Neutron (and Photon) Transport for Nuclear Reactor Problems

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Purpose

The purpose of this talk is to introduce:

- Several types of neutron transport problems in the practical arena of nuclear engineering,

- The types of computational methods that currently exist and are on the drawing board for solving these problems.

I will try to emphasize the *special features* of practical neutron transport problems and algorithms that differ from those in other areas of physics.

Outline

A. Mathematical Description

B. Characteristics of Typical Physical & Problem Data

C. Three Typical Neutron Transport Nuclear Reactor Problems

D. Monte Carlo Methods

E. Deterministic (S_N) Methods

F. Current Research

Steady-State Neutron Transport Problems

The *Linear Boltzmann* (or *Neutron Transport*) Equation:

$$\underline{\Omega}\cdot\underline{\nabla}\psi(\underline{r},\underline{\Omega},E)+\Sigma_t(\underline{r},E)\psi(\underline{r},\underline{\Omega},E)$$

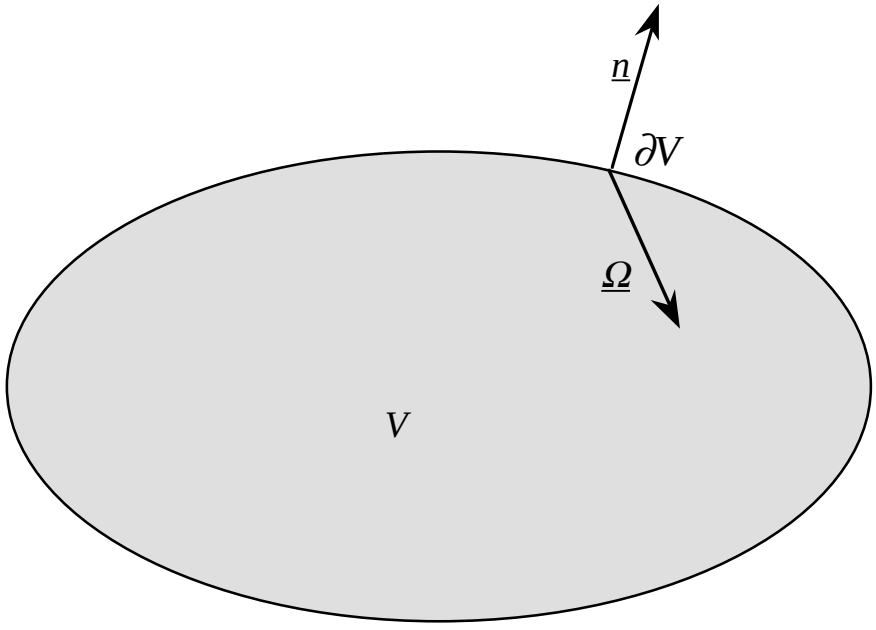
$$=\int_0^\infty\int_{4\pi}\Sigma_s(\underline{r},\underline{\Omega}'\cdot\underline{\Omega},E'\to E)\psi(\underline{r},\underline{\Omega}',E')\,d\Omega' dE'$$

$$+\frac{\chi(\underline{r},E)}{4\pi}\int_0^\infty\int_{4\pi}\nu\Sigma_f(\underline{r},E')\psi(\underline{r},\underline{\Omega}',E')\,d\Omega' dE'+\frac{Q(\underline{r},E)}{4\pi}\ ,$$

$$\underline{r}\in V\ ,\ \underline{\Omega}\in 4\pi\ ,\ 0<E<\infty\ \ , \qquad (1a)$$

Boundary Condition:

$$\psi(\underline{r},\underline{\Omega},E)=\psi^b(\underline{r},\underline{\Omega},E)\ ,\ \underline{r}\in\partial V\ ,\ \underline{\Omega}\cdot\underline{n}<0\ ,\ 0<E<\infty\ . \qquad (1b)$$



Definitions

$$\underline{\Omega}\cdot\underline{\nabla}\psi(\underline{r},\underline{\Omega},E)+\Sigma_t(\underline{r},E)\psi(\underline{r},\underline{\Omega},E)$$
$$=\int_0^\infty\int_{4\pi}\Sigma_s(\underline{r},\underline{\Omega}'\cdot\underline{\Omega},E'\to E)\psi(\underline{r},\underline{\Omega}',E')\,d\Omega'dE'$$
$$+\frac{\chi(\underline{r},E)}{4\pi}\int_0^\infty\int_{4\pi}\nu\Sigma_f(\underline{r},E')\psi(\underline{r},\underline{\Omega}',E')\,d\Omega'dE'+\frac{Q(\underline{r},E)}{4\pi}\ .$$

Independent variables (*6-D phase space*):

$\underline{r}=(x,y,z)=$ space ,

$\underline{\Omega}=(\Omega_x,\Omega_y,\Omega_z)=(\sqrt{1-\mu^2}\cos\gamma,\sqrt{1-\mu^2}\sin\gamma,\mu)=$ direction-of-flight (or *angle*),

$E=$ energy ,

Dependent variable:

$\psi(\underline{r},\underline{\Omega},E)=$ angular flux $\quad\left(\dfrac{\psi}{\nu}=\text{neutron density}\right)$,

Known problem data:

$\Sigma_t(E)=\Sigma_s(E)+\Sigma_f(E)+\Sigma_\gamma(E)=$ total cross section ,

$\Sigma_s(\underline{r},\underline{\Omega}'\cdot\underline{\Omega},E'\to E)=$ differential scattering cross section ,

$\Sigma_s(E)=\int_0^\infty\int_{4\pi}\Sigma_s(\underline{r},\underline{\Omega}\cdot\underline{\Omega}',E\to E')d\Omega'dE'=$ scattering cross section ,

$\Sigma_f(E)=$ fission cross section ,

$\Sigma_\gamma(E)=$ capture cross section ,

$\nu=$ mean number of neutrons emitted per fission event ,

$\chi(E)=$ fission spectrum $\left(\int_0^\infty\chi(E)dE=1\right)$,

$Q(\underline{r},E)=$ interior source ,

$\psi^b(\underline{r},\underline{\Omega},E)=$ boundary angular flux ,

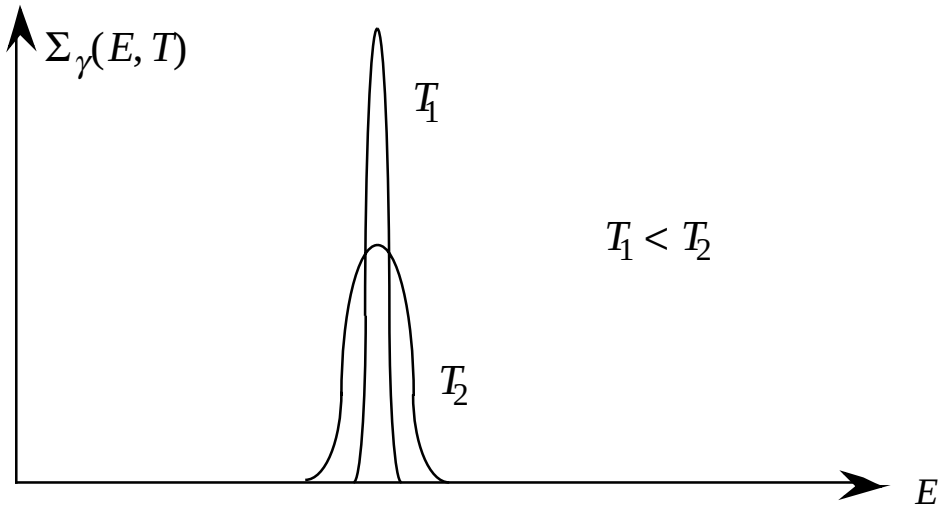
Other Relevant Physics

- Time-Dependence (Delayed Neutrons)

$$\begin{cases} \psi(\underline{r},\underline{\Omega},E,t) \\ C_j(\underline{r},\underline{\Omega},E,t) \quad , \quad 1 \le j \le 6 \end{cases}$$

- Temperature-Dependence

$$\begin{cases} \psi(\underline{r},\underline{\Omega},E) \\ T(\underline{r}) \\ \Sigma(\underline{r},E,T) \quad (known) \end{cases}$$



Doppler-Broadening of Cross Sections

- Inelastic Neutron Scattering & Fission $\rightarrow$ Photons

$$\begin{cases} \psi_{neutron}(\underline{r},\underline{\Omega},E) \\ \psi_{photon}(\underline{r},\underline{\Omega},E) \end{cases}$$

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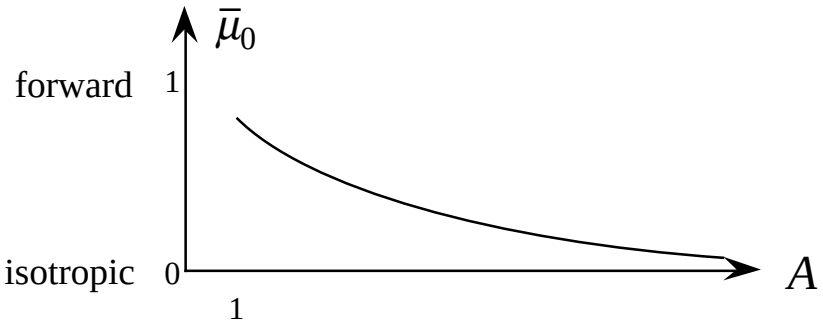
Characteristics of the Physical Data

$0.1\,\text{cm}^{-1} < \Sigma_t < 10.0\ \text{cm}^{-1}$ $\qquad \left(\text{Mean free path } = \dfrac{1}{\Sigma_t} \approx 1.0\ \text{cm}\right)$

Mean scattering cosine (low-E elastic scattering) $= \bar{\mu}_0 = \dfrac{2}{3A}$

$A = \textit{Mass Number} = \#\,(\text{neutrons} + \text{protons})$



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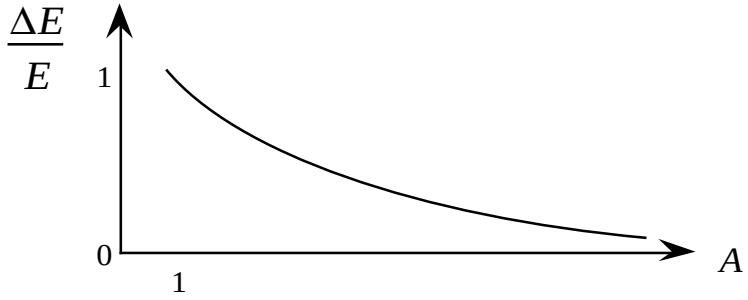
low$-E$ elastic scattering: $\dfrac{\Delta E}{E} \approx \dfrac{2A}{(1+A)^2}$ $\qquad 10^{-2}\text{ev} < E < 10^{7}\text{ev}$

$$\#\ \text{Collisions}\ (10^{7}\text{ev} \rightarrow 10^{-2}\text{ev}) \approx \begin{cases} 30 & A = 1 \quad \text{(hydrogen)} \\ 2475 & A = 238 \quad \text{(uranium)} \end{cases}$$



Characteristics of the Problem & Data

Mean free path $\approx$ 1 cm (large compared to e^- & high-*E* photons) ,

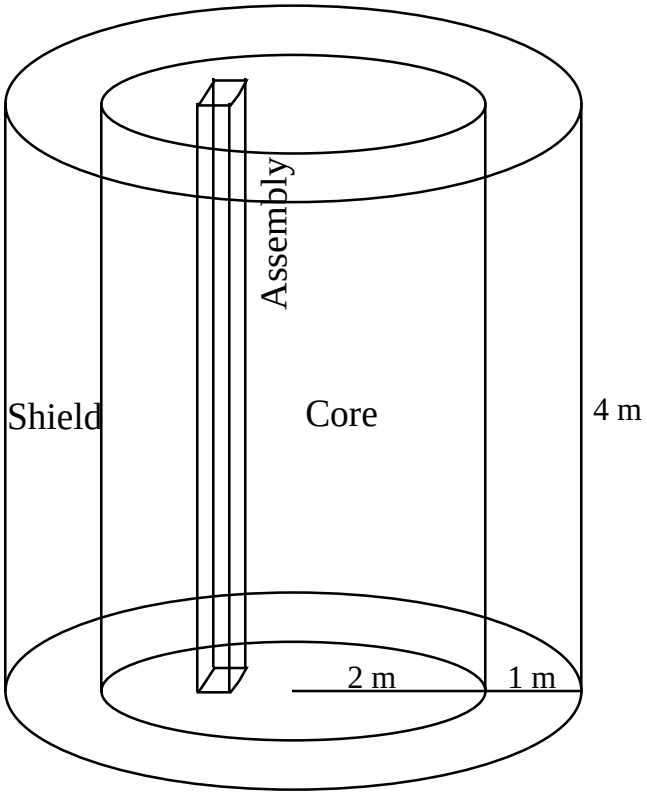
Scattering is not strongly anisotropic (as it is for e^-) ,

Existence of *capture* ,

Energy change per collision is large (compared to e^-) ,

Neutron density in a reactor core $\approx 10^9$ neutrons/ cm^3 .

Cartoon of a reactor:



Shielding and structure also exist above & below the core (reactor head).
Pipes carrying coolant penetrate through the shield and core.
The core contains a lot of mechanical structure – it is *not* homogeneous.

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Three Typical Calculations: I. Eigenvalue

Eigenvalue problems are governed by the transport equation with no interior source:

$$\underline{\Omega}\cdot\underline{\nabla}\psi(\underline{r},\underline{\Omega},E)+\Sigma_t(\underline{r},E)\psi(\underline{r},\underline{\Omega},E)$$

$$=\int_0^\infty\int_{4\pi}\Sigma_s(\underline{r},\underline{\Omega}'\cdot\underline{\Omega},E'\to E)\psi(\underline{r},\underline{\Omega}',E')\,d\Omega'dE'$$

$$+\frac{1}{k}\frac{\chi(\underline{r},E)}{4\pi}\int_0^\infty\int_{4\pi}\nu\Sigma_f(\underline{r},E')\psi(\underline{r},\underline{\Omega}',E')\,d\Omega'dE'\ ,$$

$$\underline{r}\in V\ ,\ \underline{\Omega}\in 4\pi\ ,\ 0<E<\infty\ \ , \qquad (2a)$$

and with a *vacuum* boundary condition:

$$\psi(\underline{r},\underline{\Omega},E)=0\quad ,\quad \underline{r}\in\partial V\ ,\ \underline{\Omega}\cdot\underline{n}<0\ ,\ 0<E<\infty\ . \qquad (2b)$$

In principle, V is the entire reactor (core + shield).

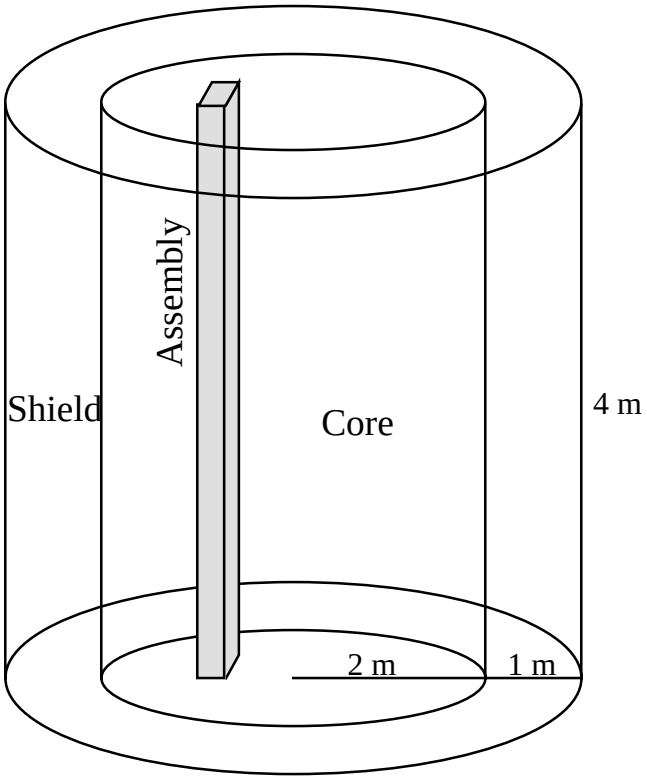
The eigenvalue *k* is the *reactor multiplication factor*.

$$k=\begin{cases}>1 & \text{supercritical}\\ =1 & \text{critical}\\ <1 & \text{subcritical}\end{cases}\ .$$

It is necessary to calculate *k* with accuracy to 4 decimal places.

"Global" reactor calculations are often performed by a diffusion code with *homogenized cross sections* obtained from *assembly* calculations (described next).

Three Typical Calculations: II. Assembly



$$\underline{\Omega}\cdot\underline{\nabla}\psi(\underline{r},\underline{\Omega},E)+\Sigma_t(\underline{r},E)\psi(\underline{r},\underline{\Omega},E)$$

$$=\int_0^\infty\int_{4\pi}\Sigma_s(\underline{r},\underline{\Omega}'\cdot\underline{\Omega},E'\to E)\psi(\underline{r},\underline{\Omega}',E')\,d\Omega'dE'$$

$$+\frac{1}{k}\frac{\chi(\underline{r},E)}{4\pi}\int_0^\infty\int_{4\pi}\nu\Sigma_f(\underline{r},E')\psi(\underline{r},\underline{\Omega}',E')\,d\Omega'dE'\ ,$$

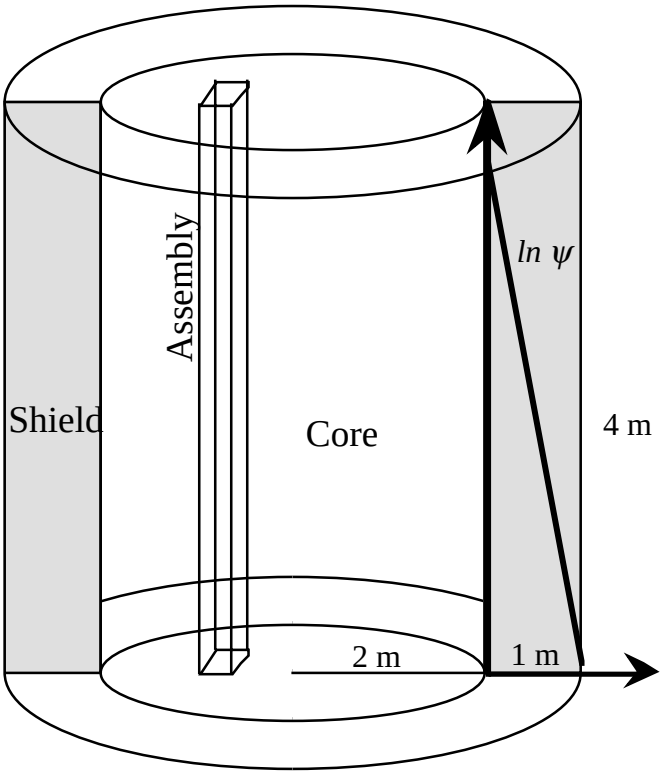
$$\underline{r}\in V\ ,\ \underline{\Omega}\in 4\pi\ ,\ 0<E<\infty\ \ , \qquad (3a)$$

$$\psi(\underline{r},\underline{\Omega},E)=\psi(\underline{r},\underline{\Omega}_r,E)\quad ,\quad \underline{r}\in\partial V\ ,\ \underline{\Omega}\cdot\underline{n}<0\ ,\ 0<E<\infty\ . \qquad (3b)$$

Now V (and k) pertain to a single assembly within the core.

Results from an assembly calculation are used to generate homogenized diffusion coefficients for the assembly [see MLA talk].

Three Typical Calculations: III. Shielding



$$\underline{\Omega}\cdot\underline{\nabla}\psi(\underline{r},\underline{\Omega},E)+\Sigma_t(\underline{r},E)\psi(\underline{r},\underline{\Omega},E)$$

$$=\int_0^\infty\int_{4\pi}\Sigma_s(\underline{r},\underline{\Omega}'\cdot\underline{\Omega},E'\to E)\psi(\underline{r},\underline{\Omega}',E')\,d\Omega' dE' \ ,$$

$$\underline{r}\in V \ , \ \underline{\Omega}\in 4\pi \ , \ 0<E<\infty \ , \qquad (4a)$$

$$\psi(\underline{r},\underline{\Omega},E)=\begin{cases}\psi^b(\underline{r},\underline{\Omega},E) \ , & \underline{r}\in\partial V_{core} \ , \ \underline{\Omega}\cdot\underline{n}<0 \ , \ 0<E<\infty, \\ 0 \ , & \underline{r}\in\partial V_{ext} \ , \ \underline{\Omega}\cdot\underline{n}<0 \ , \ 0<E<\infty. \end{cases} \qquad (4b)$$

$\Sigma_f = 0$ in shields.

The neutron density changes by *many* (> 9) orders of magnitude across a shield.

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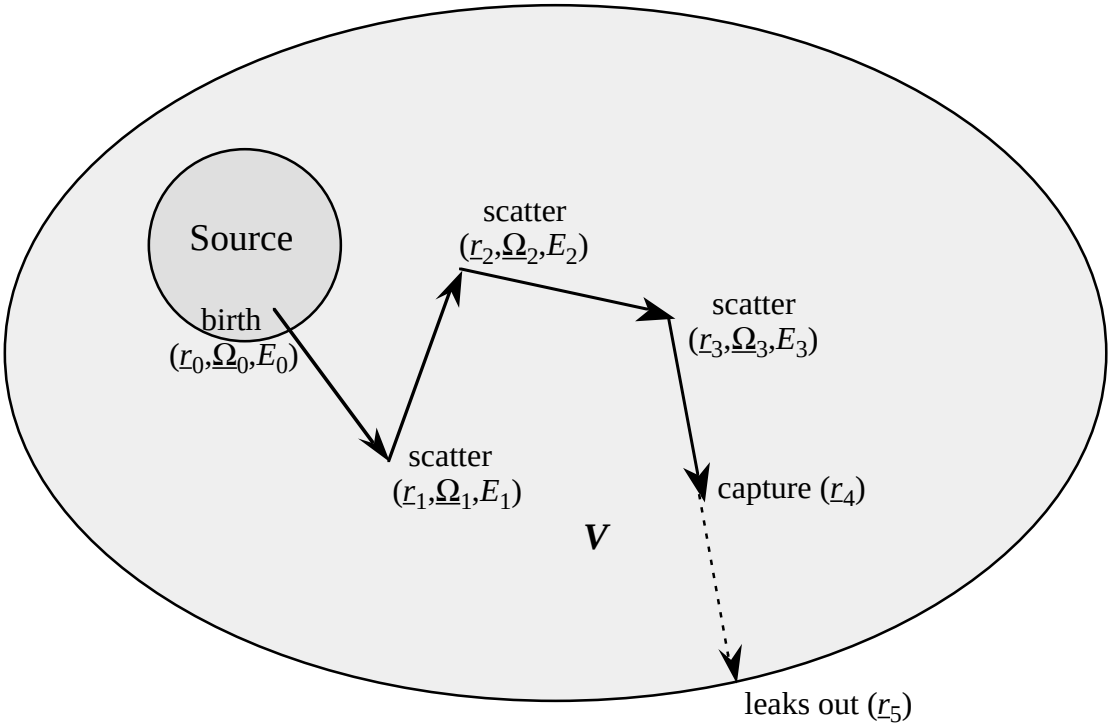
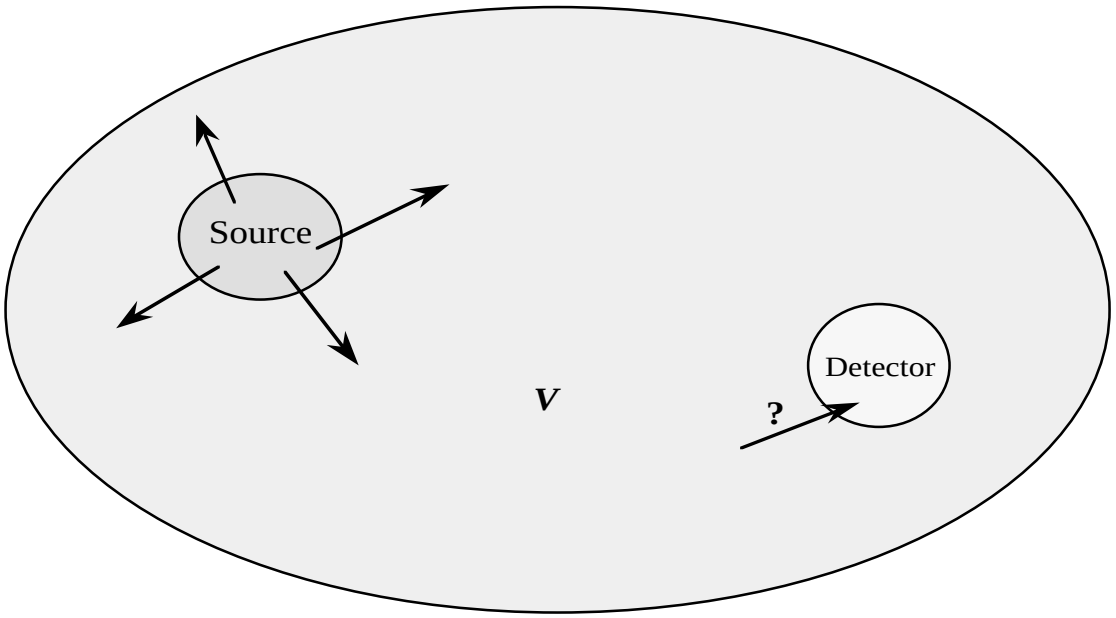
A Single Neutron "History"



Random Events (governed by probability distribution functions):

- Birthpoint (in 6-D phase space) of the neutron.
- Distance the neutron travels to a collision (or does it leak out?).
- Is the collision a scattering, a capture, or a fission event?
- If the neutrons scatters, what are its outgoing direction and energy?
- If a fission event occurs, how many neutrons are released, and what are their directions and energies?

The Basics of Analog Monte Carlo (I)



$$\text{Detector Response} = R = \int_{Detector} \int_{0}^{\infty} \int_{4\pi} \Sigma_{\gamma}(E)\psi(\underline{r},\underline{\Omega},E)\,d\Omega\,dE\,dV = ?$$

1. Generate a large number (N) of Monte Carlo particle histories.
2. Calculate N_D = the number of histories that end (with the Monte Carlo particle being captured) in the detector region.
3. Then,

$$p = \frac{N_D}{N} \approx \text{probability that a MC particle will be captured in the detector.}$$

4. If Q_S = source rate, then

$$Q_D = Q_S \frac{N_D}{N} \approx \text{rate at which particles are captured in the detector.}$$

The Basics of Analog Monte Carlo (II)

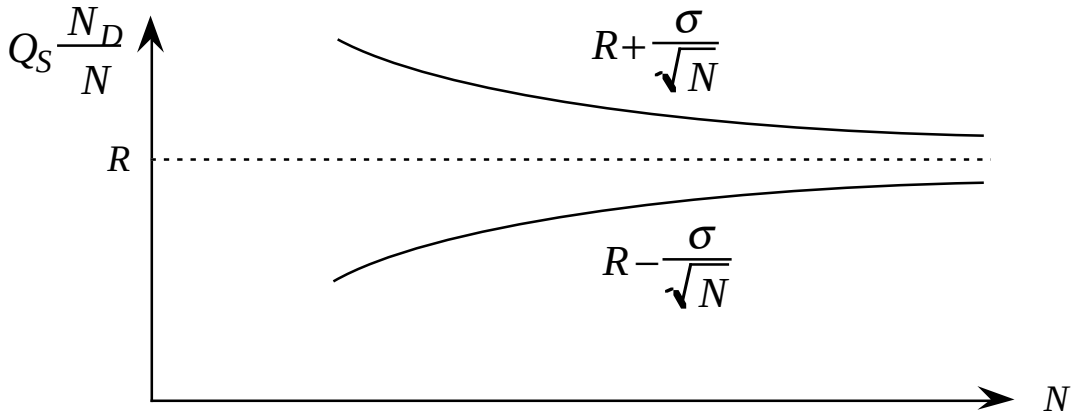
The *Central Limit Theorem*:

For large N,

$$\text{Prob}\left(\left|R - Q_S \frac{N_D}{N}\right| < \frac{\sigma}{\sqrt{N}}\right) \approx 0.67 \ ,$$

where:

σ = *standard deviation* .



We may define:

$$\text{Monte Carlo "error"} = \frac{\sigma}{\sqrt{N}} \ .$$

Consequence: To reduce the "error" by a factor of 10, one must increase the number of Monte Carlo histories – and the cost of the calculation – by a factor of 100.

A different way to reduce the error is to modify the "rules of the game" so that the estimate of R is unbiased, but σ is reduced (*nonanalog* Monte Carlo). This procedure is advantageous for estimating a *rare event*.

Estimation of Rare Events

Relative Error = $O\left(\frac{\sigma}{\sqrt{N_D}}\right)$.

If p is small, then a large number of MC particles $(N >> 1)$ are needed to achieve one "hit" $(N_D = 1)$.

To achieve a small relative error, many "hits" are required $(N_D >> 1)$.

Conclusion: If p is small, an impractical number of MC particles can be required to achieve a desired relative error in the estimate of a detector response.

Nonanalog Monte Carlo (Survival Biasing) (I)

Modify the rules of the game. Assign a new (unphysical) property to a MC particle: *w* = *weight*.

- MC particles are born with $w = 1$.
- When a MC particle undergoes a collision, it is not captured. Instead, it automatically scatters (assume $\Sigma_f = 0$), but its weight is modified (reduced) by

$$w_{new} = \left(\frac{\Sigma_S}{\Sigma_S + \Sigma_\gamma} \right) w_{old} \ .$$

  [MC particle histories are now longer than before.]

- If a MC particle undergoes a collision in the detector region, it is captured with probability

$$p_{capture} = \frac{\Sigma_\gamma}{\Sigma_S + \Sigma_\gamma} \ .$$

- If the particle is captured, its weight w_D contributes to the talley via:

$$R \approx Q_S \left(\frac{1}{N} \sum_1^N w_D \right) .$$

It is now more expensive to process *N* Monte Carlo particles. However, many more MC particles will *score* in the detector region.

Nonanalog Monte Carlo (Survival Biasing) (II)

The resulting estimate of R is unbiased:

$$R = \lim_{N\to\infty} Q_S\left(\frac{1}{N}\sum_{1}^{N} w_D^{SB}\right) .$$

Also, the Central Limit Theorem holds, and

$$\text{Error}_{SB} = \frac{\sigma_{SB}}{\sqrt{N}} \quad ,$$

with (usually)

$$\sigma_{SB} < \sigma_{\text{analog}} \quad .$$

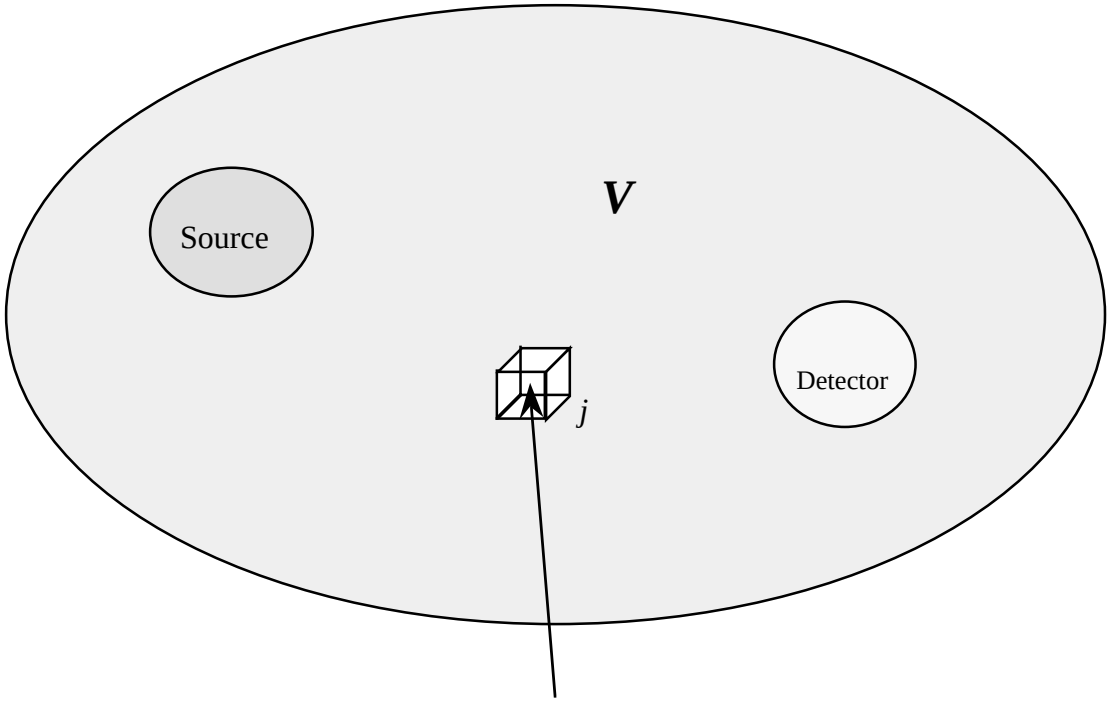
If σ_{SB} is sufficiently smaller than σ_{analog}, the SB calculation will be more efficient than the analog calculation.

Nonanalog Monte Carlo (Weight Windows)

In rare-event calculations, σ_{SB} is often not sufficiently small.

Reason: when MC particles score, their weights have a large variance.

A cure: Install a *Weight Window*:



When a MC particle is in spatial cell j, require:

$$w_j^-(\underline{\Omega}, E) < w < w_j^+(\underline{\Omega}, E) \ ,$$

by using:

$$\begin{cases} \text{Splitting} & \text{if} \quad w > w_j^+ \ , \\ \text{Russian Roulette} & \text{if} \quad w < w_j^- \ . \end{cases}$$

Properties of Weight Window Monte Carlo

- The Weight Window (WW) technique is *unbiased*. No matter how well or how poorly the weights are chosen, one has:

$$R = \lim_{N\to\infty} Q_S\left(\frac{1}{N}\sum_{1}^{N} w_D^{WW}\right) .$$

- If the Weight Windows are chosen well, the WW calculation has a smaller Monte Carlo error than the SB calculation:

$$\text{Error}_{WW} = \frac{\sigma_{WW}}{\sqrt{N}} \quad \text{and} \quad \sigma_{\text{WW}} < \sigma_{\text{SB}} < \sigma_{\text{analog}} .$$

- The computational cost (per particle) of implementing the weight window is significant.

- If σ_{WW} is sufficiently smaller than σ_{analog}, the WW calculation will be more efficient than the analog calculation.

- Large, difficult problems require many (upper and lower) weights, which are usually specified by the code-user (a lengthy and expensive task). Experience and luck are often required.

- Consequence: In addition to the standard physical problem data, the MC code user must provide good *biasing parameters* (weight windows) in order for the code to run with reasonable efficiency. Nonanalog Monte Carlo calculations that require the user to input a large number of biasing parameters are *NOT user-friendly*.

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Discretization of the Transport Equation (I)

The Linear Boltzmann (Neutron Transport) Equation:

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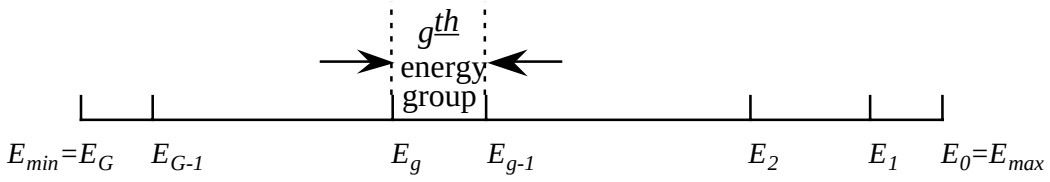
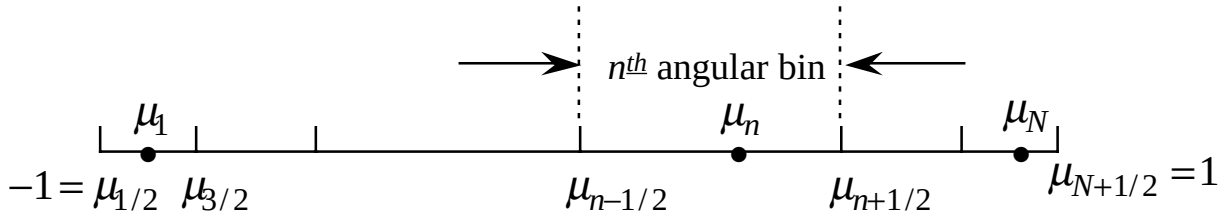
$$=\int_0^\infty\int_{4\pi}\Sigma_s(\underline{r},\underline{\Omega}'\cdot\underline{\Omega},E'\to E)\psi(\underline{r},\underline{\Omega}',E')\,d\Omega'dE'+\frac{Q(\underline{r},E)}{4\pi}\ .$$

Discretization of Energy (Multigroup):



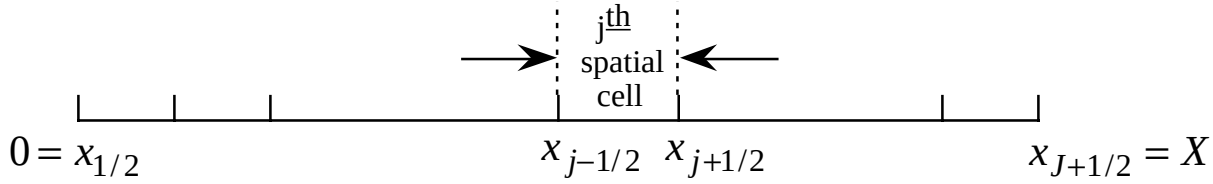
$$\psi(\underline{r},\underline{\Omega},E)\approx\psi_g(\underline{r},\underline{\Omega})/(E_{g-1}-E_g)$$

Discretization of Angle (S_N = Discrete Ordinates):



$$\psi_g(\underline{r},\underline{\Omega})\approx\psi_{g,n}(\underline{r})$$

Discretization of Space (Finite Difference, Finite Element):



$$\psi_{g,n}(\underline{r})=\psi_{g,n,j}+(x-x_j)\hat{\psi}_{g,n,j}$$

Discretization of the Boltzmann Equation (II)

- The energy-angle-space discretization of the Boltzmann equation yields a large algebraic system of equations.

  Example: If each of the 6 independent variables is discretized on a grid with 10^2 cells, the number of unknowns = $O(10^2)^6 = O(10^{12})$.

- Generally, *iterative methods* must be used to obtain solutions of the discrete equations.

- If $\Sigma_s = \Sigma_f = 0$, the discrete Boltzmann equation

  $$L\psi = (\underline{\Omega} \cdot \underline{\nabla} + \Sigma_t)\psi = Q$$

  can be directly solved by *sweeping* across the spatial grid in the directions of particle flow.

- If $\Sigma_f = 0$ but $\Sigma_s > 0$, one can *Source-Iterate* (SI):

  $$L\psi^{n+1} = S\psi^n + Q \ .$$

- SI will always converge. However, if the probability of scattering is large (≈ 1) and the system is large, SI will converge *very* slowly.

Physics-Based Aceleration: DSA (I)

The exact problem:

$$L\psi = S\psi + Q \ . \tag{5}$$

One SI sweep:

$$\boxed{L\psi^{n+1/2} = S\psi^{n} + Q \ .} \tag{6}$$

Subtract: Eq. (5)-Eq. (6):

$$L\left(\psi - \psi^{n+1/2}\right) = S\left(\psi - \psi^{n}\right) = S\left(\psi - \psi^{n+1/2} + \psi^{n+1/2} - \psi^{n}\right) \ .$$

This yields an exact equation for the error $\psi - \psi^{n+1/2}$:

$$(L - S)\left(\psi - \psi^{n+1/2}\right) = S\left(\psi^{n+1/2} - \psi^{n}\right) \ .$$

Replace the Boltzmann operator $L - S$ by its diffusion approximation:

$$\boxed{(L - S)_D\left(\psi - \psi^{n+1/2}\right)_D = S\left(\psi^{n+1/2} - \psi^{n}\right) \ .} \tag{7}$$

After solving this equation, define ψ^{n+1} via:

$$\boxed{\psi^{n+1} = \psi^{n+1/2} + \left(\psi - \psi^{n+1/2}\right)_D \ .} \tag{8}$$

Eqs. (6) - (8) constitute one *Diffusion Synthetic Acceleration* (DSA) iteration.

Physics-Based Acceleration: DSA (II)

- DSA can be *much* more efficient than SI. (Problems that with SI require 100's or 1000's of iterations require < 10 DSA iterations.)

  Reason: The spectral radius of SI becomes arbitrarily close to 1.0 as the system becomes larger and more scattering-dominated. The spectral radius of DSA is bounded less than 1.0.

- However, the calculation of the *discrete* diffusion operator $(L-S)_D$ has been – and remains – problematic. Unless $(L-S)_D$ is chosen to be *consistent* with the discrete transport operator $L-S$, the resulting iteration scheme can be unstable if $\Sigma_t \Delta x > 1$.

- In the last 25 years, much effort in the computational nuclear engineering community has gone into the development of stable and efficient DSA methods.

- Fortunately, neutron transport problems generally have $\Sigma_t \Delta x < 1$. Thus, the problem of consistent discretization with neutron transport is not as severe as it is with other transport problems, where commonly $\Sigma_t \Delta x > 1$.

- Algebraic iterations (Krylov) using DSA as a preconditioner have recently been shown to be effective.

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Current Status of Monte Carlo

Monte Carlo codes model "exact" geometries (curved surfaces) and "exact" physics (no multigroup approximation). MC codes are most efficient when limited information (a reaction rate, an eigenvalue) are sought, and are least efficient when global information is sought. Neutron MC solutions have statistical errors but no truncation errors. Often, MC codes are expensive to run and require significant user input. Current research topics include:

- More efficient nonanalog (variance reduction) techniques.
- More reliable (statistical) techniques for estimating Monte Carlo sampling errors (and bias in *k*-eigenvalue calculations).

Current Status of Deterministic (S_N) Methods

S_N codes have a limited (but expanding) capability of modeling complex geometries. These codes automatically produce global solutions. S_N solutions have truncation errors, but no statistical errors. Generally, S_N codes are less expensive to run than MC codes, and require less user input. Current research topics include:

- Greater accuracy from discretization methods
  * Ray (angular discretization) effects
  * Noncartesian spatial grids
- Greater efficiency from iterative acceleration methods
  * Effect of unstructured grids on stability
  * Krylov methods

(Current Research in) "Hybrid" Monte Carlo-Deterministic Methods

- MC and S_N methods are based on completely different mathematical (and philosophical) approximations. Yet, these methods solve the same physical problem.

- The MC and S_N communities have existed for about 50 years. They are nearly disjoint, and have had no influence on one another.

- Advances in MC methods have had no effect on S_N methods – and vice versa – until recently.

- In the last 10 years, researchers have learned that it can be advantageous to use a relatively inexpensive deterministic code to calculate the biasing parameters for a complicated Monte Carlo simulation (MCBEND, TRIPOLI, AVATAR/MCNP, A^{3}MCNP,...)

- Advantages: This removes the burden from the code user to develop a large set of biasing parameters. Also, the computer-generated biasing parameters are usually much more efficient than human-generated biasing parameters.

- Disadvantage: The code user must use two different codes to solve the problem.

- The merging of Monte Carlo and Deterministic techniques – to obtain new *hybrid* computational methods that enhance the strengths and suppress the individual weaknesses of the individual MC and S_N approaches – is largely unexplored.

Conclusions

- Current research in neutron transport aims to make practical calculations more realistic, accurate, robust, user-friendly, and efficient.

- Lessons learned and techniques developed in neutron transport may be useful in other areas, and vice versa. Hopefully, this workshop will facilitate the transfer of information among different scientific communities in which particle transport is a major concern.

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