Monte Carlo Theory & Practice (MCNP)

For Radiation Transport Solutions

Lecture 3

Dr Dennis Allen

Lecture 3 Summary

- Random numbers
- Probability distribution sampling
- Particle interactions
- More on tallies

Random Number Generation

- What is Monte Carlo famous for?
- Random number generation
  - The heart of any Monte Carlo method

“Random number generation is too important to be left to chance”

Robert R Coveyou, Research Mathematician, ORNL

Pseudo-random number generation

Pseudo RNG (or deterministic RNG)

Algorithm for generating a sequence of numbers whose distribution appears to be random

Needs to be “seeded” to start the sequence

Can we ever have a true RNG?

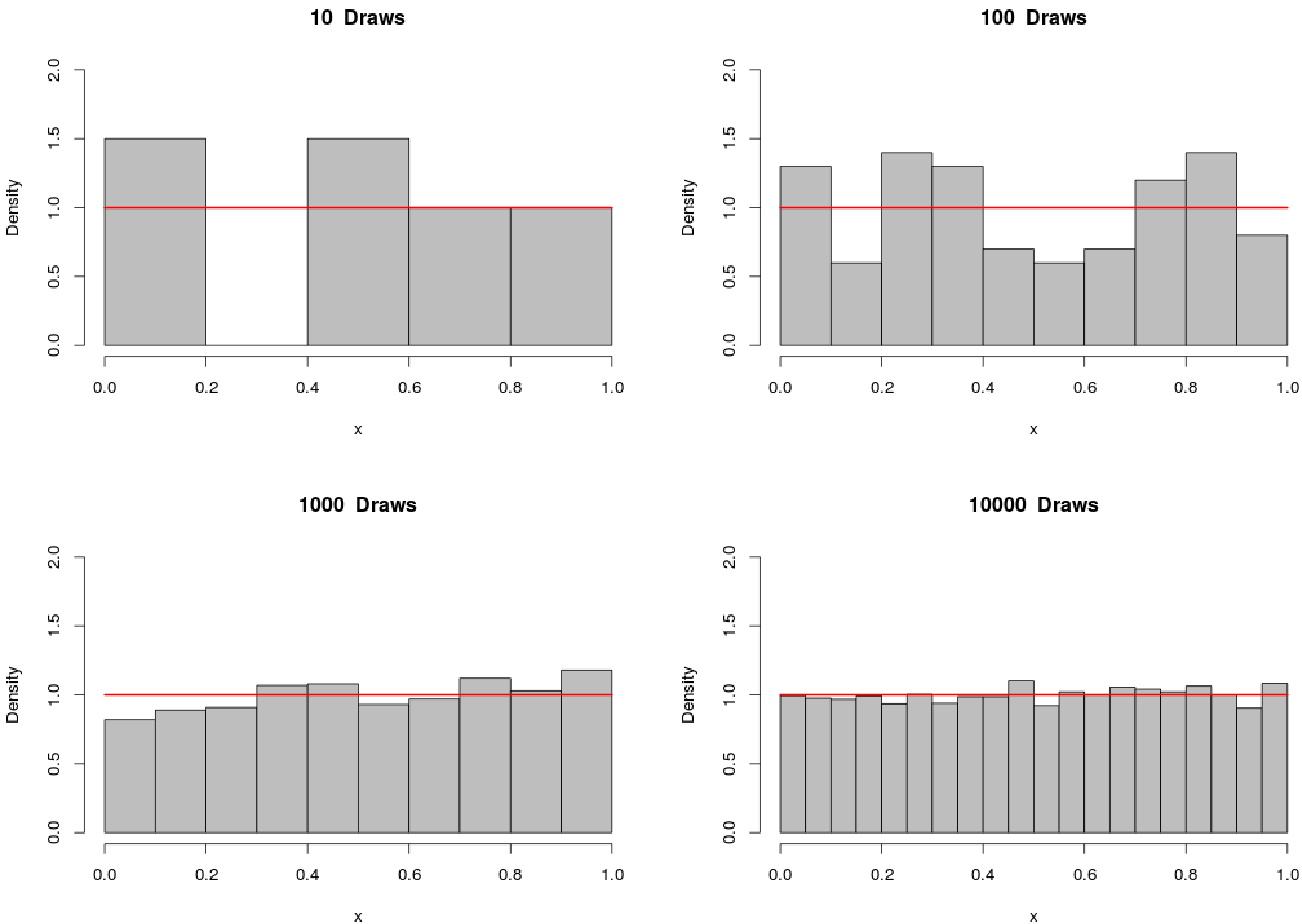
MCNP RNG

- MCNP uses a pseudo-RNG
- The implementation uses 48-bit integers and has a "period" of 2^{46} values ~7.04×10^{13}
- This can be exceeded for some problems!
- Random number "stride"
  - The number of random numbers between those used to select source particles

Random Number Generation

- RNGs aim to generate a sequence of random numbers within a fixed range whose distribution is uniform
- ξ generated “random” number
  - Usually within the unit interval $0 \leq \xi < 1$
- *P(*ξ*)* the probability of selecting ξ
- Clearly *P(*ξ*)* is chosen so that

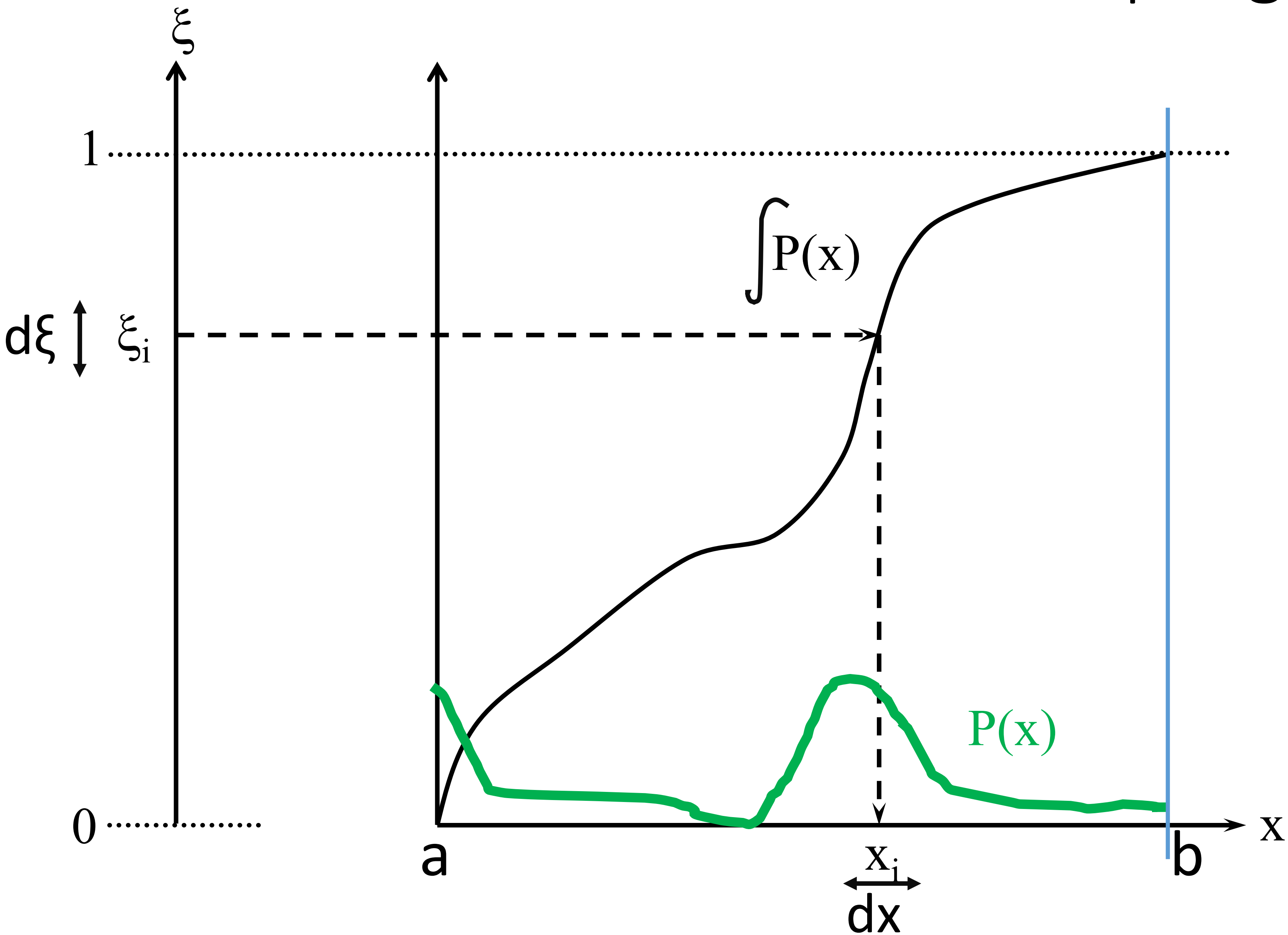
$$\int_0^1 P(\xi)d\xi = 1$$


10 Draws
100 Draws
1000 Draws
10000 Draws
Density
x
0.0
0.2
0.4
0.6
0.8
1.0
0.5
1.5
2.0

Non-Uniform Sampling

- Random variable x defined in the range $a \leq x \leq b$
- We think we know the probability distribution $P(x)$
- Wish to generate a series of random values of x to match this distribution
- We have a pseudo-RNG to generate ξ within the range $0 \leq \xi < 1$

Non-Uniform Sampling



Non-Uniform Sampling

- Transform from ξ space to x space by equating

  probability of obtaining x' in range dx' about x'

  = probability of obtaining ξ in range dξ about ξ

  Integrate from lower limit to a value x

$$\int_a^x P(x')dx' = \int_0^{\xi} d\xi' = \xi$$

- Random Sampling Rule

Applied to Radiation Transport

- The cross-section
- Describes the probability of a particle interaction

$$\Sigma_T = \Sigma_s + \Sigma_a$$

- Macroscopic cross-sections are required

$$\Sigma(\mathrm{cm}^{-1}) = \sigma(\mathrm{cm}^2)\ n(\mathrm{atoms/cm}^3)$$

$$n(\mathrm{atoms/cm}^3) = \rho(\mathrm{g/cm}^3)\ N_A \div A(\mathrm{g/mol})$$

Distance to Next Collision

- Basic Monte Carlo question
  - Where is the next collision?
  - *Diagram of scatter point*
- Probability of collision within dr' about r' is $P(r')dr'$

$$P(r') = \Sigma_T \, e^{-\Sigma_T r'}$$

- Use random sampling rule

$$\int_0^r P(r')dr' = \int_0^{\xi} d\xi' = \xi$$

Distance to Next Collision

$$\int_0^r \Sigma_T e^{-\Sigma_T r'} dr' = \int_0^{\xi} d\xi' = \xi$$

$$= 1 - e^{-\Sigma_T r}$$

- Rearrange to

$$r = \frac{-ln(1-\xi)}{\Sigma_T} \equiv \frac{-ln(\xi)}{\Sigma_T}$$

Where is the Collision?

- Distance to cell boundary = d
- If $r < d$ collision occurs within cell
- If $r > d$ particle leaves cell and enters next one
  - Need to recalculate new d and next collision distance (r)
  - New cell may have different cross-sections

Then What?

- We know where is collides, but what happens next?
- Choose which atom it collides with
  - For a material composed of several types of atom
  - a, b, c, … (isotopes considered separately for neutrons)

$$\Sigma_T = \Sigma_{Ta} + \Sigma_{Tb} + \Sigma_{Tc} + \ldots$$

Normalise by dividing by Σ_T so sum now = 1

Generate ξ and select from a, b, c, etc.

Then What?

- Depends on particle type – photon, neutron, low energy neutron
- Select type of collision in the same way
- E.g. for photon we have to choose from:
    - Compton scatter, photo-electric absorption & pair production

$$\Sigma_T = \Sigma_{cs} + \Sigma_{pe} + \Sigma_{pp}$$

Normalise by dividing by Σ_T so sum now = 1

Generate ξ and select from cs, pe & pp

Neutron Interactions

- For neutrons, in general there are many to choose from:
  - Elastic scatter (n,n)
  - Inelastic scatter (n,n')
  - Absorption (n,abs) – (n,γ), (n,α), (n,d), (n,t), (n,p), …
  - Multiplication (n,2n), (n,3n) …
  - Fission (n,f) - this too implies further neutron production
- The collision isotope determines which ones are available and what the cross-sections are
  - Also depends on neutron energy

Neutron Interactions - MCNP

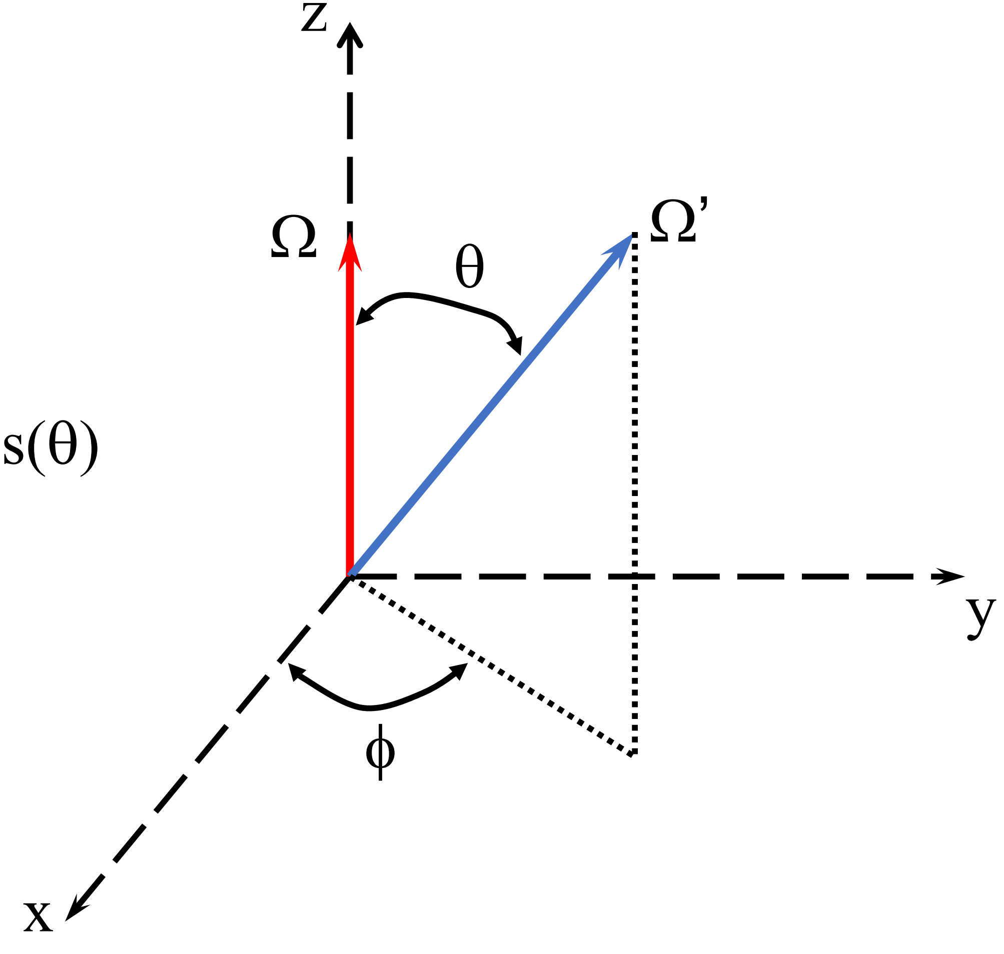
- Identify collision nuclide
- Is $S(\alpha,\beta)$ scattering required?
  - Low energy neutrons only – material dependent
- Are any photons generated?
  - Depends on mode of problem and collision type.
- Is neutron captured?
- Is collision elastic, inelastic or a fission event
  - Determines energy of ongoing neutron
  - Whether more particles (photons & neutrons) are generated
- For neutrons E<4eV, need to take thermal motion of collision atoms into account.
  - Temperature matters
  - Target nuclide velocity sampling required – subtracted from velocity of incoming neutron

Absorption

- Can lead to a number of potential events.
  - (n,γ), (n,α), (n,p), (n,d), (n,2n), (n,f), ….
- Gammas are tracked (in MODE N P)
- Fissions lead to more neutrons
  - By default MCNP will track fission-generated neutrons
  - Can be switched off
- All particles generated are "banked" if required to be tracked
  - Record location of production
  - Sample direction and energy later

Scattering - Selection of Scattering Angle

Defining the scatter angles:



Define: $\mu=\cos(\theta)$

Angle of Scatter (polar)

Probability of scattering within $d\mu$ about μ

$$P(\mu) = \int_{-1}^{\mu} \frac{\Sigma_s(\mu')2\pi d\mu'}{\Sigma_s} = \int_{-1}^{\mu} \frac{d\mu'}{2} = (\mu+1)/2$$

For isotropic scattering

$\Sigma_s(\mu)$ is constant and $(\mu+1)/2 = \xi$

$\Sigma_s(\mu)/\Sigma_s = 1/4\pi$ $\qquad$ $\mu = 2\xi - 1$

For non-isotropic scatter use random sampling rule

$$\int_a^x P(x')dx' = \int_0^{\xi} d\xi' = \xi$$

Azimuthal Scattering Angle

$$P(\phi) = \int_0^{\phi} \frac{1}{2\pi} \cdot d\phi' = \frac{\phi}{2\pi}$$

$$\frac{\phi}{2\pi} = \xi$$

$$\phi = 2\pi\xi$$

Energy After Collision

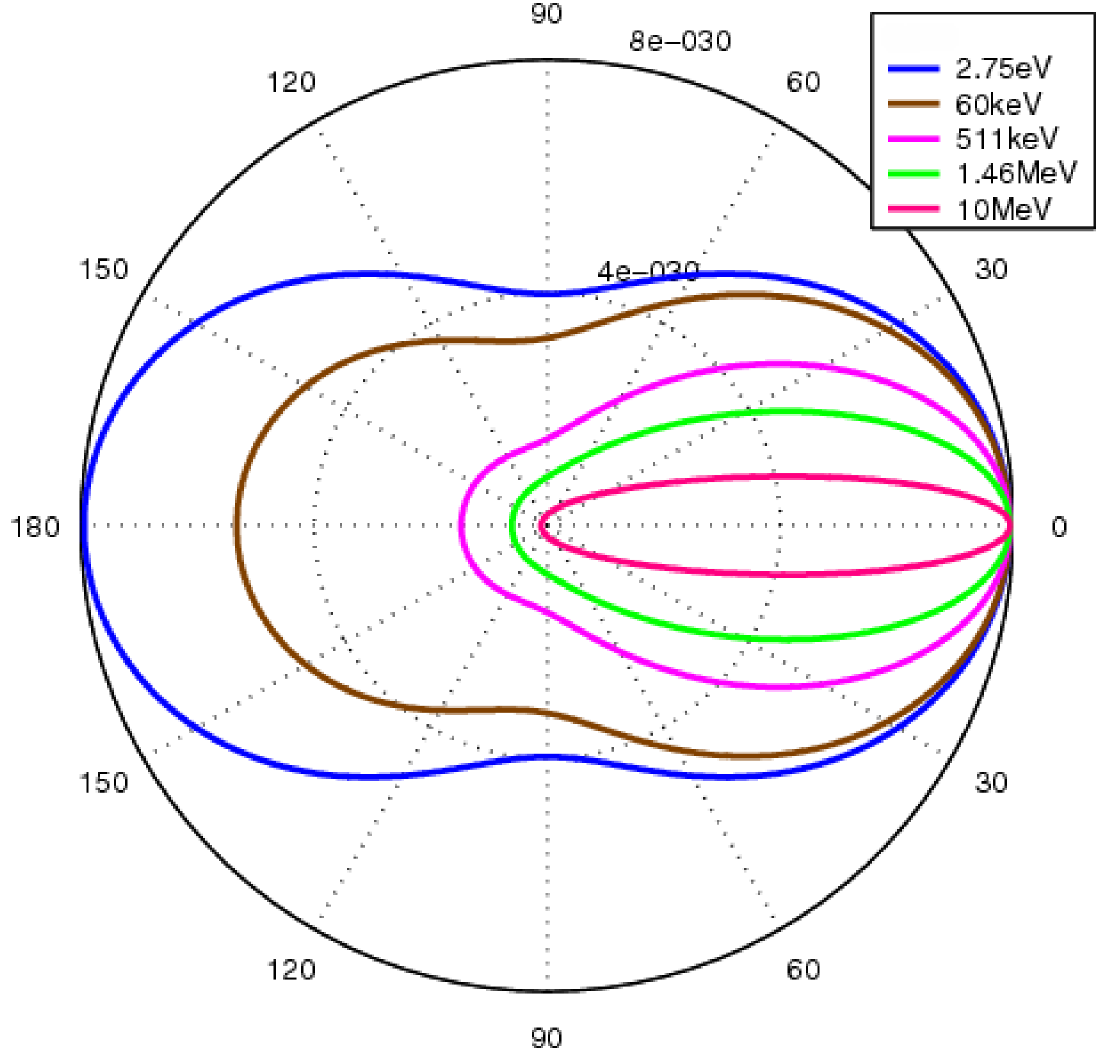
- For neutrons (elastic scatter)

$$E = E_{in}\left[\frac{1 + A^2 + 2Acos\theta}{(1 + A)^2}\right]$$

- For photons – Klein Nishina formula

$$\frac{d\sigma}{d\Omega} = \alpha^2 r_c^2 P(E_\gamma, \theta)^2 [P(E_\gamma, \theta) + P(E_\gamma, \theta)^{-1} - 1 + \cos^2(\theta)]/2$$

$$P(E_\gamma, \theta) = \frac{1}{1 + (E_\gamma/m_e c^2)(1 - \cos\theta)}$$



90
8e−030
120
60
4e−030
150
30
180
0
150
30
120
60
90
2.75eV
60keV
511keV
1.46MeV
10MeV

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

$$\phi = \frac{1}{VN} \sum_i S_i W_i$$

Variations on Tallies

Fn4 - cell flux (track length)

*Fn4 – **cell energy-weighted flux**

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

$$\phi = \frac{1}{VN_i} \sum E_i s_i w_i$$

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				

Response Functions

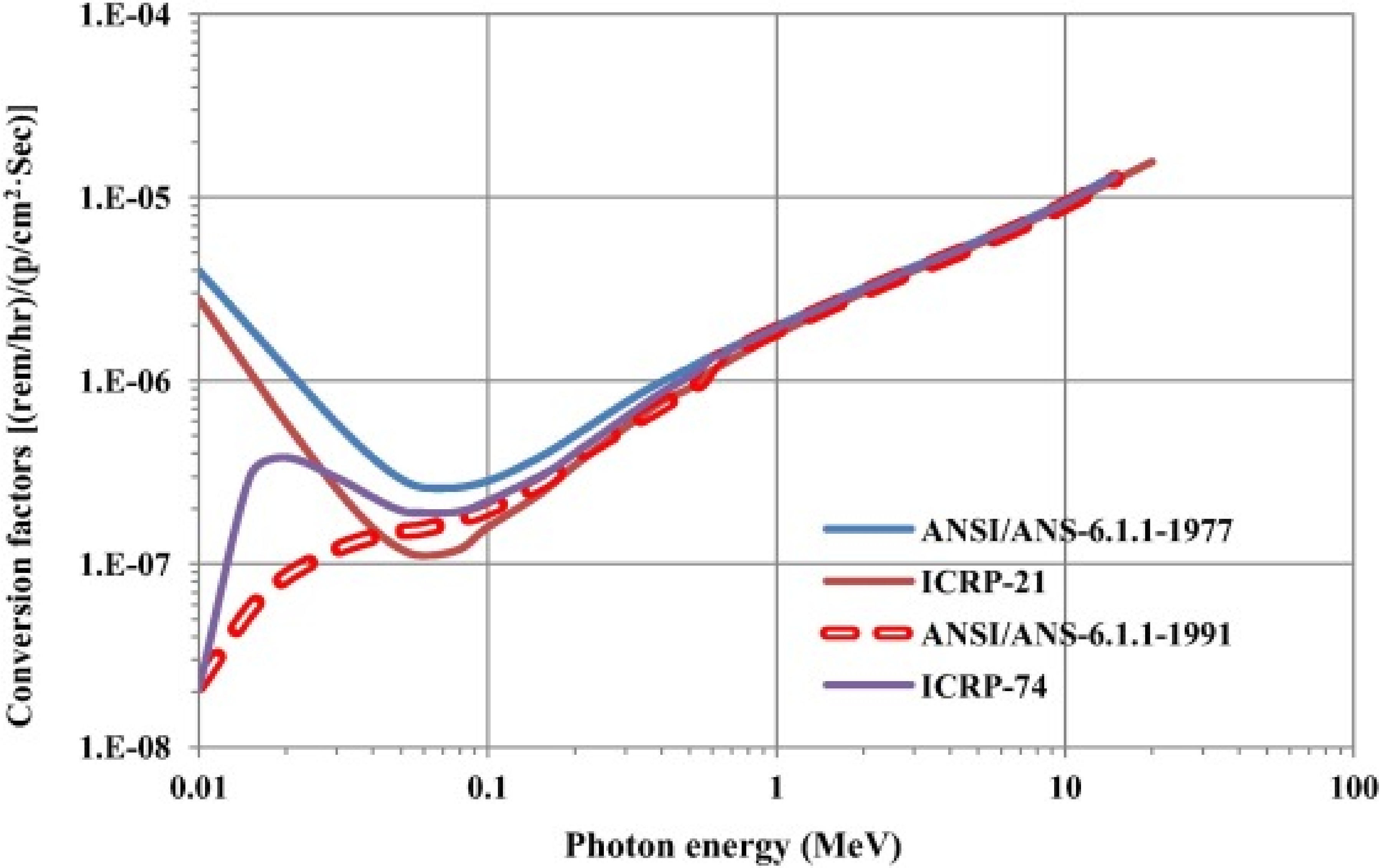
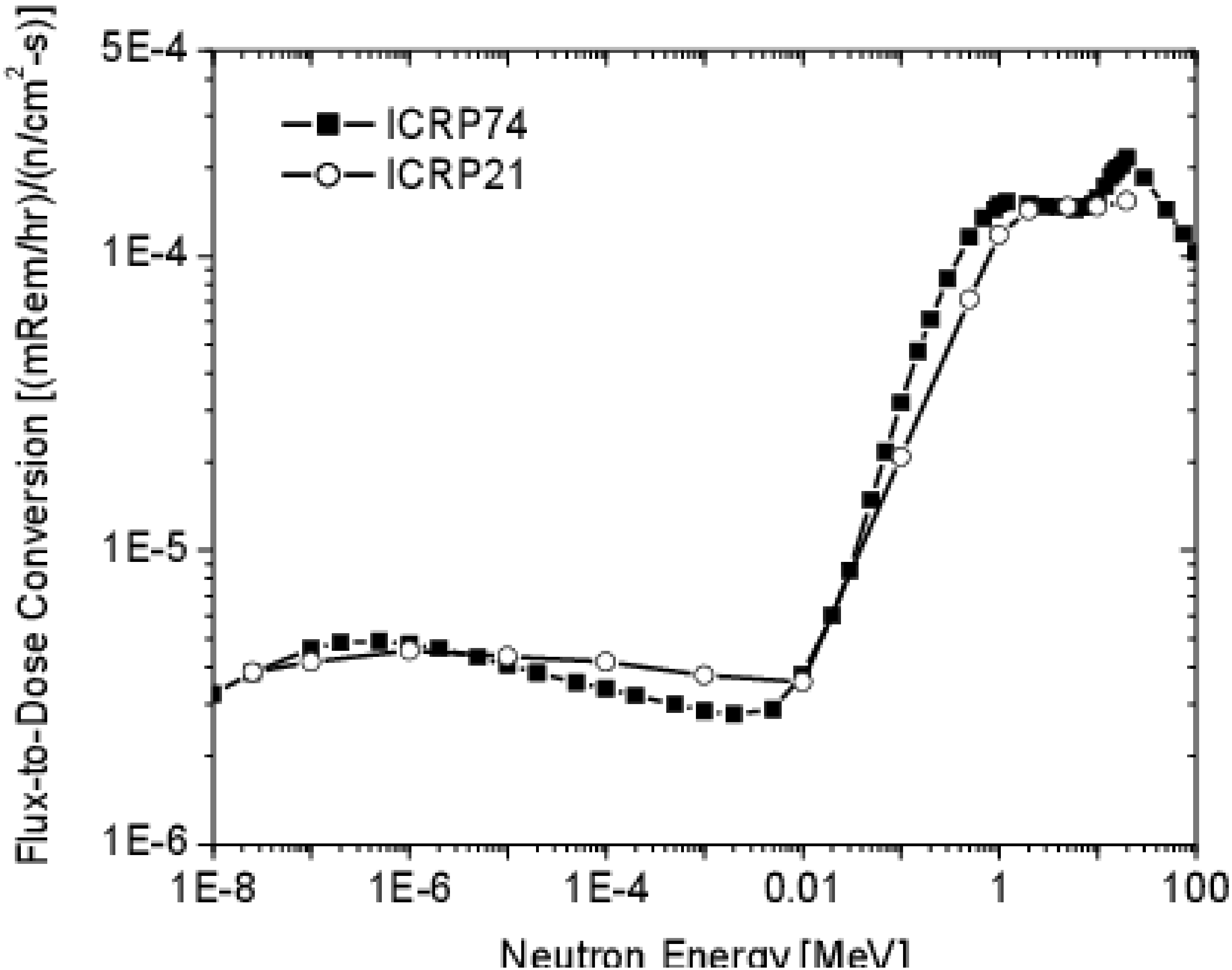


Table H.2
Photon Flux-to-Dose Rate Conversion Factors

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



Flux-to-Dose Conversion [(mRem/hr)/(n/cm^2-s)]
5E-4
1E-4
1E-5
1E-6
ICRP74
ICRP21
1E-8
1E-6
1E-4
0.01
1
100
Neutron Energy [MeV]

Response Functions

- 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

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

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

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

Other Tally Multipliers

- Energy multiplier

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

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

  - 0 tally bin multipliers apply to all tallies unless specifically overridden by another EM, TM or CM card