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A PROPOSED MONTE CARLO METHOD FOR COMPUTING THE BASIC LATTICE PARAMETERS AND THE SPACE DEPENDENT NEUTRON SPECTRA

By

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INTRODUCTION

The problem of neutron transport is basically concerned with random events. The most that can be said about any given interaction is the probability for the various kinds of events. In many of these events, the outcome (i.e., direction of neutron scattering and emergent energies) can be specified only in terms of probability distributions.

In a Monte Carlo calculation these stochastic processes are simulated on a computer by following essentially individual neutron histories. Random numbers are used to determine the outcome of the various processes.

The Monte Carlo method differs from numerical methods in that the neutrons are treated as discrete particles, while phase space is treated as a continuum (numerical methods treat the neutron population as a continuum, while phase space is represented by a set of discrete points).

The Monte Carlo method proposed here follows neutron histories through many generations. The total number of histories followed depends on the statistical uncertainty desired.

The major differences in the Monte Carlo scheme proposed here and previous Monte Carlo calculations are as follows:

1. The routine for the calculation of the fast fission factor is essentially the same as the code developed at Hanford by the author. The major difference is that the use of neutron weights has been introduced. The use of neutron weights provides an estimate of this parameter for every history followed and reduces the statistical error significantly.

2. The calculation of the resonance escape probability follows the general outline used by R. D. Richtmeyer.[1] However, an improved sampling technique is used to decrease the machine time required for each neutron history. The major innovation here is the use of doubling surfaces in the moderator.

3. The computation of the thermal utilization is a new procedure. A Monte Carlo scheme for calculating this parameter in water-uranium lattices has been developed by A. Rotenberg.[2] However, Rotenberg assumes that the thermal neutron spectrum is of the usual Wigner-Wilkins form. In the Monte Carlo method proposed here, no assumptions are made about the neutron spectra. The neutron spectrum is calculated for every region. With this calculation, the effects of spectral hardening and also epithermal fission will be included in the calculation of the thermal regeneration factor.

4. The neutron flux is calculated in a somewhat different manner. The definition that the neutron flux is proportional to the sum of the path lengths per cubic centimeter per second has been utilized. The neutron flux is recorded for 100 neutron energy groups, 25 thermal groups, 50 resonance groups, and 25 fast groups. The concept of groups has been introduced only as a convenience in recording the output. Below 100 kev, the processes take place on a continuous basis in phase space; the use of neutron groups is limited solely to the recording of the output. Above 100 kev, the neutron cross sections vary enough so that the neutrons are assumed to exist in various groups. Scatterings are followed from group to group rather than following a continuous energy degradation.

5. A generalized geometry routine is incorporated so that any type of lattice cell which can be specified by conic sections can be studied.

6. At the present time, there are no Monte Carlo codes that will compute the neutron spectra in complex lattices. Brown,[3] and Coveyou and Bates have applied the Monte Carlo method to computing thermal neutron spectra in a homogeneous infinite medium, and the proposed method extends the procedure to heterogeneous lattices.

The Monte Carlo method proposed here represents perhaps the most rigorous cell calculation that can be made; for example:

1. All transport effects are included.

2. The effect of epithermal fission on reactivity is included.

3. Spectral hardening is included.

4. No assumptions are made about the neutron spectrum.

5. In the calculation of the resonance escape probability, the following effects are included:

a. Slowing down by heavy as well as light atoms is included.

b. No assumptions are made that the transport mean-free path is small compared with the dimensions of the cell or the fuel rod.

c. No assumptions are made about the angular distributions of flux entering the fuel rod.

d. It is not necessary to approximate the cell with a cylinder.

e. Resonance scattering is included along with interference between resonance and potential scattering.

f. The Doppler broadening of all resonances is included, including both absorption and scattering.

g. It is not assumed that the slowing down density is a constant in the moderator.

6. In the calculation of the fast fission effect, the following effects are included that are usually neglected:

a. Back-scattering from the moderator is included; that is, some fission neutrons can escape from the fuel rod, make a collision in the moderator, and re-enter a fuel rod with sufficient energy to cause a fast fission in uranium-238.

b. The interaction fast effect, which may amount to a few tenths of a percent in reactivity in a graphite lattice, is included. That is, the fractional increase in the fast fission effect due to neutrons born in adjacent fuel rods or cells is included.

OVER-ALL METHOD

A neutron is assumed to be born due to thermal fission in one of the fuel rods. Initially, a uniform source distribution is assumed. The initial neutron energy is picked at random from the appropriate fission distribution. The initial direction parameters are chosen at random. (The neutron is emitted isotropically from the fission event.) This neutron is then followed as it slows down, and all pertinent events that occur are recorded. By the use of weights (this technique will be described later), the neutron can be thought of as a large assembly of neutrons all following a given trajectory. When an

absorption occurs, only a fraction of the neutrons are lost. If the original neutron weight was W_o, then after a collision occurs

$W_o \frac{\sum_a}{\sum_T}$, neutrons are absorbed,

$W_o \frac{\sum_e}{\sum_T}$, neutrons are elastically scattered,

$W_o \frac{\sum_{in}}{\sum_T}$, neutrons are inelastically scattered,

and so on.

For neutron energy above one electron volt, the scattering (elastic) mechanics are evaluated on the basis that the scattering nuclei are stationary.

If the neutron energy is less than one electron volt, the scattering nuclei are assumed to have a Maxwell-Boltzman distribution. The scattering mass used is an effective scattering mass such that the proper transfer functions which allow for chemical binding will be obtained.

The output of the Monte Carlo code will be as follows:

1. The average flux in each region for each neutron energy group.
2. The resonance escape probability.
3. The thermal utilization.
4. The fast fission effect.
5. The neutron regeneration factor, η.
6. The infinite neutron multiplication factor.
7. The statistical uncertainty for each of the above parameters.

If the lattice to be studied contains graphite, a priori knowledge of the importance functions is assumed. Work done elsewhere indicates that thermal neutrons might make several hundred collisions before entering the fuel. This difficulty can be alleviated by the use of doubling surfaces. Each time a neutron passes through a doubling surface in the outward direction, the neutron weight is increased by n (n = integer) and 1/n neutrons followed. If the neutron survives a game of Russian Roulette, a random number ξ is generated; if $\xi < 1/n$, the neutron survives; if $\xi > 1/n$, the neutron history is terminated. If the neutron passes through the doubling surface on the inward direction, the weight is decreased by n, and n neutrons are followed. These surfaces are placed at λ , $2\lambda \rightarrow n\lambda$ from the process tube or channel.

λ = mean-free path for graphite.

The optimum value of n will be determined during trial runs of the program. The optimum value is defined as the maximum n, for which the answer remains the same. Once this factor has been determined, it will be permanently incorporated into the program.

SAMPLING METHOD

The sampling technique used in this program is somewhat different from the usual straightforward procedures, such as diminishing weights. After each collision, the neutron weight is examined to determine if it is less than the cut-off value W_c. If not, the history continues, but once the weight has been reduced below W_c, a random

number ζ is chosen. If $\zeta > W_c$, the history is terminated and the tallies made. If $\zeta \leq W_c$, the history is continued, but the weight is increased by multiplying by $1/W_c$. Thus, histories are regenerated n times with probability W_c^n. For coding purposes, the procedure is altered somewhat. After each collision, a random number is chosen and tested against the actual weight W'.

$$W' = W_o \frac{\sum_s}{\sum_t}$$

If $\zeta > W'$, the history is terminated and the tallies made. If $\zeta < W'$, the weight is increased to W_o and the history is continued. The optimum value of W_o is approximately unity, and it has been shown that both procedures are statistically correct.

GEOMETRY

In general, surfaces of the following forms can be recognized:

1. $(x-x_o)^2 + (y-y_o)^2 - K = 0$
2. $x-K = 0$
3. $y-K = 0$
4. $z-K = 0$
5. $y = m\,x + b$

Surfaces are assigned one of the forms (1-5) by use of an index D_α ($\alpha = 1,2,3,4,5$). A microscopic region α is identified by listing the values of D_α that bound it. It is also necessary to identify both bounding surfaces and doubling surfaces by $D_{\alpha\,b}$ or $D_{\alpha\,n}$. A further parameter is needed to specify the types of materials in region α.

The first step in the geometry routine (the initial source routine is a separate entity) is to determine the distance to a collision. This can be written[4] (see Appendix C)

$$\ell = -\lambda_{\alpha}^{G} \ln \xi$$

ξ = a random number in the range $[0,1]$

λ_{α}^{G} = mean-free path in material α for neutrons with energy G

The distance to the nearest boundary is then calculated for a neutron with coordinates x_1, y_1, z_1, and direction cosines u, v, and w where

$u = \cos \alpha$

$v = \cos \beta$

$w = \cos \gamma$

and α, β, and γ are the angles made by the line of flight with the x, y, and z axes respectively.

The distance to a boundary of the type

$$(x-x_o)^2 + (y-y_o)^2 - K = 0$$

can be calculated by substituting into the above equation

$$x = d\,u + x_1$$

$$y = d\,v + y_1$$

The results would be:

$$d = -\frac{b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$b = 2(ux_1 + vy_1 - x_o u - y_o v)$$

$$c = (x_1^2 + x_o^2 - 2\,x_o x_1 + y_1^2 + y_o^2 - 2\,y_o y_1 - K_\alpha)$$

$$a = u^2 + v^2.$$

For boundaries of the form,

2. $X - K_\alpha = 0$

3. $y - K_\alpha = 0$

4. $z - K_\alpha = 0$

5. $y = m_\alpha x + b_\alpha$,

the solutions are

2. $d = -\dfrac{x_1 - K}{u}$ if $\dfrac{x - K}{u}$ 0

3. $d = -\dfrac{y_1 - K}{v}$ if $\dfrac{y - K}{v}$ 0

4. $d = -\dfrac{z_1 - K}{w}$ if $\dfrac{x - K}{w}$ 0

5. $d = \dfrac{b - y_1 + m\,x_1}{v - m\,u}$.

The smallest positive value of d being accepted as the distance to region α'. A check is then made to determine if

1. $\ell \leq d$

2. $\ell > d$

If the first equality holds, a collision occurs in region α, and the collision routine is called. If the second statement is true, then the neutron is advanced to:

$$x = du + x_1$$

$$y = dv + y_1$$

$$z = dw + z_1$$

A check is now made to determine if the new region D_α' is a doubling surface or a boundary. If D_α' is a doubling surface which is described by an equation

$$x^2 + y^2 - K = 0,$$

a further check is made to determine if

1. $x_1^2 + y_1^2 \leq K$
2. $x_1^2 + y_1^2 > K.$

If the neutrons original position was such that

$$x_1^2 + y_1^2 \leq K,$$

the weight of the neutron is increased by n if the neutron survives the game of Russian Roulette. If $x^2 + y^2 > K$, the neutrons weight is decreased by n and n neutrons followed. If the surface D_α is a boundary, then

$x = -x$, for type 2, 3, and 4 surfaces

$x = -x$)
) for type 5 surfaces
$y = -y'$)

and the neutron history is continued.

When the neutron has been advanced to its new position, (if $\ell > d$) a new ℓ is calculated

$$\ell = -\lambda_\alpha^G 1 \ell n \left(1 - \frac{\gamma}{P(d)}\right)$$

$$P(d) = e^{-\Sigma_\alpha d}$$

and the collision routine is called. The neutrons new position is:

$$x' = \ell u + x$$

$$y' = \ell v + y$$

$$z' = \ell w + z$$

Before the collision routine is called, the neutron track length in region λ and λ' is recorded. The neutron flux for any energy group can be defined as the sum of the track lengths per cubic centimeter per sec. Thus, the average flux in each region can be calculated by

$$\bar{\phi}(E) = \sum_{n=1}^{N} W_n \ell_n(E)$$

where

W_n = neutron weight

$\ell(E)$ = track length per collision for a neutron of energy E.

COLLISION ROUTINE

Two cases are considered for elastic scattering.

1. If the neutron energy is above E min (E min = 1 ev), the moderating atoms are considered to be at rest. In this case, the energy loss can be readily calculated as follows:

$$E' = E(S_c + T_c \mu)$$

$$\mu = \cos\psi' = 2\xi - 1$$

Ψ' = angle of deflection in the center of mass system from the original line of flight.

E = original neutron energy

E' = new neutron energy

$S_e = 1/2\ (1+re)$

$T_e = 1/2\ (1-re)$

$re = (A-1)^2/(A+1)^2$

ζ = random number in the range (0,1)

The cosine of the angle of deflection in the laboratory system from the original line of flight can be calculated as follows:

$$\cos\psi = \frac{1 + A\mu}{(1 + A^2 + 2A\mu)^{1/2}}$$

The direction parameters after collision are then calculated by[5]

$$u' = \frac{b\,c\,w\,u - b\,d\,v}{1 - w^2} + a\,u$$

$$v' = \frac{b\,c\,w\,v + b\,d\,u}{1 - w^2} + a\,v$$

$$w' = \frac{-\,b\,c}{1 - w^2} + a\,u$$

where

$a = \cos\psi$

$b = \sqrt{1 - a^2} \qquad 0 \leq \psi \leq \pi$

$c = \cos\delta$

$d = \sin\delta = \pm\sqrt{1 - c^2}$

$\delta = \pi\,(2\zeta - 1)$

If w' is close to unity, that is if $1 - w' - 2^{-n} < 1$, the formulas become indeterminate, and the following is used:

$$u' = b\,c$$

$$v' = b\,d$$

$$w' = a\,w$$

2. If the neutron energy is less than E_{min}, the moderator atoms are considered to have a Maxwell-Boltzman distribution of velocities.

The probability p of a collision between a neutron of velocity $\vec{v}$ and a target of velocity $\vec{v}_2$ and with $\vec{v}_r = \vec{v} - \vec{v}_2$ depends upon the relative velocity and the distribution of target velocities. The probability of a collision with a moderator atom is obtained by integrating over all $\vec{v}_2$

$$\int p\, d\vec{v}_2 = \int_0^w \sigma(|\vec{v} - \vec{v}_2|)\, m(\vec{v}_2)\, d\vec{v}_2$$

The assumption is made that the scattering cross section is constant in this region. Then

$$\int p\, d\vec{v}_2 = \sigma \left[\frac{e^{-\alpha v^2}}{\sqrt{\pi \alpha}\, v} + \left(1 + \frac{1}{2\alpha v^2}\right) \operatorname{erf} \sqrt{\alpha}\, v \right]$$

with

$$\alpha = \frac{A}{2kT}$$

Since the integral probability is complex, it is much more convenient to deal with the differential probability. The selection of v_2 is made with a rejection technique.[3] An upper bound of the

integrand is $v + v_2$; the upper bound of the probability is then

$$\int_{p}^{max} d\vec{v}_2 = v\int m(v_2)\, dv_2 + \int v_2\, m(v_2)\, dv_2$$

$$= v + I$$

$$I = V_o\sqrt{\frac{T}{T_o}\ \frac{4}{\pi}}$$

A random number ζ in the range (0,1) is drawn. If $\zeta \leq v/(v + I)$, a value of v_2 is chosen from a Maxwellian distribution (see Appendix B). If $\zeta > v/(v+I)$, v_2 is selected from the distribution $v_2 m(v_2)$.

The v_2 so obtained is representative of the upper bound probability p(max), the actual probability is more restrictive. Every velocity v_2 is chosen too frequently by the method because each velocity is chosen with maximum probability. The frequency should be reduced by the fraction which p(max) exceeds the actual p. Thus, a second random number ζ is drawn to test the choice of v_2. If $\zeta \leq |\vec{v} - \vec{v}_2| / |\vec{v} + \vec{v}_2|$, v_2 is accepted; otherwise, the sample is rejected and the process is repeated.

The value of μ is selected by choosing a random number ζ in the range (0,1) and

$$\mu = 2\zeta - 1$$

If the scattering is accepted, the calculation proceeds in the usual manner.

For any collision one has

$$\gamma\,\vec{v} + \beta\,\vec{v}_2 = \gamma\,\vec{v}' + \beta\,\vec{v}_2' = \vec{V}_c$$

where $\vec{v}_c$ is the velocity in the center of mass, and the primed and unprimed quantities refer to the post and pre-collision velocities. Since for elastic collisions

$$|\vec{v} - \vec{v}_2| = |\vec{v}' - \vec{v}_2'|,$$

the new neutron speed is

$$|v'| = |\beta |\vec{v} - \vec{v}_2| + \vec{v}_c|$$

$$= \sqrt{\beta^2 |\vec{v}-\vec{v}_2|^2 + \vec{v}_c^2 + 2 (v-v_2) V_c \lambda}$$

$$\lambda = 2 \xi - 1$$

$$\gamma = 1/(1 + A_{eff})$$

$$\beta = A_{eff}/(1 + A_{eff})$$

$$V_c = (V^2 + 2 A_{eff} v v_2 + A_{eff}^2 v_2^2)^{1/2} (A_{eff} + 1)^{-1}$$

$$|\vec{v}_r| = \sqrt{v^2 + v_2^2 - 2 \mu v v_2}$$

The direction parameters after collision can be calculated in the usual manner except that

$$\cos \psi = \cos \psi' \cos \psi'' - \sin \psi' \sin \psi''$$

$$\cos \psi' = \frac{|\vec{v}_c| + |\vec{v}-\vec{v}_c|}{|\vec{v}'|}$$

$$\cos \psi'' = \frac{v'_2 + A_{eff} |\vec{v}| |\vec{v}_2| \mu}{(A_{eff} + 1) |\vec{v}| |\vec{v}_c|}$$

$$\left| \vec{v} - \vec{v}_c \right| = (v_c^2 - v_2^2 - 2 A v v_2 \mu)^{1/2}$$

ψ' = angle between $\vec{v}_c$ and $\vec{v}'$

ψ'' = angle between $\vec{v}_c$ and $\vec{v}$

In the above calculations for elastic scattering, it was assumed that scattering was isotropic in the center of mass system. If the appropriate differential scattering cross sections were known, the effect of anisotropic scattering collision in the center of mass system could easily be calculated.

In the case of inelastic scattering, the emergent neutron energy is chosen from the evaporation model.[6]

$$N(E') = E' \exp^{-E'/\theta}$$

$$\theta = 2 E^{1/2}/B$$

$$B \approx 0.62 \sqrt{A}$$

A random number ζ in the range (0,1) is calculated and

$$E_1 = -\frac{1}{\theta} \ln \zeta$$

A second random number in the same range is chosen and

$$E_2 = -\frac{1}{\theta} \ln \zeta$$

then

$$E' = E_1 + E_2 \quad \text{(see Appendix E)}$$

After the scattering mechanics have been calculated, the appropriate quantities are recorded and the history either continues or is terminated. If the history has been terminated, the program selects a neutron from the born storage portion of the program. If none is available, the program returns to initial start.

CROSS SECTION ROUTINE

The neutron cross sections are divided into finite energy groups except in the range 0.45 ev to 100 kev. In all ranges, the neutron energy may vary continuously although the absorptions and fluxes are recorded in finite groups. In this energy range resonance absorption in uranium -238 predominates. The U-238 resonance region consists of three loosely defined sub-regions:

1. Resolved region
2. Statistical region
3. Region above $\sim$ 10,000 ev

For the first two cases (including interference between resonance scattering and absorption and the thermal motion of the target atoms), the cross sections for absorption and scattering can be written as

$$\sigma_a (E,T) = \sigma_{r\,a}\, \psi(x,\theta)$$

$$\sigma_s (E,T) = \sigma_{r\,s}\, \psi(x,\theta) + 2\left(\frac{1+A}{A}\right)\sqrt{\sigma_p\, \sigma_{r\,s}}\, \chi(X,\theta)$$

$$\sigma_f (E,T) = \sigma_f \psi(x,\theta) \quad \text{(for U-235)}$$

(See Appendix A for the calculation of the ψ and χ functions.)

where

$$\sigma_{ra} = \frac{2.607}{E_o} \left(\frac{1+A}{A}\right)^{3/2} \left(\frac{E_o}{E}\right)^{1/2} \frac{\Gamma_n \Gamma_\gamma}{\Gamma^2} \times 10^{-18} \text{ cm}^2$$

$$\sigma_s = \frac{2.607}{E_o} \left(\frac{1+A}{A}\right) \frac{\Gamma_n^2}{\Gamma^2} \times 10^{-10} \text{ cm}^2$$

$$\sigma_f = \frac{2.607}{E_o} \left(\frac{1+A}{A}\right)^{3/2} \left(\frac{E_o}{E}\right)^{1/2} \frac{\Gamma_n \Gamma_f}{\Gamma^2} \times 10^{-18} \text{ cm}^2$$

$$\psi(x, \theta) = \frac{1}{2\sqrt{\pi\theta}} \int_{-\infty}^{\infty} \frac{dy}{1+y^2} e^{-(x-y)^2/4\theta}$$

$$\chi(x, \theta) = \frac{1}{2\sqrt{\pi\theta}} \int_{-\infty}^{\infty} \frac{dy}{1+y^2} 2y\, e^{-(x-y)^2/4\theta}$$

$$x = \frac{2}{\Gamma} \left(\frac{E}{1+A} - E_o\right)$$

$$\theta = \left(\frac{A}{1+A}\right)^2 \frac{4 E kT}{A^2} = \frac{34.44 \times 10^{-5} T E}{A^2} \left(\frac{A}{1+A}\right)^2$$

E = energy of the neutron

E_o = energy of the neutron at the center of the resonance

A = nuclear mass

k = Boltzman constant

T = absolute temperature

σ pot = constant potential scattering cross section

Γ_n and Γ_γ are the neutron and x-ray half widths.

The cross-sections for a nuclide that has resonances are

$$\sigma_a(E) = \sigma_a(E,T) + k/\sqrt{E}$$

$$\sigma_s = \sigma_s(E,T) + \sigma \text{ pot}$$

When a neutron of energy E has a collision, a calculation is made on the energy scale to determine the two nearest resonances. Let these resonances be at E_o and E_o' such that

$$E_o \leq E \leq E_o' \quad .$$

The cross-sections for the reaction are then taken as the sum of the background cross-sections and thecontribution from these two resonances.

For the statistical region it is assumed that

1) The resonances are uniformly spaced
2) They have constant radiation width
3) The neutron widths are distributed with a Porter-Thomas distribution.

The probability that

$$x = \left(\frac{\Gamma_{no}}{\Gamma_{no_{ave}}}\right)^{1/2}$$

be between x and x + dx is given by

$$P(x)\,dx = \sqrt{\frac{2}{\pi}}\, e^{-x^2/2}\, dx \quad .$$

Then

$$\Gamma_n = \Gamma_{no}\sqrt{E_o} \quad .$$

The procedure used to select from the Porter-Thomas distribution is first select two random numbers and define (see appendix D)

$$\beta_1 = -\ln \xi_1$$

$$\beta_2 = -\ln \xi_2$$

if $(\beta_1 - 1)^2 \leq 2\,\beta_2$, $x = \beta_1$. Otherwise two more random numbers are drawn until the criteria is satisfied.

In the region above $\sim$ 10,000 ev, where higher angular momenta effects become important, (n, γ) cross-sections are taken from BNL-325.[7] The assumption is made that self-shielding is negligible in this region.

In U^{235} the neutron fission widths are distributed as[8]

$$d\,P(v) = e^{-v}\,dv$$

$$v = \frac{\Gamma_f}{\Gamma_{f_{ave}}}$$

Selection of v is then the same as the selection of the distance to a collision.

INITIATING PROCEDURE

To start the program ν_{25} neutrons are assumed to be born in one of the fuel rods from thermal fission. The initial position is first picked from a uniform distribution in the fuel rod. An initial neutron energy is picked at random from the Cranberg fission spectrum (see appendix E). Then ν_{25} neutrons of this energy and initial position

are stored in the born storage. Then one neutron is picked from born storage and its history is traced. If this neutron is lost before it causes further fissions, the born storage is searched and another neutron is followed. If no neutrons are in born storage then the program returns to start. If the initial neutron is not lost before it causes further fission, the new fission neutrons are stored in born storage to await their turn. Thus, the assumption that the thermal fission distribution is uniform is rectified.

The initial neutron's position and direction cosines are calculated in the following manner. Chose a random number ζ in the range (0,1)

$$R = \zeta\sqrt{K\alpha}$$

another random number is chosen and

$$\phi = \pi(2\zeta - 1) \quad .$$

Then

$$x' = R \cos \Theta$$

$$y' = R \sin \Theta$$

and

$$x = x' + x_o$$

$$y = y' + y_o \quad .$$

Another random number ζ is chosen in the range (0,1), and

$$w = 2\zeta - 1$$

$$\zeta = \sqrt{1 - w^2}$$

Again, a random number is chosen and

$$\theta = \pi(2\zeta - 1)$$

$$u = \rho \cos \theta$$

$$v = \rho \sin \theta$$

GENERATION OF RANDOM NUMBERS[9,10]

The sequence

$$\zeta_{i+1} = (2^a + 1)\ \zeta_i + C \qquad \text{mod } 2^{36}$$

has been shown to be satisfactory if $a \geq 2$ and c is odd.

This sequence generates a full period of 2^{35} random numbers before repeating the sequence.

APPENDIX

A. Calculation of $\Psi(x, \theta)$ and $\chi(x, \theta)$[11,12]

The convergent series are

$$\Psi_c(x, \theta) = e^{\frac{-x^2}{40}} \sum_{n=0}^{N} \left(\frac{x}{40}\right)^{2n} \alpha_n(40)$$

$$\alpha_n(40) = \frac{\Gamma_n(40)}{n!}$$

and $\Gamma_o(40)$ is the tabulated incomplete gamma function.

$$\chi_c(x, \theta) = \frac{x}{40} \sum_{n=0}^{N} \left(\frac{x}{40}\right)^{2n} \alpha'_n(40)$$

$$\alpha'_n(40) = \frac{\Gamma_{n+1}(40)}{n!} \quad .$$

The values of n at which the series are terminated is defined as

$$\left\{ \left[\left(\frac{x}{40}\right)^{2n} \alpha_n(40) \right] \sum_{n=0}^{n-1} \left(\frac{x}{40}\right)^{2n} \alpha_n(40) \right\} \leq 0.00156 \quad .$$

The asymptotic series are

$$\Psi_a(x, \theta) = \sum_{n=0}^{4} \left[\frac{40}{x^2+1} \right]^n \beta_n(x)$$

$$\beta_0(x) = \frac{1}{x^2+1}$$

$$\beta_1(x) = 1/2\ \beta_0(x) \left[3-4\ \beta_0(x) \right]$$

$$\beta_2(x) = 3/4\ \beta_0(x) \left[5-20\ \beta_0(x) + 16\ \beta_0^2(x) \right]$$

$$\beta_3(x) = \frac{15}{8}\ \beta_0(x) \left[7-56\ \beta_0(x) + 112\ \beta_0^2(x) - 64\ \beta_0^3(x) \right]$$

$$\beta_4(x) = \frac{105}{16}\ \beta_0(x) \left[9-120\ \beta_0(x) + 432\ \beta_0^2(x) - 576\ \beta_0^3(x) + 256\ \beta_0^8(x) \right]$$

$$\gamma_A(x, \Theta) = \sum_{n=0}^{4} \left(\frac{4\Theta}{x^2+1}\right)^n \beta_n'(x)$$

$$\beta_0'(x) = \frac{x}{x^2+1}$$

$$\beta_2'(x) = -1/2\ \beta_0'(x) \left[3-4x\ \beta_0'(x) \right]$$

$$\beta_2'(x) = 3/4\ \beta_0'(x) \left[5-20\ x\ \beta_0'(x) + 16x^2\ \beta_0^2(x) \right]$$

$$\beta_3'(x) = -\frac{15}{8}\ \beta_0'(x) \left[7-56\ x\ \beta_0'(x) + 112\ x^2\ \beta_0^2(x) - 64x^3\ \beta_0^3(x) \right]$$

$$\beta_4'(x) = \frac{105}{16}\ \beta_0'(x) \left[9-120\ x\ \beta_0'(x) + 432x^2\ \beta_0'^2(x) - 576x^3\ \beta_0'^1(x) + 256x^4\ \beta_0'^4\ x \right]$$

The conditions under which the convergent series are used is:

$0 \leq x < 1.2$ and $4\Theta \geq 0.275x^2 + 0.05$

$1.2 \leq x < 10$ and $4\Theta \geq 0.12x^2 + 0.28$

$10 \leq x < 100$ and $4\Theta \geq 0.105x^2 + 1.75$

$100 \leq x < 200$ and $4\Theta \geq 0.95x^2 + 100$

The coefficients β_n and β_n' have been determined by E. J. Leshan.

B. Selection From a Maxwell Boltzman Distribution

A useful device employed by von Neuman is used here. A random number ζ is generated in the range $[0,1]$.

$$\zeta V_{max} = V$$

Then $M(V_p)$ is calculated, where V_p is the most probable velocity. A second random number is generated, and if

$$\zeta M(V_p) \leq M(\zeta V_{max})$$

the velocity is accepted as V; if the inequality is not satisfied, the procedure is repeated until the criteria is satisfied.

B. Selection of the Distance to a Collision

The probability density is

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

and

$$P(l) = \int_0^l p(l)dl = 1 - e^{-\Sigma l}$$

is the corresponding distribution function for a first collision at l.

$$\zeta = 1 - e^{-\Sigma l}$$

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

Since $1 - \zeta$ is equi-distributed in the range $[0, 1]$ if ζ is

$$l = -\tau \ln \zeta$$

D. Selection of Resonance Partial Widths[13]

The reduced neutron width is distributed as

$$dp(x) = \sqrt{\frac{2}{\pi}}\ e^{-x^2/2}\ dx$$

where

$$x = \left(\frac{\Gamma_{no}}{\Gamma_{no_{ave}}}\right)^{1/2}$$

The probability that β_i will be obtained and accepted is

$$P(\beta_i) = \int_{(\beta_1-1)^2/2}^{\infty} P(\beta_i)\ P(\beta_2)\ d\beta_2$$

$$P(\beta_i) = \int_{(\beta_1-1)^2/2}^{\infty} e^{-\beta_1}\ e^{-\beta_2}\ d\beta_2$$

$$= e^{-\beta_1} \int_{(\beta_1-1)^2/2}^{\infty} e^{-\beta_2}\ d\beta_2 = \frac{1}{e}\ d^{-1/2\ \beta_1^2}$$

which has the required distribution.

E. Selection from the Evaporation Model Spectrum

The probability distribution is

$$dp(E) = CE\ e^{-E/T} \quad .$$

The sum of two random logarithms has the distribution

$$P(x) = \int_0^x e^{-Y}\ e^{-(x-Y)}\ dY = xe^{-x} \quad .$$

The sum of two numbers each distributed as $e^{E/T}$ has the distribution required.

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