    $ Void cell outside surface 2

C  The Surface Cards
1   SO    10.0           $ Sphere centred on origin, rad=10.0
2   SO    15.0           $ Sphere centred on origin, rad=15.0

C Data Cards – just a single material card in this case
MODE  P
IMP:P 1 1 0
M1      13000   1.0   $ Aluminium, 100% pure
```

A simple model of an iron cylinder

C Model created 19/11/16 by DA Allen, last modified 19/11/16

C The Cell Cards

```
1    1   -7.6  -1  2  -3    $ Cylinder of m1, ρ=7.5g/cc
2    0              1:-2:3  $ Void cell outside surface 2
```

C The Surface Cards

```
1   CX    5.0     $ Cylinder along x axis, radius=5.0
2   PX    0.0     $ Plane perpendicular to x axis at x=0.0
3   PX    20.0    $ Plane perpendicular to x axis at x=20.0
```

C Data Cards – just a single material card in this case

```
MODE  P
IMP:P 1  0
M1     26000   1.0   $ Iron, 100% pure
```

Data Cards - Materials

Mm $\quad$ *$ZAID_1$ $fraction_1$ $ZAID_2$ $fraction_2$* ....

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

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*