THE PHASE SPACE TIME EVOLUTION METHOD APPLIED TO MULTIGROUP NEUTRON TRANSPORT

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I. INTRODUCTION

In performing reactor physics calculations on the level of sophistication of transport theory or diffusion theory, the primary quantity of interest is the neutron density. Depending on the problem and accuracy desired, one can obtain this variable as a function of space, angular direction, energy, and time. The linearized Boltzmann equation is essentially the starting point for all calculations of this type and represents an analytical formulation of conservation of points in phase space. Although the formalism is elegant, exact solutions are seldom obtained, and computer oriented numerical methods are used in solving the complex integro-differential equation. Tavel and Zucker[1] suggested that instead of burdening the computer with the task of solving the transport equation directly, perhaps a simpler and more efficient method would be to use the computer memory as a library to store and keep track of neutrons moving through phase space. In this way the neutron density at any position, direction, and energy could be observed by displaying the computer memory at any time. In order to keep this inventory, Tavel and Zucker[1] introduced a two-dimensional (space, direction) discretized phase space considering only the one-speed approximation. Cordaro[2] expanded the coordinate system by using a three-dimensional discretized grid; the third dimension was energy. However, he considered electron transport where the majority of the collisions were not catastrophic in energy or direction, thus allowing a finely divided energy dimension to account for space and energy changes. In the multigroup neutron transport formulation, the three dimensional (space, direction, energy) grid is similar to Cordaro and Tavel's

system in the first two coordinates, but the energy dimension is arbitrarily discretized. Each energy plane represents a different velocity group. Transfer between these energy planes represents up or down scattering and is dependent upon the cross sections and degree of anisotropy used.

Only one space dimension is considered in this analysis. However, two or three space coordinates could be constructed. Also other geometries could be introduced. The Phase Space Time Evolution (PSTE) method is essentially geometry independent. A complex geometry only adds to the programming difficulty.

One of the most significant aspects of this method is the inclusion of time as a variable. By keeping track of neutrons traveling through a scattering medium with their equations of motion given by Newton's Laws, the effective time evolution of the neutron population can be displayed at any given time step. It will be shown that the time increment depends on the energy region involved in a particular problem. Two examples: 1) if fast neutrons are being considered, the time interval would lie within the range needed to observe the time evolution of the neutron density in a nuclear explosive; 2) if thermal neutrons are of interest, the time evolution of a reactor approaching criticality could be considered with some allowances made for slowing down.[1]

II. BASIC THEORY

Only one spatial dimension will be considered in this analysis. It is possible to extend this method to two or three spatial dimension problems, however the programming complexity is increased. Also since most transport problems of interest involve medium discontinuities, a three region configuration is used. For simplicity, slab geometry is considered and, hence the total physical problem takes the form of a slab of finite dimensions sandwiched between two regions which can either be considered finite or infinite.

The spatial dimension labeled X in Figure 1 is divided into a mesh whose increment (ΔX) is in general a function of material and energy. This will be described later. The X dimension is measured in terms of mean free paths primarily because the motion of neutrons through a medium is relative to the mean distance between interactions. The vertical axis is μ, the angular variable of neutron density. Since the geometry is one dimensional, this axis represents the direction of neutron motion such that

$$\mu = \cos\theta \qquad -1 \leq \mu \leq 1 \tag{1}$$

where

$$\theta = \cos^{-1}\frac{V_x}{V} \tag{1b}$$

V_x: X component of velocity

V: magnitude of velocity.

Azimuthal symmetry is assumed so that all neutrons on a cone of half angle θ are considered the same by the method. Depending upon the accuracy of the calculation, the vertical axis can be divided into as many equal increments $\Delta\mu$ as required.

Consider a given 'box' in Figure 1 outlined by a certain $\Delta\mu$ and ΔX. For the computer memory, each increment of μ corresponds to a given J value and similarly each X increment to an I value. Every box is therefore located by four pairs of coordinates. (See Figure 1). However if one pair is known the others may be calculated. For convenience, the upper right coordinate set is used to identify the position of the box. In Figure 1, this would be the set (I,J). In Figure 2, corresponding to each energy, there is a phase space grid to describe neutron motion at that energy.

The density in the box or phase space element corresponding to coordinates (I,J) in some energy plane E_k is $N(I,J,E_k,t)$. Time is an implicit parameter as will be shown later in this section. The density is assumed constant throughout the box.

Also in Figure 2 the spatial axes are X_{E_1}, X_{E_2},..., X_{E_N}. The reason and effect of this fact will be discussed later in this section. It will suffice for now to notice that the spatial dimension (which is measured in total mean free paths) in general varies with energy.

To be exact, the distance between the planes should be proportional to the energy itself. In this multi-group formulation, however, neutrons can only possess discrete energies and therefore the distance between the planes has no meaning as far as the computations are concerned. A continuous energy dimension has been considered,[2] but for electron transport with the assumptions of only down scattering and no catastrophic collisions, i.e., collisions which do not result in large energy or angle changes. While this is a good assumption for electron transport, neutron motion is of a different nature; large energy and angle changes occur

frequently. The multi-group formulation allows both up and down scattering, has no restrictions on the energy loss involved in collisions within the framework of the energy planes, and permits large angle changes in collisions.

A logical question to ask at this point is since neutron motion is being described directly without solving the transport equation, what is the physical significance of a box in phase space and how does it relate to neutron transport? This question must be answered in two parts. First, the physical meaning of a 'box' in phase space will be explained.

Consider a one dimensional medium with a source located somewhere in its interior. The density of neutrons in the direction $\Delta\mu$ about μ within the spatial interval X and X + ΔX would coincide with the neutron density of a particular box in every energy plane. Furthermore, if the neutrons in this medium were assumed to possess a finite number of discrete energies, say E_1, E_2, E_3,..., E_N, then a 'box' in some energy plane E_k would represent the neutron density on some interval X and X + ΔX in some direction $\Delta\mu$ about μ, and at some energy E_k. This is for a given time. However, neutrons are moving through space and experiencing interactions which, in general, alter their direction μ and energy E_i. This leads to the second part of the question: How does a phase space box element behave in neutron transport? The general equation in the PSTE method which describes uncollided particle motion at a given energy E_k is

$$X(E_k,t + \Delta t) = X(E_k,t) + V(J,E_k)\Delta t \qquad (2)$$

where

$X(E_k,t + \Delta t)$: position in energy plane E_k at time $t + \Delta t$

$X(E_k,t)$: position at time t in plane E_k

$V(J,E_k)$: velocity corresponding to E_k in direction J.

As a phase space element moves along the X axis according to Eqn. (2), it deforms into the shape of a parallelogram. To redefine the density of the grid elements with that of the sheared box, the fraction of the total area of the parallelogram which overlaps each grid element is the amount of the initial density that is evenly distributed in that element. In other words, if the box is halfway between two elements, then the density of each element would be redefined with half of the density of the sheared box. (See Figure 3).

Next, the neutrons which experience interactions in traveling through a time increment Δt will be considered.

The probability that a neutron traveling with velocity $V(E_k)$ will experience an interaction in a time Δt is

$$P(E_k,\Delta t) = 1 - e^{-\Sigma(E_k)V(E_k)\Delta t} \qquad (3)$$

where

$\Sigma(E_k)$: energy dependent total cross section

$V(E_k)$: velocity (cm/sec) corresponding to energy E_k

Δt: time (sec).

The collision density is essentially a continuous function, and in the PSTE method interactions are only observed after a finite time step. Therefore in order to approximate nature only 10% of the particles in a phase space element are arbitrarily permitted to experience an interaction in time Δt. This makes multiple scattering at most a 1% correction.

In the multigroup formulation one tenth of the neutrons in the energy group corresponding to the highest velocity in total mean free paths per second is allowed to interact. Hence from Equation (3):

$$\Delta t = \frac{-\ell n(0.9)}{(\Sigma V)_{max}}. \qquad (4)$$

This insures that the time interval will be small enough so that transport in all other groups will obey this restriction.

Referring to Eqn. (4), in general, the total cross section Σ is a function of energy in the medium under consideration. The velocity V in centimeters per second is only dependent upon the energy. Since a three region configuration is used presently in the code the maximum implied in Eqn. (4) refers to the product of the largest total cross section found in the problem and the highest velocity. The program is so designed as to search for the maximum automatically without any special instructions from the user.

To better approximate nature, the Δt in Eqn. (4) is itself subdivided into five increments. At the end of each of these increments the moving phase space element pauses and the fraction which has interacted during that time is calculated. Of this fraction, the portion that experiences scattering events is redistributed in angle. This corresponds to forming identical replicas of the sheared box above and below it in the μ direction.

In general, a known fraction will scatter into every direction and into every energy, hence in each energy plane, replicas of the original box are formed and the actual fraction transferred is determined by the

group transfer cross probabilities. Once the neutrons transfer to another group, they travel for the remainder of the time step with the velocity corresponding to their new energy. The apportionment and redistribution is the same as with the unscattered neutron case discussed earlier. (See Figure 3).

Another important grid parameter to be discussed is the spatial mesh interval. This quantity is related to the major source of error of the PSTE method. In the apportioning process, the density portion of the sheared box that lies in each phase space element is evenly redistributed among those elements. By so doing some neutrons are effectively speeded up and some slowed down from their actual motion. To be exact, only the portion of the phase space element that the sheared box occupies should be redefined by this apportioning process. Tavel and Zucker[1] suggested a method that would eliminate this error and make the apportioning exact. However, it is an additional complexity and will be only mentioned here. Nevertheless it should be considered in later studies of the PSTE method.

In order to best approximate neutron transport in a digitized phase space, a considerable amount of care must be taken in determining the mesh spacing. The mesh interval must be chosen to yield the maximum accuracy with the minimum requirement of computer storage. The particular increment of interest is that of the lowest energy group E_N. It will be shown later that a simple relationship exists between the mesh spacing of each group in a given medium. Since neutron transport is in terms of the distance traveled in a time step, it follows that the mesh spacing should be some fraction of that distance. The mesh interval of the lowest energy

group ΔX_N can be represented as

$$\Delta X_N = \alpha V(E_N)\Delta t \tag{5}$$

where α is some constant yet to be determined, Δt is the time step from Eqn. (4) and $V(E_N)$ is the velocity in terms of total mean free paths of the lowest energy group in a given medium.

To illustrate the trend of thought used in determining the α in Eqn. (5), consider Figure 4. In part a, the mesh interval ΔX_a was made small relative to the distance traveled in the time step. The apportioning process here would yield little error since the sheared box is slanted so much that no large change in position takes place upon redistribution. However another factor comes into play here, namely computer storage. Since in the multigroup formulation, neutrons can assume different velocities, boxes in the largest energy plane, E_1 will travel much further than boxes in the smallest energy E_N. Hence a fine grid would significantly increase storage requirements. In part b of Figure 4 the second alternative is shown. This example shows a large mesh interval. The apportioning error is much larger here since the fraction lying in the second element must be redistributed over a large region. This size would require less computer storage, but the associated error would be unsatisfactory. In part c, the sheared box traveled such a distance relative to the mesh spacing as to be divided evenly between two grid elements. Here the apportioning error is minimized. Each half of the box is redistributed essentially over the same amount of space. The configuration yields $\alpha = 1/3$. This value produces the best combination of required computer storage and minimum apportionment error.

The mesh interval of each energy plane can now be easily derived. Each energy plane contains the same number of mesh points and for simplicity it is required that each mesh interval represent the same distance in centimeters along the X axis. If this were not the case, a different number of mesh points would be required at each energy to yield the actual space dimension of the given medium. With the mesh interval of the lowest energy group ΔX_N now known, and the total mean free path λ_k (cm) $[= \Sigma_k^{-1}]$ at each energy E_k, ΔX_k can be found by observing:

$$\Delta X_1 \lambda_1 = \Delta X_2 \lambda_2 = \Delta X_3 \lambda_3 = \ldots = \Delta X_N \lambda_N. \tag{6}$$

Solving for ΔX_k in Eqn. (6) yields

$$\Delta X_k = \Delta X_N \left(\frac{\lambda_k}{\lambda_N}\right), \quad k = 1,2,3,\ldots,N. \tag{7}$$

The quantity $\left(\frac{\lambda_k}{\lambda_N}\right)$ represents the relative flight distance between interactions at an energy different from E_N. If the total cross section was constant with respect to energy, then from Eqn. (7), obviously the mesh interval in each group would be the same. However, in general this is not the case, and the code was designed to utilize Eqn. (7) and other mesh dependent factors to allow for energy dependent cross sections.

Now that the spatial mesh has been defined, the distance traveled at energy E_k relative to E_N must be studied. Consider the energy ratio, $(E_1/E_N) = 10^8$. This value is not unusual in neutron slowing down problems. Since the corresponding velocity ratio varies as the square root of the energy, $\frac{V_1}{V_N} = 10^4$. This implies that neutrons in the fastest group will travel 10,000 times further than neutrons in the slowest group.

In terms of mesh points, recall in the slowest group the mesh interval was determined such that the box would travel 3 elements in the time step Δt. To describe for the present mono-directional neutron transport in the fastest group, 3×10^4 mesh elements would be needed. The amount of storage necessary for a multigroup study with such a large number of mesh elements could be obtained, but the execution time required would be extremely large and for the most part impractical. At this point a trade-off was made. In a search for a physically suitable energy ratio and number of energy groups, Edlund and Zweifel[3] suggested that 4 groups and $\frac{V_1}{V_N} = 8$ would be versatile enough to study thermal energy distributions as well as to analyze the fission region of the fast reactor energy spectrum. The code as of this writing is dimensioned to this capacity.

Another important grid parameter is the energy flight envelope. This quantity represents the maximum number of phase space elements a given box could span in traveling a distance $V(E_k)\Delta t$. To study this parameter, consider first the trivial case, $V = 0$. In this situation, the box does not move, but it still occupies a mesh interval in the grid, hence the envelope is one. For a more realistic example, let $V = 1$ cm/sec and assume this is the slowest speed. It has been shown that the box will travel a maximum distance of three elements in the direction which corresponds to $\mu = 1$. The box could also travel three elements in the $\mu = -1$ direction, hence the envelope for the energy group is seven. If in another group relative to the preceding example, $V = 2$ cm/sec, then the box would travel twice as far as in the previous case, therefore counting the element where the box originated, the envelope is thirteen. Table 1 summarizes these facts and presents sample envelopes for typical speeds.

III. INTERFACE PARAMETERS

In dealing with problems where abrupt material changes occur, diffusion theory at best can yield a first approximation. Transport theory is the primary tool for obtaining accurate results in problems of this type. For this reason most problems in transport theory involve more than one region. In the PSTE method, Tavel and Zucker[1] initially considered a three region problem in slab geometry. The multigroup formulation utilizes the same geometry and configuration. However, interface complications do arise.

Figure 5 displays the configuration and the variables used in the computer code to recognize certain positions in the one space-dimensional mesh. The two variables IAB and IBC determine the number of phase space elements between the three regions. A stipulation imposed on the width of medium B requires it be at least as wide as the largest flight envelope. This prevents any boxes from freely passing entirely through medium 2 without experiencing any interactions. It would be a relatively simple extension however to release this restriction if desired.

The other variables IBAB, IBBA, etc. indicate the boundaries of the buffer regions. All elements in these regions are treated by special parts of the code.

Complications arise at the interface because, in general, there is a space and velocity discontinuity at these points. The problem exists because the mesh interval and the velocity varies with the total mean free path of the region. In general the material properties and hence the total mean free path varies with the medium as well as with energy. Conse-

quently the mesh interval and the velocity at each energy in every medium is different.

To illustrate the complexity of the interface problem, Figure 6 shows a typical situation. For simplicity only two directions, $\mu = \pm 1$ and one energy will be considered.

Fortunately the vertical grid μ is constant with energy and material so it presents no problem. Consider the box denoted by the coordinates (I,J,E). Assume this box has the direction $\mu = -1$ and travels toward the medium interface. There are four possibilities for future positions of the box.

The easiest case is for the box not to reach the interface so that apportionment is performed as previously explained. Any box in the buffer region will eventually traverse the interface. Recall that the time step Δt is subdivided into smaller intervals. Presently the subdivision is $\frac{\Delta t}{5}$. Neutrons are only allowed to experience interactions once per time step Δt. After the first subdivision of time $\frac{\Delta t}{5}$, a fraction of the initial particles have experienced some interactions. These particles then travel the remaining distance, namely $\frac{4\Delta t}{5}$ without incident. This procedure allows for apportionment after relatively little box movement and as a result, this case is a common occurrence.

In Figure 6b the second possibility is shown. The box labeled (I,J,E) has traveled completely into the other medium. Due to the interface discontinuities, the final position of the box must be computed in a special way. Let γ be the fraction of the total range traveled in medium 2 and β equal the fraction traversed in medium 1.

$$\gamma + \beta = 1 \tag{8}$$

If $V_1\Delta t$, $V_2\Delta t$ denote the total range of the box in medium 1 and 2 respectively, γ can be represented as

$$\gamma = \frac{|\underline{\overline{X}} - X_I|}{V_2\Delta t} \tag{9}$$

where $|\underline{\overline{X}} - X_I|$ is the distance from the box coordinate X_I to the interface mesh position $\underline{\overline{X}}$. Similarly for the fraction of the range traversed in medium 1

$$\beta = \frac{|\underline{\overline{X}} - X_{I'}|}{V_1\Delta t} \tag{10}$$

where $X_{I'}$ is the final position of the box in medium 1. Substitution of Eqn. (10) into (8) yields:

$$X_{I'} = |\underline{\overline{X}} - V_1\Delta t(1 - \gamma)| . \tag{11}$$

This case is handled with relatively little difficulty. The computer must simply recognize that the box has completely entered a different medium and then calculate the final position by (11).

Figure 6c displays the third case. Here the box has sheared across the boundary. Since the final positions are calculated in finite time steps, the shear is continuous across the boundary and the width of the box is the same as the mesh interval in the originating medium. The actual shape of the box in medium 1 would be something like the dotted lines displayed in the figure. It is impossible in the practical sense to calculate the position of the box with the discontinuity of slope present. The sheared box outlined by solid lines in Figure 6c is calculated by using the mesh interval of the originating medium and the velocity of the receiving medium. The apportionment procedure is performed, and the area

fractions are then used to redefine the density of the phase space elements the box occupied. The author admits this is an inaccuracy. The two parts of the parallelogram divided by the material boundary should travel at the velocity corresponding to their respective regions. The entire distance traversed should not be governed by the velocity of the incident medium. Nevertheless the author feels it is a satisfactory approximation in considering the computer factors as well as the physical inaccuracy itself.

The fourth and final case is a combination of the last two situations discussed. The box initially located at (I,J,E) first completely traverses the interface, and the box position is calculated by Eqn. (11). Then in the remainder of the time step Δt, it starts back toward medium 2 and occupies elements on both sides of the interface. The apportionment is performed by the procedure previously discussed, however, now the velocity in medium 2 is used in determining its final position. The box is incident on the region from which it initially originated.

More combinations could be formed from the four situations explained above. Due to the double discontinuity which in general exists at all interfaces in the multigroup formulation of the PSTE method, the buffer subroutines which perform the above calculations are the most complex parts of the code. In the development of the method more time was spent on interface problems than any other facet of the program.

IV. ANISOTROPY

When the PSTE method was first constituted, only isotropic scattering was included. Later Cordaro,[2] for applications in electron transport, considered anisotropic scattering by formulating a probability distribution which was a function of the incident and outgoing directions. A brief discussion of Cordaro's derivation as applied to neutron transport will be given here.

Figure 7 displays the geometry involved in a general scattering event. The unit vector $\vec{n}_i$ represents the incident direction of the neutron and relative to $\vec{n}_x$ a unit vector in the X direction subtends a polar angle θ_i. The direction of the scattered neutron $\vec{n}_s$ subtends an angle θ_s relative to the plane determined by $\vec{n}_i$ and $\vec{n}_x$. The polar angle $\vec{n}_x$ makes with $\vec{n}_s$ is denoted θ_s. The azimuthal angle θ_x, corresponds to the reference of the plane formed by $\vec{n}_x$ and $\vec{n}_s$ to the Y axis. Similarly θ_i is the angle between the plane determined by $\vec{n}_x$ and $\vec{n}_i$ and the Y axis. Finally θ_s is azimuthal reference angle of the plane formed by $\vec{n}_x$, $\vec{n}_i$ to the plane determined by $\vec{n}_x$ and $\vec{n}_s$.

In this general three space dimensional configuration, the object is to obtain a probability distribution which is solely a function of the projections of $\vec{n}_s$ and $\vec{n}_i$ on $\vec{n}_x$. Since only unit vectors are involved, the following projections are defined:

$$\mu_x = \vec{n}_s \cdot \vec{n}_x = \cos \theta_x \tag{12a}$$

$$\mu_i = \vec{n}_i \cdot \vec{n}_x = \cos \theta_i \tag{12b}$$

$$\mu_s = \vec{n}_i \cdot \vec{n}_s = \cos \theta_s. \tag{12c}$$

This is a logical goal since all angles are measured from the X direction in the one space dimension considered in this discussion.

The angular dependent scattering cross section $\Sigma(\mu_s)$ is assumed to be expanded to Legendre Polynomials:

$$\Sigma(\mu_s) = \Sigma_0 p(\mu_s) = \frac{\Sigma_0}{2\pi} \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} C_\ell P_\ell(\mu_s) \tag{13}$$

where

Σ_0: amplitude (cm^{-1})

$P_\ell(\mu_s)$: Legendre polynomial of index ℓ.

The coefficients C_ℓ are given by

$$C_\ell = \int_{-1}^{1}\int_{0}^{2\pi} p(\mu_s)P_\ell(\mu_s)d\phi_s d\mu_s. \tag{14}$$

By using the "Addition Theorem" for spherical harmonics and integrating over the azimuthal reference angles ϕ_x and ϕ_i, Cordaro obtains $P(\mu_x|\mu_i)$: the normalized probability that an incident neutron with direction μ_i will depart from the scattering event with some direction μ_x.

$$p(\mu_i|\mu_x) \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} C_\ell P_\ell(\mu_x)P_\ell(\mu_i). \tag{15}$$

Eqn. (15) would be sufficient in its present form if the angular direction is continuous. A more useful form would be $p(\Delta\mu_x|\Delta\mu_i)$, i.e., the probability that an incident neutron in some range of angles $\mu_c \le \mu_i \le \mu_d$ will scatter into another range, say $\mu_b \le \mu_x \le \mu_a$. The properly normalized distribution[4] is

$$p(\Delta\mu_i|\Delta\mu_x) = \frac{\int_{\mu_c}^{\mu_d} d\mu_i \int_{\mu_b}^{\mu_a} d\mu_x p(\mu_i|\mu_x)}{\int_{\mu_c}^{\mu_d} d\mu_i \int_{-1}^{1} d\mu_x p(\mu_i|\mu_x)}. \tag{16}$$

Cordaro considered only the integration over μ_x for electron transport. Tavel extended this by performing a second integration over μ_i. These results are both stated in Eqn.

To perform this integration the following three point recussion relation was utilized.

$$P_\ell(\mu) = \frac{1}{2\ell+1}\left(\frac{dP_{\ell+1}}{d\mu}(\mu) - \frac{dP_{\ell-1}}{d\mu}(\mu)\right) \quad \text{for } \ell > 0. \tag{17}$$

Equation (16) becomes

$$p(\Delta\mu_i|\Delta\mu_x) = \tfrac{1}{2}(\mu_a - \mu_b) + \frac{1}{\mu_d - \mu_c}\sum_{\ell=1}^{\infty}\frac{C_\ell}{2(2\ell+1)}\left\{\left[(P_{\ell+1}(\mu_a) - P_{\ell+1}(\mu_b)) - (P_{\ell-1}(\mu_a) - P_{\ell-1}(\mu_b))\right]\left[(P_{\ell+1}(\mu_d) - P_{\ell+1}(\mu_c) - (P_{\ell-1}(\mu_d) - P_{\ell-1}(\mu_c))\right]\right\}. \tag{18}$$

This expression can be simplified, for example consider anisotropy. Then $p(\mu_s)$ has the form

$$p(\mu_s) = \sum_{\ell=0}^{\infty}\frac{2\ell+1}{4\pi}C_\ell P_\ell(\mu_s) = \frac{1}{4\pi}(1 + \mu_s). \tag{19}$$

The two coefficients which are nonzero are

$$C_0 = 1 \tag{20a}$$

$$C_1 = 1/3. \tag{20b}$$

Eqn. (18) reduces to

$$p(\Delta\mu_i|\Delta\mu_x) = \tfrac{1}{2}(\mu_a - \mu_b) + \frac{1}{18}\,\frac{(P_2(\mu_a) - P_2(\mu_b))(P_2(\mu_d) - P_2(\mu_c))}{\mu_d - \mu_c}. \tag{21}$$

Both $(\mu_a - \mu_b)$ and $(\mu_d - \mu_c)$ are equal to the particular increment taken for the μ axis.

The $p(\Delta\mu_i|\Delta\mu_x)$ serves as a weighting function along with the apportioning factor. Together they redistribute the scattered neutrons in space and direction.

If the anisotropic cross section for each medium is known as a function of energy and angle, the usefulness of this analysis becomes apparent. The probability distribution can be formulated for each group by expanding the cross section in terms of Legendre polynomials. Then by substitution of the Legendre coefficients C_ℓ into Eqn. (18), anisotropy to any order can be obtained to fit any particular problem. This is one of the advantages of the PSTE method. Effectively no more time is required to run the code with anisotropic scattering than with isotropic scattering. Furthermore any degree of anisotropy can be used without any noticeable effect on execution time. The accuracy of the scattering function depends mainly on knowledge of the cross section itself rather than on the method used in the analysis.

V. "DIGITIZED" GREEN'S FUNCTION

The digitized Green's function concept originated in the initial development of the PSTE method by Tavel and Zucker.[1] In the multigroup formulation the dimension of energy is the primary addition to the digitized Green's function the previous authors used.

The time evolution of the neutron distribution could be generated by the procedure described in the interface discussion. This straightforward method would determine the final position of the box, perform the apportionment calculation, and redefine the density of the phase space elements the box occupied. By repeated iterations of this process the time evolution of the initial distribution could be generated. However, this procedure needs only to be utilized when an interface is present in the envelope of the box. If the envelope of a box does not overlap the interface, then for all general purposes the neutrons in this element of phase space can be considered to exist in an infinite medium. The straightforward procedure need only be applied once to boxes in this region. The time evolved density of each phase space element which the box will have influenced in traveling through the mesh is calculated by use of the Green's function matrix. This function $G(I \rightarrow I', J \rightarrow J', E_n \rightarrow E_m)$ yields the density at time $t + \Delta t$ in the phase element (I', J', E_m) due to unit density at time t in the phase space element (I, J, E_n). The subscripts on the energy E represent the discrete energy planes. Also the Δt is the subdivided time step, namely $\frac{\Delta t}{5}$. For an arbitrary density at time t $\rho^{(t)}(I, J, E_n)$, the Green's function matrix will generate the time evolved density, at some point I', J' in energy plane E_m by the fol-

lowing equation

$$\rho^{(t+\Delta t)}(I', J', E_m) = \sum_{n,J,I} \rho^{(t)}(I, J, E_n) G(I \to I', J \to J', E_n \to E_m). \quad (18)$$

In general the group constants will change with energy and as a result a different Green's function for each energy must be calculated. Also the distance the box travels varies with the vertical axis μ, hence a Green's function for each discrete angular direction is necessary. Actually only half of the angular directions need to be considered due to the imposed symmetry about the X axis. In other words, neutrons with direction $\mu = -1$ are treated by the same Green's function as neutrons with $\mu = 1$. The procedure used to describe neutron transport in the buffer region needs only to be applied once in the calculation of the Green's function. The asset of this method comes from the fact that the time evolved neutron density for all elements that can be considered in the infinite medium region is calculated by simple matrix operations. To find the time evolution of the initial neutron distribution, each nonzero density in every phase space element need only to be multiplied by the Green's function.

The advantages of the Green's function approach is three-fold. First, all of the physics associated with the problem to be solved is embedded in the Green's function. Anisotropic scattering, fission, absorption, time dependent cross sections, etc. are incorporated into the matrix function. The basic theory of neutron transport by the PSTE method allows a wide variety of process options and all of them can be neatly formulated into a simple matrix.

The second and third advantages are related. Since computer execution time and storage requirements are of practical importance, they must also be considered essential factors. A four group analysis with $\frac{V_1}{V_N} = 8$ occupies approximately 125 K fast core storage, and total execution time is on the order of three minutes.† The core storage could be reduced significantly if tape and/or disk units were used as storage areas.

The previous statistics are relative to the IBM 360 Model 65 computer located at Virginia Polytechnic Institute and State University in Blacksburg, Virginia. Of course other computers will alter the above figures.

†A detailed breakdown of the storage requirements will be given later.

VI. INTERACTION PROCESSES

In the one speed version of the PSTE method Tavel and Zucker[1] consider the three processes: isotropic elastic scattering, absorption and fission. For isotropic scattering, the fraction that scatters into every angular direction at each time step is determined by the input macroscopic scattering cross section of the medium Σ_s. The fraction absorbed is determined by the input absorption cross section Σ_a. The fission process is described as an absorption of a neutron followed by an isotropic emission of on the average ν neutrons. The process is treated in a similar matter as elastic scattering, but instead of scattering, a certain number of particles are removed and ν times that number are replaced isotropically.

The multigroup formulation adds the option to vary the cross sections with energy. If the scattering cross section is known as a function of energy and angle, it can be utilized as simply as isotropic scattering in the one speed case. The fission process is still considered an isotropic process although the fission cross sections are now energy dependent.

One inherent advantage of the PSTE method which has yet to be utilized is the inclusion of time dependent cross sections in the computer code. This important asset is a simple extension of the method. After each time iteration the cross section has only to be redefined to whatever value of interest. The Green's functions would then contain time as an explicit parameter. It will be shown the time step is small enough to consider high transient neutron transport problems, and it is mainly in this area where the PSTE method can be used to its peak efficiency.

VII. SOLVED PROBLEM

A simple problem which exhibits the usefulness of the multigroup formulation of the PSTE method is the time evolution of an initial neutron distribution in an infinite medium.

Two energy groups are considered with the velocity magnitudes being 8 cm/sec in the fast group and 1 cm/sec in the slow group. The purely absorbing medium is divided into three parts by two parallel lines. A spatially constant isotropic source is placed in the center region. Figures 9 and 10 display the logarithm of the scalar flux of the fast and slow groups respectively for two time steps. Figures 11, 12 and 13 display the logarithm of the angular flux in the fast group in the directions indicated. The time increment is 0.0146 sec. This is the time required for 10% of the neutrons in the fastest group to experience an interaction.

VIII. PROGRAM STATISTICS

Execution time and core storage are also important factors in performing transport theory calculations. The multigroup formulation of the PSTE method requires a large computer storage capacity. Tape or disk units would fulfill this need, but fortunately the computing facilities at Virginia Polytechnic Institute and State University allow sufficient memory that external storage devices are only used as scratch files.

The code is divided into three parts. Part 1 compiles all input information and computes the Green's function as well as all spatial parameters. The core storage and execution time is negligible compared to the main section (Part two) of the program. Part 2 accepts the data calculated in Part 1 via direct access disk files and performs the major calculation. Figure 8 shows the logic used in this step. MAIN receives the information from Part 1 and is used as a control unit for the remainder of the code. MEDA, MEDB and MEDC are subroutines which utilize the Green's functions for the calculation of the neutron density. BUFAB, BUFBA, BUFBC and BUFCB compute the position of boxes experiencing a medium boundary in traversing a distance $V\Delta t$. BUFFER and APORT are used by the interface routines to perform this function. SMLOG is a semi-log plot routine and HILOW is used by SMLOG to calculate the maximum and minimum as well as the first and last nonzero points of each data set. Part 3 is a separate program of negligible size and execution time which plots and lists the angular flux for any time increment in any discrete angular direction from Part 2. The angular flux for each time step is written in an on line permanent disk file. Part 3 simply reads this file and plots

the data for any time increment and angular direction specified.

Table 3 shows a breakdown of the storage required for each component in Part 2. The dimension in the MAIN component distinguishes between the main source program and the storage required for all variables stored in common.

CONCLUSIONS

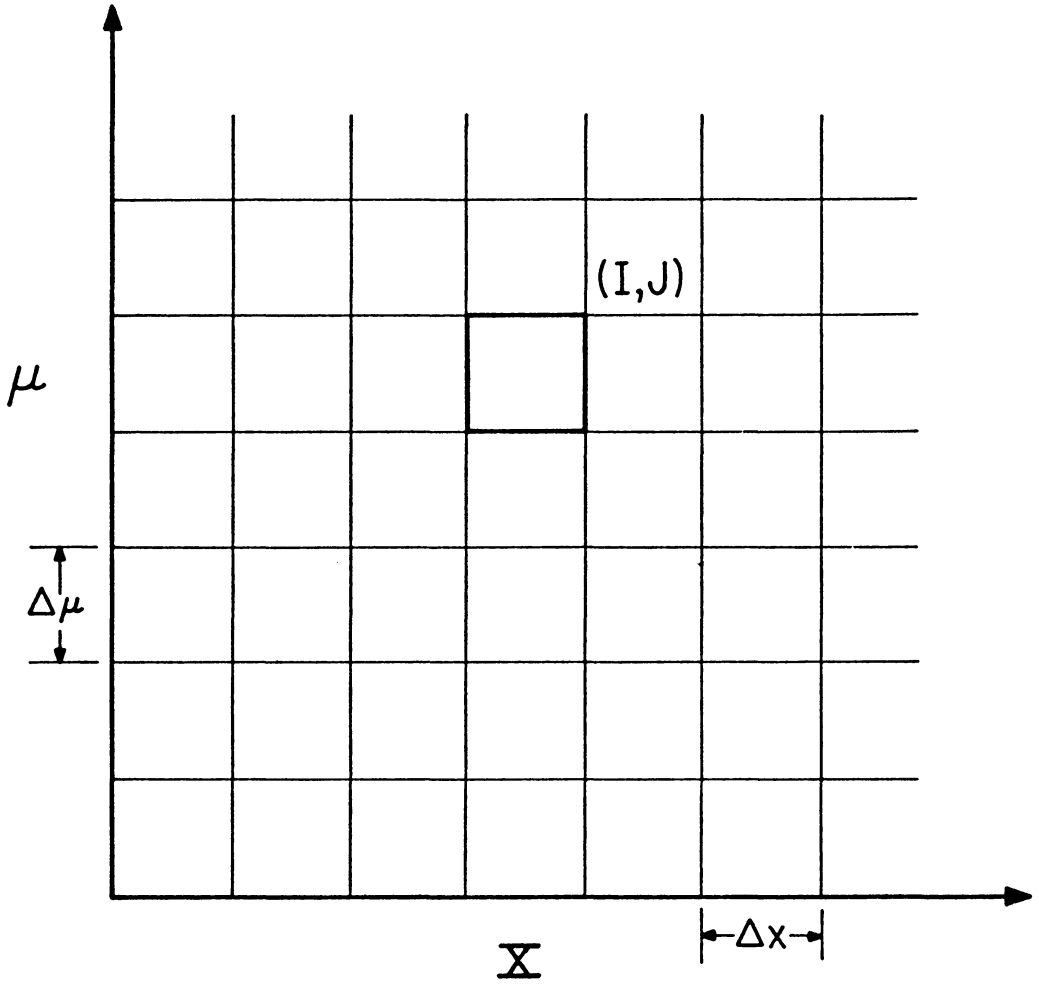
The multigroup formulation of the PSTE method is an effective task for solving high transient neutron transport problems. In general, when a medium is exposed to a transient flux, the energy dependent material properties change in time. The PSTE method offers the capabilities to change material parameters as rapidly as the transient flux itself and thus yield a better approximation to nature. Inherent in this method is the simplicity of the theory. The method can be applied to a variety of problems with little changes in the present multigroup formulation.

A standard technique for solving the linearized transport equation is the Monte Carlo Method. Here the flight path and interactions of thousands of individual neutrons must be studied. Besides being time consuming, it is restricted by the statistical limitations inherent in the method. The purpose of such a large number of events is to find the net or average behavior of the transient phenomenon. The PSTE method considers only the destiny of average neutrons and thus no statistical limitations exist. For electron transport, Cordaro compared the PSTE and Monte Carlo methods[2] and found excellent agreement. Also the execution time for the PSTE code was on the order of minutes while the Monte Carlo calculation took roughly an hour.

An area of future study for the PSTE method yet to be explored is the field of neutron spectroscopy. The neutron interactions with the unknown due to an incident flux can be measured accurately. However, to obtain the absorption spectrum of the sample, the incident energy spectra must be obtained. This is a difficult task and has not been accurately

done. The PSTE method can determine the energy distribution at some time and distance away from a known source. Thus the energy dependent angular and scalar flux incident on the sample can be calculated.

FIG. 1



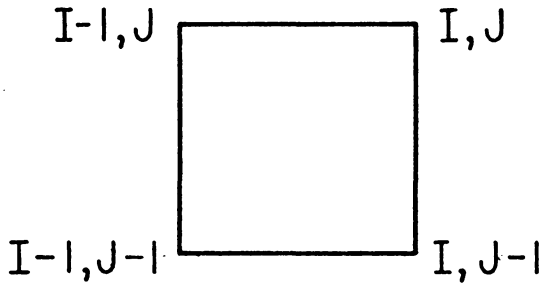
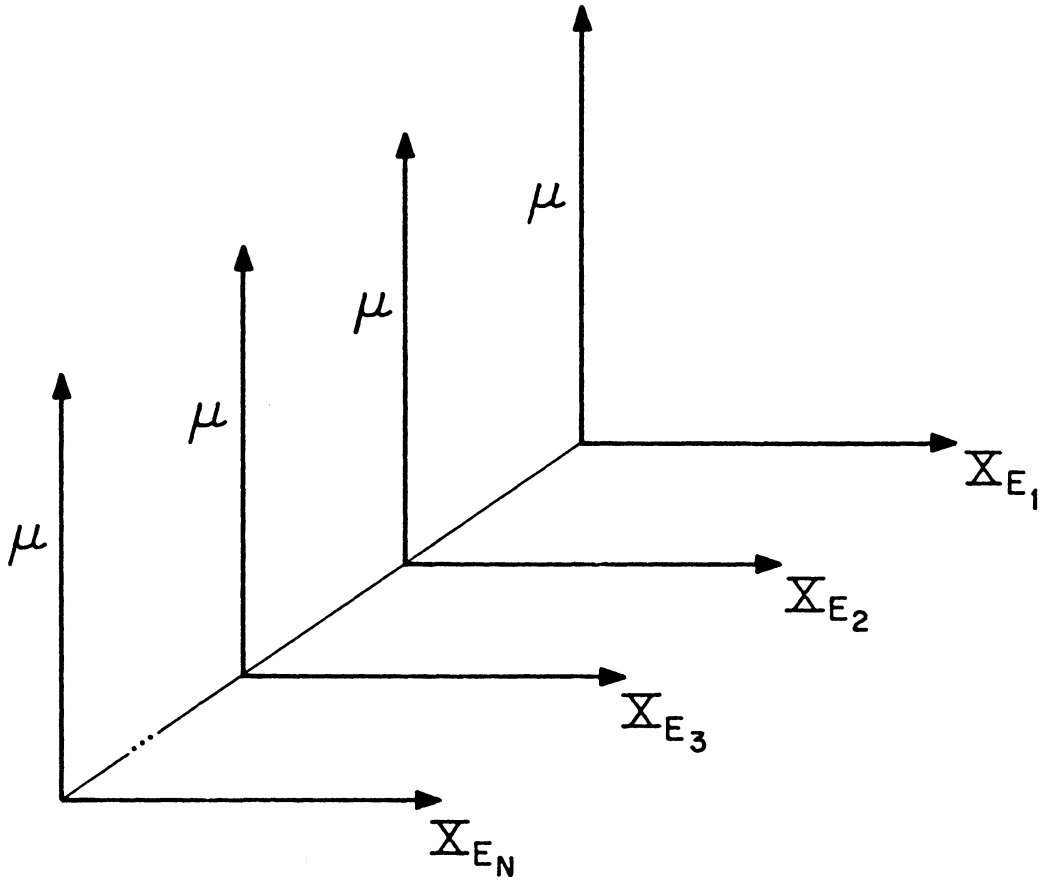
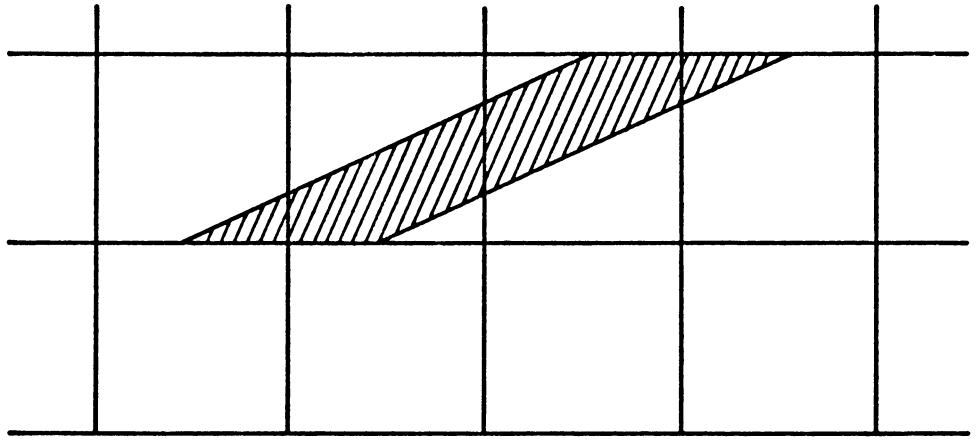


FIG. 2

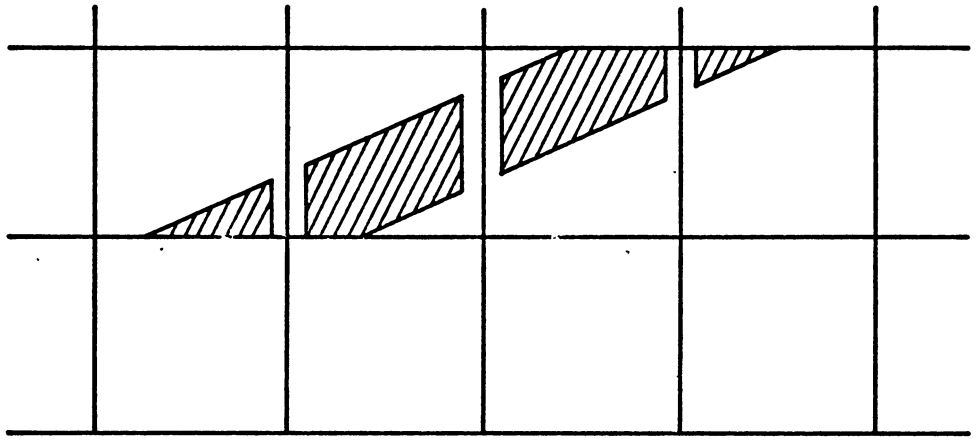


$E_1 > E_2 > E_3 > \ldots > E_N$

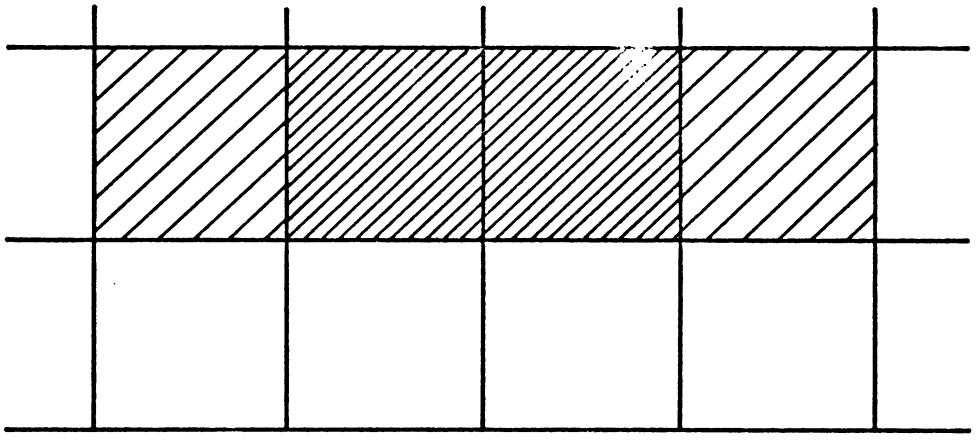
FIG. 3



FINAL POSITION OF PARALLELOGRAM



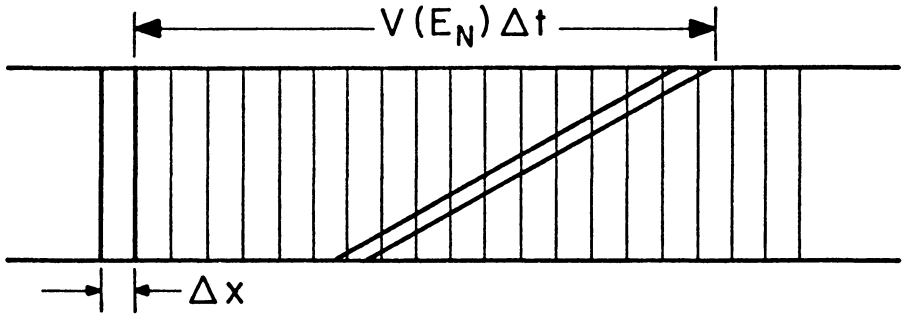
THE APPORTIONMENT



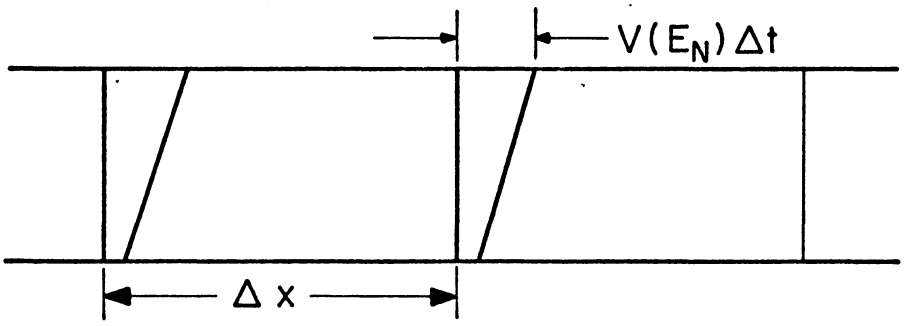
THE REDISTRIBUTION

FIG. 4

(a)



(b)



(c)

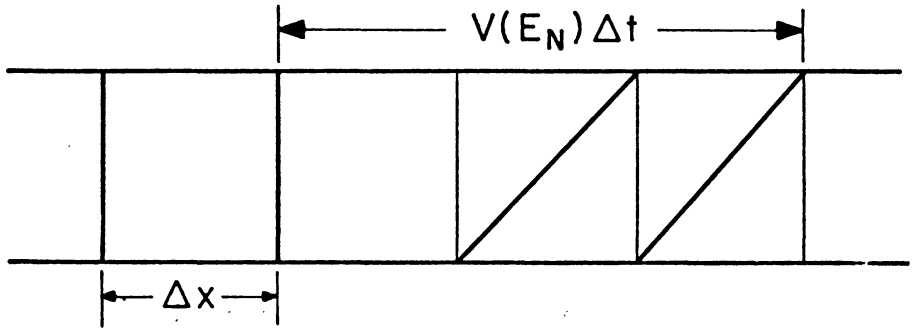


FIG. 5

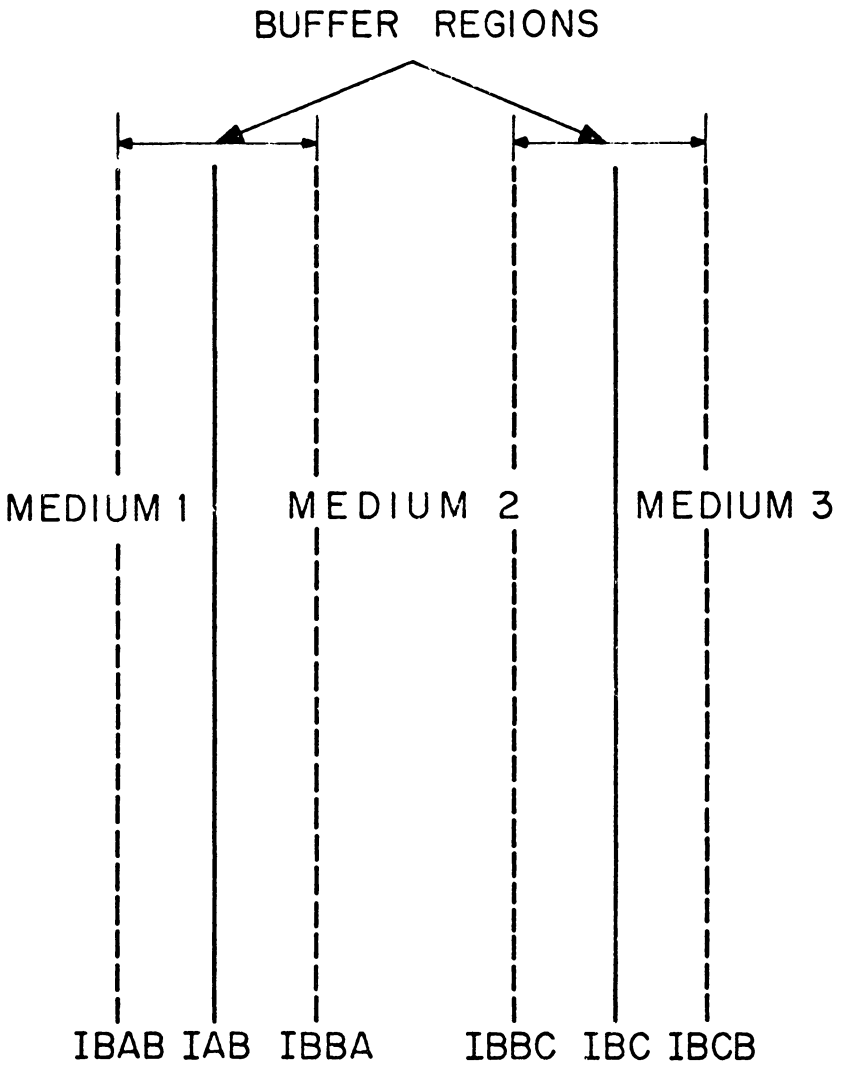

BUFFER REGIONS
MEDIUM 1
MEDIUM 2
MEDIUM 3
IBAB
IAB
IBBA
IBBC
IBC
IBCB

FIG. 6

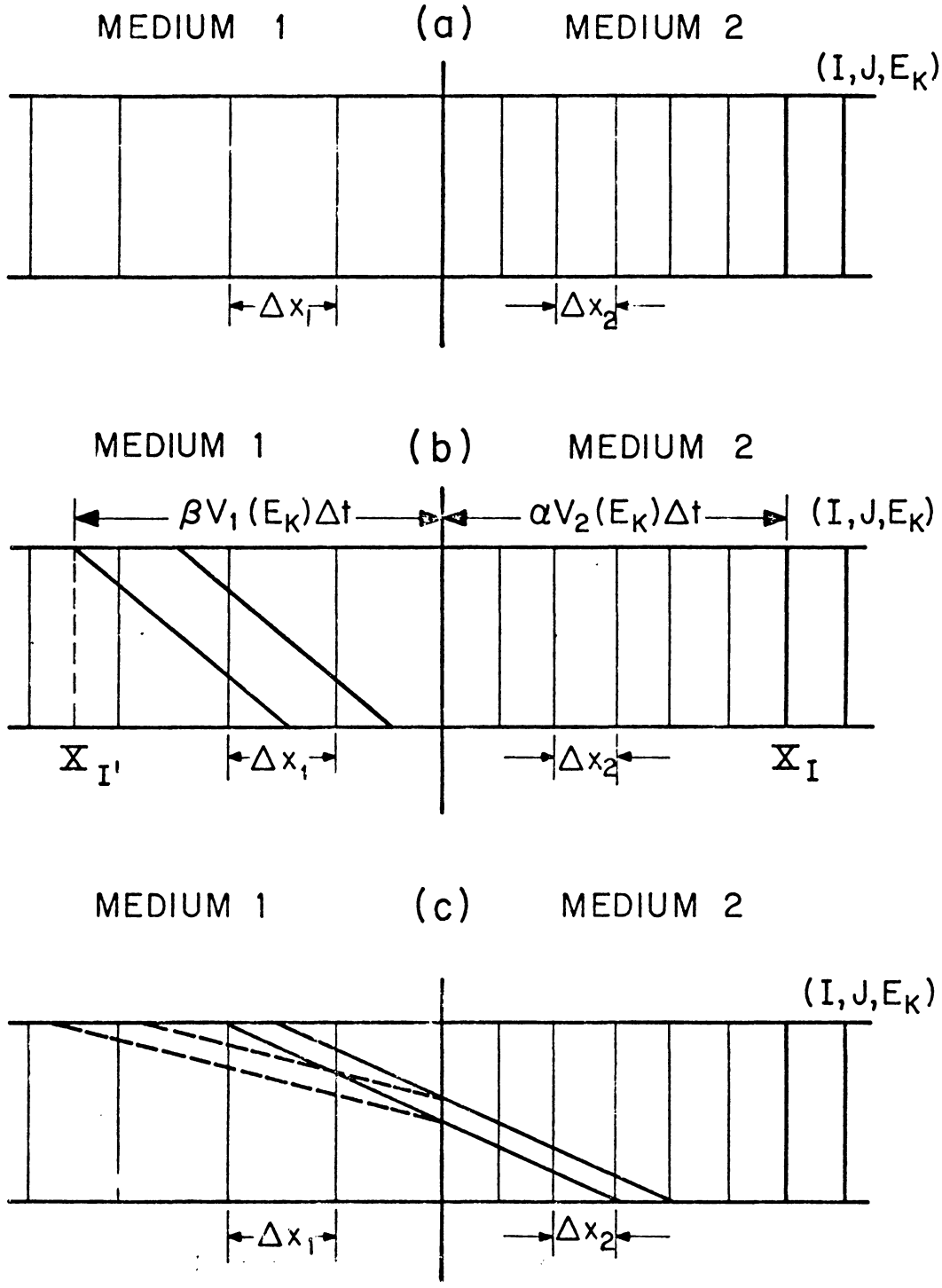

MEDIUM 1
(a)
MEDIUM 2
(I,J,E_K)
Δx_1
Δx_2
MEDIUM 1
(b)
MEDIUM 2
βV_1(E_K)Δt
αV_2(E_K)Δt
(I,J,E_K)
X_I'
Δx_1
Δx_2
X_I
MEDIUM 1
(c)
MEDIUM 2
(I,J,E_K)
Δx_1
Δx_2

FIG. 7

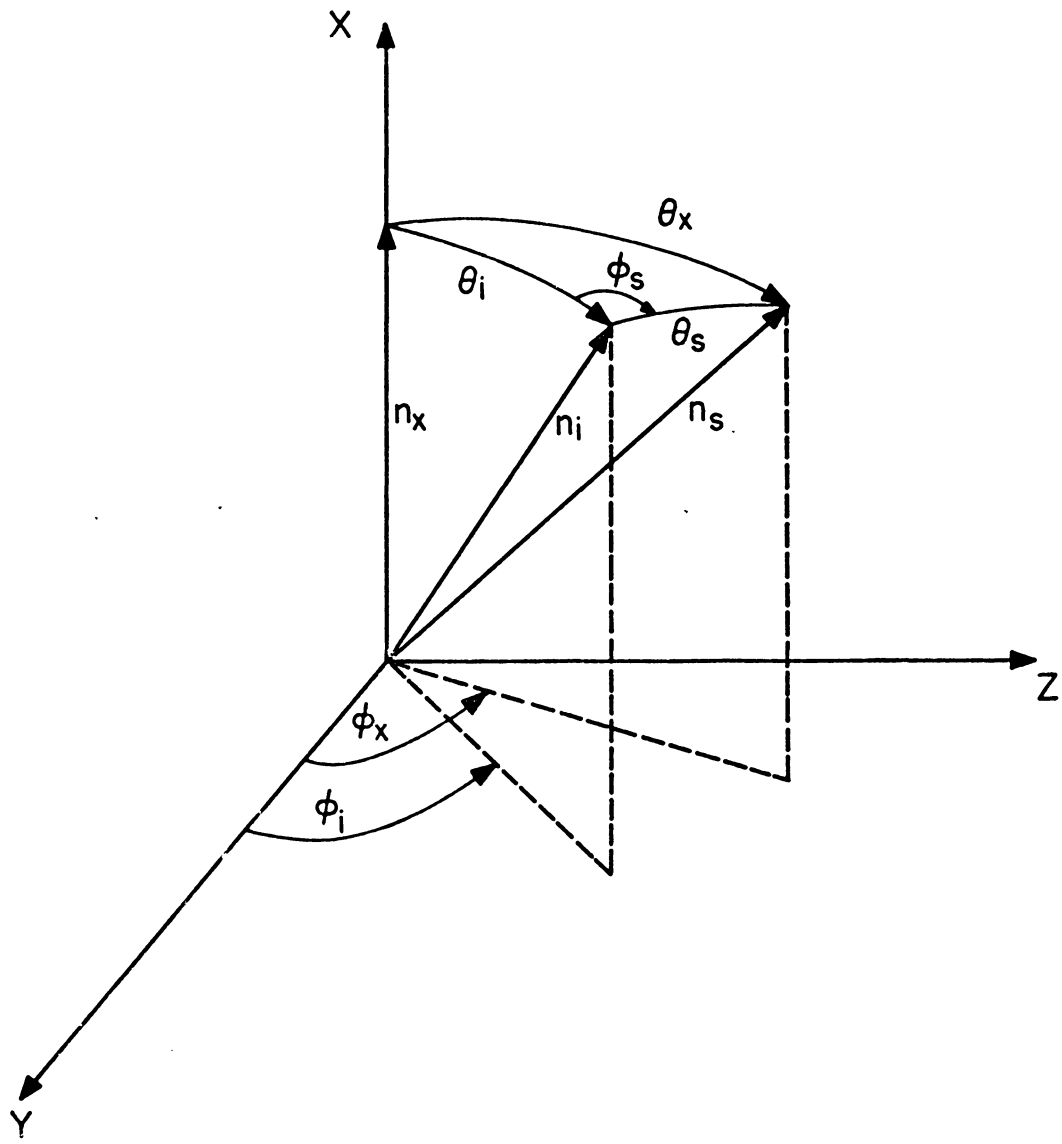
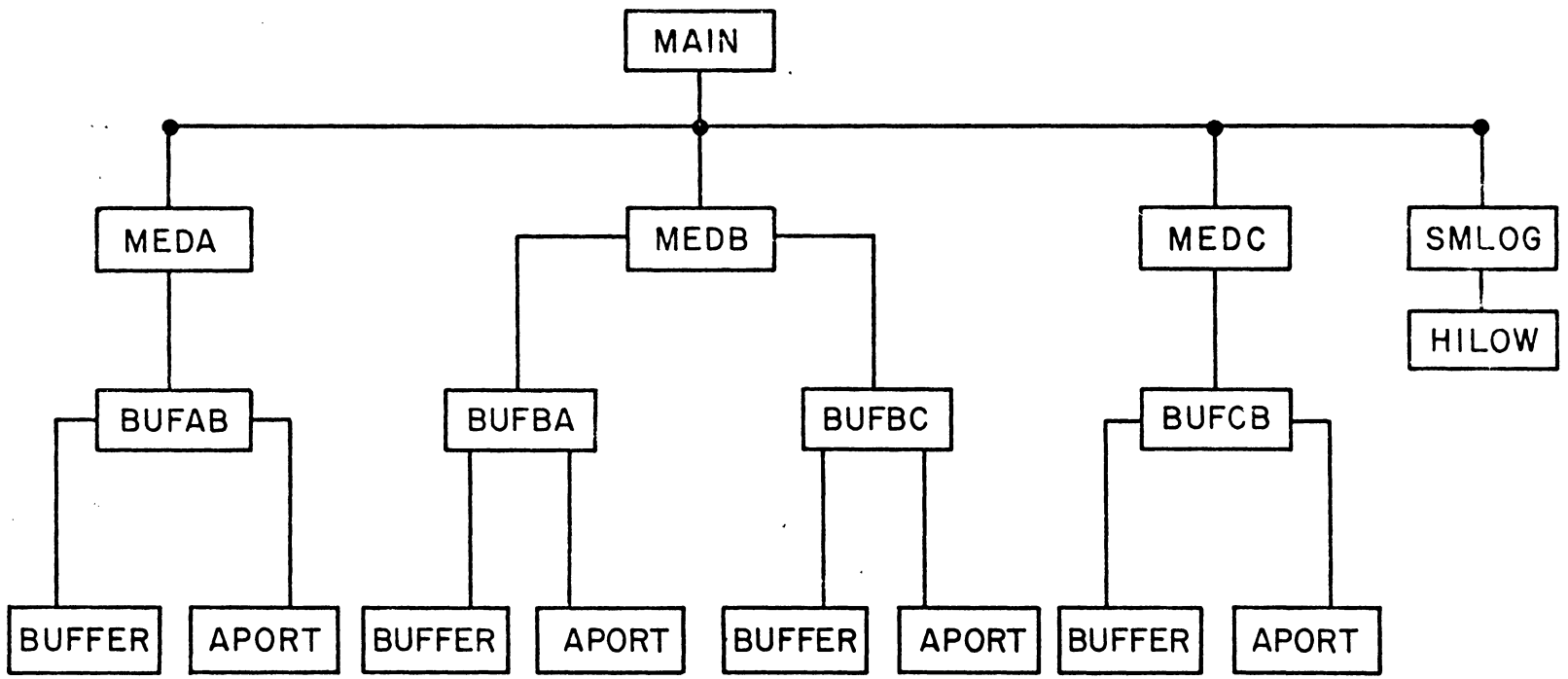


FIG. 8


MAIN
MEDA
MEDB
MEDC
SMLOG
HILOW
BUFAB
BUFBA
BUFBC
BUFCB
BUFFER
APORT
BUFFER
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BUFFER
APORT
BUFFER
APORT

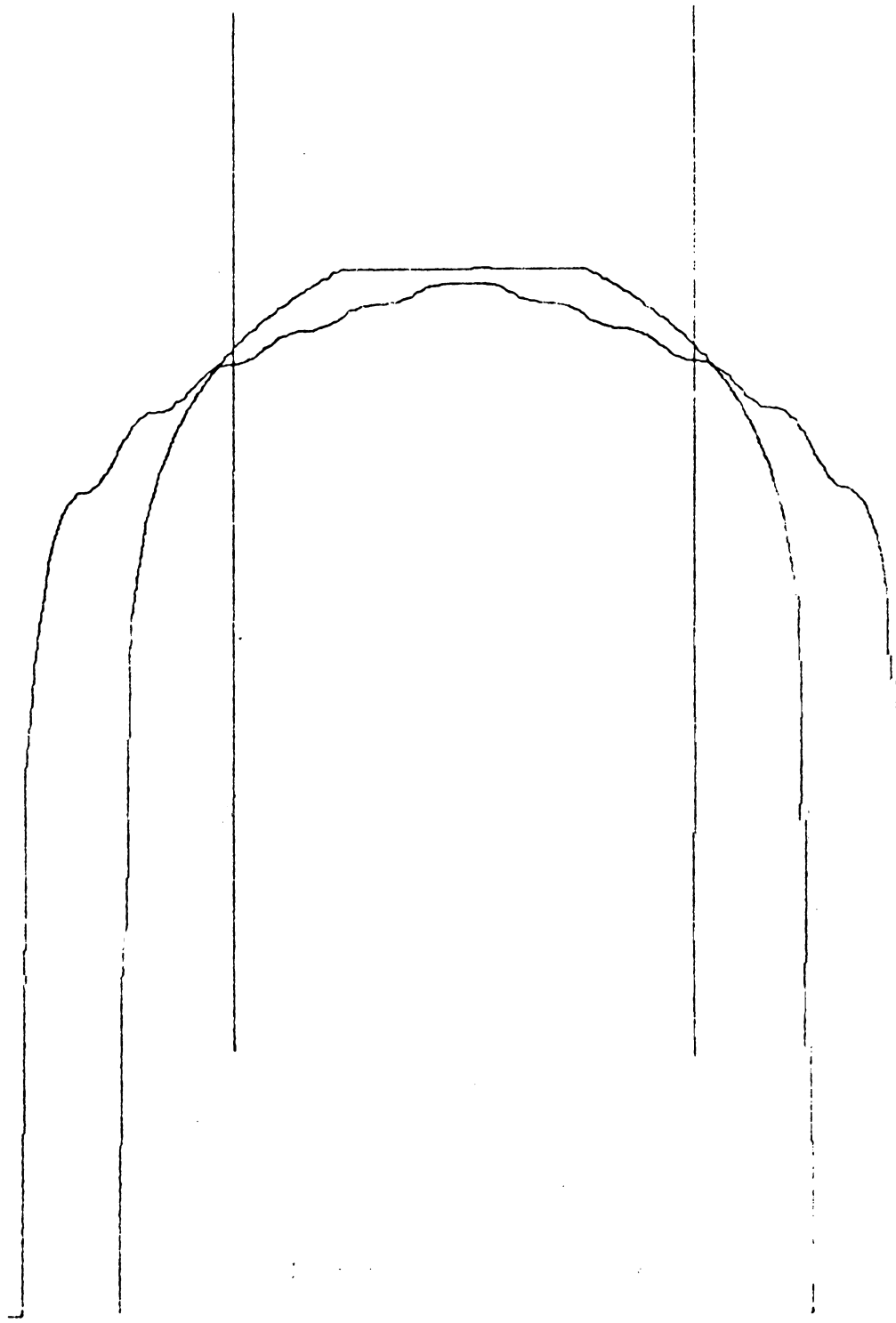

FIG. 9

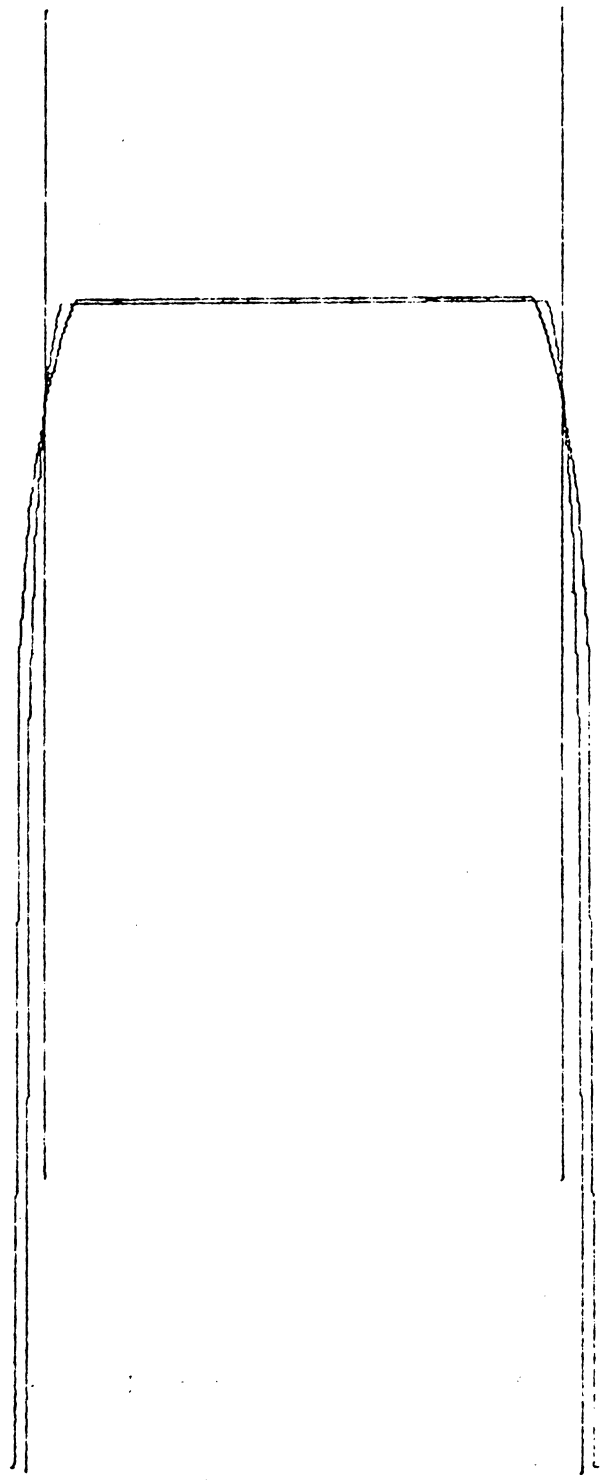

FIG. 10

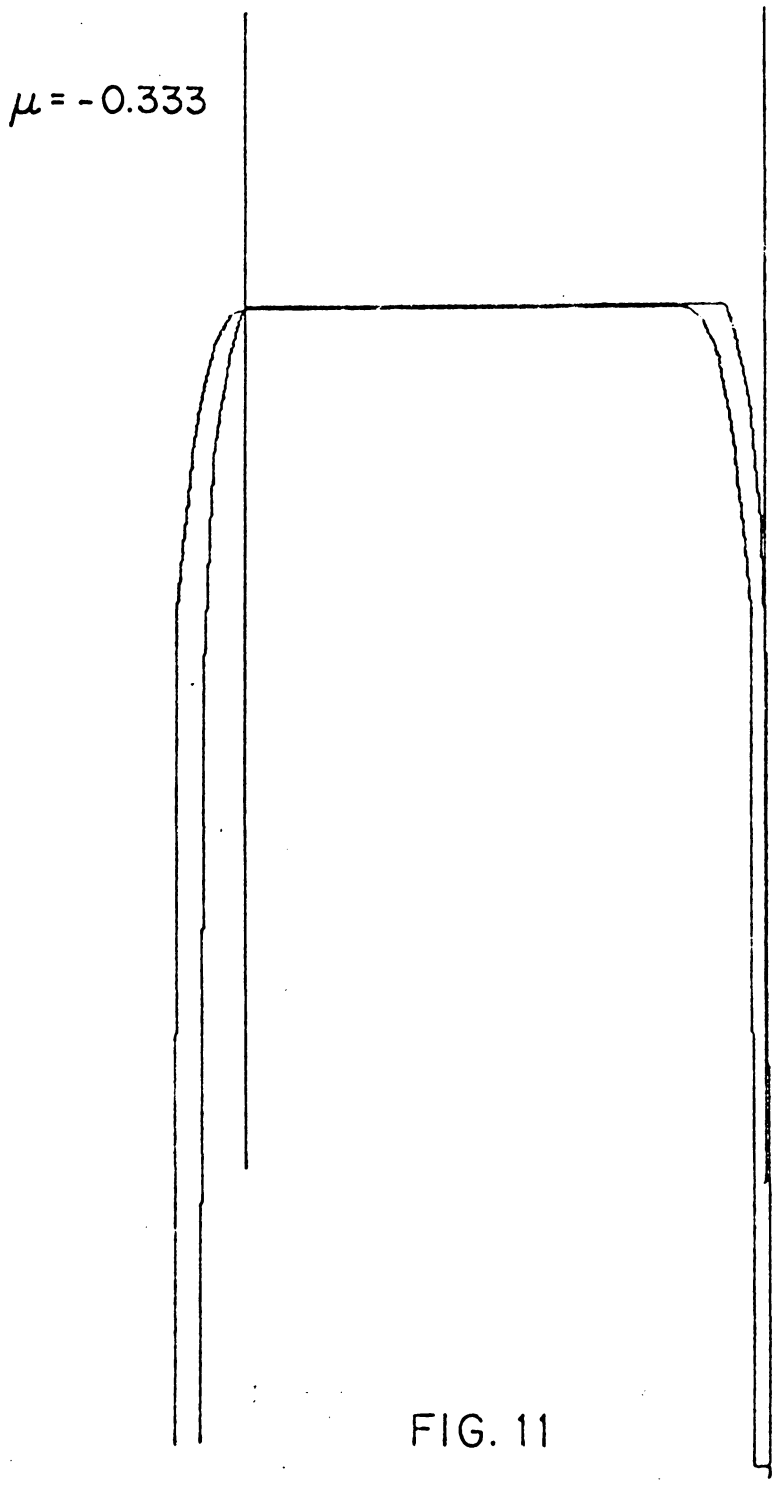

FIG. 11

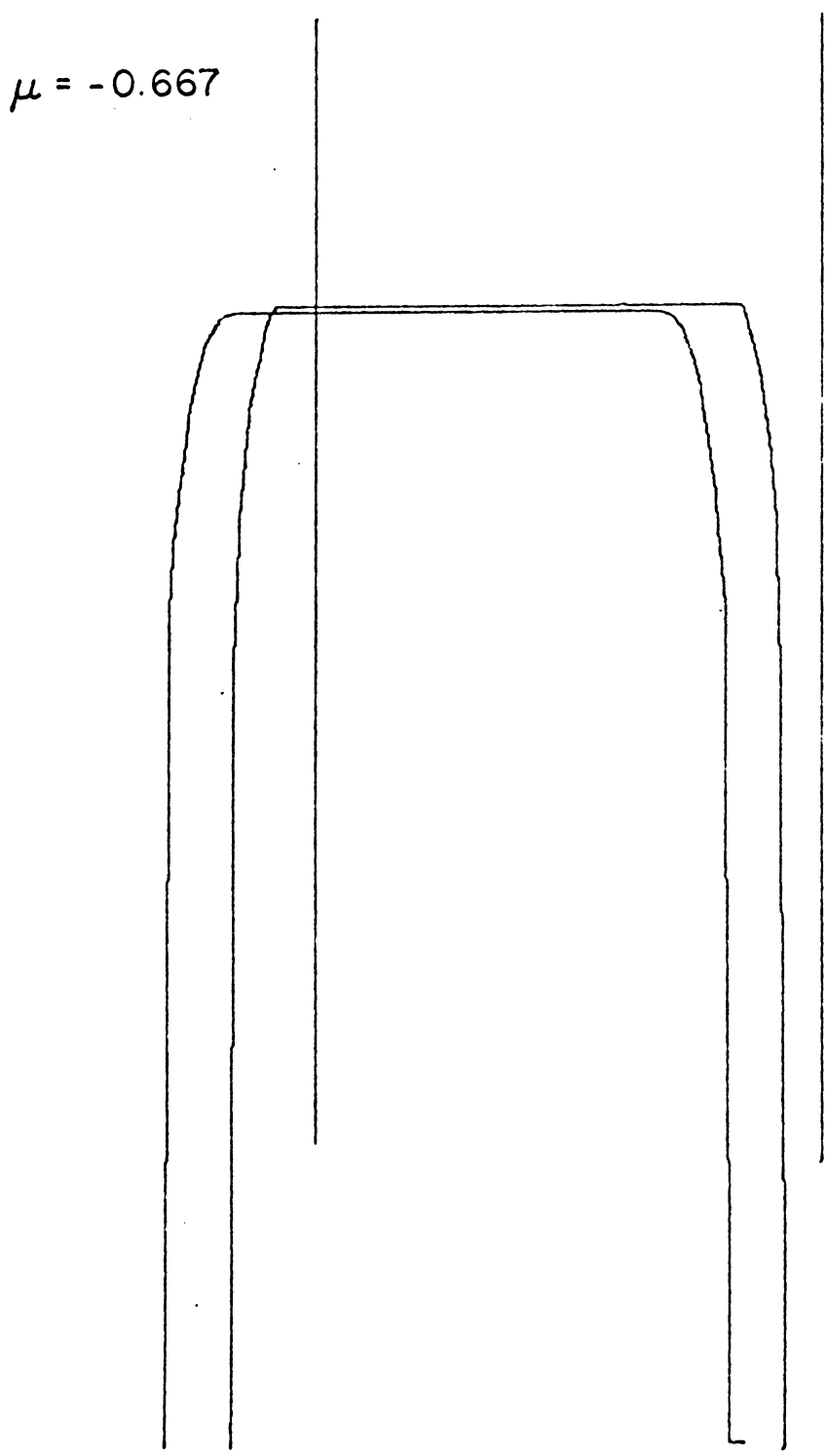

FIG. 12

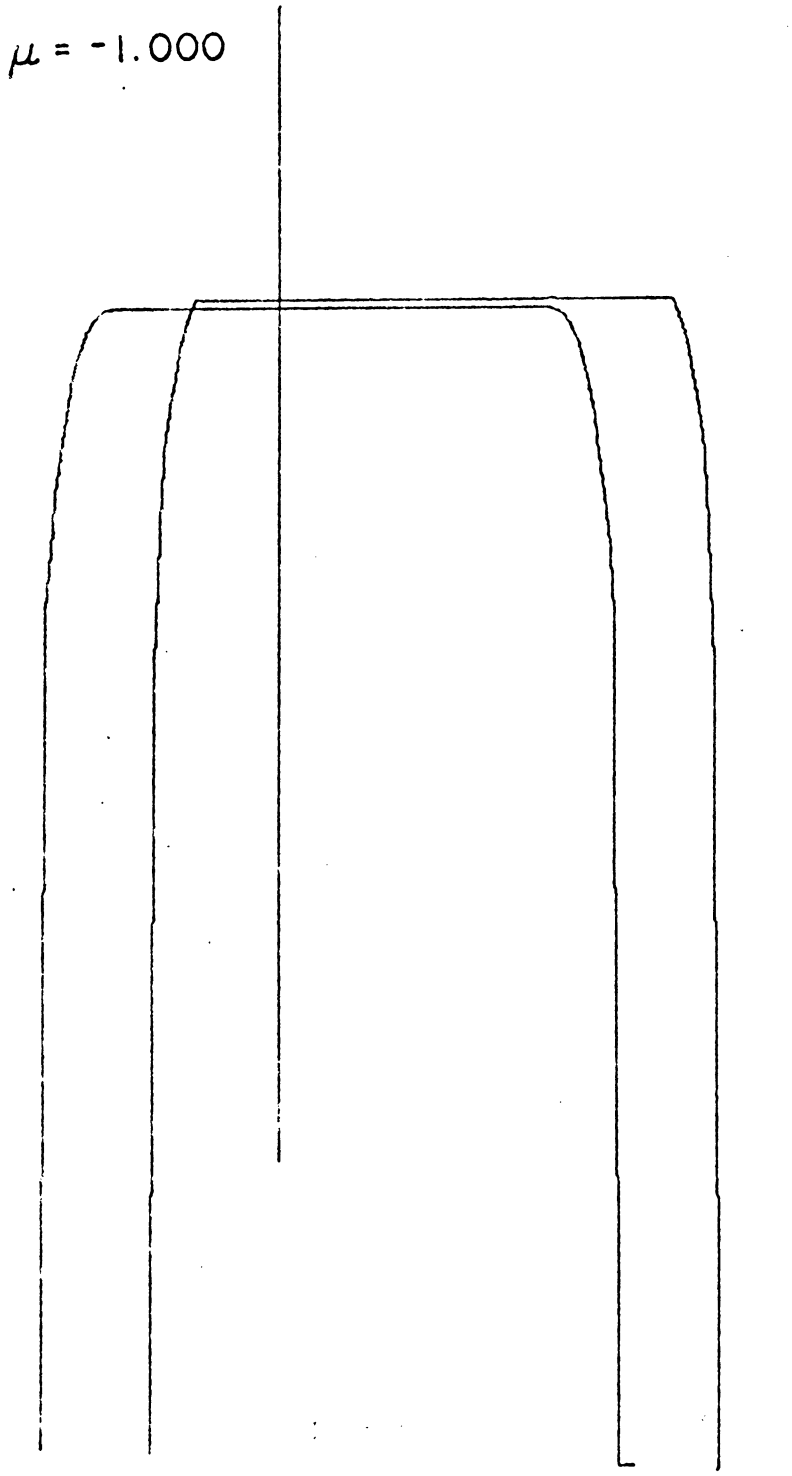

FIG. 13

TABLE I*

ENERGY FLIGHT ENVELOPES

Group Number	Velocity (cm/sec)	Envelope
1	8	49
2	4	25
3	2	13
4	1	7

*The values of the velocities in the table are irrelevant; only the relative magnitude is important here.

TABLE 2

Storage Requirements for Primary Components

Component		Storage (Bytes)	Percent of Total
MAIN	Common	181,046	66.700
	Main Source	23,414	8.630
MEDA		1,472	0.542
MEDB		1,688	0.621
MEDC		1,552	0.572
BUFAB		5,058	1.860
BUFBA		5,104	1.880
BUFBC		4,874	1.800
BUFCB		4,924	1.810
BUFFER		1,302	0.480
APORT		4,602	1.700
SMLOG		12,930	4.760
HILOW		1,044	0.385
Disk Files		22,432	8.260
	TOTAL	271,442	100.000%

REFERENCES

1. M. Tavel and M. Zucker, "The Phase Space Time Evolution Method", Brookhaven National Laboratory Report BNL-14705 (1970).

2. M. Cordaro, Ph.D. Thesis, Cooper Union College (1970).

3. M. C. Edlund and P. F. Zweifel, Virginia Polytechnic Institute and State University, Private Communication.

4. M. Tavel, Vassar College, Private Communication.

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THE PHASE SPACE TIME EVOLUTION METHOD APPLIED TO MULTIGROUP NEUTRON TRANSPORT

by

Richard Bradley Jones

(ABSTRACT)

The Phase Space Time Evolution (PSTE) method was initially developed for one speed neutrons. This discussion considers the alterations performed in transforming the one speed case to a more general multigroup code. Also the complications which arose in this transformation are discussed.

The multigroup formulation of the PSTE method calculates the energy dependent scalar and angular neutron density at very small time increments. In a reactor even slow neutrons travel at relatively high velocities and therefore to keep the distance the particles travel on the order of their mean free path, a small time increment must be used.

To illustrate the usefulness of the PSTE method, the time evolution of the neutron density of a nuclear device is modeled in slab geometry and the energy dependent scalar and angular flux is displayed as a function of time and space.