Lecture Note 7

Monte Carlo method

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Statistical Nature of Neutron Reaction

- Macroscopic Cross section

  Σ_t? Probability of reaction for a neutron traveling unit distance

$$dn = -n\Sigma_t dx$$

$$n(x) = n_0 e^{-\Sigma_t x} \qquad \left(e^{-\Sigma_t x} \text{ : survival probability after traveling } x\right)$$

- Probability to react within unit distance after traveling x

$$p(x) = e^{-\Sigma_t x} \cdot \Sigma_t$$

- Mean free path

$$\int_0^\infty x p(x) dx = \int_0^\infty x \cdot e^{-\Sigma_t x}\Sigma_t dx = \cancel{-xe^{-\Sigma_t x}\Big|_0^\infty} + \int_0^\infty e^{-\Sigma_t x} dx = \frac{1}{\Sigma_t}$$

- In core, collision probability

$p = \tilde{p}(\vec{r}, E) dV dE$: probability for a neutron born somewhere in the core to have a collision around $\vec{r}, E$ with dV, dE (phase space)

$(p \ll 1)$

Statistical Nature of Neutron Reaction

- Number of collision for N neutrons born

  – Expected value? $= N \cdot p$

  – Expected variance ?

- for k collisions out of N neutrons, possible number of occurrences

$$\eta(k, N) = {}_N C_k \, p^k (1-p)^{N-k}$$

$\Rightarrow$ a_{kN} of $(p+q)^N$: coeff of the i-th order term $(q = 1 - p)$

= probability for k neutrons (out of N neutrons) to have collisions

– Expected value of k

$$\sum_{k=0}^{N} \left[k \cdot \eta(k, N) \right] = \sum_{k=0}^{N} \left[k \cdot {}_N C_k \, p^k q^{N-k} \right] ?$$

Moment Generating Function for PDF

- The moment-generating function of a random variable X is
  - If X has a continuous probability density function $p(x)$, then the MGF is given by

$$M_X(t) = \int_{-\infty}^{\infty} e^{tx} p(x)dx \rightarrow \quad M_X(t) = E(e^{tx})$$

$$M'_X(t) = \int_{-\infty}^{\infty} xe^{tx} p(x)dx \quad \rightarrow \quad E(X) = M_X(0) = \int_{-\infty}^{\infty} xp(x)dx$$

$$M_X^{(n)}(t) = \int_{-\infty}^{\infty} x^n e^{tx} p(x)dx \quad \rightarrow \quad E(X^n) = M_X^{(n)}(0) = \int_{-\infty}^{\infty} x^n p(x)dx$$

PDF : Probability Density Function

  - If X has a discrete probability density function $p(x)$, then the MGF is given by

$$M_X(t) = \sum_{k=0}^{N} e^{tx} p(x)$$

$$M'_X(t) = \sum_{i=0}^{N} xe^{tx} p(x) \quad \rightarrow \quad E(X) = M'_X(0) = \sum_{i=0}^{N} xp(x)$$

$$M''_X(t) = \sum_{i=0}^{N} x^2 e^{tx} p(x) \quad \rightarrow \quad E(X^2) = M''_X(0) = \sum_{i=0}^{N} x^2 p(x)$$

Moment Generating Function for PDF

- Expected value of k using MGF

$$E\left(k\right) = M'_K(0) = \sum_{i=0}^{N} k\ p(k)$$

$$\begin{cases} M_K(t) = \sum_{k=0}^{N} e^{tk}\ {}_N C_k\, p^k q^{N-k} = \sum_{k=0}^{N} {}_N C_k \left(pe^t\right)^k q^{N-k} = \left(pe^t + q\right)^N \\ M'_K(t) = N\left(pe^t + q\right)^{N-1} \cdot pe^t \\ M'_K(0) = N(p+q)^{N-1} p = Np \end{cases}$$

$$\therefore E\left(k\right) = Np$$

Moment Generating Function for PDF

- Expected variance of k using MGF

$$\sigma_N^2 = \sum_{k=0}^{N}\left[\left(k-\bar{k}\right)^2 \eta(k,N)\right] = \sum_{k=0}^{N}\left[\left(k^2 - 2k\bar{k} + \bar{k}^2\right)\eta(k,N)\right]$$

$$= \sum_{k=0}^{N}\left[k^2\eta(k,N)\right] - 2\bar{k}\sum_{k=0}^{N}\left[k\eta(k,N)\right] + \bar{k}^2\sum_{k=0}^{N}\left[\eta(k,N)\right]$$

$$\left(\begin{array}{l} \sum_{k=0}^{N}\left[k\eta(k,N)\right] = \bar{k} \\ \sum_{k=0}^{N}\left[\eta(k,N)\right] = 1 \end{array}\right)$$

$$= \overline{k^2} - 2\bar{k}\cdot\bar{k} + \bar{k}^2$$

$$= \overline{k^2} - \bar{k}^2$$

$$\begin{cases} M_K(t) = \left(pe^t + q\right)^N \rightarrow M_K'(t) = N\left(pe^t + q\right)^{N-1}\cdot pe^t \\ M_K''(t) = N(N-1)\left(pe^t + q\right)^{N-2}\cdot p^2 e^{2t} + N\left(pe^t + q\right)^{N-1}\cdot pe^t \\ M_K''(0) = N(N-1)p^2 + Np \end{cases}$$

$$\sigma^2 = M_K''(0) - \left[M_K'(0)\right]^2$$

$$= N(N-1)p^2 + Np - N^2p^2$$

$$= Np(1-p)$$

$\rightarrow q \sim 1$ for $p << 1$

$\rightarrow$ Relative standard deviation: $\dfrac{\sqrt{Var(k)}}{\bar{k}} = \dfrac{\sqrt{Npq}}{Np} = \dfrac{\sqrt{q}}{\sqrt{Np}} \approx \dfrac{1}{\sqrt{Np}} \propto \dfrac{1}{\sqrt{N}}$

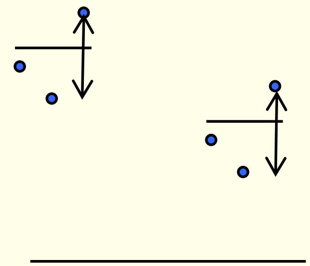
$$\therefore Var(k) = Npq$$

Estimation of p

- Estimation of p

Since p is unknown, let's find p by experiment

Repeated Simulation with n neutrons/cycle



– Let $N = n \cdot C$ (where C is the number of cycles)

$$p_i = \frac{1}{n}\sum_{j=1}^{n} p_{ij} \qquad p_{ij} = \begin{cases} 1 & \text{if collision in phase space} \\ 0 & \text{otherwise} \end{cases} \qquad (i - \text{cycle}\ ,\ j - \text{neutron})$$

$$\bar{p} = \frac{1}{C}\sum_{i=1}^{C} p_i$$

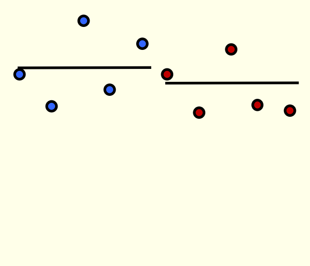
$\rightarrow$ $C-1$ for sample variance because of reduced degree of freedom due to the use in the sample mean. $\Leftarrow$ Two data $\rightarrow$ one deviation.

$$\sigma_s^2 = \frac{1}{C-1}\sum_{i=1}^{C}\left(p_i - \bar{p}\right)^2$$

(conservative estimation of the real standard dev of the population)

$$\sigma_s^2\left(\bar{p}\right) = \frac{\sigma^2\left(p_i\right)}{C}$$

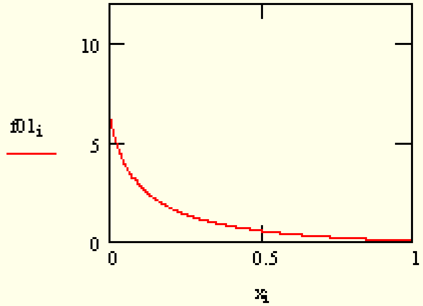
: Expected Variance of $\bar{p}$



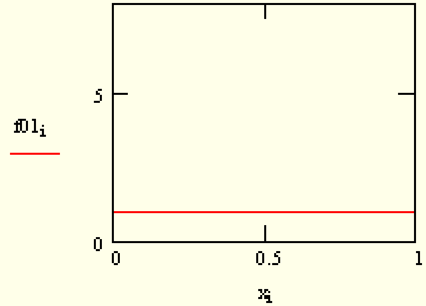
$$\therefore \sigma^2\left(\bar{p}\right) = \frac{\sum_{i=1}^{C}\left(p_i - \bar{p}\right)^2}{C\left(C-1\right)}$$

Central Limit Theorem

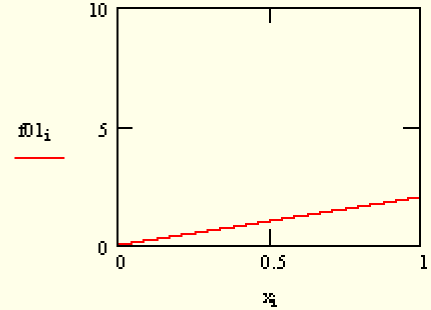
- the average of a large number of independent and identically-distributed random variables will be approximately normally distributed (i.e., following a Gaussian distribution) if the random variables have a finite variance
  - Let $x_1, x_2, x_3, \ldots$ be a set of n independent and identically distributed random variables having finite values of mean μ and variance $\sigma^2 > 0$.
  - Cetral limit theorem states that
    as the sample size n increases,
    the distribution of the sample average approaches the normal distribution
    with a mean μ and variance $\dfrac{\sigma^2}{n}$ irrespective of the shape of the original distribution.



NonNormal Distribution of X



NonNormal Distribution of X



NonNormal Distribution of X

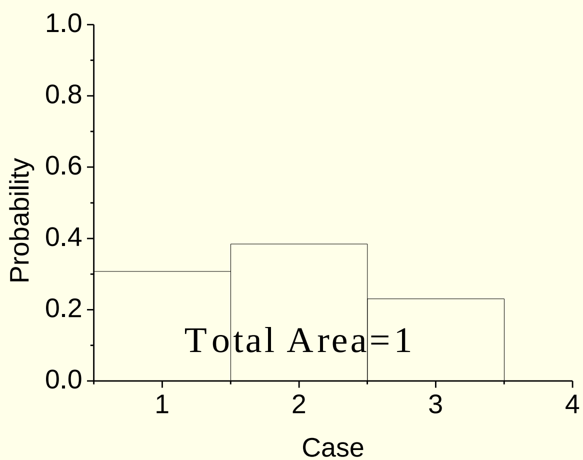
PDF, CDF and Golden Rule

- PDF : Probability Density Function

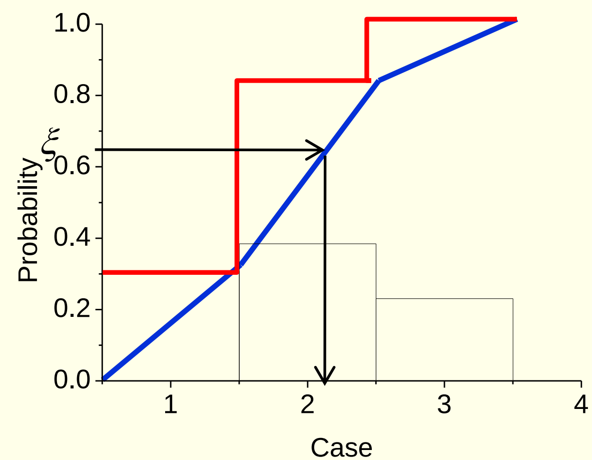
$p(x)dx$: probability

- CDF : Cumulative Distribution Function

$$\int_{-\infty}^{x} f\left(x'\right)dx'$$



PDF

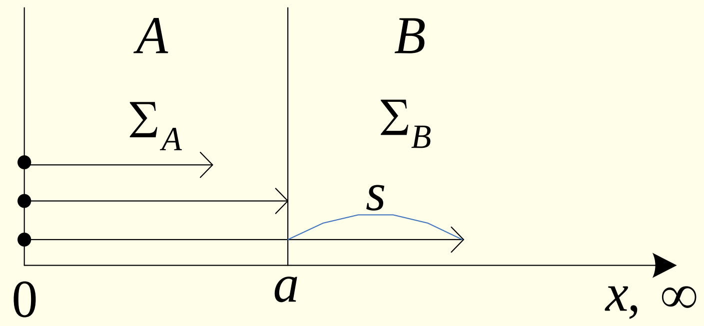


CDF

- Golden Rule

With a CDF given, an event can be picked by a random number ξ.

Probability of Collision at x with two regions



– PDF $\quad A: p(x) = \Sigma_A e^{-\Sigma_A x}$

$$B: p(x) = e^{-\Sigma_A a}\Sigma_B e^{-\Sigma_B s} \quad (s = x - a)$$

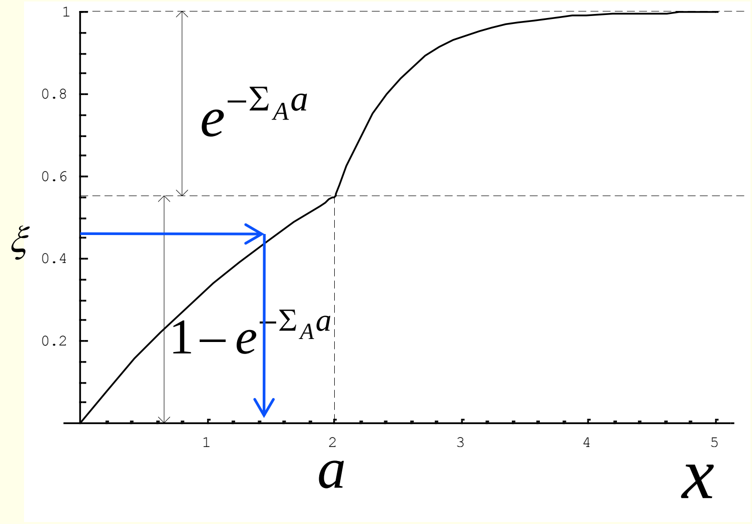
$$= e^{-\Sigma_B a} e^{-\Sigma_B s}\Sigma_B = e^{-\int_0^x \Sigma(l)dl}\Sigma_B$$

– CDF

$$P(x) = \int_0^a \Sigma_A e^{-\Sigma_A l} dl + e^{-\Sigma_A a}\int_0^s \Sigma_B e^{-\Sigma_B l} dl$$

$$= \begin{cases} 1 - e^{-\Sigma_A x} & , \ x \le a \\ \left(1 - e^{-\Sigma_A a}\right) + e^{-\Sigma_A a}\left(1 - e^{-\Sigma_B s}\right), & x > a \end{cases}$$

$\rightarrow$ Probability of collision within x



Length of Travel to first collision for a random number ξ

MC Simulation of Neutron Migration in 2D with MG Xsec

Problem Geometry

- **2D core with assembly-wise Xsec**
  - No heterogeneous configuration within Assembly
  - Constant xsec over each FA
- **Subdivision of each assembly into cells**
  - Flux averaged over each cell
- **Neutrons are moving in 3D space, but axially invariant neutron behavior**

$$\frac{\partial}{\partial z} = 0 \rightarrow \varphi(x, y, z_1) = \varphi(x, y, z_2) \text{ for any } z_1 \text{ and } z_2.$$

- **Radial BC can be either reflective or vacuum**

Cross Sections

- **Multigroup macroscoic cross sections given with scattering matrices**
- **Scattering is assumed to be isotropic**

$$\Sigma_t = \Sigma_{tr} = \frac{1}{3D} \text{ when using diffusion solver data}$$

Things to Consider in Simulating Stochastic Events Occurring a Neutron Flight

Characterization of a neutron

- Position (x,y,z)
- Moving direction (α, θ) or $(\Omega_x, \Omega_y, \Omega_z)$
- Energy (g)
- Weight (w)

Position of collision in space

- How long to move from the current position?

Type of interaction

- absorption, scattering, fission

Scattering mechanism

- Deflected angle after scattering
- Energy after scattering

Fission neutrons emitted

- Number
- Location : Source point in the next simulation

Shooting a neutron and first move

- Get the position of $i-th$ fission source neutron from the storage $\rightarrow$ determine the initial cell number
- Determine the energy group of emission using χ_g
- Determine the angle of emission assuming isotropic emisssion

  - using the angle pickup scheme on the next slide
- Determine the first travel distance

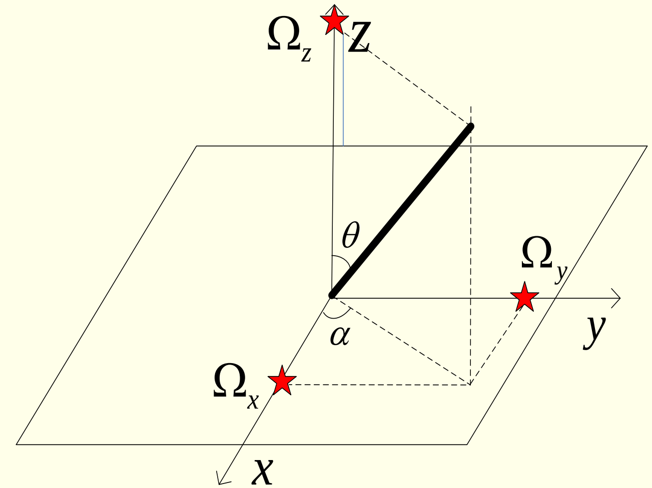
Selection of Angle

$$\Omega_x^2 + \Omega_y^2 + \Omega_z^2 = 1$$

$$\Omega_x = \sin\theta \cdot \cos\alpha$$

$$\Omega_y = \sin\theta \cdot \sin\alpha$$

$$\Omega_z = \cos\theta$$



Select α : $0 \sim 2\pi$ $\qquad \alpha = \xi \times 2\pi \quad (0 \le \xi \le 1)$

Select θ : $0 \sim \pi$

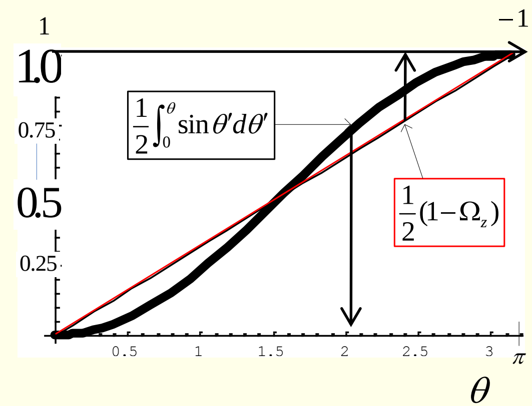
$$p(\theta)d\theta = Csin\theta d\theta$$

$$\int_0^{\pi} p(\theta)d\theta = C\int_0^{\pi} sin\theta d\theta = 2C \rightarrow C = \frac{1}{2}$$

$$CDF : P(\theta) = \int_0^{\theta} p(\theta')d\theta' = \frac{1}{2}(1 - cos\theta) = \frac{1}{2}(1 - \Omega_z) = \xi$$

$$\Omega_z = 1 - 2\xi \qquad (0 \le \xi \le 1)$$

$$\sin\theta = \sqrt{1 - (\cos\theta)^2} = \sqrt{1 - \Omega_z^{\,2}}$$



SNURPL

Distance to Move

- Straight path of distance

For given Σ_t, probality to have collision in dx after traveling s: $p(s)dx = \Sigma_t e^{-\Sigma_t s} dx$

$$C(s) = \int_0^s \Sigma_t e^{-\Sigma_t s'} ds' = -e^{-\Sigma_t s'} \Big|_0^s = 1 - e^{-\Sigma_t s}$$

C(s) : Cummulative Distribution Function

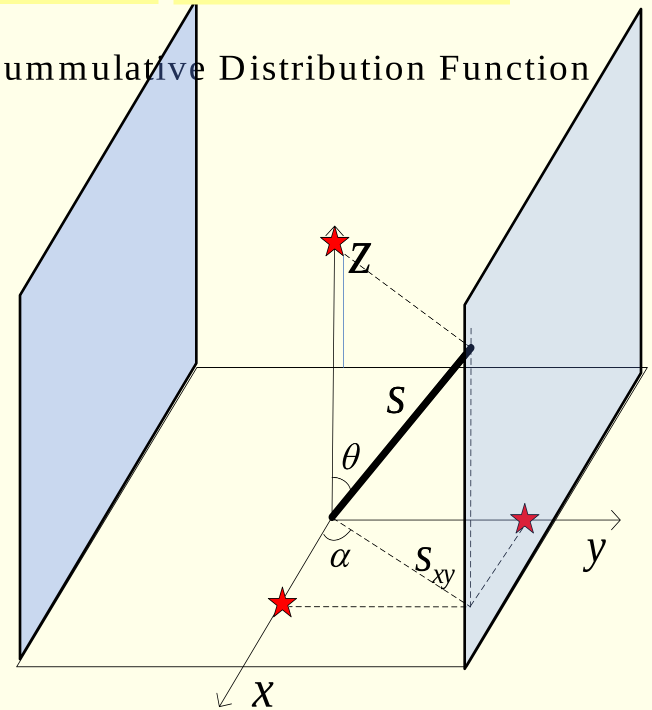
$$C(s) = \xi \quad \text{(random variable)}$$

$$1 - e^{-\Sigma_t s} = \xi$$

$$s = \frac{-\ln(1-\xi)}{\Sigma_t}, or = \frac{-\ln \xi}{\Sigma_t}$$

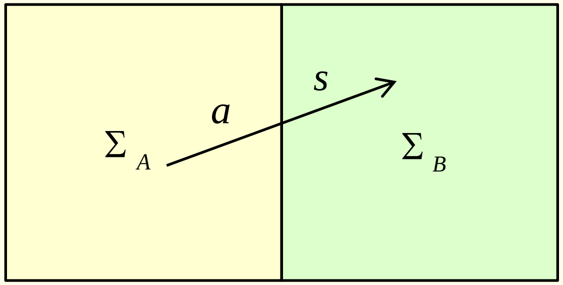
$$s_{xy} = s \times \sin\theta = s \times \sqrt{1-\cos^2\theta} = s \times \sqrt{1-(\Omega_z)^2}$$

$$\Delta_x = s_{xy}\cos\alpha;\ \Delta_y = s_{xy}\sin\alpha$$

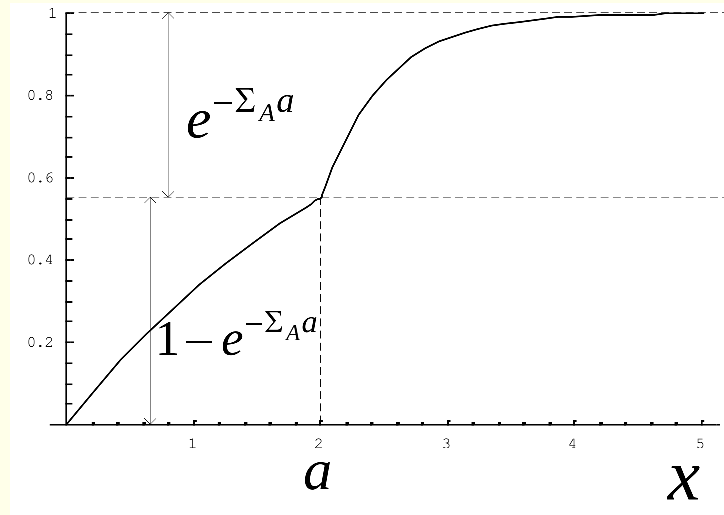


Segmented Simulation of Flight Across Cells

- Once-through simulation



  - Requires complicated CDF for more than two cells



$$P(s) = \left(1 - e^{-\Sigma_A a}\right) + e^{-\Sigma_A a}\left(1 - e^{-\Sigma_B s}\right)$$

- Segmeted simulation
  - Stop first at surface if the first random flight distance is obtained longer than the distance to surface (DTS)
    - what would be the probability to stop at surface? $P = e^{-\Sigma_A a}$
  - Pick a random number for another random flight using Σ_B

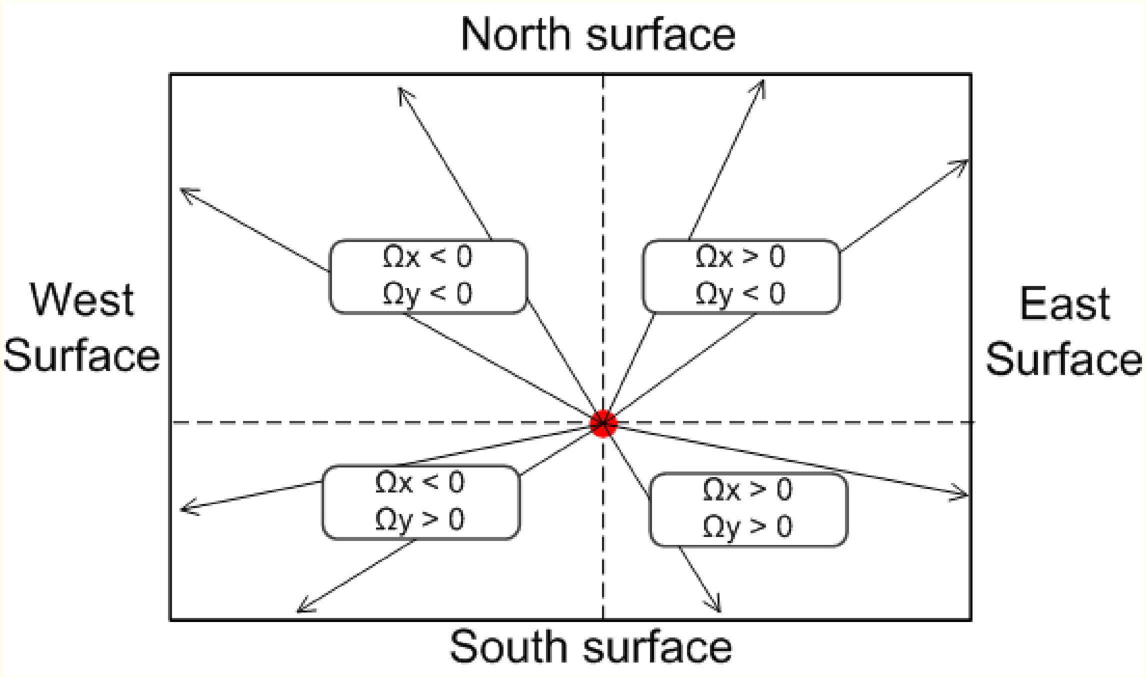
$$P(B \mid A) = e^{-\Sigma_A a}\left(1 - e^{-\Sigma_A s}\right)$$

A=Event to move to surface in cell A

B=Event to move by s in cell B

  - Much simpler

Determination of Distance to Surface



The four combination of sign of x,y directional vector ($\pm\Omega_x, \pm\Omega_y$) determines a possible surface to be reached after collision

Collision in Current Cell

Fission

Record fission for every collision for more spreaded fission sites than fission only after absorption

- can occur with a prob. $\dfrac{\Sigma_{fg}}{\Sigma_{tg}}$, ν neutrons per fission
- expected number of fission neutrons per collision $\nu \dfrac{\Sigma_{fg}}{\Sigma_{tg}}$
- integer number of fission neutrons $int\left(\nu \dfrac{\Sigma_{fg}}{\Sigma_{tg}} + \xi\right)$

$$E\left(int\left(a+\xi\right)\right) = i_a \bullet P(\xi < 1-(a-i_a)) + (i_a+1) \bullet P(\xi \geq 1-(a-i_a))$$

$$= i_a\left(1-(a-i_a)\right) + (i_a+1)(a-i_a) = a$$

Scattering

- can occur with a prob. $\dfrac{\Sigma_{ag}}{\Sigma_{tg}}$
- group transfer to g′ can occur with $\dfrac{\Sigma_{gg'}}{\Sigma_{sg}}$, need angle selection

Outscattering!

Absorption

- if not scattering, absorption.

Terminate simulation of the current neutron

Treatment of Boundary

Determine if the surface is external boundary

If vacuum surface, terminate migration

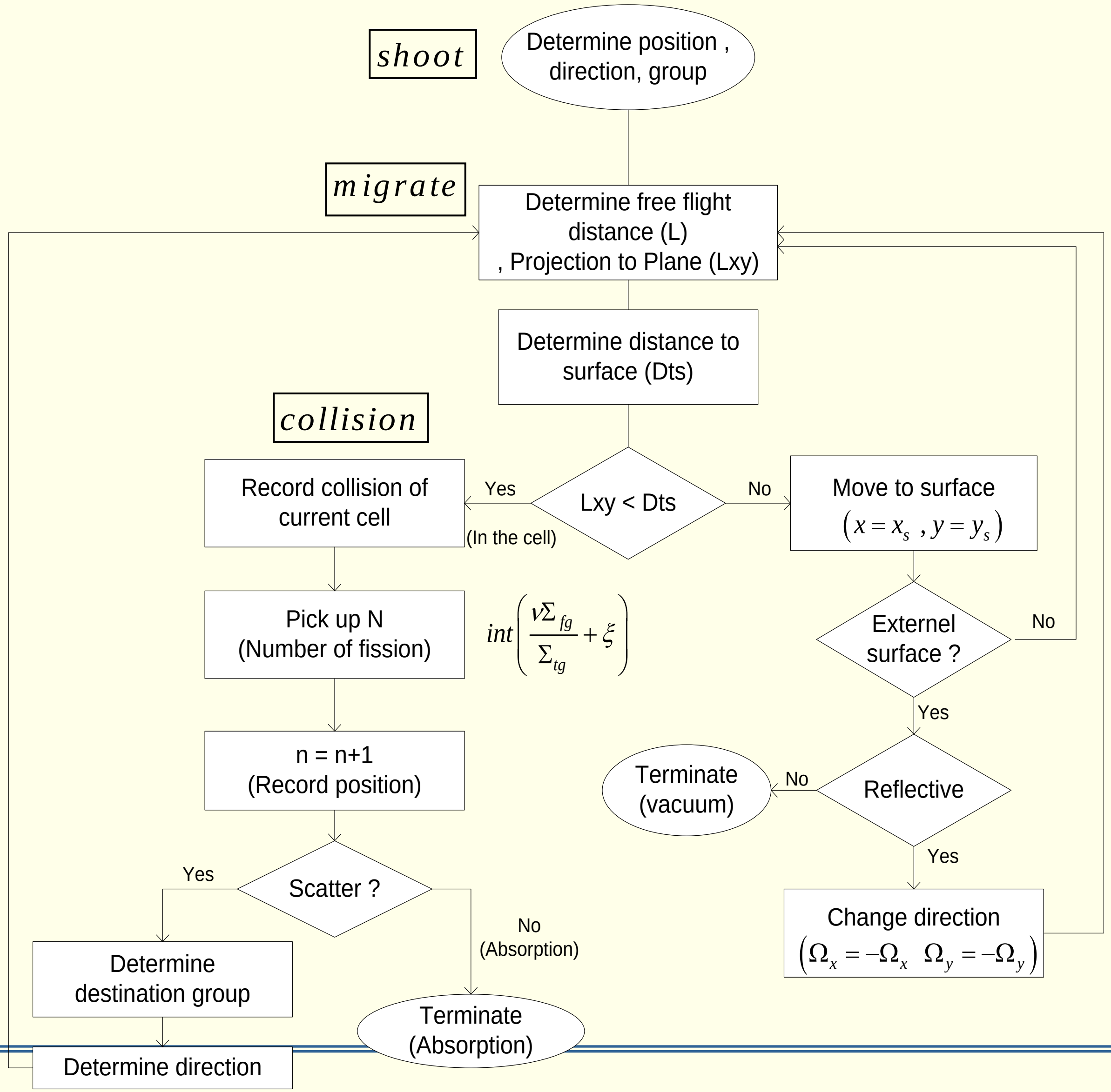
If reflective surface, change the moving direction accordingly

$$e.g.\quad \text{reflection on } y-z \text{ surface}$$

$$\Omega_x = -\Omega_x, \Omega_y = \Omega_y, \Omega_z = \Omega_z$$

- **Then sample another move**

Flow Chart of Simulation of a Neutron Migration



for i=1:C

for j=1:n(i)

migrate

end

$$k' = k\frac{n(i+1)}{n(i)}$$

end

Flux Scoring (Tally)

- Note on time dimension

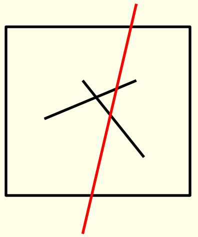
  - Although steady-state condition is simulated in MC calculation, we should adimt that source is in fact given per unit time

- Collision Estimator

  – Reaction rate of a cell : $R_g^c = \Sigma_{tg}^c \phi_g^c V_c \rightarrow \quad \phi_g^c = \dfrac{R_g^c}{V_c \Sigma_{tg}^c}$

  – Accumulate the number of collisions. Since source is given per unit time, the scored number of collisions can be regarded as collision rate. Thus dividing it by the volume and total Xsec yields flux.

- Track Length Estimator



  – Neutrons passing through a cell should contribute to flux, but missing in the collision estimator if the neutron just passes a cell, not making any collision

  – Expected number of reactions for a track of length l formed within a cell: $R_g^l = \Sigma_{tg}^c l$

  – Total number of expected reactions within a cell: $R_g = \sum_i \Sigma_{tg}^c l_i^c = \Sigma_{tg}^c \sum_i l_i^c$

  where l_i^c is the track length generated per unit time (in 3D)

  – Reaction Rate: $R_g = \Sigma_{tg}^c \phi_g^c V_c = \Sigma_{tg}^c \sum_i l_i^c \rightarrow \quad \phi_g^c = \dfrac{1}{V_c} \sum_i l_i^c \leftarrow$ track density!

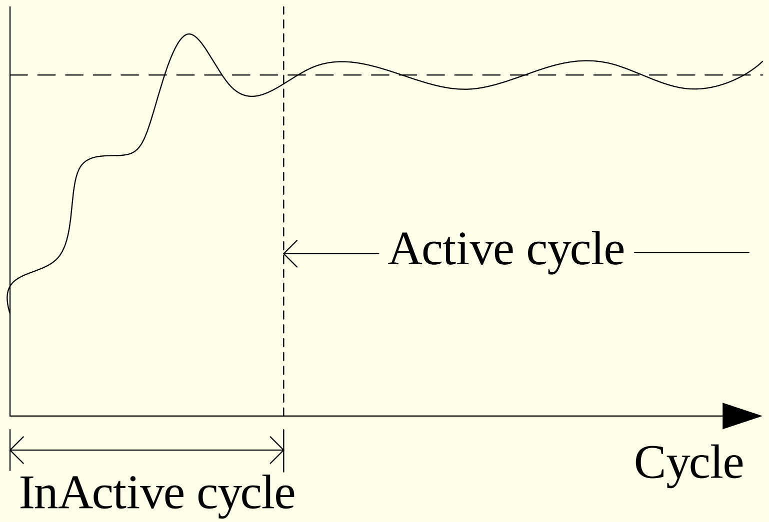
Fission Source Treatment

- Expected number of fission neutrons at the subsequent generation in a multiplying medium of $k_{eff} \neq 1$ for n particles simulated $= k_{eff}\, n$

- Adjustment of ν by $\lambda = \dfrac{1}{k^{(c-1)}}$
  - Avoid amplification by k_{eff} in advance
  - Fission neutron sampling $n_i^{(c)} = int\left(\lambda \dfrac{\nu\Sigma_{fg}}{\Sigma_{tg}} + \xi \right)$: adjust ν by λ

- New estimate of $k^{(c)}$
  - Sum up all the fission neutrons generated: $n^{(c)} = \sum_i n_i^{(c)}$
  - $k_{fis}^{(c)} = \dfrac{n^{(c)}}{n^{(c-1)}} k^{(c-1)}$ return to normal by correcting the artificial adjustment of ν by $\dfrac{1}{k^{(c-1)}}$
  - $Collision:\ n_{col}^{(c)} = \sum_i \left(\dfrac{\nu\Sigma_{fg}}{\Sigma_t} \right)_i \quad \rightarrow k_{col}^{(c)} = \dfrac{n_{col}^{(c)}}{n^{(c-1)}}$
  - $Track:\ n_{trk}^{(c)} = \sum_i l_i^{(c)} \nu\Sigma_{fg} \quad \rightarrow k_{trk}^{(c)} = \dfrac{n_{trk}^{(c)}}{n^{(c-1)}}$

Inactive vs. Active cycles



– because of the unknown source distribution, initial guess of source distribution should be given causing a lot of variation at the initial phase of cycles.

– need inactive cycles to change the spatial source distribution from the initial definition to a correct distribution for the problem

– avoid excessively large variance encountered in inactive cycles by avoiding tallies in this phase

Statistical Processing

- Sample mean and variance after C active cycle simulations

$$\bar{k}_{col} = \frac{1}{C} \sum_{c=N_{ia}+1}^{N_{ia}+C} k_{col}^{(c)}$$

$$s_{k,col}^2 = \frac{1}{C-1} \sum_{c=N_{ia}+1}^{N_{ia}+C} (k_{col}^{(c)} - \bar{k}_{col})^2$$

- Standard deviation of the sample mean

$$\sigma_{k,col} = \frac{s_{k,col}}{\sqrt{C}} \cong \frac{1}{C} \sqrt{\sum_{c=N_{ia}+1}^{N_{ia}+C} (k_{col}^{(c)} - \bar{k}_{col})^2} \quad (\because C \approx C-1)$$

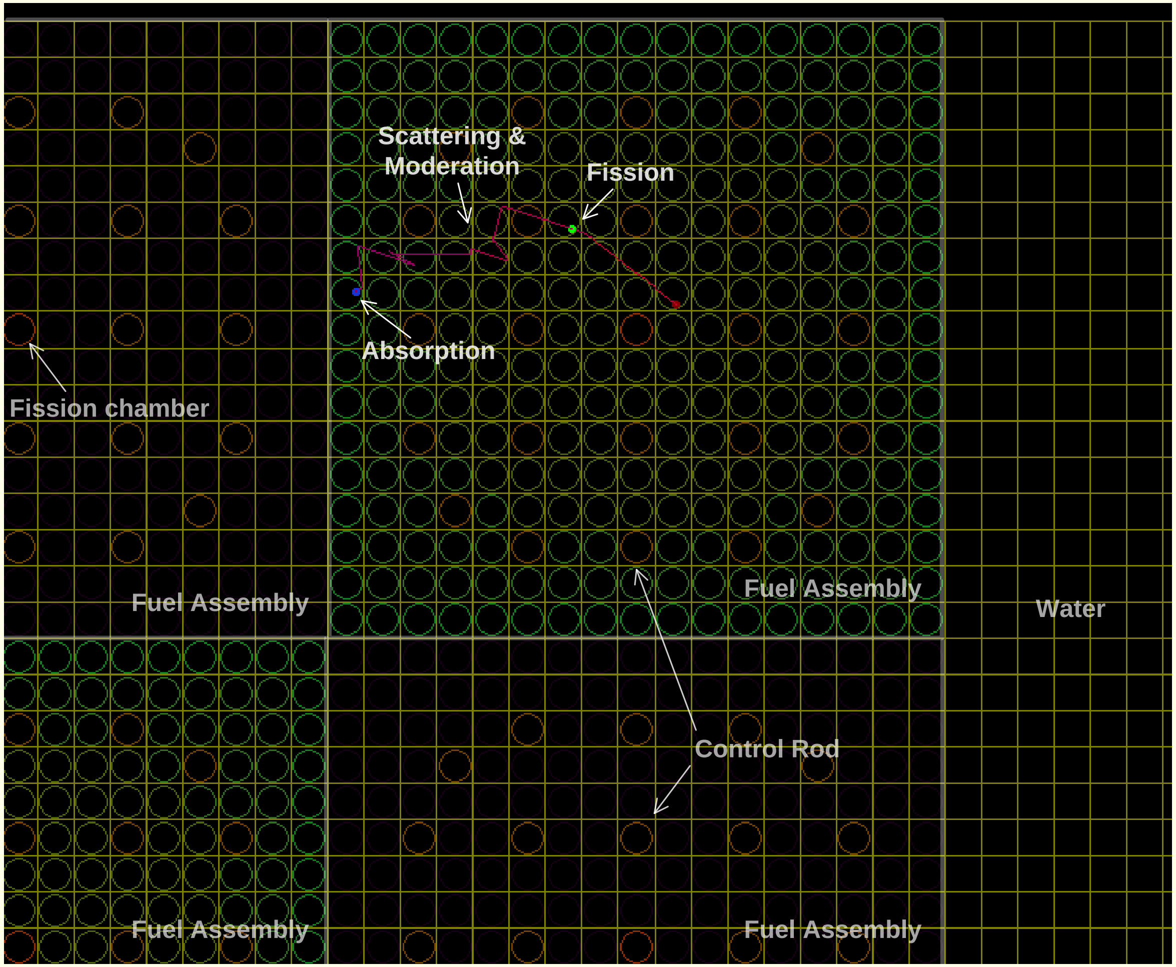
- Confidence level

$$\bar{k} \pm \sigma : 68.3\%$$

$$\bar{k} \pm 2\sigma : 95.4\%$$

$$\bar{k} \pm 3\sigma : 99.7\%$$

Example of particle tracing



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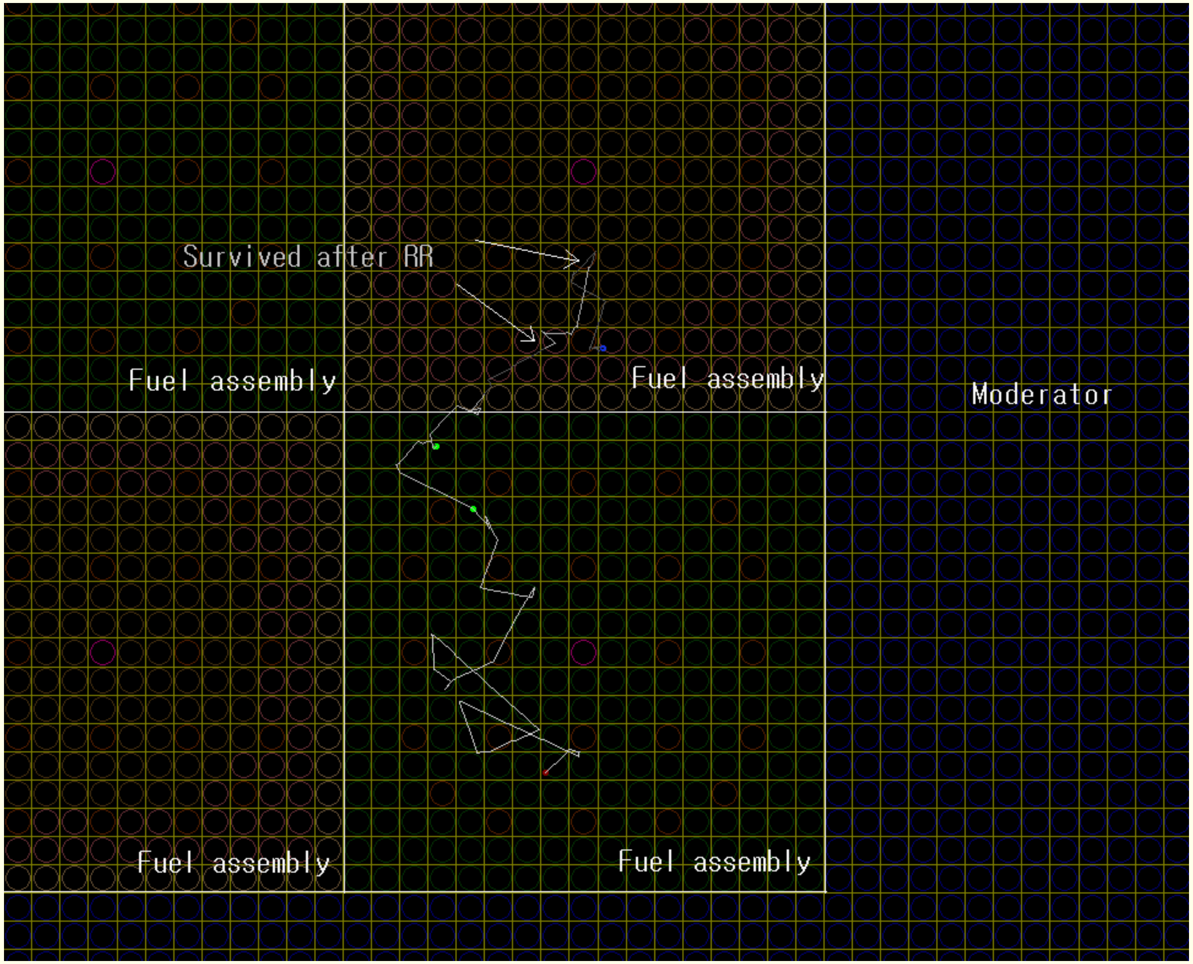
Example of particle tracing



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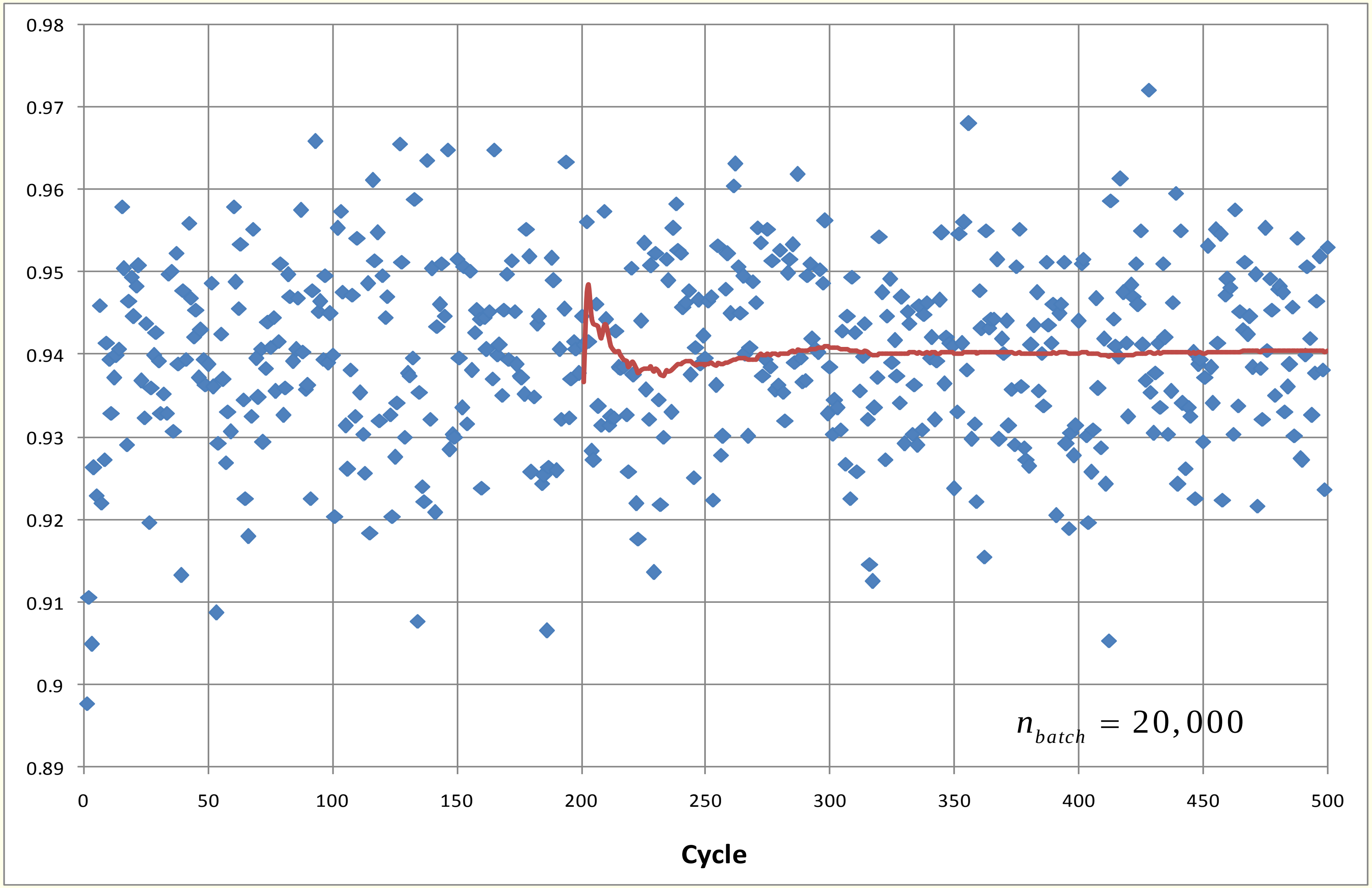
K-eff variation for C5G2 Model Problem



Variance Reduction Methods

Need and Approach

- **Reduce the variances of tallies by modifying neutron behavior**
  - Save neutrons as much as possible instead of killing them while conserving the mean values of tallies
- **Analogue vs. Non-Analogue Monte Carlo**

Typical Methods

- **Weight Window Method**
- **Implicit Capture**

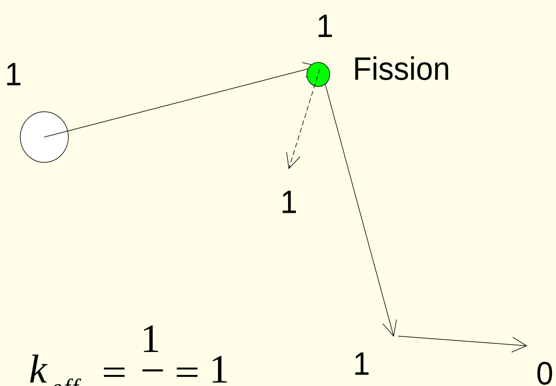
Particle Weight

Concept

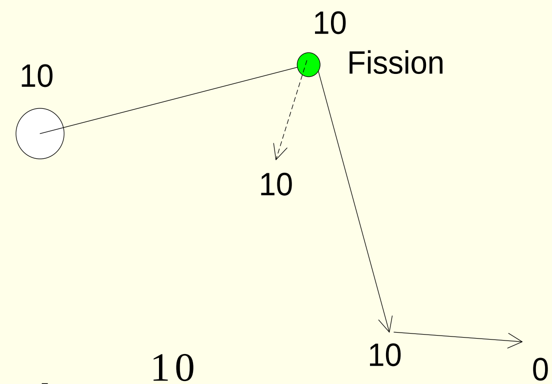
- A single particle being traced in MC simulation is not a single neutron, rather a group of neutrons
- The number of neutrons may be adjusted during the simulation by introducing weight for each particle

Weight

- Relative number of neutrons represented by a particle



$$k_{eff} = \frac{1}{1} = 1$$



$$k_{eff} = \frac{10}{10} = 1$$

Implicit Capture

Background

- When an absorption reaction occurs, all the neutrons represented by the particle disappears at once in analogue MC. This can magnify the variance of MC calculation

Implementation

- Do not kill the particle when absorption is selected. Instead, make it survive with less weight

- Weight reduction with survival probability

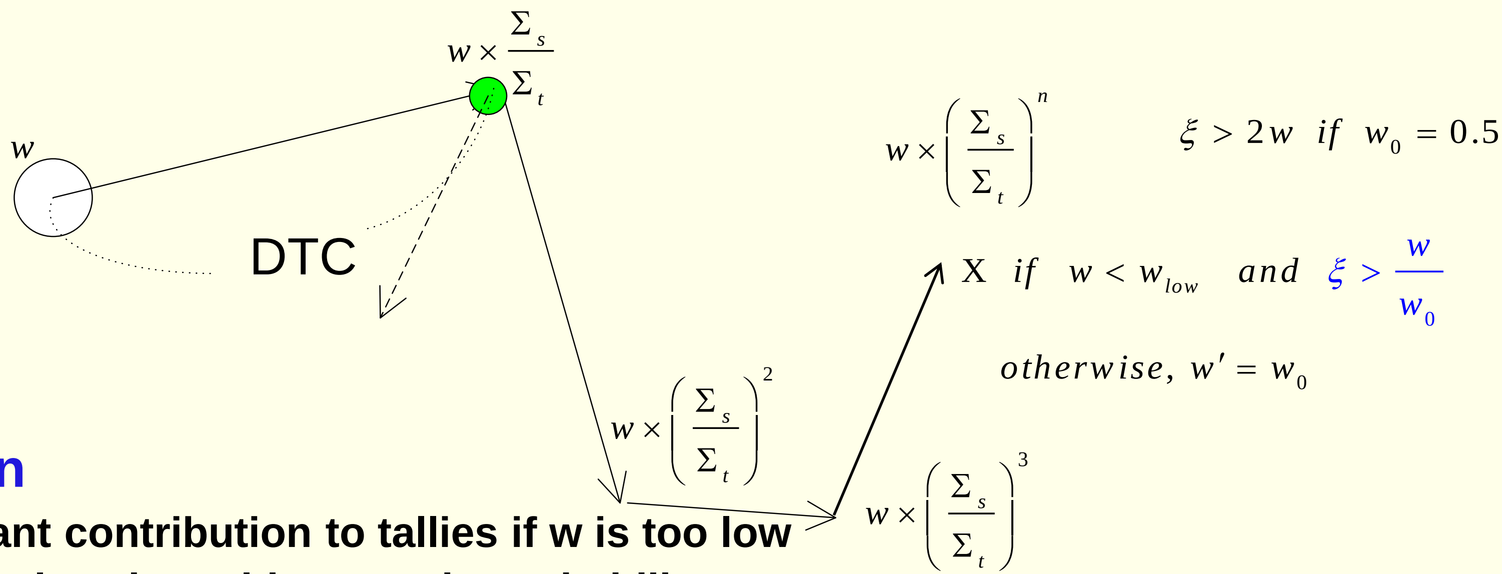
$$w' = w \times \left(1 - \frac{\Sigma_a}{\Sigma_t} \right) = w \times \frac{\Sigma_s}{\Sigma_t}$$

- Collision / Track length / Fission Neutron adjustment

$$e.g.\ P_{fis} = \frac{\lambda \nu \Sigma_f}{\Sigma_t} \times w$$

Termination of Implicit Capture

Deterministic weight reduction after each collision



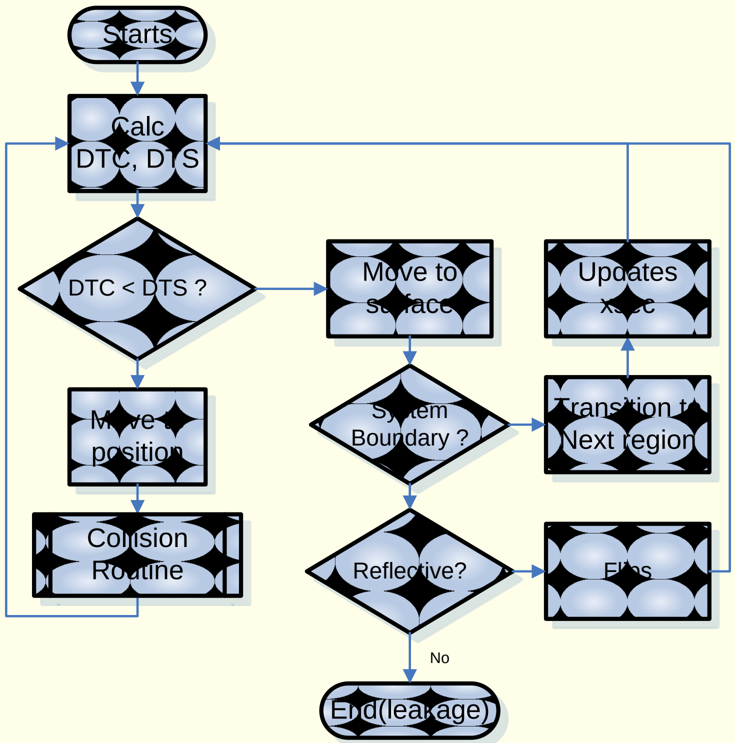
Termination

- **Insignificant contribution to tallies if w is too low**
- **Kill if w<w_low, but with a certain probability**

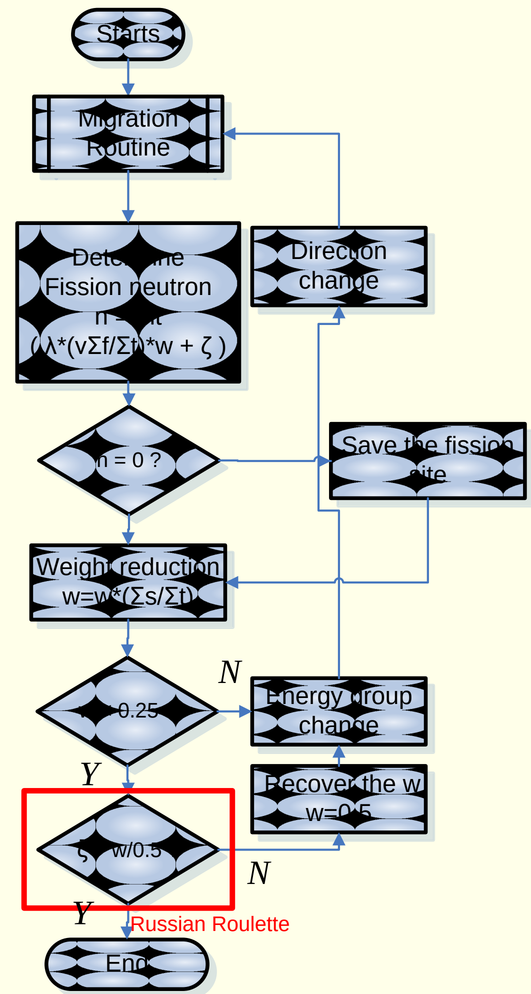
$$w < w_{low}\,(0.25) \quad and \quad \xi > \xi_S\,(0.4)$$

- **Weight adjustment to conserve the weight**
  - Adjusted weight can potentially lower then the limit $w' = \frac{w}{\xi_S} \leftarrow E(w) = \frac{w}{\xi_S}\xi_S + 0 \cdot (1 - \xi_S)$
- **Fixed Adjusted Weight (w_0)**
  - Adjust survival probability to $\frac{w}{w_0} \leftarrow E(w) = w_0 \frac{w}{w_0} + 0 \cdot (1 - \frac{w}{w_0})$

Modified Calculation Flow for Implicit Capture

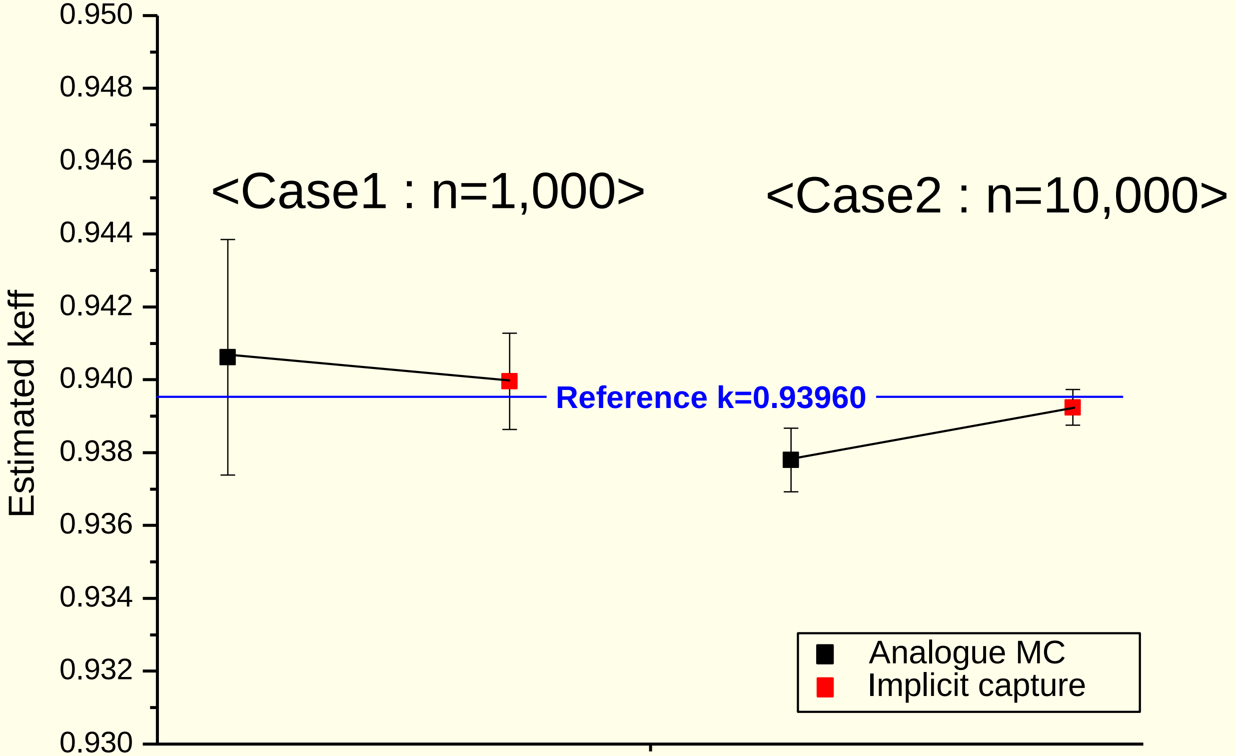


< migration routine>



< collision routine>

Effectiveness of Implicit Capture



< Result of L336C5G2>