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# Cockcroft Institute Postgraduate Lectures
# Numerical Methods and Lattice Design

## Lecture 3: Monte Carlo Particle Transport

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# The Course Syllabus and Projects

- Recap on programming languages for physics; MATLAB and Python; summary of commands;
- Introduction to numerical computing; errors in computer calculations;
- Numerical integration methods; Euler's method; higher-order methods;
- Precision vs. accuracy; validation;
- Phase space; conserved quantities;
- Introduction to mappings and nonlinear systems;
- *Example: Methods for solving the linear and non-linear simple harmonic oscillator.*
- Introduction to Monte Carlo methods; Monte Carlo integration; classical problems;
- Pseudorandom and quasirandom sampling; methods of sampling; generation of distributions;
- Particle transport simulation; nuclear cross sections; particle histories; applications of Monte Carlo transport;
- *Example: Simulation of penetration of neutrons through shielding.*
- From mappings to linear optics; the concept of lattices;
- Transfer matrices and periodic solutions; propagation of linear optics parameters;
- Classic optical systems: the FODO, the double-bend achromat;
- Matching and optimisation; penalty/objective functions;
- Hill-climbing methods: Cauchy's method, Nelder-Mead, simulated annealing;
- Variables and constraints; under- and over-constrained problems;
- *Example: MAD8 matching of FODO Twiss values;*
- Multiple-configuration methods; genetic algorithms and evolutionary algorithms;
- A bestiary of codes; choosing the right code;
- Common pitfalls;
- *Example: Particle tracking in MAD8;*

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*'The true logic of this world is the calculus of probabilities.'*

***James Clerk Maxwell***

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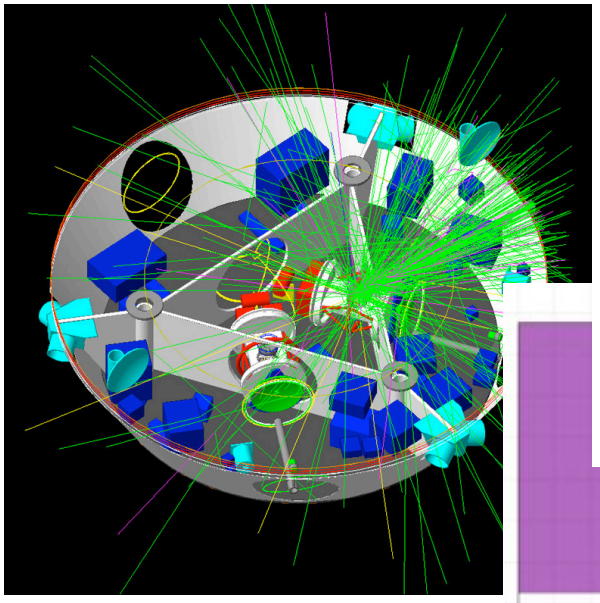
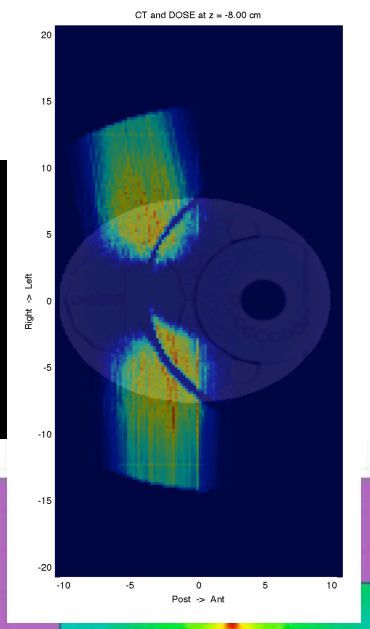
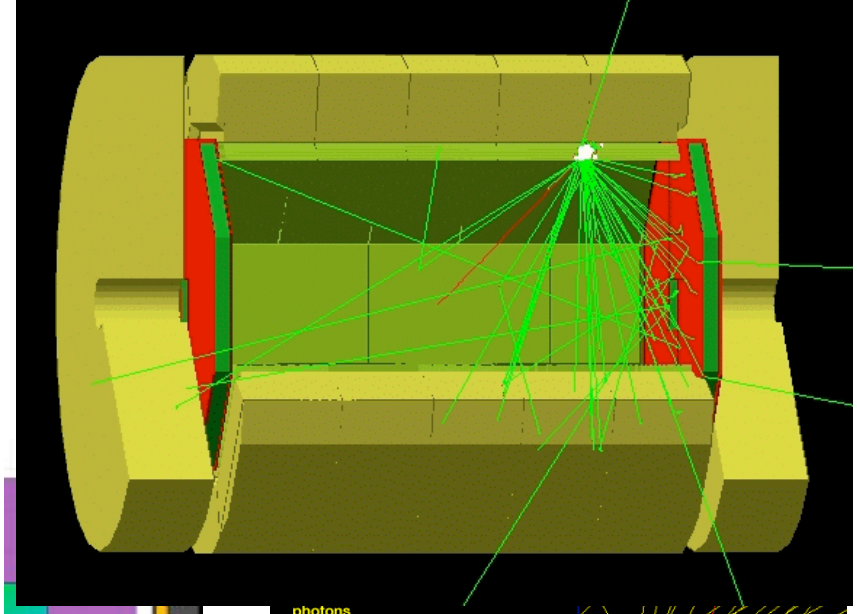
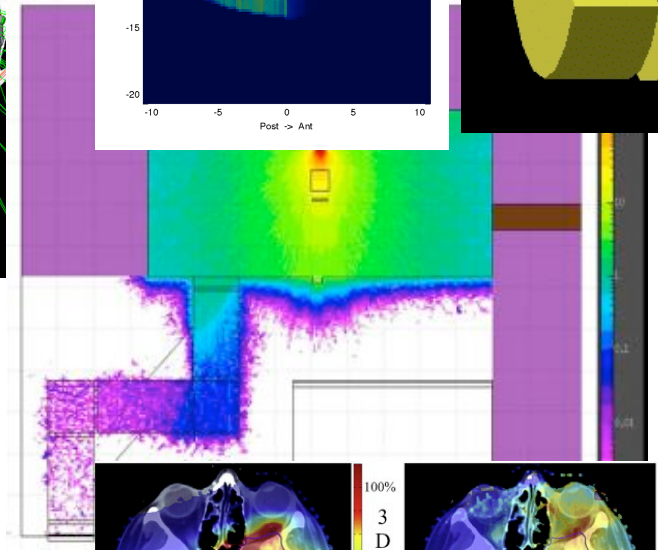
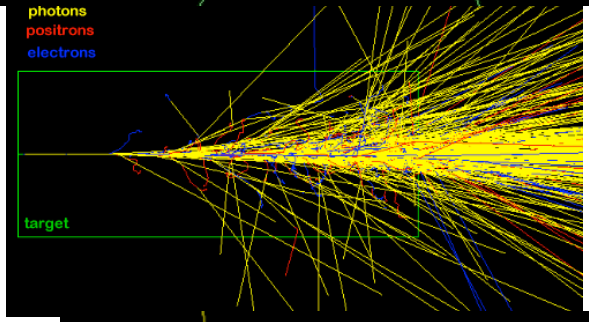
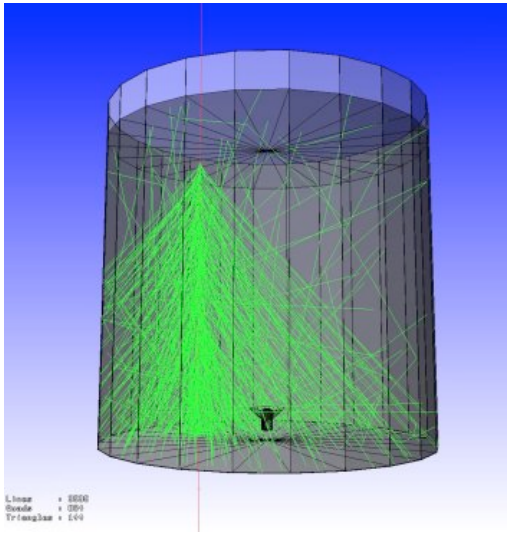


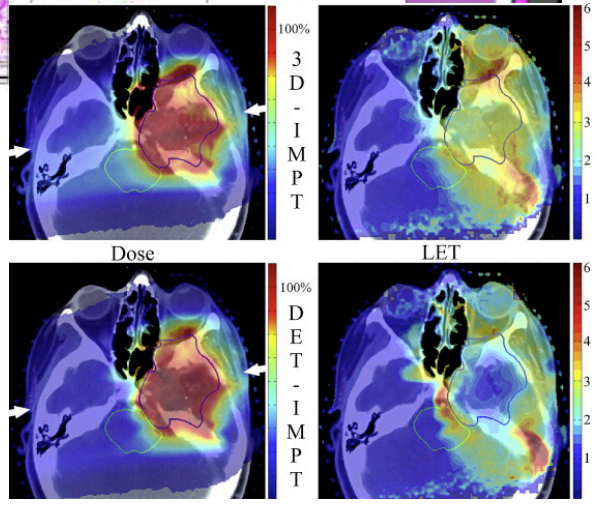


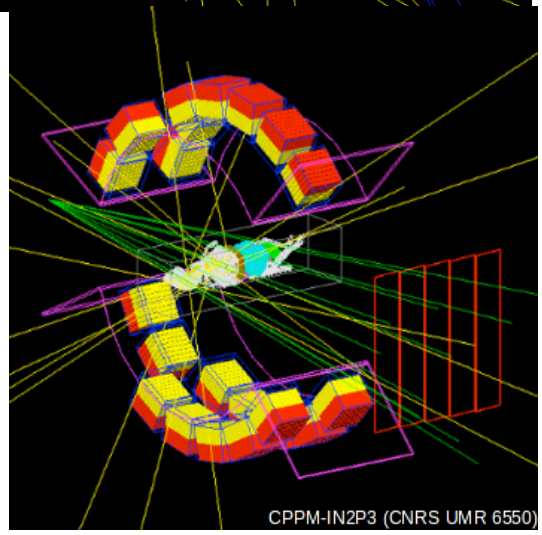







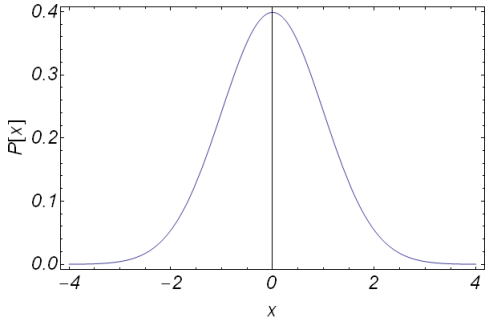



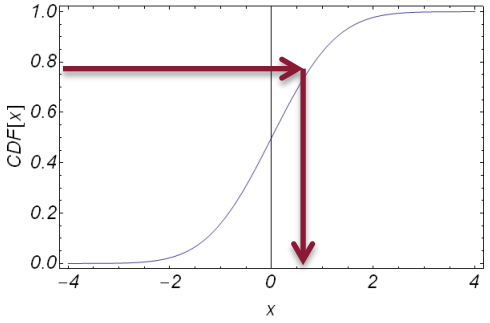


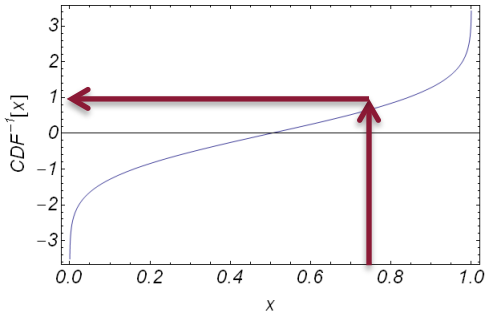



# Inverse distribution sampling/cumulative distribution sampling

The inverse distribution method is quite simple – integrate the **probability density function** of the distribution you want to sample from, and then invert it to form the **inverse cumulative distribution** function. Multiply a uniformly-distributed variable by the inverse CDF to get a distribution distributed according to your original PDF.

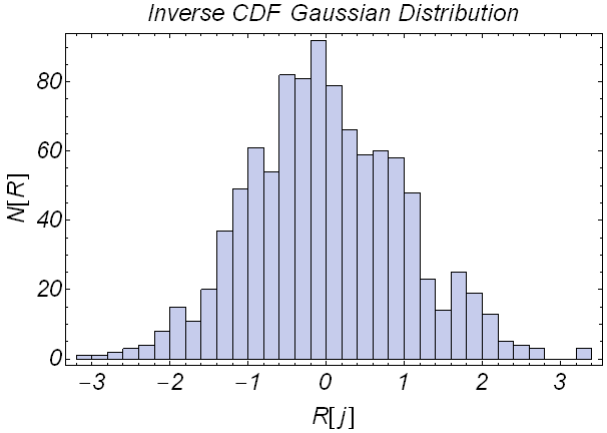



$$\mathrm{cdf}^{-1}(x) = \sqrt{2}\mathrm{erf}^{-1}(2x-1)$$

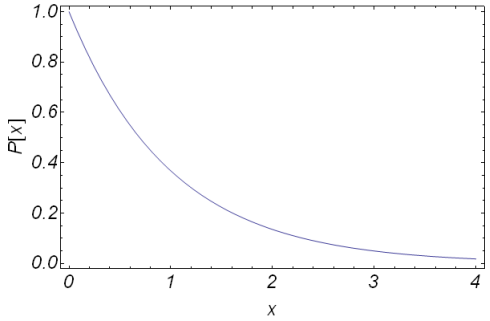
$$\mathrm{erf}^{-1}(x) = \frac{1}{2}\sqrt{\pi}\left(x + \frac{\pi}{12}x^3 + \frac{7\pi^2}{480}x^5 + \frac{127\pi^3}{40320}x^7 + \frac{4369\pi^4}{5806080}x^9 + \frac{34807\pi^5}{182476800}x^{11} + \cdots\right).$$



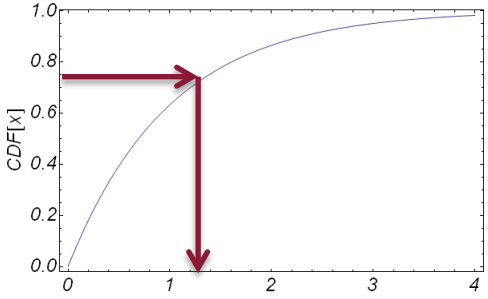

Works just great for a Gaussian (again….)

# Sampling the Exponential Distribution

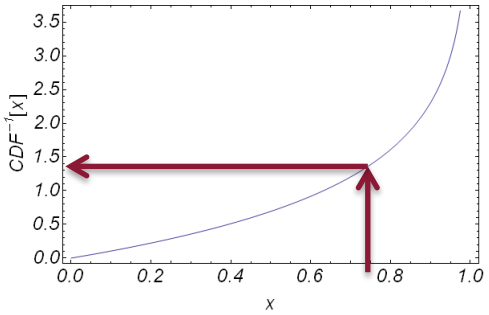
- Sampling functions is straightforward, provided the inverse CDF can be found.



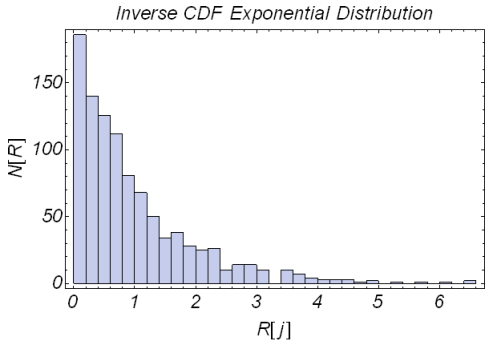

$$\mathrm{pdf}(x) = e^{-x}$$




$$\mathrm{cdf}(x) = \int_0^x \mathrm{pdf}(x) = 1 - e^{-x}$$

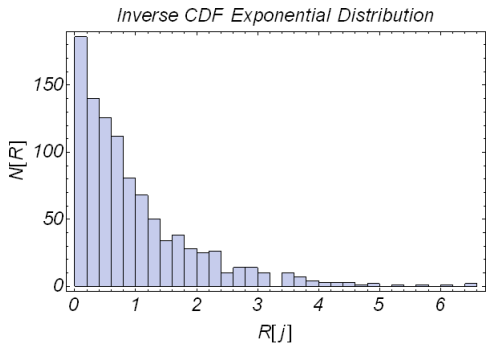



$$\mathrm{cdf}^{-1}(z) = -\ln(1-z)$$




This is really important! Pay attention here!

# Exponential Distribution via Normal and Antithetic Variates




$$\mathrm{cdf}^{-1}(x) = -\log(1-x)$$

$$x_i = -\log(1-u_i)$$

$$x_i = -\log(u_i)$$

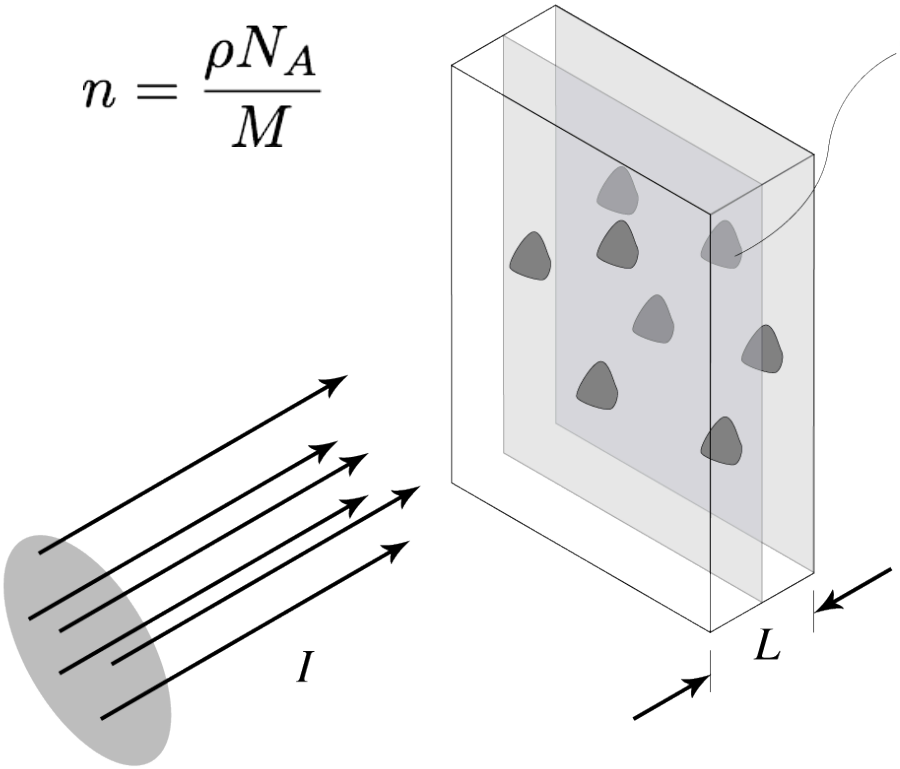
For mean free path λ

$$P[x] = e^{-x/\lambda}$$

$$s_i = -\lambda \log(u_i)$$

# Particle Absorption, and Other Interactions

$$n = \frac{\rho N_A}{M}$$




Number absorbed in thin layer

$$N_L = n\sigma I L$$

Rate of absorption per unit thickness

$$R = -\frac{dI}{dx} = n\sigma I$$

Intensity variation with thickness

$$I(x) = e^{-n\sigma x}$$

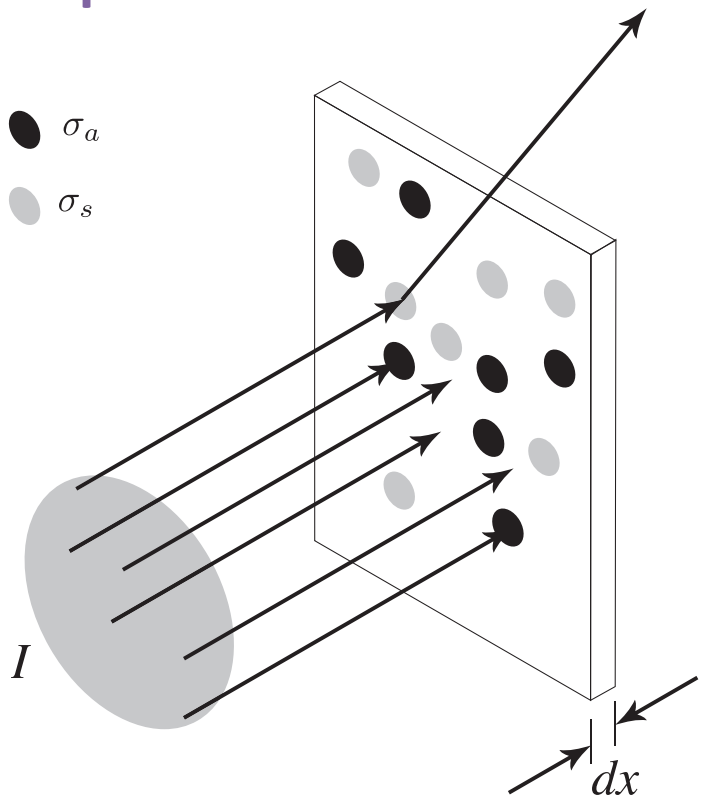
$$\Sigma = n\sigma \qquad \lambda = 1/\Sigma \qquad I(x) = e^{-x/\lambda}$$

Macroscopic x-section

Microscopic x-section

Mean Free Path

# Multiple Processes




$$P[j] = \frac{\Sigma_j}{\Sigma_T}$$

a or b?

$$u < \frac{\Sigma_a}{\Sigma_a + \Sigma_b} \quad ?$$

a b

$$\Sigma_T = \Sigma_1 + \Sigma_2 + \Sigma_3 + \ldots = n_1\sigma_1 + n_2\sigma_2 + n_3\sigma_3 + \ldots.$$

*on so on... to GEANT4*

$$\lambda_T = \frac{1}{\Sigma_T}$$

For mean free path λ

$$P[x] = e^{-x/\lambda}$$

$$s_i = -\lambda \log(u_i)$$

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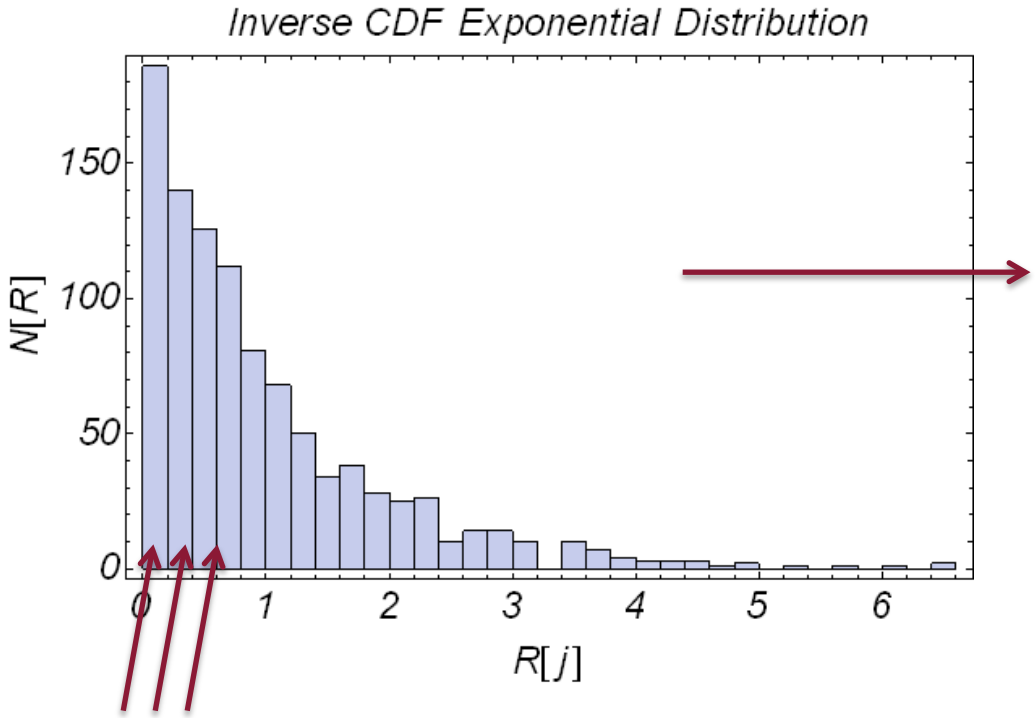
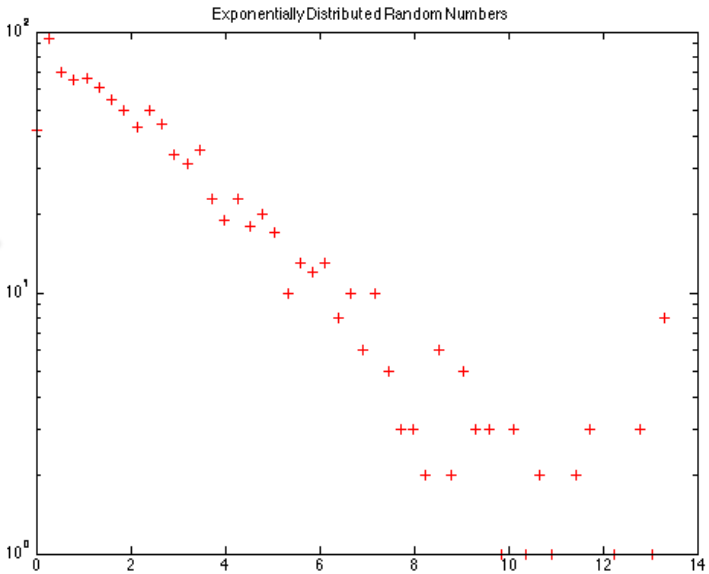
## Doing the fit (you should of course know how to do this!)

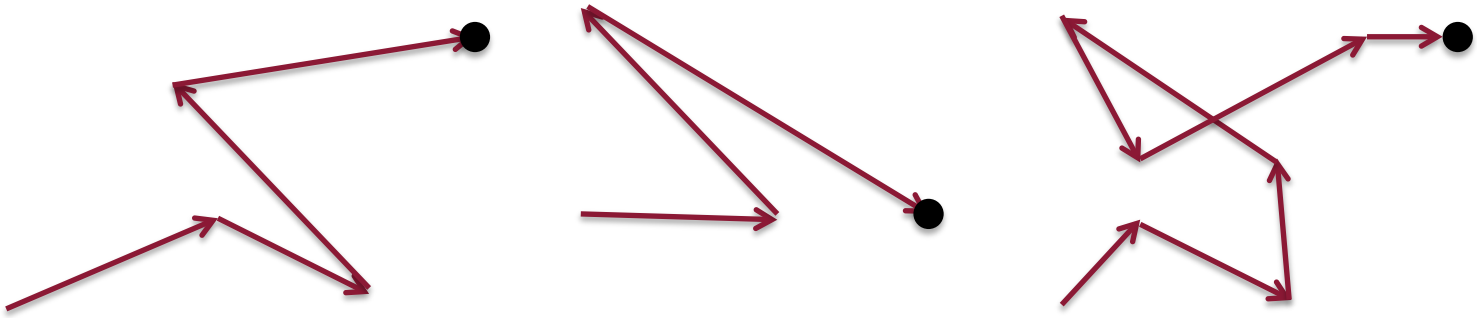



hist() function gives bin heights

- Get bin heights; these are numbers of particles absorbed at that depth
- Plot log(number of particles) versus depth, and fit a line
- The gradient gives the mean free path (which in this case is the same as the characteristic attenuation length)

# Particle Histories



- A particle history is the path taken by a particle until it stops (is absorbed)
- At each step, choose amongst possible processes $\sum_i$
- If scattering (i.e. continue moving), then take another step
- Else absorbed, and stop

- We assume each successive step is isotropic in direction (see later), but whose step length is distributed according to **exp(-x/λ)**
- This is an another example of Markov Chain Monte Carlo

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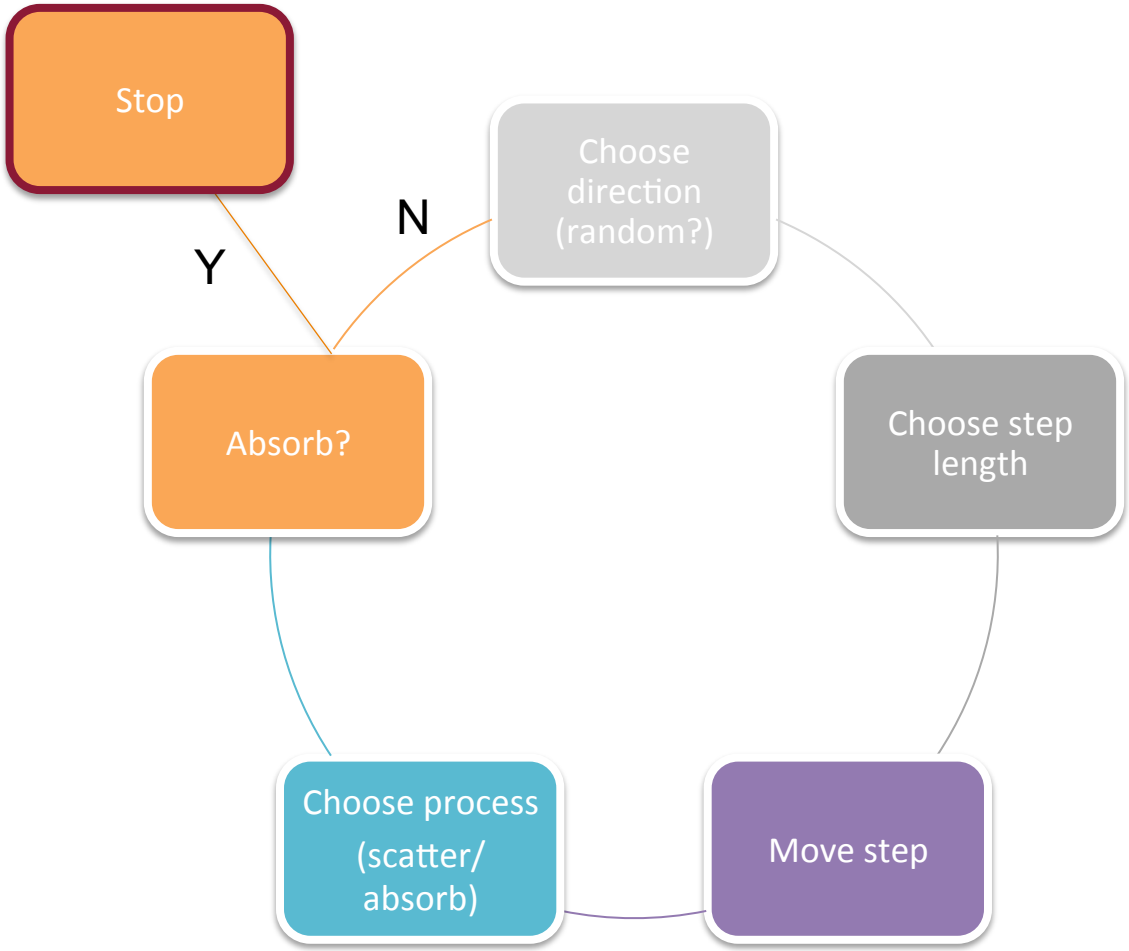
# Flowchart of Neutron History Calculation (Infinite Medium)



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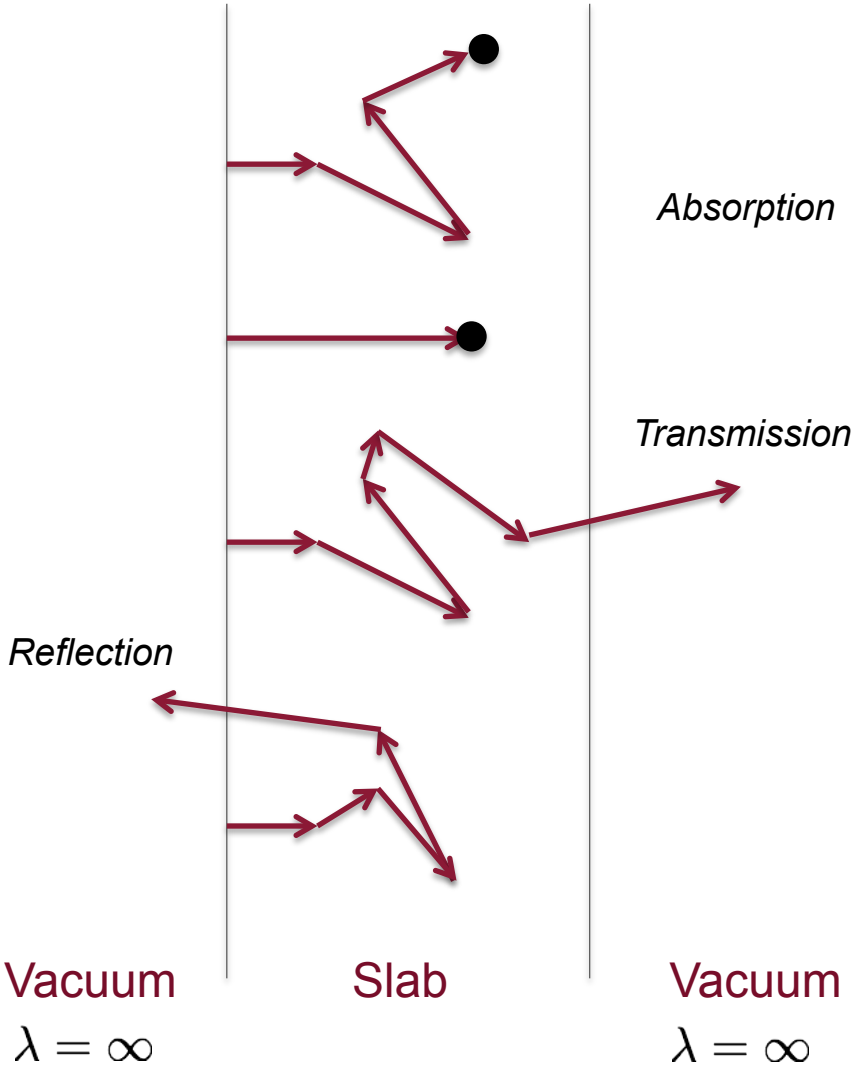
# Example: Passage Through a Finite Medium – Slab Calculation

- As well as absorption, particle can leave interesting regions.
  - E.g. Exit a slab of material
- We may wish to then ignore further calculations
  - This is called 'killing' the particle history
- Neutrons may be scattered or absorbed in a slab of material

  OR

  They may exit
  - in code 'parlance' this is called leaving the world volume, or when the importance is set to zero



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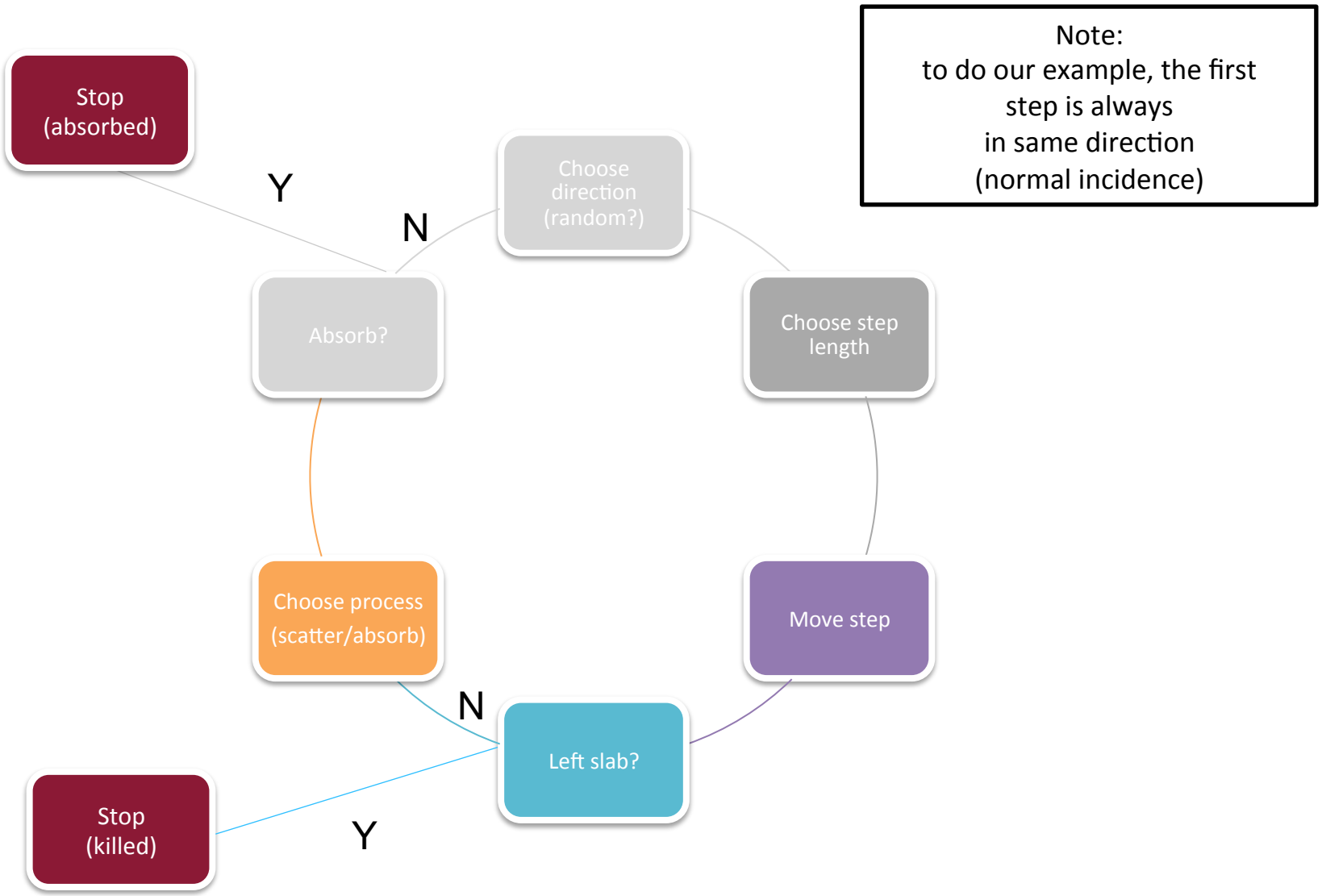
# Flowchart of Neutron History Calculation (Finite Slab)




Note:
to do our example, the first step is always in same direction (normal incidence)

# Exercise for the interested....

- You can develop a simulation of penetration of neutrons through a slab of thickness T
- Thermal neutrons only
  - Use a single, averaged cross section for each process
- Only absorption or isotropic scattering

- Like all good nuclear physicists, we work in c.g.s. units!

| | Water | Lead | Graphite |
|---|---|---|---|
| *Absorption $\sigma_a$/barn* | 0.6652 | 0.158 | 0.0045 |
| *Scattering $\sigma_s$/barn* | 103.0 | 11.221 | 4.74 |
| *Density /g cm$^{-3}$* | 1.00 | 11.35 | 1.67 |

- Typical nucleus $R \sim 6$ fm , therefore $\pi R^2 \sim 1$ barn

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# Calculations to perform

- Percentage absorption/transmission/reflection in 10cm of water, lead, graphite

- Variation of absorption/transmission/reflection with slab thickness for water, lead, graphite
  - Determine characteristic attenuation lengths when scattering is included
  - This will be different from the 'absorption only' value

- Should include error bars
  - Have a think what this value should be!

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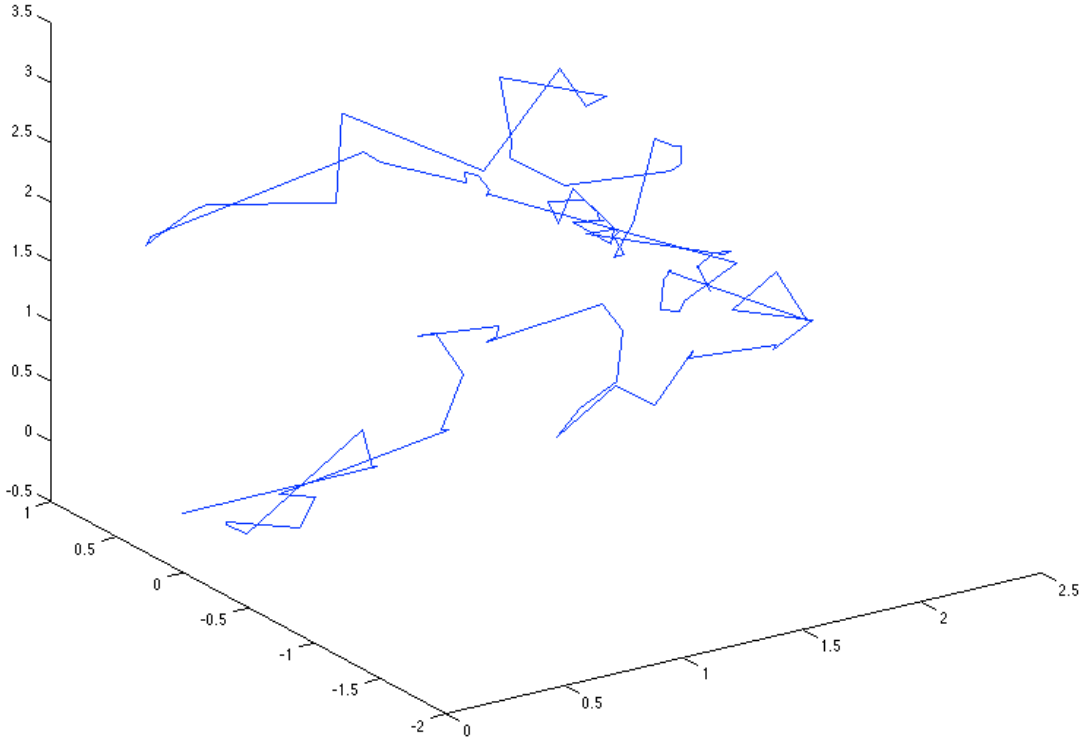
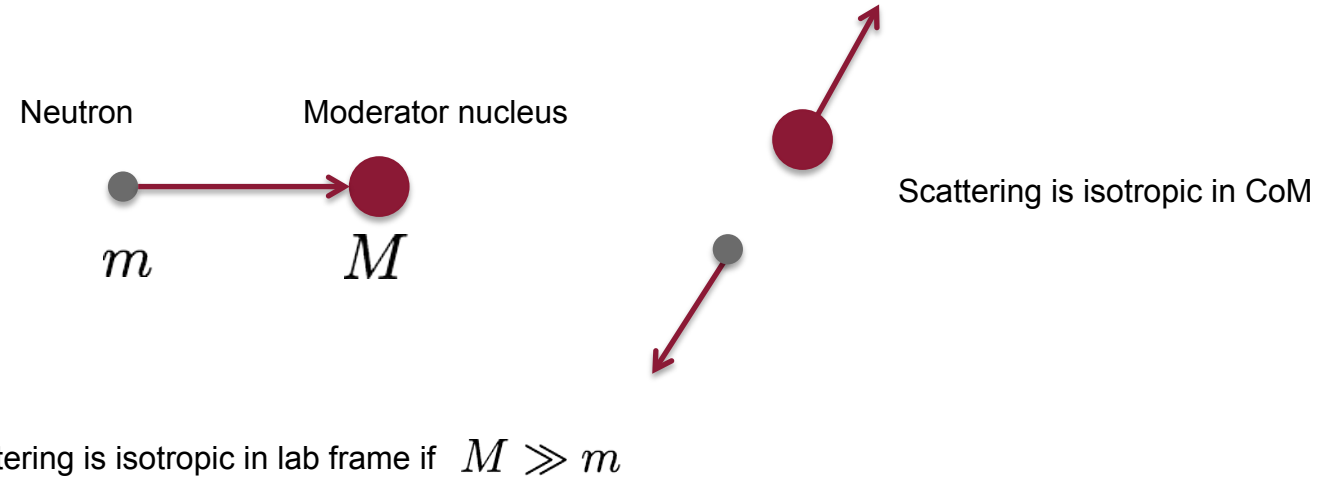
# Doing Random Walks in 3D



# Neutron Scattering

- Thermal neutrons arise in any system where there are many more scattering events than absorptions: $\sigma_s \gg \sigma_a$
- The neutrons obtain the same kinetic energy as their surroundings
  - Equilibrium energy $E \sim \frac{3}{2}kT$
  - (How many eV?)




Scattering is isotropic in lab frame if $M \gg m$

*Q: At what rate do initially fast particles slow down in a scattering medium (e.g. a moderator) and achieve thermal energies?*
*Hint: Calculate the typical number of scatters*

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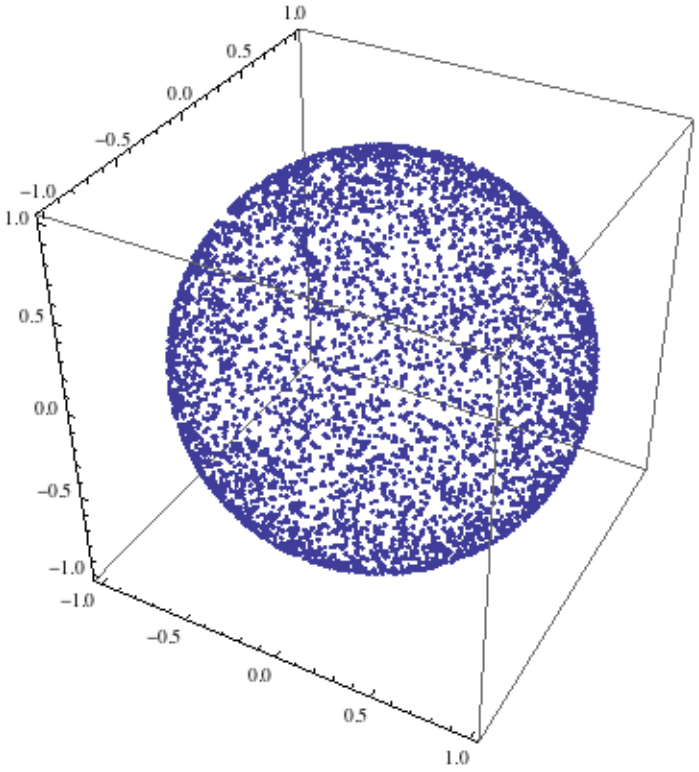
# Points on a Sphere

- *Problem:*

  How to generate points which are uniformly distributed on a sphere?

- Ideas?



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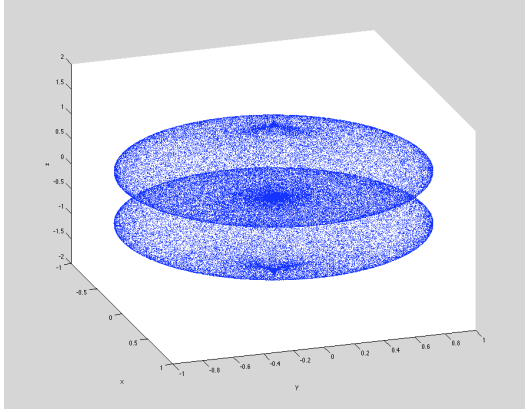
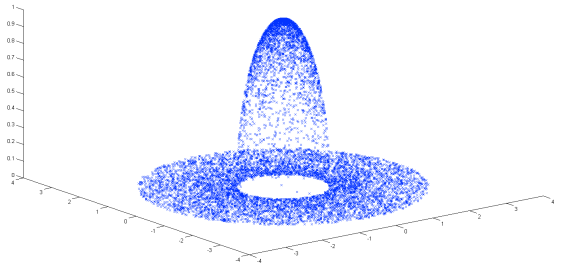
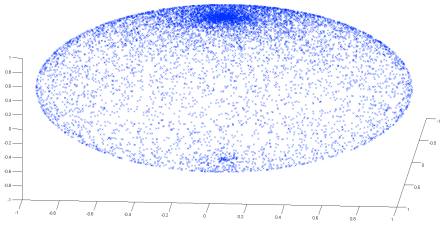
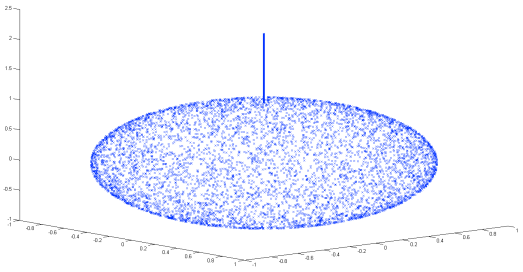
# Isotropic Unit Vector

- There are a few ways to do this…

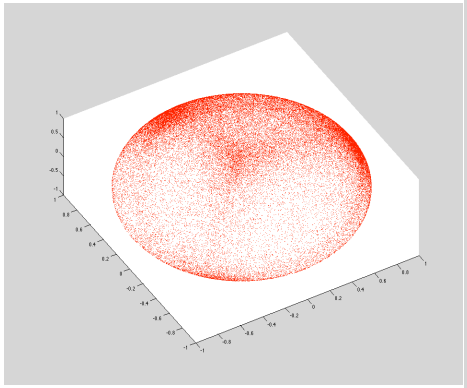


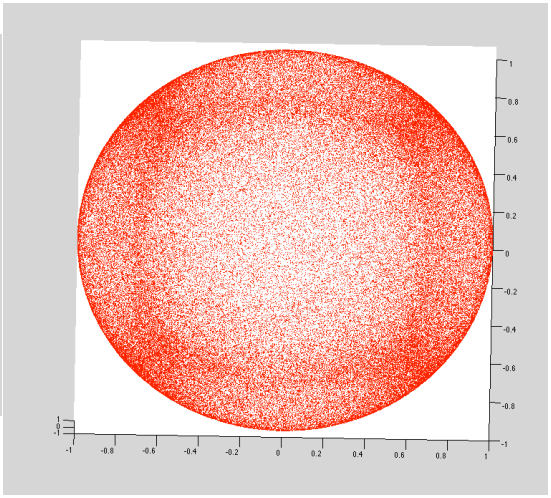


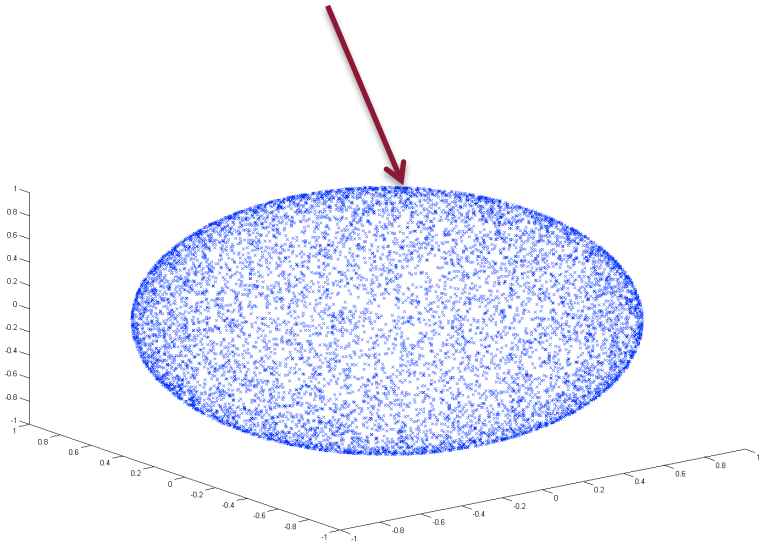




Want this one!







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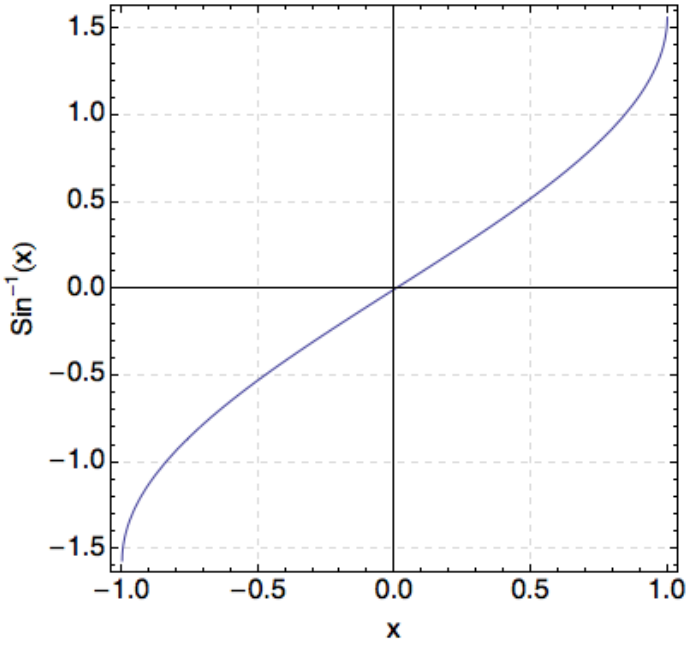
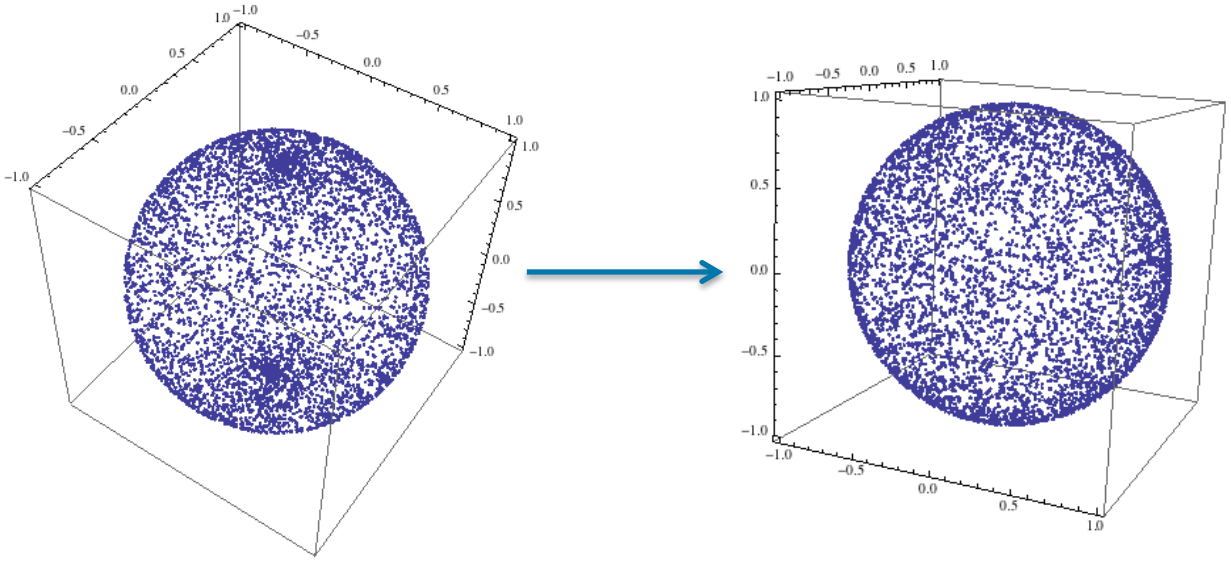
# Eliminating those Pesky Poles

- $r = 1$
- Sample $\theta$ and $\phi$ over $-\pi$ to $\pi$
- Spherical -> Cartesian conversion
- Doesn't work because samples are concentrated at the poles




- Clue: can use inverse CDF method again

$$\theta_i = sin^{-1}(u_i)$$



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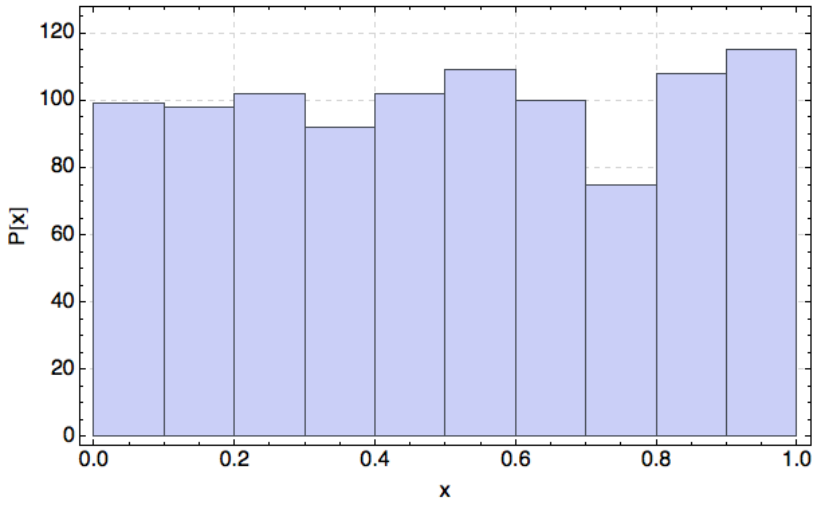
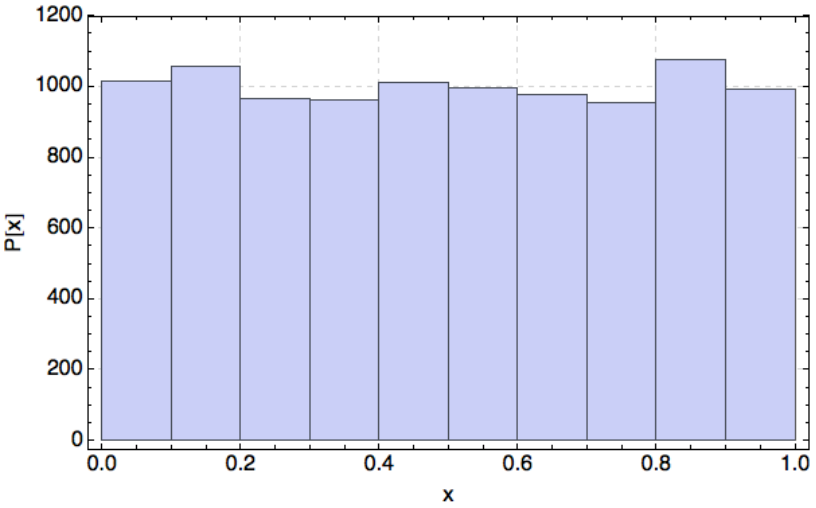
# Uniform or not?




1,000 samples




10,000 samples

- The probability of each bin having a certain height is approximately Gaussian-distributed

- We expect each bin to have fluctuation around $\sigma = \sqrt{\mu}$
- (The exact value is smaller, and is binomially-distributed)

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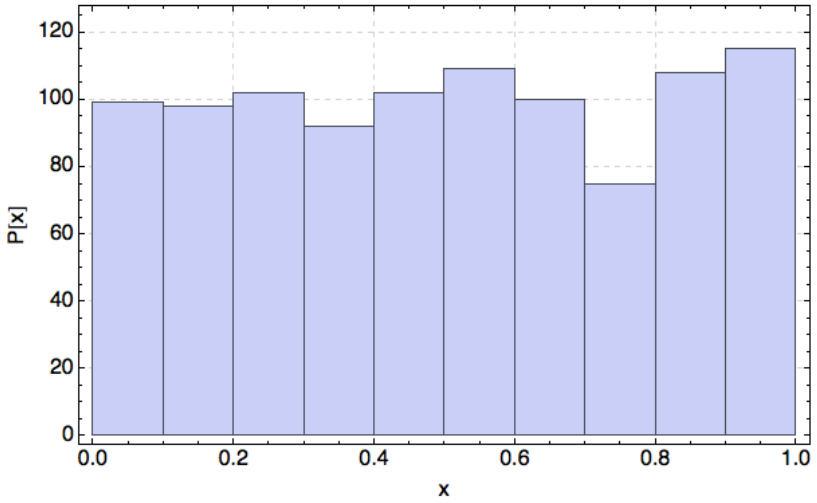
# Estimating variances

$$n = 1000$$
$$p = 0.1$$
$$a = np = 100$$




$$\sigma_a \simeq \sqrt{100} = 10$$

Normal (approximation)

$$Var(a) = np(1-p) = a(1-\frac{a}{n})$$

Binomial

$$\sigma_a = \sqrt{np(1-p)} = \sqrt{\frac{a(n-a)}{n}} = \sqrt{90} \simeq 9.5$$

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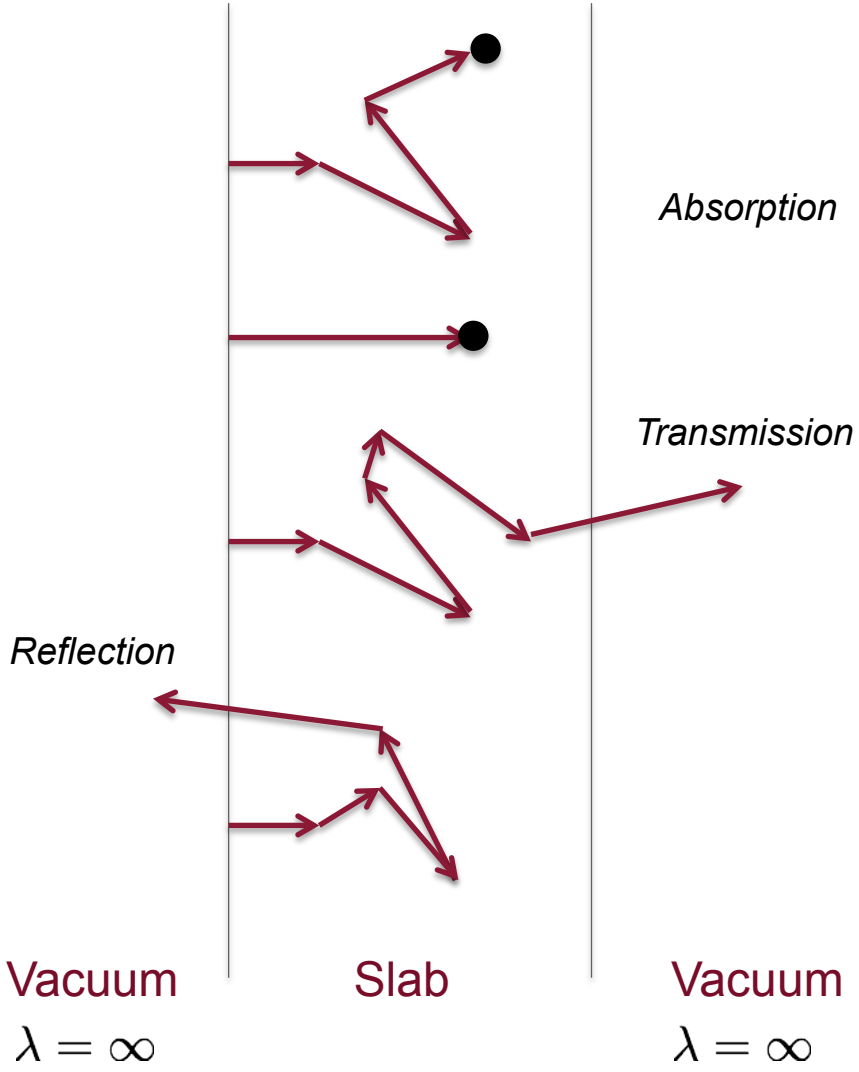
# Tallies

- Each neutron history has 1 of 3 possible results
  - Absorption
  - Transmission
  - Reflection
- We calculate the result of 1 history
  - Add 1 to the appropriate tally



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# Tally Errors

- Each history is a ‘throw into a bucket’
- N throws

- % transmission is A/N, R/N, T/N
- Error of A is approximately $\sqrt{A}$ (for small A).

# Another Way to Check Tally Errors

- Run your calculation n times
  - e.g. 10 times
- Calculate the mean and standard deviation of each of the tallies A, R, T
- You have a direct estimate of the simulation error

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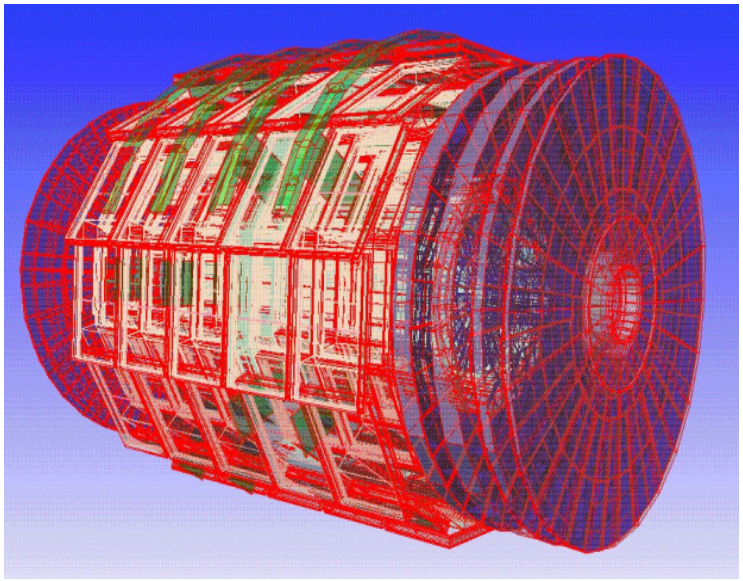
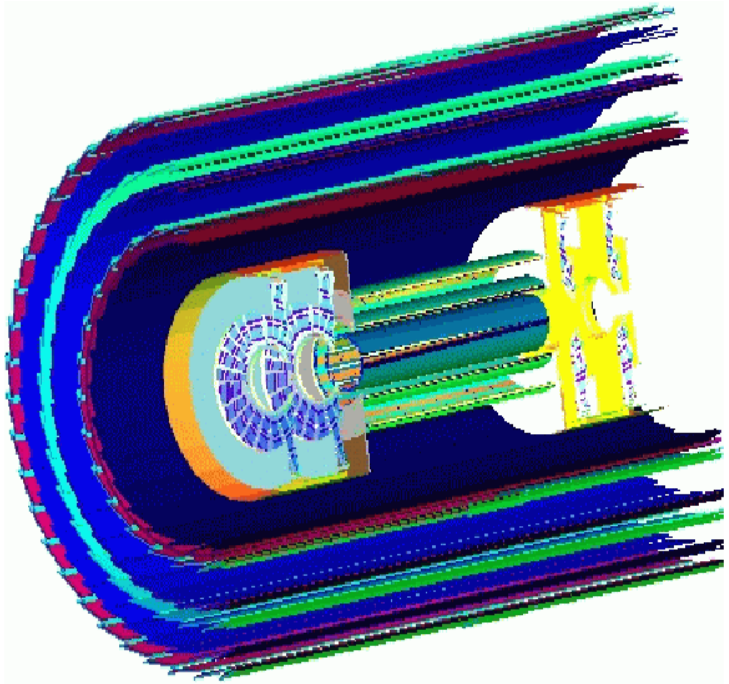
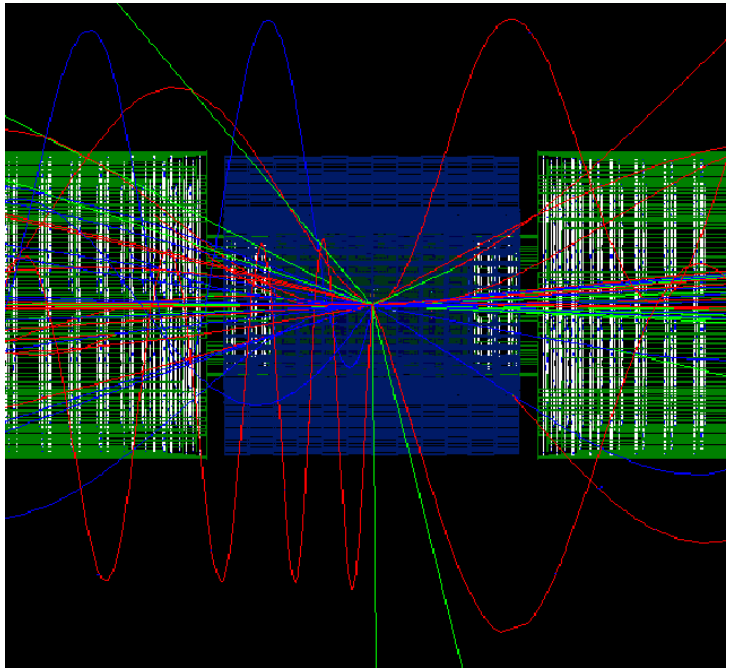
# Some Details: Material Boundaries

- Obviously, cases of interest are not limited to single slabs of material lying in a vacuum







- Much of a code's operation is in geometry definition, navigation, and boundary crossing

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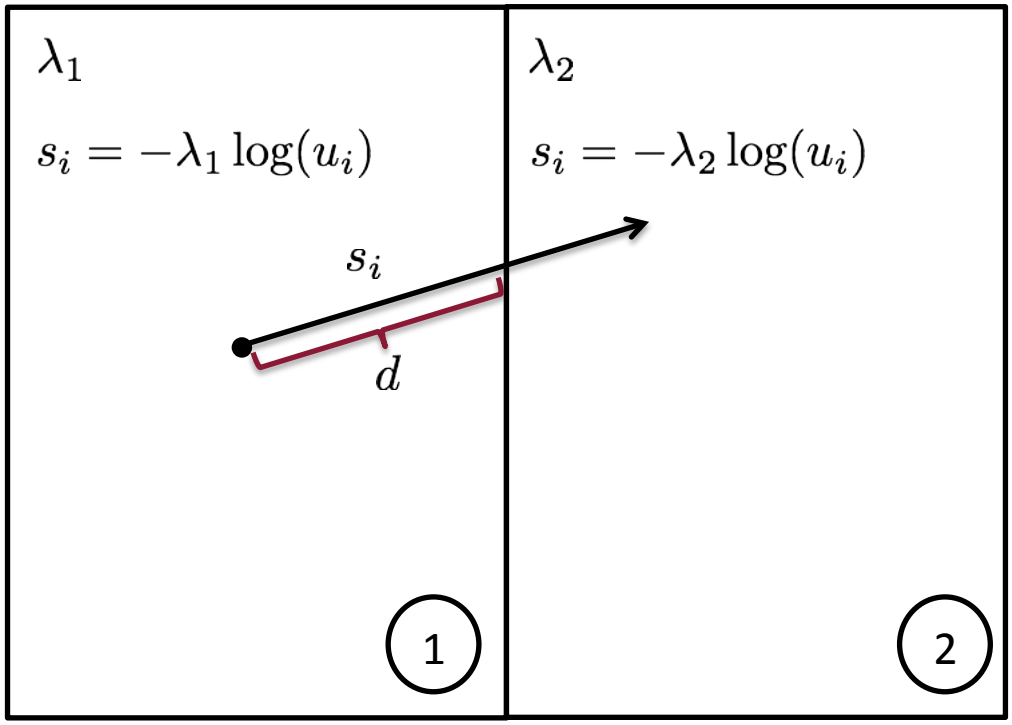
# Description of the Geometry Problem



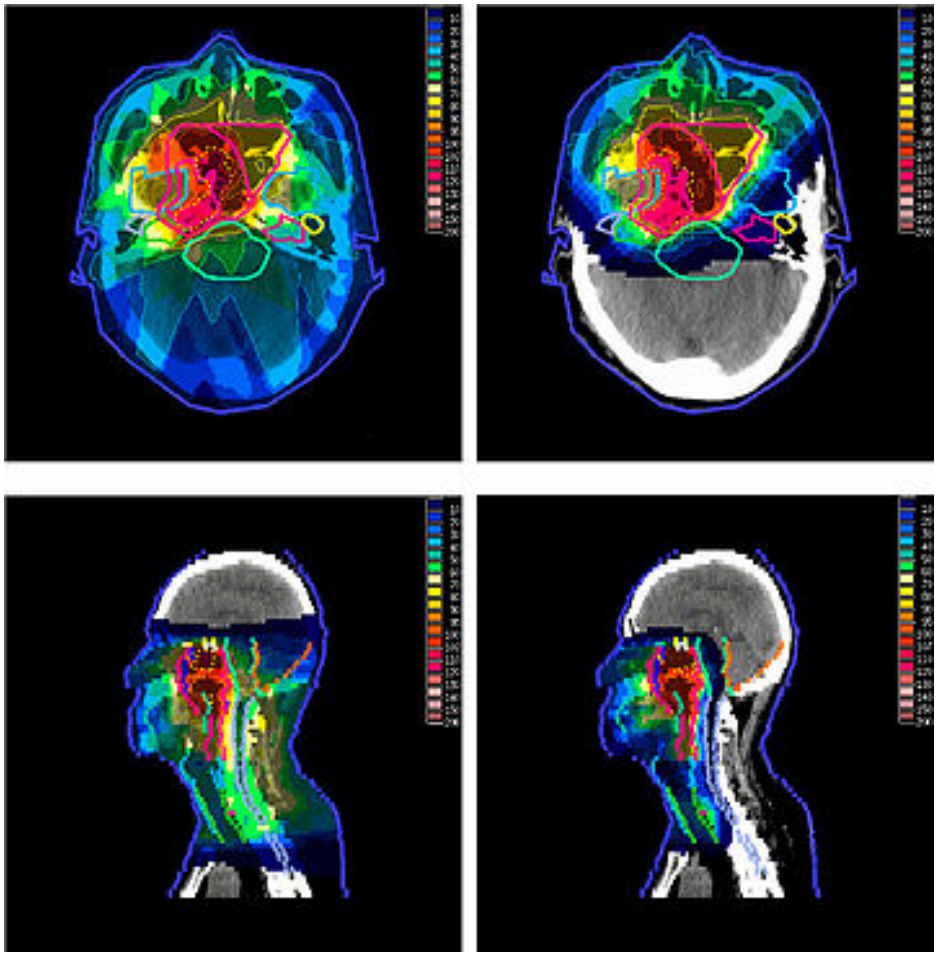

Region 1/Material 1 Region 2/Material 2

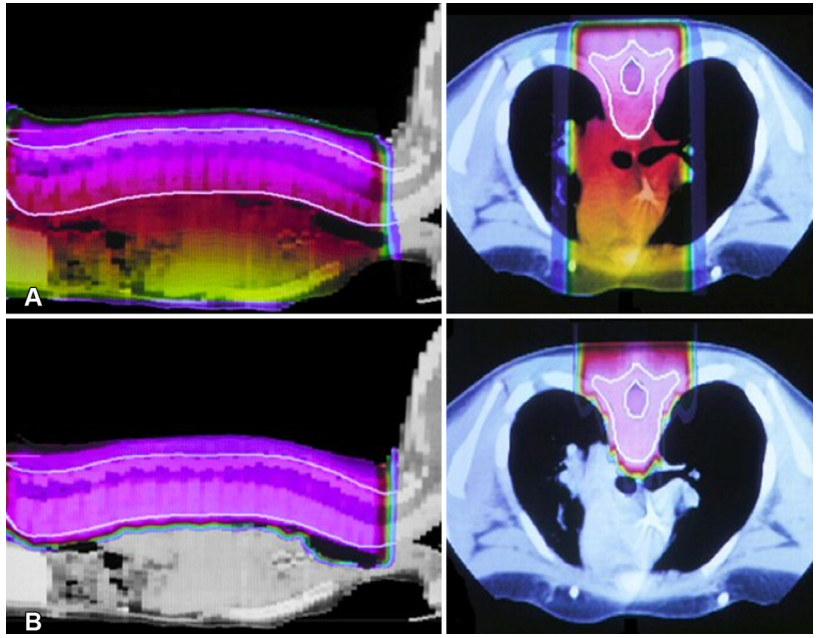
*d* is distance to boundary

- The step is the wrong length in Region 2
- Introduces statistical bias into the steps
- Also goes wrong if stepping the other way

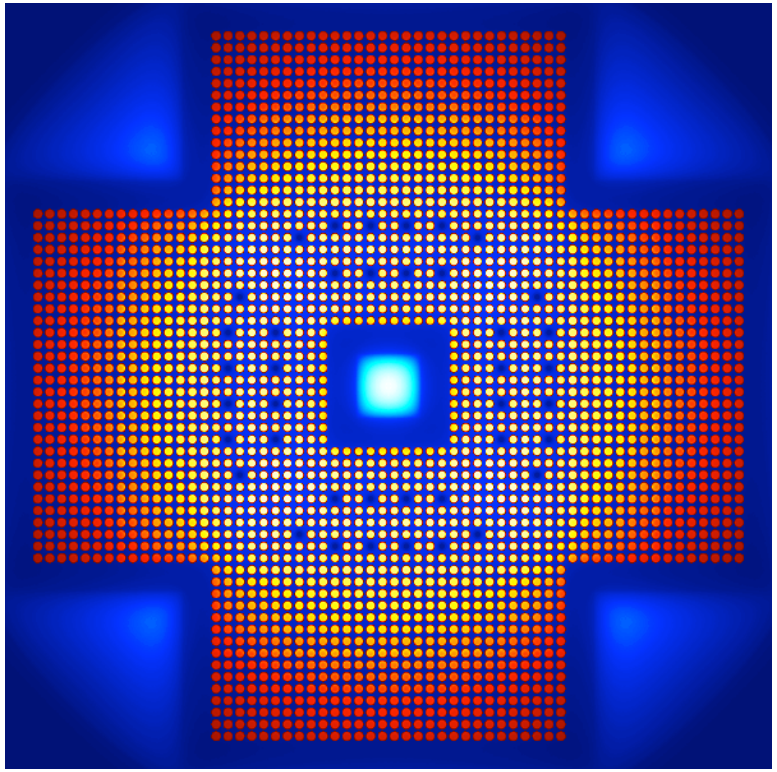
- Can get round this by calculating *d*, then stopping the step and starting again
  - This is the method used, but it involves lots of geometry calculations

# Application Example: Radiotherapy





# Application Example: Tracking neutrons through a reactor



- The regular geometry of a typical reactor lends itself to efficient navigation
  - i.e. a simple formula for working out where you are at the end of the step
  - one example of these is hole geometries, an important concept in particle tracking

# Standard vs EGS Sampling

- Standard Sampling:
- Calculate total Mean Free Path:

$$\frac{1}{\lambda_T} = \frac{1}{\lambda_a} + \frac{1}{\lambda_s}$$

- Take 1 step: $P[x] = e^{-x/\lambda_T}$

$$s_i = -\lambda_T \log(u_i)$$

- Choose process according to the branching ratio

$$P[j] = \frac{\Sigma_j}{\Sigma_T}$$

- EGS Sampling:
- Propose a step length for each process: $P[x_a] = e^{-x/\lambda_a}$ $P[x_s] = e^{-x/\lambda_s}$

$$s_a = -\lambda_a \log(u_i)$$
$$s_s = -\lambda_s \log(u_j)$$

- The shortest step length wins:

$$s_i = \min[s_a, s_s]$$

then that is the process that occurs (with P=1)

This is the method used in most codes you will encounter (GEANT4, EGS, FLUKA etc.), although MCNP uses 'Standard' sampling.
Try to figure out why.

*EGS means 'Electron-Gamma Shower', the name of a code*

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*'Sir,*

*In your otherwise beautiful poem (The Vision of Sin) there is a verse which reads:*

*"Every moment dies a man, every moment one is born."*

*Obviously, this cannot be true and I suggest that in the next edition you have it read:*

*"Every moment dies a man, every moment 1 1/16 is born."*

*Even this value is slightly in error but should be sufficiently accurate for poetry.*'

***Charles Babbage (in a letter to Lord Tennyson)***

# Example: Nuclear Reactor Criticality

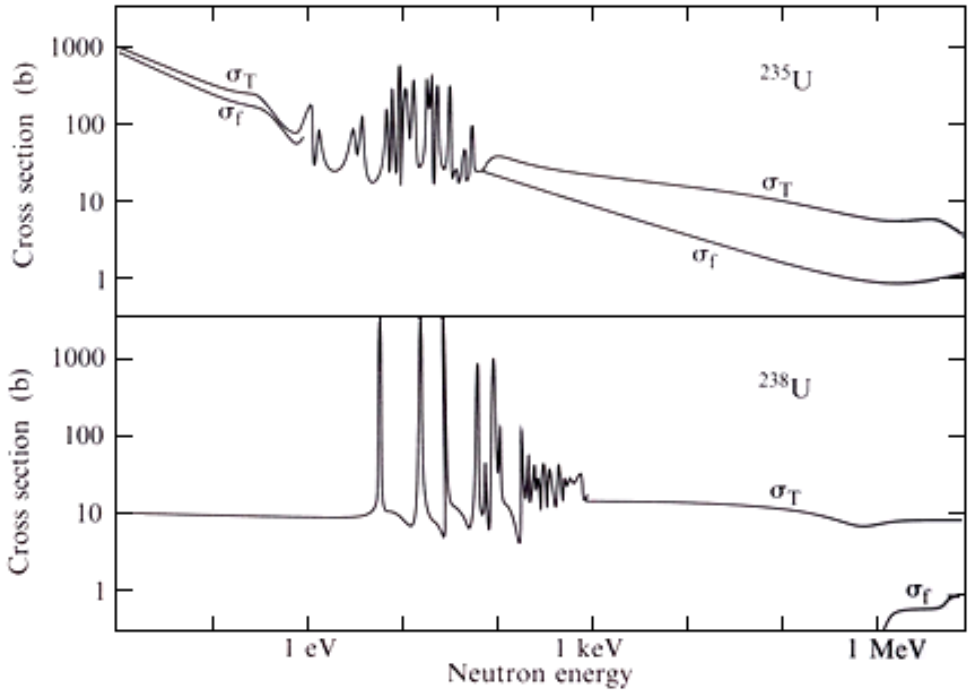
$$\sigma_T = \sigma_s + \sigma_c + \sigma_f$$

Total = Scattering (elastic) + Capture (radiative) + Fission

Can also define an absorption cross section:

$$\sigma_a = \sigma_c + \sigma_f$$

The values for all these cross sections are often highly-dependent on the incoming neutron energy



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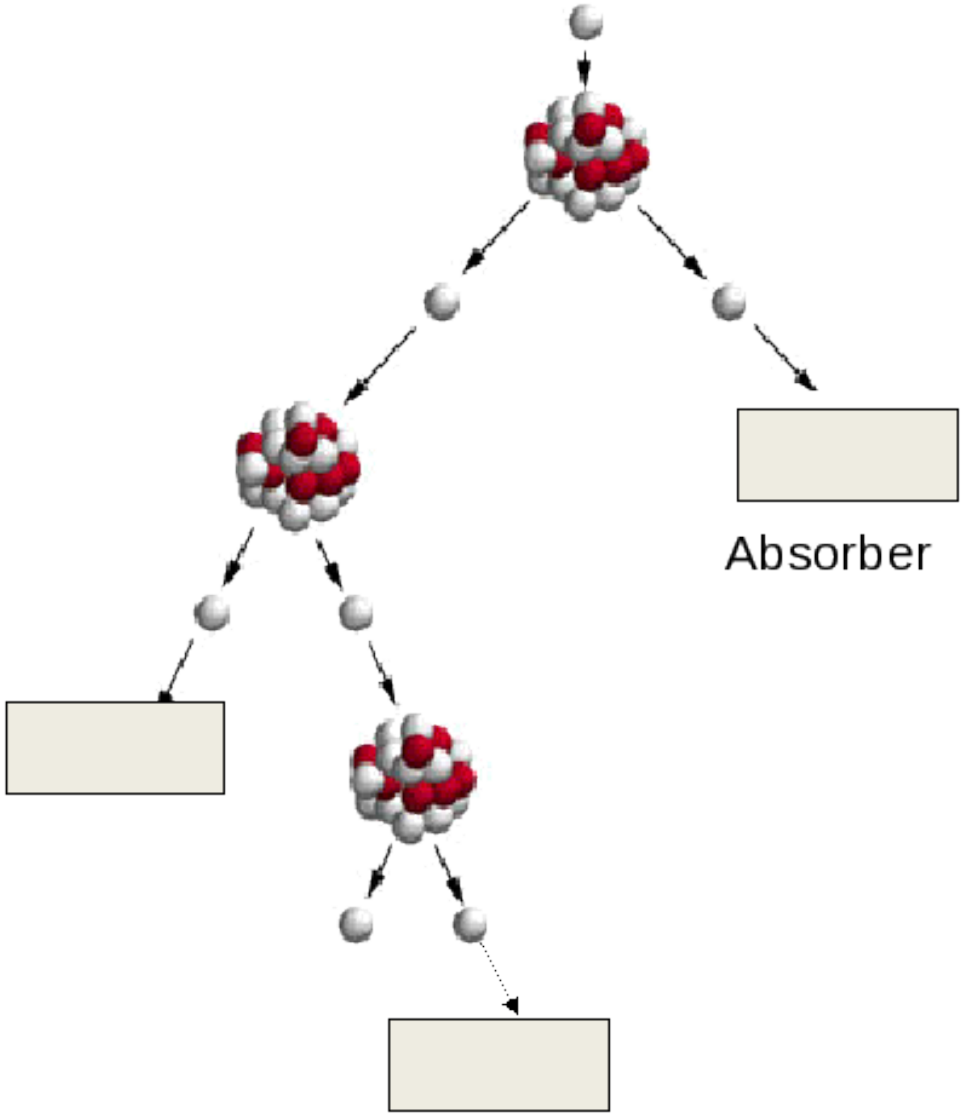
# Neutron Multiplication Factor k

- k < 1; Sub-critical, reaction unsustainable
- k = 1; Critical, chain reaction stable and maintained by (e.g.) control rods
- k > 1; Super-critical, reaction rate increases
- All are neutron multiplying systems
  - One initial neutron makes many more



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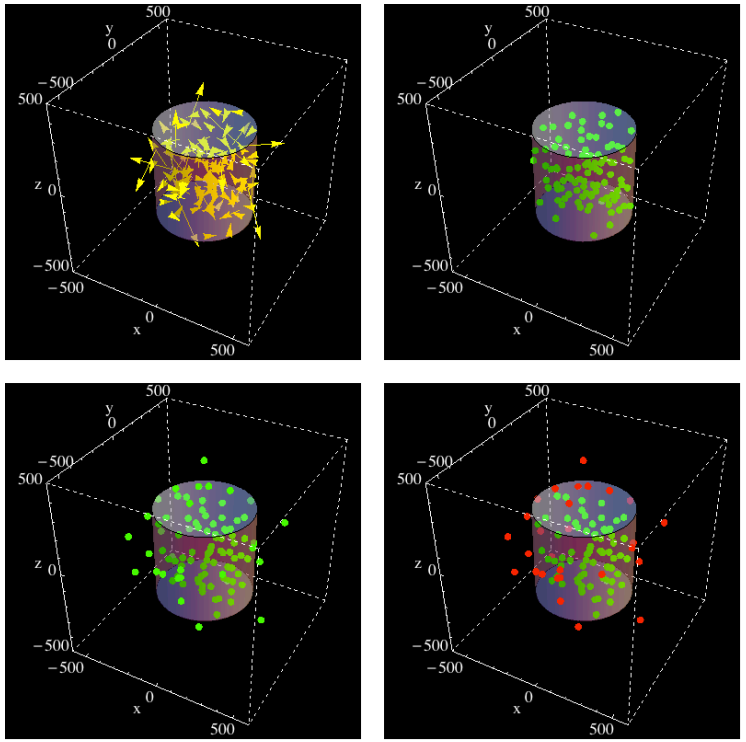
$$\eta = \frac{\nu\sigma_f^F}{\sigma_a^F}$$

$$f = \frac{\Sigma_a^F}{\Sigma_a}$$

$$k_\infty = \epsilon p f \eta$$

$$k_{eff} = \epsilon p f \eta P_{NL} P_{NLth}$$



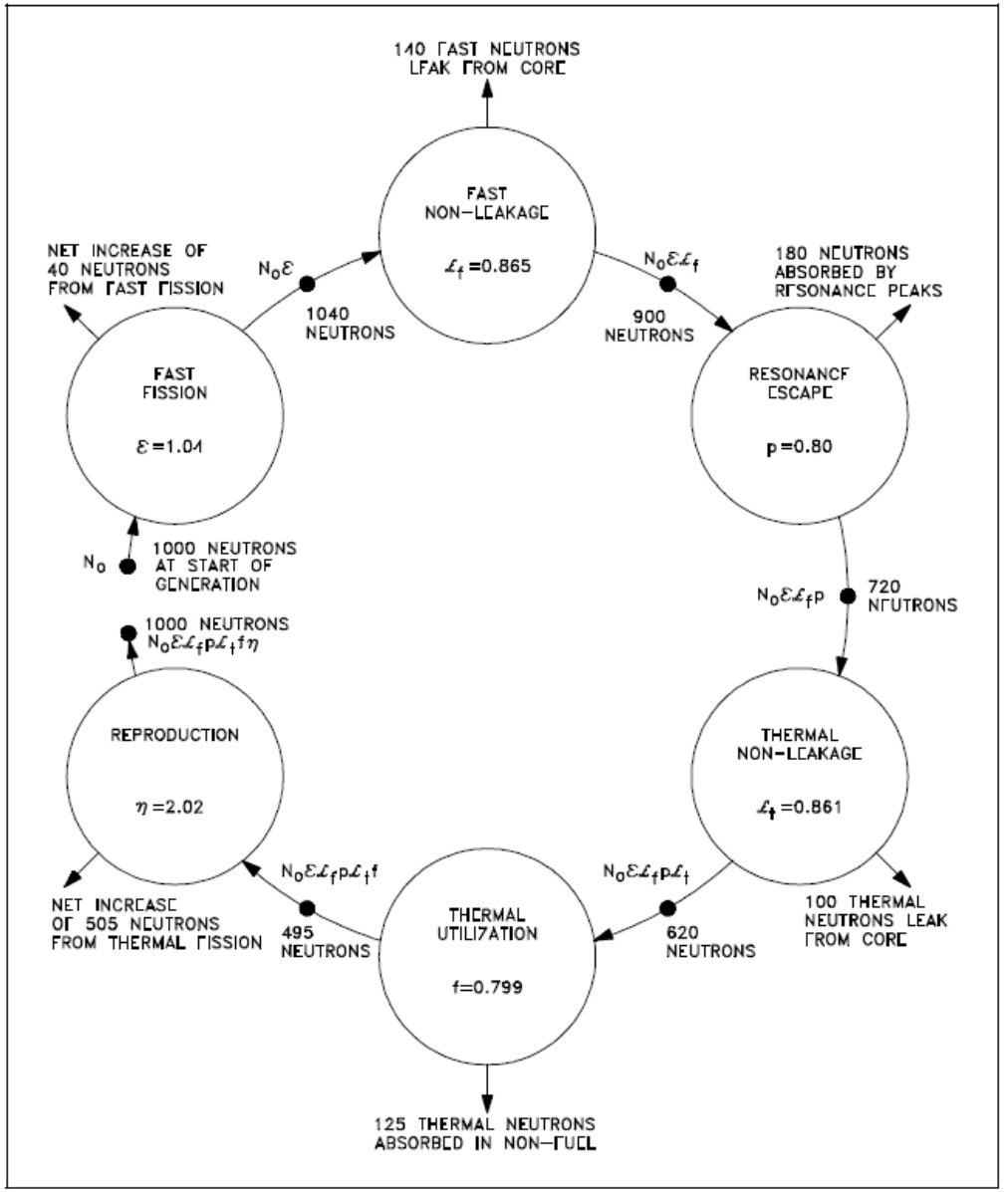



Figure 1 Neutron Life Cycle with $k_{eff} = 1$

$$n_{chain} = 1 + k_\infty + k_\infty^2 + k_\infty^3 + \cdots + k_\infty^n + \cdots = \frac{1}{1 - k_\infty}$$