Monte Carlo Methods for nuclear particles transport .

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Monte Carlo Methods

The physical properties of a complex system are stochastic : Their values belong from the statistical behavior of the system micro-states population.

Monte Carlo Methods

When a physical property is estimated (measured) with a proper sample population its mean is not affected by high fluctuations.

Deterministic Models.
Systems of differential equation on partial derivatives.
Strong regularization and convergence conditions.
Fast and elegant codes that work on simple or simplified systems.

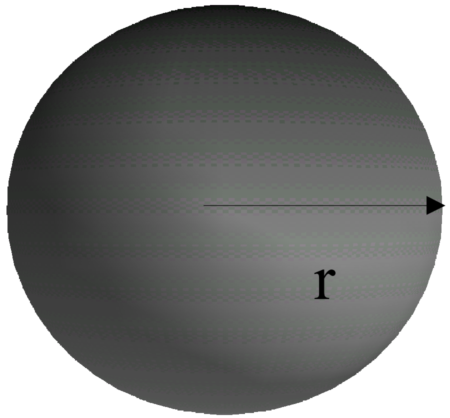
Monte Carlo Methods

Monte Carlo models.
Sampling of microscopic and/or macroscopic variables distributions to simulate the system behavior.
The approach is general and permits to simulate complex systems.
The computer codes are slow than the deterministic ones.

Monte Carlo Methods

Calculation of the volume of a sphere:
"Deterministic Method".

$$V = \frac{4}{3}\pi r^3$$

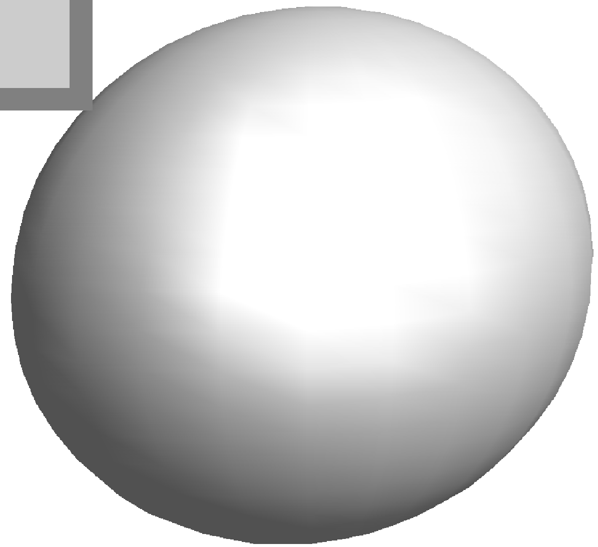


The knowledge of the radius r permits the calculation of the volume V !!!!

Monte Carlo Methods

Calculation of the volume of a sphere: "Monte Carlo Method".

$$V = \frac{\sum_i P_i l_i}{N} = \pi R^2 \frac{\sum_i l_i}{N}$$



- Define a second sphere, with radius R, that completely contains the first.
- N emission points, with score πR^2 each, are sampled on the second sphere surface.
- For each point an inner trajectory, with random direction, is sampled.
- All the trajectories segment of length l that cross the sphere under measurement were "tallied" .

Monte Carlo Methods

Volume estimation of a sphere (r=05 cm) by Monte Carlo.

"True" Volume= 0.523598 cm3

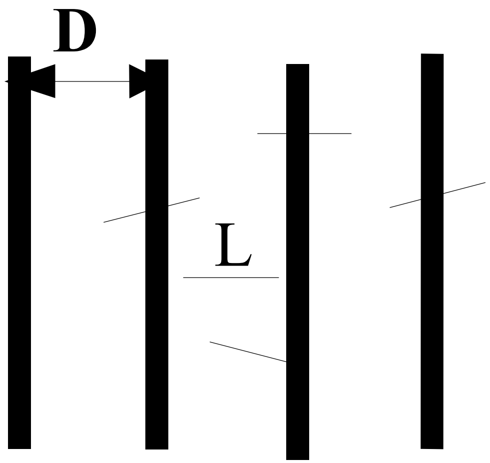
Nps	Volume(cm3)	Standard Dev.
10	0.00000E+00	0.0000
100	4.40285E-01	1.68E-01
1000	4.82744E-01	5.37E-02
10000	5.28167E-01	1.75E-02
100000	5.27829E-01	5.54E-03
1000000	5.21010E-01	1.72E-03

M.C. Method is not the best choice!!!

Monte Carlo Methods

An M. C. method is able to estimate volume and surface of an object like this!!!!

Monte Carlo Methods



1707: DeBuffon experimentally verify the probability P of intersection between a segment of length L, randomly oriented, and a set parallel lines spaced with a period D:

$$P = \frac{L/D}{\Pi/2}$$

First Monte Carlo "experiment"

Monte Carlo Methods

1886
Laplace suggests a random sampling method for the calculation of Π .

Lord Kelvin integrates the gas kinetic equations through random sampling (More than 5000 collisions were hand-sampled!!!).

1940
Monte Carlo method make its debut in Nuclear Physics during the II world war at Los Alamos.

Monte Carlo Methods

The first Computers were build:
Monte Carlo, a tedious and time consuming technique, became affordable.
Since 1947 a lot of neutronic diffusion problems were simulated by Monte Carlo.
The progressive growth of the computational power encourage the development and the use of the M.C. Simulations.

Monte Carlo Methods

- **Sampling a probability distribution:**

X is a random variable that is distributed with a non-decreasing, continuos and differentiable cumulative function:

$$Prob\{X \leq x\} = F_X(x)$$

The probability density function of X can be defined as

$$f_X(x) = \frac{dF_X(x)}{dx}$$

and

$$f_X(x) \geq 0$$

Monte Carlo Methods

- **Random generate the number sequence {X}={X_1,X_2,..,X_N}, where N »1.**
- **Sort, in increasing order, the sequence {X}.**
- **If *n* is the number of values of {X} that fall in the bin Δx « Xmax-Xmin then, for each bin:**

$$\frac{n}{N} \approx \int_{\Delta x} f_X(x)\, dx$$

The frequency histogram estimates the probability distribution function:

$$f_X(x)$$

- **This is still true for very large periodic {X} sequences.**

Monte Carlo Methods

Sampling by inverse transform.

The uniform distribution, defined on the set [0,1] as
U[0,1)
may be used to sampling random variables that obey to different distributions .

$$R = \int_{-\infty}^{X} f_X(x)\, dx$$

Every number R, sampled on $U_R[0,1)$, correspond to a value X distributed in $F_X(x)$.

Monte Carlo Methods

Diffusion of a neutron of energy E in a isotropic and homogeneous media.

Estimate the collision probability of the neutron in the path from l to l + dl along the direction of propagation.

$$p(l)\,dl = e^{-\Sigma_t l}\,\Sigma_t\,dl,$$

Probability of collision.

$$\Sigma_t$$

Total macroscopic cross section: probability of collision per length unit.

Monte Carlo Methods

Diffusion of a neutron of energy E in a isotropic and homogeneous media.

The sampling of the random variable ζ, uniformly distributed on [0,1), by inverse transform yield:

$$\zeta = \int_0^l e^{-\Sigma_t s} \Sigma_t \, ds = 1 - e^{-\Sigma_t l}$$

$$l = -\frac{1}{\Sigma_t} \ln(1-\zeta)$$

and

$$l = -\frac{1}{\Sigma_t} \ln(\zeta)$$

The last relation is the well known relation for the distance of collision.

Monte Carlo Methods

Engine of Monte Carlo simulation

Set of decisions taken sampling experimental (evaluated) probability distribution functions of the physical properties (such as cross sections) peculiar of system under simulation.

Monte Carlo Methods

An Example of M.C. Decision chain:

- A neutron diffuses in a media.
- Check the probability density function for collision.
- A collision after l cm of path is sampled.
- Check of the total cross section of the media nuclides .
- A nuclide is sampled for collision.
- Check of the cross section of the selected nuclide (Scattering, Capture, Fission..).
- A reaction is sampled.
- The optional event of photons production is sampled.

Monte Carlo Methods

Each event selected has a statistic weight in the sample population of the system under investigation.

Monte Carlo simulations are statistic investigations on system behavior.
The consistency between sample population and target population must be always checked.

Is my sample a realistic representation of the entire system?

Monte Carlo Methods

MCNP
Monte Carlo N Particles
Los Alamos National Laboratory

A Monte Carlo code for transport neutrons, photons and electrons.
It solves transport complex problems.

How many complex ?

Monte Carlo Methods

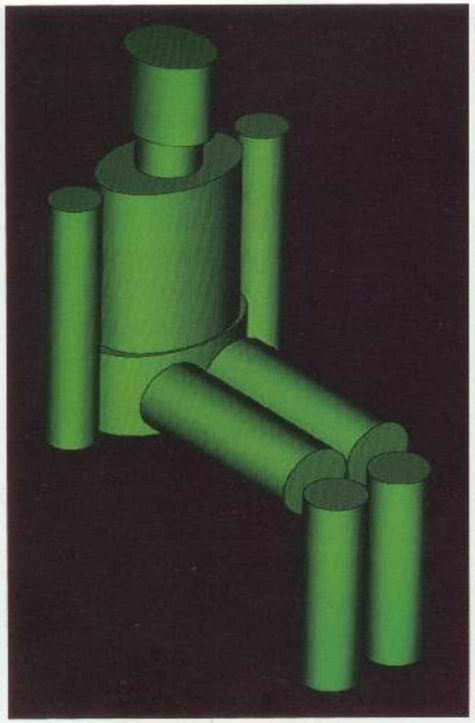


Fig.3: Sitting BOMAB phantom.

Fig.4: Skeleton of the ADAM phantom.

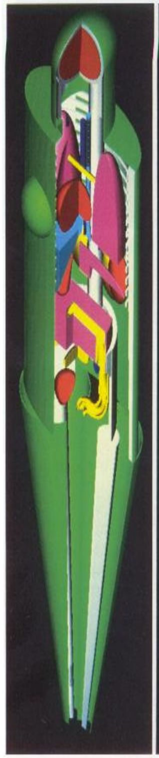


Fig.9: Sectional view of the EVA phantom with internal organs

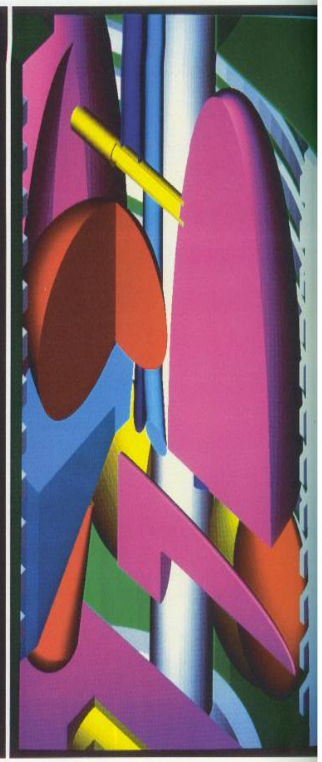
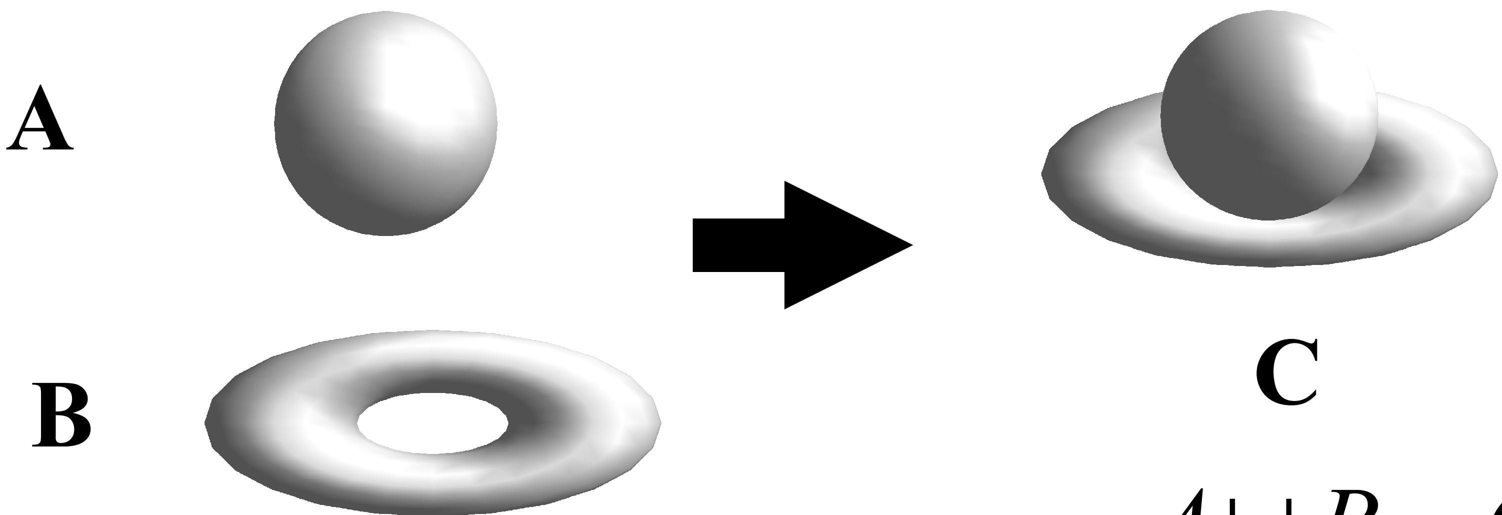


Fig.10: Zoom of fig.9

Monte Carlo Methods

MCNP combinatorial geometry:

Sets of space points defined by surfaces bound and body are combined together by means of combinatorial operators such as union, intersection and exclusion to define cells.

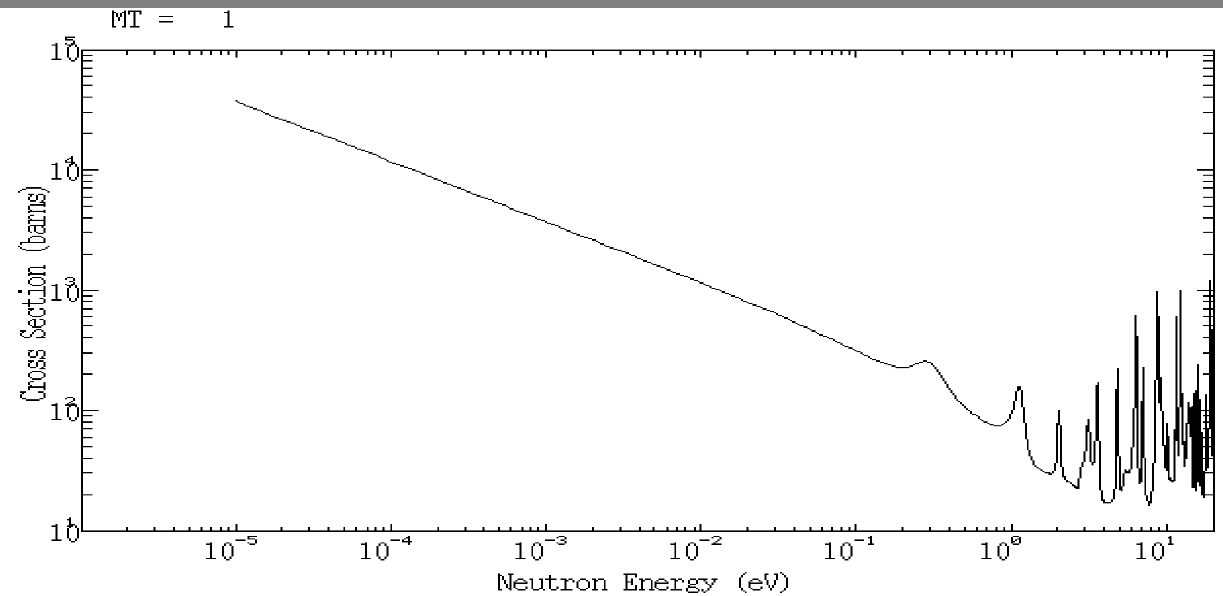


$$A \cup B = C$$

Monte Carlo Methods

MCNP materials definition:

The MCNP cells could be filled with users defined materials. The materials composition can be expressed at isotopic level. The macroscopic transport properties of each material are calculated from microscopic, continuos, cross section data stored in the MCNP libraries (Mainly ENDF-B-VI).



Monte Carlo Methods

MCNP Source definition:

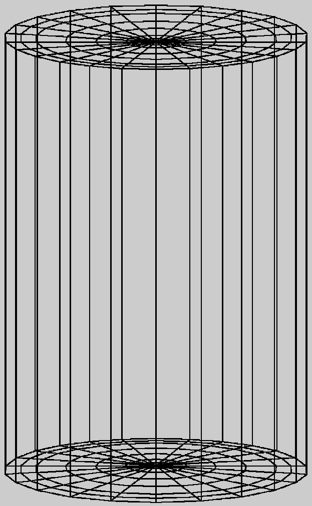
All the phase-space parameter of particles source can be defined through user defined distribution or build-in function:

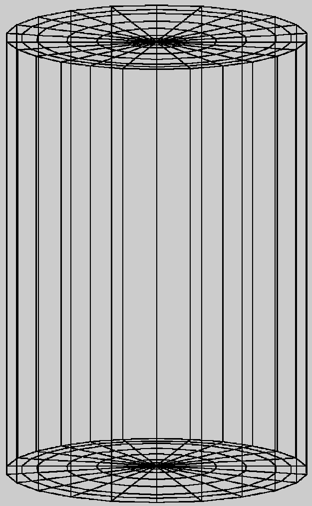
·A cell, surface or point source with its own spatial p.d.f .

·The energetic spectrum of the particles.

·The initial direction.

·The time of emission.



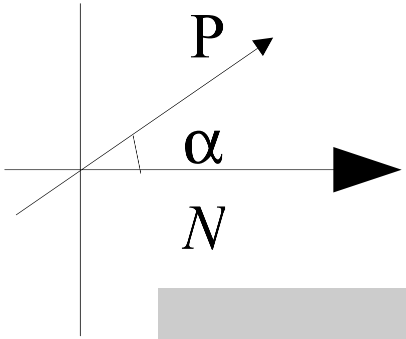


Each one of this variables can be expressed in function of the others by a multi-level source definition that allows the possibility to decompose very complex problem in more simple steps.

Monte Carlo Methods

MCNP estimation of quantities (tallies):

•**Particle current tally estimates the following quantity:**



$$F1 = \int_A \int_\mu \int_t \int_E J(\vec{r}, E, t, \mu)\, dE\, dt\, d\mu\, dA$$

$$\mu = \cos(\alpha) \qquad J(\vec{r}, E, t, \mu) = |\mu|\, \Phi(\vec{r}, E, t)$$

That is the number of particles crossing a surface

The range of integration over area,energy,time, angle and the vector relative to which μ is calculated could be controlled by user input.

Monte Carlo Methods

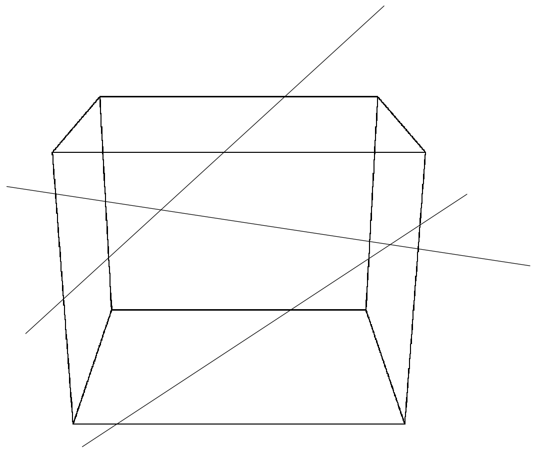
MCNP estimation of quantities (tallies):

Track length estimate of cell flux:

$$F4=\int_V \int_t \int_E \Phi(\vec{r},E,t)\, dE\, dt \frac{dV}{V}=\int_V \int_s \int_E N(\vec{r},E,t)\, ds\, dE \frac{dV}{V}$$

$$N(\vec{r},E,t)\, ds = track\ lenght\ density$$

$$ds = v\, dt$$



MCNP estimates this integral by summing WT_l/V for all particles tracks in the cell.

Monte Carlo Methods

MCNP "measurement" :

- They belongs from sampling on all possible particle paths (random walk).
- They are afflicted by statistical fluctuations.

Monte Carlo Methods

Let f(x) be the probability density function of the quantity x associated with a particles population . The true mean of x can be expressed as:

$$E(x) = \int x\, f(x)\, dx = true\, mean$$

Because of the implicit sampling of f(x) performed through random walk the Monte Carlo estimates the true mean as:

$$\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

Where N is actual number of history and x_i the tally score.

The relationship between E(x) and $\bar{x}$ is given by The Strong Law of Large Numbers.

$$\lim_{N \to \infty} \bar{x} = E(x)$$

Monte Carlo Methods

Variance of the true value E(x)

$$\sigma^2 = \int (x - E(x))^2 f(x)\, dx = E(x^2) - E(x)^2$$

M.C. Variance estimation:

$$S^2 = \frac{\sum_{i=1}^{N} (x_i - \bar{x})^2}{N - 1} \approx \overline{x^2} - \bar{x}^2$$ **Where** $$\overline{x^2} = \frac{1}{N} \sum_{i=1}^{N} x_i^2$$

This formulation holds for every kind of distribution of x and its mean for which E(x) and σ^2 exist and are finite values.

Monte Carlo Methods

The variance of the estimated mean $\bar{x}$ is:

$$S_{\bar{x}}^2 = \frac{S^2}{N}$$ **Where** $$S_{\bar{x}} \propto \frac{1}{\sqrt{N}}$$

- **The quantity S_x can be reduced:**
- **Increasing the number of history N.**
- **Reducing the spread of S at constant N.**

Monte Carlo Methods

Precision and accuracy

Precision

The uncertainty in $\bar{x}$ caused by statistical fluctuations.

Affecting Factors:
a) code; b)problem modeling; c)user;

Accuracy

A measure of the closeness of $\bar{x}$ to E(x).

Affecting Factors:
a) Tally type; b)variance reduction; c)Number of history

Monte Carlo Methods

Tally estimated relative error

$$R \equiv \frac{S_{\bar{x}}}{\bar{x}}$$

R is the relative error and represents the statistical precision (at 1σ level) as fractional result with respect to the estimated tally mean.

***Guidelines for interpreting the Relative error R**

Range of R	Quality of the Tally
0.5 to 1.	Garbage
0.2 to 0.5	Factor of a few
0.1 to 0.2	Questionable
< 0.1	Generally reliable

* From MCNP manual.

Monte Carlo Methods

MCNP Figure of Merit.

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

R=Estimated relative error($\propto$ N^{-1}).

T = Computer time in minutes ($\propto$ N).

If a tally is well behaved FOM should approximately constant during the problem (except in the early stages).

FOM has 3 uses:

- **If not constant the confidence interval may not overlap the expected score value.**
- **FOM compare the efficiency of M.C. by with various variance reduction technique .**
- **FOM estimates the computer time required to reach a desired R.**