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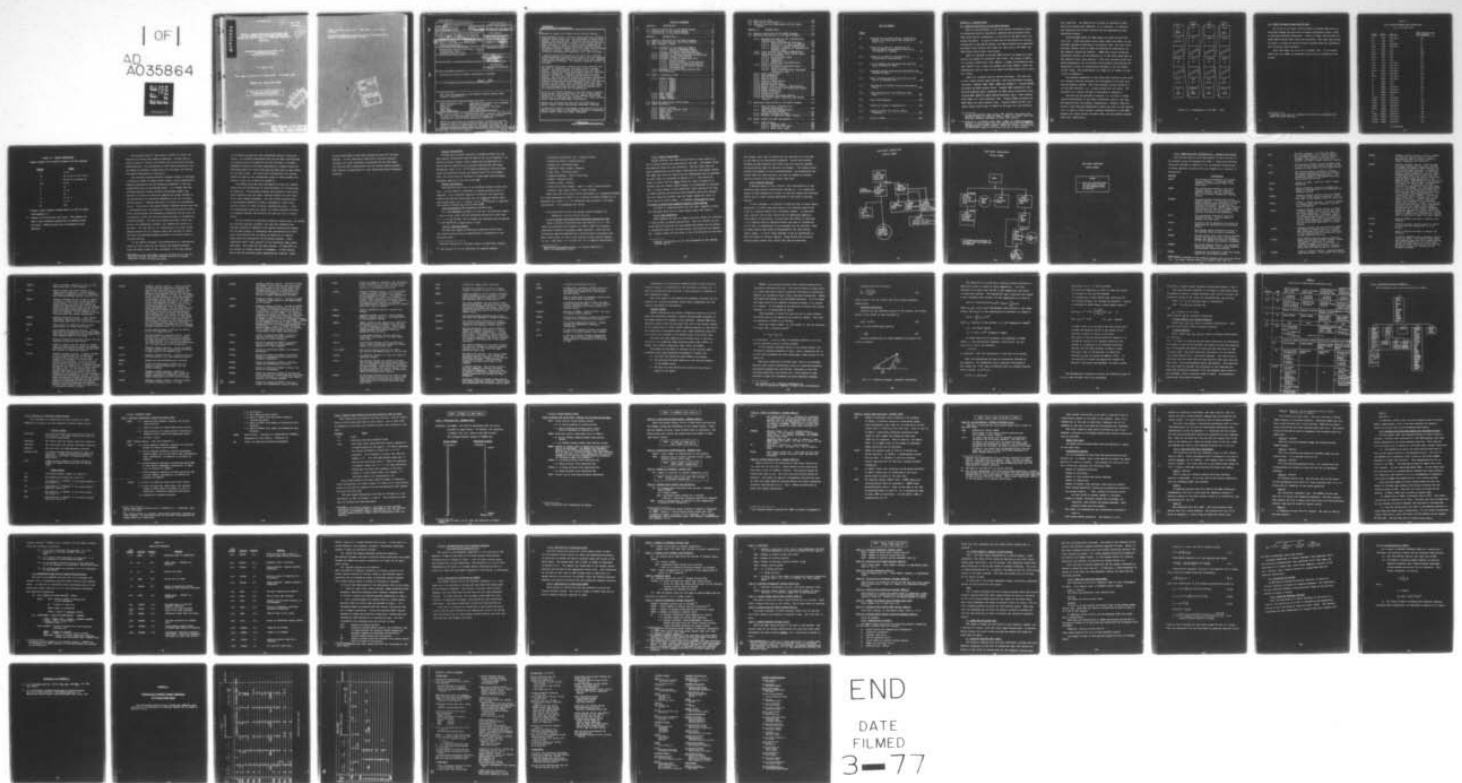
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**EAM-CE: A THREE DIMENSIONAL MONTY CARLO CODE
FOR THE SOLUTION OF THE FORWARD NEUTRON AND
FORWARD AND ADJOINT GAMMA RAY TRANSPORT EQUATIONS -
REVISION D**

Mathematical Applications Group, Inc.
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Elmsford, New York 10523

31 October 1975

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The SAM-CE system is a FORTRAN Monte Carlo computer code designed to solve the time-dependent neutron and gamma ray transport equations in complex three-dimensional geometries. SAM-CE is applicable for forward neutron calculations and for forward as well as adjoint primary gamma ray calculations. In addition, SAM-CE is applicable for the gamma ray stage of the coupled neutron-secondary gamma ray problem, which also may be		

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solved in either the forward or the adjoint mode.

Time-dependent fluxes, and flux functionals such as dose, heating, count rates, etc., are calculated as function of energy, time and position. Multiple scoring regions are permitted and these may be either finite volume regions or point detectors or both. Scores at point detectors are made by a special "bounded estimation" procedure which eliminates unbounded scores due to the usual inverse-square estimation process. Other scores of interest, e.g., collision and absorption densities, etc., are also made.

A special feature of SAM-CE is its use of the "combinatorial geometry" technique which affords the user geometric capabilities exceeding those available with other commonly used geometric packages. An automatic geometry checker is included.

All nuclear interaction cross section data (derived from the ENDF IV libraries) are tabulated in point energy meshes. The energy meshes for neutrons are internally derived, based on built-in convergence criteria and user-supplied tolerances. Tabulated neutron data for each distinct nuclide are in unique and appropriate energy meshes. Both resolved and unresolved resonance parameters from ENDF data files are treated automatically and extremely precise and detailed descriptions of cross section behavior is permitted. Such treatment avoids the ambiguities usually associated with multi-group codes, which use flux-averaged cross sections based on assumed flux distributions which may not be appropriate.

By use of the "band" feature of the code, which automatically splits cross section data into two or more energy ranges to be treated one at a time, SAM-CE affords one the ability to consider many nuclides, in a given configuration, each being described in much detail.

SAM-CE also provides the user with the opportunity to employ energy, region and angular importance sampling.

An extensive library of processed cross sections for use in SAM-CE is available at the Radiation Shielding Information Center (RSIC), ORNL, Oak Ridge, Tennessee.

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SECTION 2 - PROGRAM SAM-X

2.1 General Description of the SAM-X Program

With the establishment of the Cross Section Evaluation Center at Brookhaven National Laboratory, detailed and up-to-date evaluated cross section information, in the form of the ENDF files, has become available. In order to make use of this wealth of accurate information in the SAM-CE System, the SAM-X program which generates processed cross section data tapes for later use in the SAM-F and SAM-A Monte Carlo codes, was written.

SAM-X is designed to process ENDF neutron and gamma ray cross section and gamma ray production data files. The output of SAM-X is a neutron element data tape (NEDT)*, a gamma ray production data tape (GPDT)*, and a gamma ray element data tape (GEDT)*, which are subsequently used as input to the SAM-F and SAM-A Monte Carlo transport codes.

SAM-X is a program with an overlay structure. The code comprises a small driver (main overlay), and five processors (primary overlays): NUTRON, PEND, WEED, GAMMA and BCDEAN.** Program NUTRON processes the ENDF neutron files. Program PEND (Production from Evaluated Nuclear Data) processes the ENDF photon production files. Program WEED (Weed-out Extra Energy-dependent Data), which complements PEND, is a data reduction code. Program GAMMA processes the ENDF gamma ray cross section files. Program BCDEAN converts the normal binary mode output of SAM-X to BCD mode for inter-facility

* In the descriptions that follow, EDT (element data tape) will generally refer to either an NEDT, a GPDT, or a GEDT, where the specific reference intended is clear from context.

** Referred to as NUTRON, PEND, WEED, GAMMA and BCDEAN throughout Section 2, these primary overlay programs are actually coded as PROGRAM OVER10, OVER20, OVER30, OVER40 and OVER50, respectively, as convenient flags in switching from CDC to IBM versions.

data reduction. But WEED may be utilized to reprocess a GPDT which has already been "WEED-ed", if so required. In addition, the internally set default criteria may be superseded by user-specified criteria.

Program GAMMA reads the ENDF gamma ray cross section file (File 23). Since both Monte Carlo codes, SAM-F and SAM-A, do not consider coherent scattering at the present time, the total cross sections (MT=501) given by ENDF are modified by subtracting out the coherent scattering (MT=502). GAMMA then treats incoherent scattering (MT=504) and re-tabulates it in the same energy mesh as the modified total cross sections. Note that the Monte Carlo programs subsequently use the classic Klein-Nishina distribution for scattering so that an inconsistency develops in the low energy (x-ray) range. The organization of a GEDT for an element is described in Appendix B.

The machine dependence of the binary EDT produced by the first four primary overlays motivated the development of the post processing program, BCDEAN. This fifth primary overlay serves as a two way EDT converter, i.e., binary-to-BCD and vice versa. The structure of a typical BCD EDT is described in Appendix N.

The user may now proceed to Section 2.5, 2.6 and 2.7 which contain descriptions of the input, additional notes to the user, and tape and file utilization, respectively. However, those desiring a more thorough background of SAM-X may wish to read Section 2.2, 2.3 and 2.4 which contain a general description of the ENDF System, the theory behind the SAM-X code, and the program information flow, respectively.

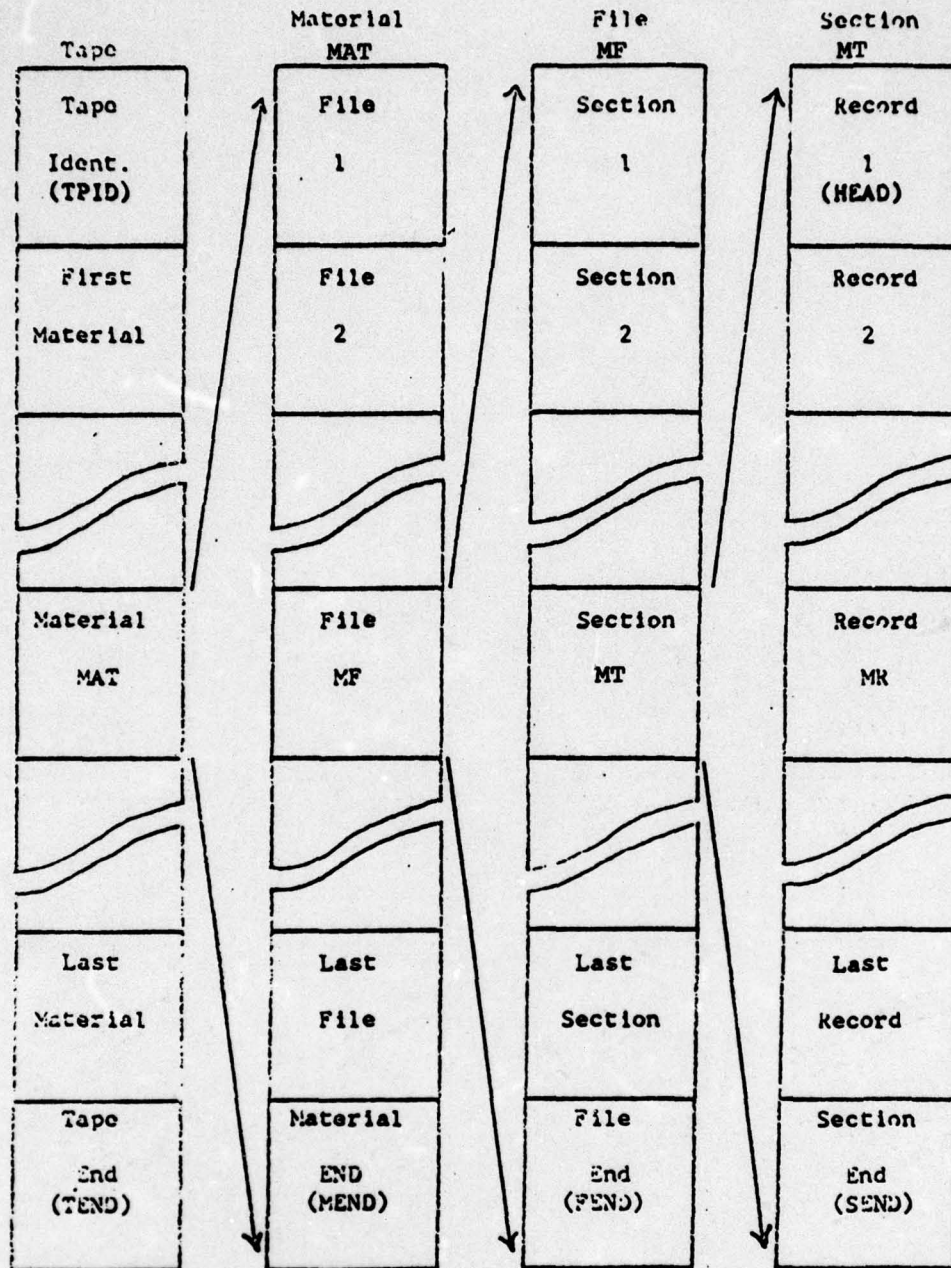


Figure 2.1 - Arrangement of an ENDF Tape

2.5 SAM-X Processed Cross Section Data

As an aid to the user, files of SAM-X processed ENDF data are available through the Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory. Table 2.6 shows the nuclides for which SAM-X neutron data files are available. The right hand column of Table 2.6 shows for which of these nuclides gamma ray production data files are also available.*

Note that Table 2.6 is as of 31 October 1975. It is anticipated that the number of processed files will be increased in the future.

* A complete file, for all elements (Z=1 to 94) is available for gamma ray cross sections.

TABLE 2.6

SAM-X PROCESSED NEUTRON CROSS SECTION DATA

(as of 31 October 1975)

<u>IDENT.</u>	<u>ZZAAA</u>	<u>ENDF I.D.</u>	<u>GAMMA PRODUCTION DATA ALSO AVAILABLE</u>
H-1	1001	4148 Mod 2	Yes
H-2	1002	1120	No
H-3	1003	4169 Mod 1	No
He-4	2004	4504 Mod 0	No
Li-6	3006	1271	Yes
Li-7	3007	1272	Yes
Be-9*	4009	1289	Yes*
B-10	5010	1273	Yes
B-11	5011	1160	No
C-12	6012	4274 Mod 0	Yes
N-14	7014	4133 Mod 4	Yes
O-16	8016	4134 Mod 2	Yes
Na-23	11023	4156 Mod 0	No
Mg	12000	4512 Mod 1	Yes
Al-27	13027	4135 Mod 2	Yes
Si	14000	4151 Mod 2	Yes
Cl	17000	1149	Yes
K	19000	1150	No
Ca	20000	4152 Mod 3	Yes
Fe	26000	4180 Mod 2	Yes
Cu	29000	4529 Mod 1	No
Cd	48000	1281	No
Ta-181	73181	4179 Mod 3	No
W-182	74182	4582 Mod 2	Yes
W-183	74183	4583 Mod 2	Yes
W-184	74184	4584 Mod 2	Yes
W-186	74186	4586 Mod 2	Yes
Pb	82000	4136 Mod 5	Yes
U-235	92235	4188 Mod 1	Yes
U-238	92238	4187 Mod 1	Yes
Pu-239	94239	4539 Mod 0	No
Pu-240	94240	4540 Mod 0	No

* In processing

TABLE II - REGION DESCRIPTION

(region numbers are circled on Figure 3.4c for clarity)

<u>REGION</u>	<u>INPUT</u>
1	+1 -2
2*	+2 -3 -4 -5 -6 -7 -8 -9
3	OR +3 -5 -6 -10 OR +4
4**	+5 -6
5	+6
6	+7 -9
7	+8
8	+9 -2 -7
9	+7 +9
10	+10

* Bodies 5 and 6 project outside body 3 in the X-Y plane
(see Appendix P)

** Bodies 5 and 6 buttress each other. The negation of
body 6 here eliminates possibility of machine round
off error. Negation might not be necessary on CDC
machines.

One possible type of input error is shown in figure 3.5b wherein the overlap area remains undefined. Another type of error is shown in figure 3.5c wherein the overlap area has been double-defined. The correctness of this region description can be tested by choosing a single point in the region and testing the region description at this point.

The checking routines provide a general method of obtaining a sufficient number of check points within a given combinatorial geometry description and the checking procedures to test the single definition of the problem space. It is based upon the following general theorem relating the minimum number (and location) of points at which the regions are singly defined to the specification of the entire geometry as the sum of singly defined regions. Consider each pair or triplet of intersecting bodies. From each of the bodies choose a bounded surface such that a corresponding pair or triplet of intersecting surfaces occurs. Choose single points infinitesimally displaced from the point of intersection within each of the volumes enclosed by neighboring bounded surfaces. For each non-intersecting body, choose two points, one immediately interior, one immediately exterior to the body. If, and only if, all these points lie within singly defined regions for all singlet, pairs and triplets of bodies and their corresponding bounded surfaces, the problem space is uniquely defined.

In the SAM-CE technique, the determination of intersection points is found either by ray tracing (by standard methods) along the edges formed by the intersection of two body planes*

*Ray tracing along body edges is also utilized by the code to establish whether two bodies composed entirely of planes buttress or truly overlap each other.

or by direct solution for the intersection point of three surfaces. It is easily established that for two body intersections, ray tracing can be utilized for all but one case - a bounded quadratic surface of one body intersecting a bounded surface of the second body in a curve that does not abut upon an edge formed by two body planes. For three body intersections ray tracing cannot be used for the intersection point of three bounded surfaces at least two of which are quadratic.

The method which has been developed and coded into SAM-CE, solves for the intersection of three surfaces; all of which may be quadratic. The procedure reduces the problem of three quadratic equations into one which involves finding the real roots of an eight degree polynomial. For two surface intersections, a minimization procedure is used to determine a third intersecting surface in order to obtain intersection points. Once the intersection points are found, ray tracing methods are used to determine whether they actually lie upon all (two or three) bodies.

In the interests of shortening computer running time, the procedure utilizes whenever possible, the less time consuming ray tracing technique as opposed to the surface intersection method. For the same reason, it eliminates from consideration all body pairs and triplets that can easily be shown not to overlap. These goals are obtained by the following sequence. Place "Equivalent RPPs" (axes parallel to the coordinate axes) about each body. Test these for two body overlap. If these RPPs do not overlap no further testing is necessary. If RPP overlap does occur the enclosed bodies themselves may overlap. Place

close fitting ARBs or BOXs about bodies and test for two body overlap. If this additional check still indicates possible overlap, the longer procedure is required and the code tests for true two body intersections (by ray tracing where possible). Test triplet intersections for only those bodies which intersect pairwise.

Angular Distribution

Sources may be either isotropic or monodirectional but the same angular distribution must be used in all source regions.* (It should be noted, however, that a source may be generated in a finite cone by specifying an isotropic distribution and using exceedingly high, (e.g., 10^{10}) angular weights to kill particles which are generated outside the desired cone.)** At the present time, the source must be isotropic if uncollided flux-at-a-point estimates (Section 3.2.8) are to be made.

Energy Distribution

The code has built into it the Cranberg fission neutron spectrum. If this option is selected, no energy spectrum input is required. If an arbitrary spectrum is desired, the input must contain the desired energy mesh and the integrated source above each energy point (i.e., a table of E vs $\int_E^{E_{\max}} S(E) dE$ is required). Monoenergetic sources may also be specified.

Time Distribution (Time-dependent problems only)

If a time-dependent problem is to be run, the user must supply a table of time values and the integrated source up to each time (i.e., t vs $\int_0^t S(t) dt$). As an option, all radiation may be emitted at a user-specified single value of time.

3.2.4.2 External Source

The user may supply an externally generated source tape. Each source particle must be described by 14 parameters in the following order:

* Angular biasing of an isotropic source is permitted, however.

** See Section 3.2.10 for discussion of angular weights.

3 Cartesian Coordinates (cm.) (floating point)
 3 direction cosines (floating point)
 1 energy (ev) (floating point)
 1 geometric region number (integer)
 1 time (sec.) (floating point)
 1 unused parameter; enter a zero here.
 1 weight (floating point)
 1 history number (integer)
 1 extra carry along weight; enter a 1 here (floating point)
 1 particle type index; enter a 1 here (integer)

These data must have been written previously, by a separate program, on a file designated as tape 15, as a series of binary records for 35 particles at a time; i.e., (14 parameters per particle) x (35 particles/record) = 490 parameters per record.

Given the array A(14,35) the proper output statement is*

```
WRITE(15) ((A(I,J),I=1,14),J=1,35).
```

3.2.4.3 Source from Previously Generated Interaction Tape

Using a neutron interaction tape (see Section 3.2.1), and gamma ray production data supplied by SAM-X, SAM-F can generate, internally, sources of secondary gamma radiation. Note that the interaction tape was generated by a previous SAM-F calculation and has a form similar to that of the external source tape of Section 3.2.4.2. (See Table 3.1, on page 207, for a complete description.)

* Experienced programmers prefer, of course, WRITE(15) A which is considerably faster.

3.2.5 Output Energy Mesh

During tracking, the code stores fluxes in each region in a set of energy output bins specified by the user. The number (≤ 100) and width of these bins are arbitrary. The bin limits must be given consecutively in the input, starting with the highest energy. The upper and lower bin limits for all supergroups must be preceded by minus signs as explained in Section 3.2.3. Care should be taken to insure that the upper energy bin limit is equal to or greater than the highest source energy to be generated in the problem. A cutoff energy is also specified, which instructs the code to cease tracking any particle which degrades below this energy.* The user should be certain that the lowest energy bin limit is lower than the cutoff energy. In essence, there must be a bin available to store every possible energy in the problem.

(In order to simplify matters for the user, Appendix E gives the hierarchy table for all input energy limits and tables.)

3.2.6 Time Dependence

SAM-F enables the user to compute particle fluxes as a function of time as well as energy and position. The user selects any desired time bin structure for the problem and enters the bin limits in consecutive order on the input forms, starting with the highest bin. Output fluxes will be given in this bin structure in the edit.

* However, see Section 3.2.11, for discussion of the thermal neutron option.

The longest time, used in specifying the time bins, will be used by the code as the time-cutoff parameter. During the tracking process the code computes the flight time of a particle between collision points from its velocity (or energy). All nuclear interactions are assumed to occur instantaneously. By accumulating the flight times for each particle, the code is capable of storing particle fluxes in the proper output time bins.

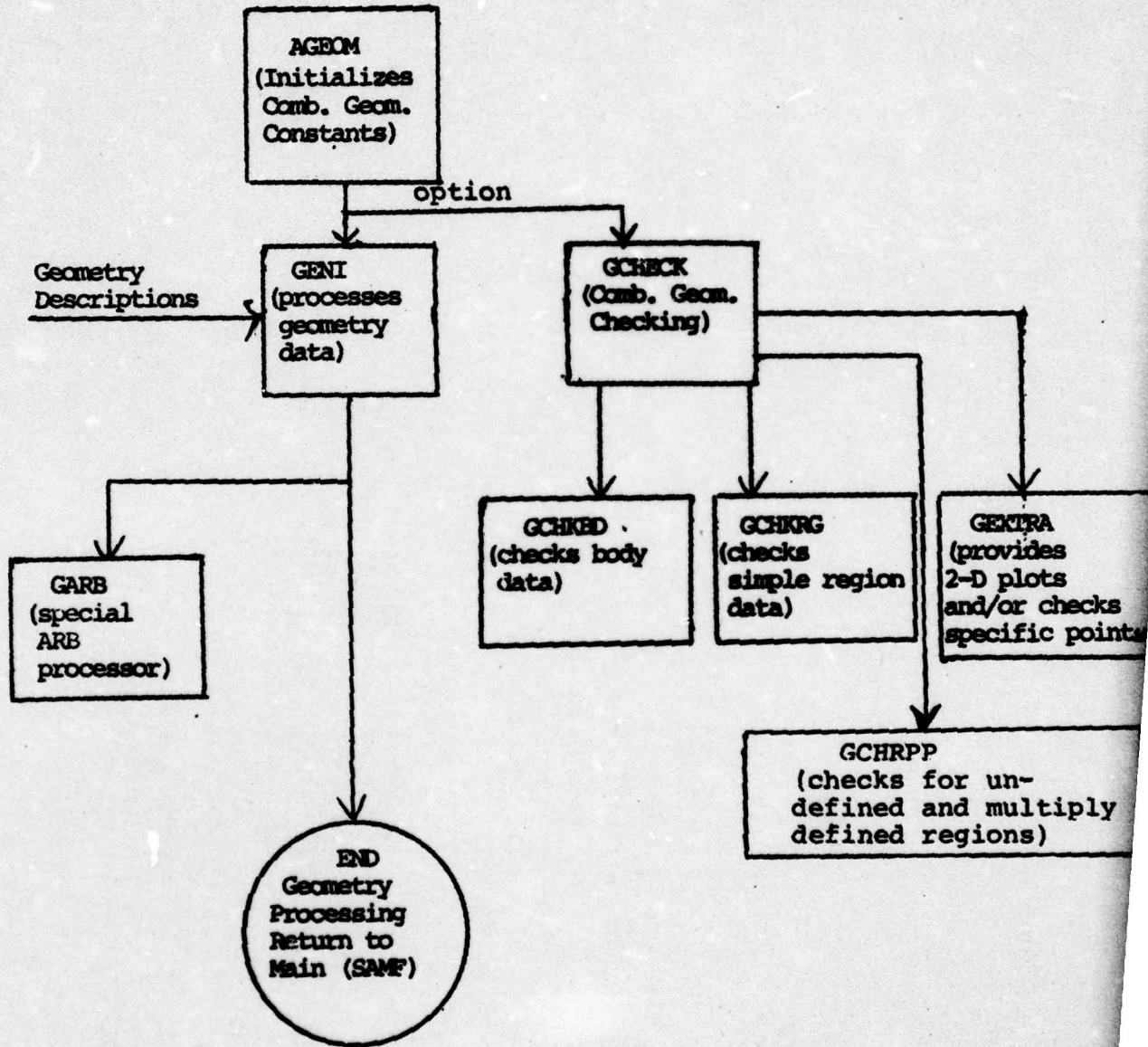
3.2.7 Scoring Regions

A scoring region is one in which a flux contribution is computed for each particle which passes through it. In a nonscoring region no such computation is made, so that the output edit provides fluxes only in those regions designated in the input as scoring regions.

In some problems it is desired to know the flux in every region separately, in which case each region in the problem would be defined as a scoring region with a different number. In some problems, however, two or more regions may be completely symmetric with respect to the source, in which case the fluxes in these symmetric regions could be combined without any loss of information, and in fact, an improvement in the accuracy will be obtained. Each of these regions then would be designated by the same scoring region number. In still other problems it may be unnecessary to know the fluxes in certain regions. These should then be given scoring region number zero, which tabs them as nonscoring.

FLOW CHART (Simplified)

Overlay AGEOM

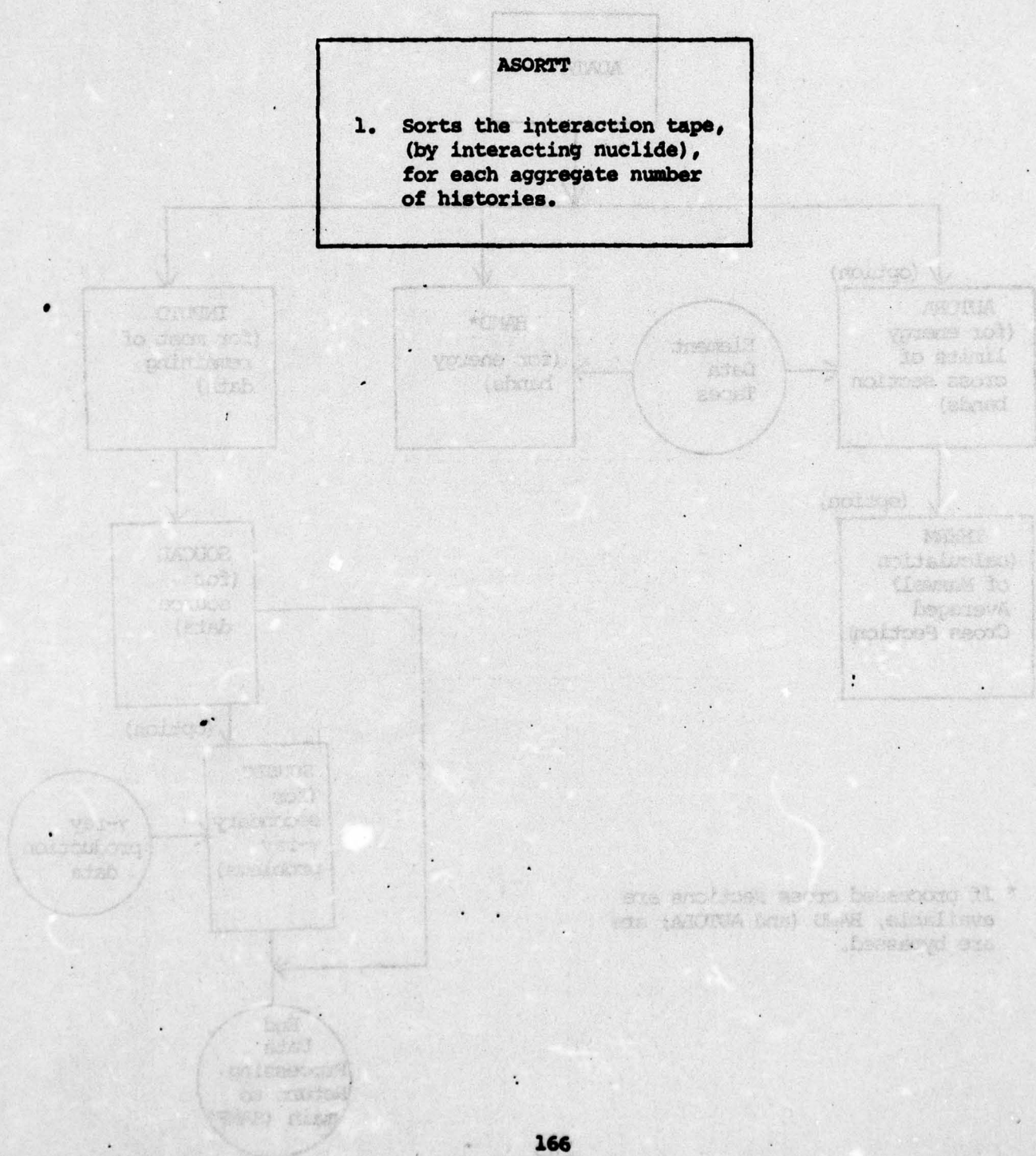


FLOW CHART (Simplified)

Overlay ASORTT

ASORTT

1. Sorts the interaction tape,
(by interacting nuclide),
for each aggregate number
of histories.



3.3.1 SAM-F Routines (Alphabetical) - General Description

This section gives a brief description of every routine in the program, given in alphabetical order.* These brief descriptions are followed, in Section 3.3.2, by detailed descriptions of those important routines which are flagged by an asterisk (*) superscript.

<u>Routine</u>	<u>Description</u>
ADATA	The controlling program of the second primary overlay. It oversees three secondary overlays which read in the input data.
AGEOM	The controlling program of the first primary overlay. In this overlay, geometry data is read in, organized, and, as an option, checked for logical errors.
AMONTE*	The controlling program of the fourth primary overlay. It oversees the routines which generate source particles, do the tracking and scoring and perform the tallying of results. AMONTE also controls the shuttling in and out of banded cross section data and the organization of the particle histories into aggregates.
AMOUT	The controlling program of the fifth primary overlay. It calls SUBED to perform the final edit.
ANISOT	Called by DR3 to determine the center of mass angle of scattering for anisotropic events.
ARG*	The general angle reselection routine of the bounded flux-at-a-point procedure.
ARPREP	Called by ARG, as an aid in angle reselection for two special cases: (1) neutron energy just above the inelastic threshold or (2) for neutron scattering by hydrogen.
ASORTT*	The third primary overlay. For secondary gamma ray problems, this routine presorts the precursor interaction events.
AUTOBA	Calculates and supplies to BAND the energy limits for cross section bands.

*All routines involved in the geometry package begin with the letter "G". All other routines begin with letters other than "G".

EDIT The edit routine. It prints out flux and flux-dependent (e.g., dose) answers as functions of energy, time and scoring regions. The routine also prints out "point" and "small volume" detector results.

FILL An auxiliary routine, called by BAND, used to fill in the cross section arrays and the scattering data tables in the banded arrays.

FLUP* The flux-at-a-point estimation routine. The routine calculates scores as functions of energy, time and detector point. The scores are stored in the MASTER array and are printed out by EDIT.

FLUPV* Similar to FLUP. Used for "small volume" detectors.

GARB Special geometry routine to process the input for the ARB body of the Combinatorial Geometry package.

GARBER Geometry checker routine called by GARBOX to store planar surface parameters of RPP, BOX, RAW, in the MASTER array for later use.

GARBIN Geometry checker routine. Called by GCHECK to convert ARB plane parameters into ARB point parameters.

GARBOX Geometry checker routine called by GCHRPP to place closest fitting BOX or ARB about each body containing a quadratic surface. It stores these data, the normal vector, and distance from origin to the planes of a body containing a quadratic surface for use in region checking. GARBER is called to store the plane parameters for planar bodies.

GATHER Geometry checker routine called by GTSURF and GTQDPT to gather terms of a rotated and translated "principle axis" equation to form coefficients of the general transformed quadratic surfaces.

GCHECK Main geometry checker routine called by AGEOM for routines (GCHKBD, GCHKRG, GCHRPP and GEXTRA - see below) to perform geometry checking of various types. It also calls GARBIN (see above) to store point data for ARBs needed for checking.

GCHKBD Geometry checker routine. Performs various body data checks. Calls GEQUIV (see below).

GCHKRG Geometry checker routine called by GCHECK to check for simple errors in region descriptions and to provide a table of region references for each body.

GCHRPP Geometry checker routine. Once the body and simple region data have been checked by GCHKBD and GCHKRG, GCHRPP examines the RPPs placed about each body to establish possible two body overlaps. If RPP overlapping occurs, GARBOX is called to place an equivalent BOX or ARB about each non-planar body of the pair and to store these data and body plane parameters in the MASTER array. Overlapping of the equivalent body pairs and the two body intersections (involving a planar body) are then checked (via ray tracing along body edges) by a call to GIRTWB. For overlapping body pairs, a call to GIRTWC then checks the remaining two body intersection points for no or multiple region specification. For intersecting pairs, GARBOX is called for third bodies which intersect each of the bodies of the pair. GIRTWC then checks three body intersections for improper region specification. Printout of the two and three body overlaps (TBO), buttressing surfaces for two planar bodies (BSTB), equivalent BOX or ARB overlap (EBOXARBO), equivalent RPP overlap (ERPPPO) occurs for values of IORPP=0...3 respectively. Higher values of IORPP lead to printout of the new case in addition to those for lower numbers.

GCROSS Used by checker routines to compute cross products.

GDETER Geometry checker routine called by GTPLPT to calculate the determinant of a 3x3 matrix.

GDOT Used by checker routines to compute dot products.

GENI The major geometry input processing routine called by AGEOM. The routine first reads body geometry data then calls GFREE to read the region description (in a free field format) and puts the data into the FPD and MA arrays in the form required by the tracking routines.

GEQUIV Used by checker routines to place an RPP about each body in the geometry.

GETIR Used to locate the region number of a given spatial location. During geometry checking it identifies points in undefined and multiply-defined regions (see Fig. 3.5).

GETXB Geometry checker routine called by GTQDPT to test if a point lies on each of two or three bodies. It first calls GTBDPT to obtain an interior point for each of the bodies and then tests to see if the distance from this point to the body surface is the same as distance from this point to the point of interest. If so, GTIRNT is called to check point for region correctness.

GEXTRA Geometry checking routine. Calls GPOINT (see below) and also sets up the two-dimensional point grid for picture printouts.

GFREE This routine is called by GENI to read region data in a free field format.

GG The distance calculating routine. Given a position \bar{X} and direction \bar{W} and a body number, this routine computes the two distances RIN, ROUT measured from \bar{X} to the body.

GGTEC Special distance calculating routine for the truncated elliptical cone (TEC).

GIROB Geometry checker routine called by GCHRPP. Used to locate points to check for possible undefined and multiply-defined regions near the surface of individual bodies.

GIRTWB Geometry checker routine. Called by GCHRPP to find intersections of two bodies by tracing along or parallel to the edge formed by two planes of a planar body. It operates in two modes. In the first, ray tracing along the edges of an equivalent ARB or BOX of a body with a quadratic surface determines any overlap with a second equivalent ARB or BOX. In the second mode, the intersection points of a planar body with another body (not necessarily planar) are obtained by ray tracing in the four quadrants formed by two intersecting planes. By this means intersection points and buttress points (buttress points are obtained for two planar bodies) are obtained for the two bodies. Identification of undefined and multiply-defined region specification at these points is obtained by calls to GETIR.

GIRTWC

Geometry checker routine. Called by GCHRPP to check two and three body intersection points which are found by ray tracing (by a call to GG) along all edges formed by all possible plane surfaces taken one from each of two of the bodies. It uses (at a starting point outside the bodies) four rays parallel to the edge, one in each of the four quadrants formed by the two planes, in order not to miss buttressing surfaces. If a point along a ray falls on all the bodies, a call to GTIRNT checks the point for correct region specification. For two body checking the check point chosen along the ray is at the entry of the ray into the second body after passage into the first body surface. For three bodies, ray tracing is done along edges formed by planes of two of the bodies. Therefore, both the last entry and first exit points along the ray are region checked. By this means, points along all possible two plane surface intersections are obtained. Further checking occurs via a call to GTQDPT.

GP

An auxiliary routine, called as an option by G1, for debug printout.

G1

The main geometry tracking routine. Given a position \bar{X} , a direction \bar{W} , and a region IR, the routine will calculate the distance "S" from the point \bar{X} to the next region in the direction \bar{W} . The routine also determines IR', the next region to be encountered.

GPACK

Geometry checker routine. Called by GCHRPP to pack overlap and intersection information of body pairs in the MASTER array.

GPOINT

Geometry checker routine. Locates and prints out the region of all user-supplied points.

GRAFIC

Prints out the two-dimensional pictures.

GRID

Finds the proper region number for all points in the two-dimensional grid for picture display.

GTARBX

Geometry checker routine. Called by GIRTWB to store equivalent ARB or BOX for bodies containing a quadratic surface in unused locations of the FPD and MA arrays.

GTBDPT

Geometry checker routine. Called by GETXB to obtain interior point of a body.

GTIRNT Geometry checker routine. Called by GIRTWC and GTQDPT to set RIN and ROUT parameters stored for each of the two or three intersecting bodies so that a subsequent call to GETIR effectively involves points in each of the quadrants or octants formed by two or three intersecting surfaces.

GTPLPT Geometry checker routine. Called by GIRTWC to obtain a space point on the edge formed by two planes.

GTQDPT Geometry checker routine. Called by GIRTWC to obtain intersection points of all pairs or triplets of surfaces from each of two or three bodies, no more than one of which is a plane, via calls to GTRQU. All possible intersection points are found for three surfaces and a minimization procedure called by GRTQU is used to obtain a sufficient number of check points prior to calling GTRQU. GTSURF and/or GATHER are called to obtain surface parameters from the stored body parameters for two surfaces. A call to GETXB determines whether these points lie on all the bodies. If so, GETXB calls GTIRNT to check the correctness of the region descriptions.

GTRQA5 Called by subroutine GRTQU to perform a partial reduction of three quadratic equations of three unknowns.

GTRQB3 Called by subroutine GTRQU to perform a partial reduction of three quadratic equations of three unknowns.

GTRQFN Called by subroutine GTRQPL to evaluate a polynomial.

GTRQLN Called by subroutine GTRQU to determine whether the equations being solved are linearly independent.

GTRQMX Called by subroutine GTRQU to perform a random four-dimensional rotation.

GTRQPL Called by subroutine GTRQU to obtain the roots of a polynomial.

GTRQR3 Called by subroutine GTRQU to perform the final reduction of three quadratic equations of three unknowns to a single eight degree equation of a single unknown.

GTRQSF Called by subroutine GTRQU to set up a random four-dimensional rotation matrix.

GTRQU Called by GTQDPT to determine the coordinates of the intersection of three quadratic surfaces, or of selected points on the intersection of two quadratic surfaces.

GTSURF Geometry checker routine. Called by GTQDPT to obtain surface parameters for bodies having quadratic surfaces. The method used is to consider all terms of a quadratic surface with a specific position and orientation. The contribution of these terms to the quadratic of interest is obtained utilizing rotation and translation of coordinates via a call to GATHER.

GUNIT Used by checker routines to compute unit vector.

GVECTR Geometry checker routine. Checks angles made by various vectors in the description of the geometric bodies.

INPUTD Reads in most of the Monte Carlo input data and stores it in the MASTER array for use by the calculation routines. Region specification, importance sampling data, output energy meshes, and detector data are handled by this routine.

INPUTE An auxiliary routine used to flag very distinctly all errors in the Monte Carlo input data.

LENTHS An auxiliary routine called by BAND and FILL. Used to determine lengths of energy tables in a given energy band.

MAIN* (SAMF) The overall control routine for SAM-F. The size of the MASTER array is set by SAMF.

NDQSET An auxiliary function to find the length of specified arrays.

PICK* The control routine for superbin latents. This routine stores particles whose energies are not included in the superbin currently being processed. These particles are stored by PICK in either the central memory or on tapes depending on the amount of core available for the particular problem.

RANDW An auxiliary routine called by FILL to read binary blocks of data from the element data tape (EDT) and to write binary blocks of reduced data on the banded organized data tape (ODT).

RANF A built-in random number generator.

REFD An auxiliary routine to read in binary arrays, or partial arrays, very rapidly.

SEEK* Given an array, A, with elements monotonically decreasing and a variable, X, this routine will search through the A array and determine the bin containing X.

SOUCAL* The input processor for the source information required by the Monte Carlo routines for primary transport problems. The routine processes energy and time spectra data, and source region data which are stored in the MASTER array.

SOUGAM* The routine which generates the source particles for secondary transport problems.

SOUGEN* The routine which generates the source particles for primary transport problems - except for the external source option.

SOUPIC* The routine which calls either SOUGAM or SOUGEN to generate secondary or primary source particles, respectively. It will also read in source data from an external source tape. In addition, SOUPIC controls the angle of emission reselection procedure for problems involving one or more point detectors.

SOUSEC The input processor for the gamma production data for secondary transport problems. Creates file 13, the organized gamma production data tape.

SUBED The main edit routine. The routine reads the answer arrays from the statistical aggregate tape and prepares it for editing by the EDIT routine. Flux-dependent responses are also calculated in this program.

TALLY* A summary routine. The routine prints a one line summary of results for each statistical aggregate. Quantities such as number of collisions, absorptions, and energy deposition are printed for each aggregate.

TDIFIN Called by INPUTD if thermal neutron diffusion option has been involved. TDIFIN reads and preprocesses the diffusion option input.

TERP A linear interpolation routine.

THERM A subroutine, called by AUTOBA, which pre-calculates cross sections averaged over the Maxwellian spectrum for the thermal neutron option.

TIMEX Used to keep track of computer running time during Monte Carlo execution.

TRALA* A tracking routine used by FLUP, the main flux-at-a-point routine. It tracks from an initial collision (or source) point to a detector point.

TRALAV* Similar to TRALA. Used by FLUPV, the flux-in-a-small-volume routine.

TROPIC A routine to generate a vector of direction cosines from an isotropic distribution.

VCALC The volume computation routine. Region volumes are computed by numerical integration.

WRIT An auxiliary routine to write out binary arrays, or partial arrays, very rapidly.

WRT14 A routine to write 14-word records onto tape. The routine is called whenever a transmission or interaction is to be put on tape.

Subsequent to the direction checking stage, at most one live detector sphere is intersected by the originally selected ray. If such an intersection has survived, a new direction is selected in the reselection stage.

The final stage in the reselection procedure involves the calculation of a weight adjustment factor which compensates for the biasing introduced by reselection.

Program ASORTT

ASORTT reorganizes the neutron interaction tape so as to provide (for secondary problems) a memory saving scheme analogous to the BAND feature for transport cross sections. Whereas BAND automatically splits cross section data into two or more energy ranges, to be treated one at a time, ASORTT makes provisions so that during the generation of secondary gamma rays, gamma production data for one element only resides in the MASTER array at any given time.

The basis for this memory-saving process lies in the prior creation of an organized gamma production data tape (OGPDT) by SOUSEC and a sorted interaction tape, (SIT), by ASORTT.

The format of the OGPDT is similar to the original gamma production data tape described in Appendix D, except that:

- a) the first two words for each element are dropped,
- b) the pointers are made relative to the starting address in the MASTER array,
- c) the data for each element are written as one logical record on the OGPDT.

AMONTE, the controlling Monte Carlo overlay program first considers a potential new ray. This can be either a source particle (read from source tape or generated internally by subroutine SOUPIC) or a picked up latent from a previous interaction. AMONTE next tests the energy of the considered particle. If it is below the lower bound of the superbin currently treated, it is stored as a latent. If the energy of the particle is within the current superbin, it is transmitted to CARLO.

CARLO proceeds to track the particle and to score answers. Collisions made by the particle are stored by CARSCA. The tracking procedure in CARLO is as follows.

Given the region number, IR, the energy, E, and the direction of flight, \overline{WB} , a sampling weight*

$$W = W_{IR} \times W_E \times W_{\Omega}$$

is calculated. A test is made to determine whether or not the thermal diffusion option is being invoked.

If the thermal diffusion option is not being invoked, the "ordinary" tracking procedure is used. First, subroutine DR1 is called, which provides the total macroscopic cross section in the region IR.

When point detectors are being used, (and if the extended particle path passes sufficiently close to a specified detector) preliminary geometrical calculations, necessary to bias the collision positions, are carried out. This biasing is that required to make flux estimates for point detectors bounded.

* See Appendix F for a detailed discussion of the use of importance sampling in Monte Carlo calculations.

Invoking the law of cosines,

$$\frac{E'}{E} = \frac{1+A^2+2A\omega_C}{(1+A)^2} \quad (37)$$

where E and E' are the initial and final neutron energies, respectively.

Inelastic Scattering

Letting Q be the excitation energy of the nucleus, the kinetic energy in the center of mass decreases to

$$\frac{1}{2}\mu v_r^2 = \frac{1}{2}\mu v^2 - Q \quad (38)$$

where μ is the reduced mass given by

$$\mu = \frac{A}{A+1} \quad (39)$$

Invoking conservation of linear momentum one obtains the velocity diagram:

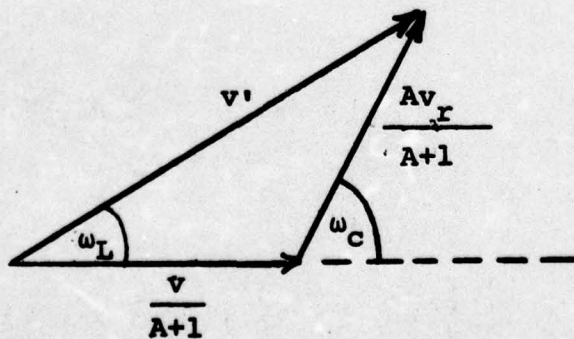


Fig. 3.7 - Velocity Diagram - Inelastic Scattering

The subroutine is called when a particle enters collision at some point within a region of given composition. Its first function is to select the nuclide in the composition with which the particle collides. The probability that a particle with energy E will interact with nuclide k of the composition R is given by

$$p(k,R) = C(k,R)\sigma_T(k,E)/\mu_{T,R}(E); P(K,R) = \sum_{n=1}^K p(n,R)$$

where $\mu_{T,R}(E)$ is the total macroscopic cross section of the composition, and $C(k,R)$ is the concentration of nuclide k in region R.

$$C(k,R) = \frac{\rho_k}{A_k} N_0 \times 10^{-24}$$

where ρ_k = density of the nuclide, k, in the composition (gm/cm^3)

A_k = its atomic weight

$N_0 = 0.6023 \times 10^{24}$; Avogadro's number

By normal Monte Carlo procedure, DR3 generates a random number, ξ , and successively compares ξ with $P(k,R)$, for all values of k, until the condition

$$\xi < P(k,R)$$

is satisfied. Then the interaction is with that k-th nuclide.

Next, DR3 determines the type of interaction suffered by the particle. The probability that a particle with energy E will suffer the "i-th" type interaction with the already selected "k-th" nuclide, is given by:

$$P(i,k) = \sigma_i(E)/\sigma_T(E)$$

path from S to I. If the ray misses the detector completely no score is made and control is returned to the calling program.

6. If interception is made TRALAV next calculates \overline{IJ} the flight distance (cm) through the detector. Control is returned to FLUPV where a track length score of

$$WT \times g_S \times e^{-\lambda} \times \overline{IJ} \times \left[\frac{1 - e^{-\lambda_d}}{\lambda_d} \right] \text{ for } \lambda_d > 0 \quad \text{or}$$

$$WT \times g_S \times e^{-\lambda} \times \overline{IJ} \quad \text{for } \lambda_d = 0 \quad (\text{vacuum})$$

is made, where λ_d is the mean free path flight path through the detector and WT is the weight of the particle at point S, prior to collision.

7. Note that if the ray starts inside the sphere it is allowed to scatter in an unbiased direction (non-source) or to proceed in its original direction (source) and the same estimate as above is made with $g_S=1$, and, if the particle is inside the detector as well as inside the sphere, $e^{-\lambda} \rightarrow 1$. If the particle is inside the sphere but outside the detector, and misses the detector, no score is made.

The mathematical technique to select the scattering angle at S is of some interest and is now presented.

where ξ is a random number uniformly distributed between 0. and 1.

Once $\cos\alpha$ has been selected it is simple by usual Monte Carlo procedures to select a random azimuthal angle and to calculate the direction cosines of $\overline{S_1}$, which are designated W_{x_2} , W_{y_2} and W_{z_2} .

Then, if θ is the selected angle of scattering:

$$\cos\theta = W_{x_1} \cdot W_{x_2} + W_{y_1} \cdot W_{y_2} + W_{z_1} \cdot W_{z_2}$$

and

$$g_S = g(\cos\theta) \times 2\pi(1-\cos\psi)$$

where $g(\cos\theta) = \frac{1}{4\pi}$ for isotropic scattering.

S inside sphere, but outside detector

Select W_{x_2} , W_{y_2} , W_{z_2} from an isotropic distribution. Then $g_S=1$ and score only if path intersects detector.

S inside detector

Again, select W_{x_2} , W_{y_2} and W_{z_2} from an isotropic distribution and then $g_S=1$.

Note: In order to increase calculational efficiency (by decreasing the number of rays which intercept the sphere but miss the detector) MAGI investigated the effects of splitting the cone into an inner and outer cone. The inner cone goes from angle 0 to $\psi/2$ and the outer cone from $\psi/2$ to ψ , (see above diagram). The code forces 3 particles into the inner cone for each particle that goes into the outer cone - with corresponding weight adjustments. This modification does seem to increase the efficiency of the technique for cubic and cylindrical detectors (with the diameter about equal to the altitude), and is currently coded in SAM-F. Investigations along these lines should continue.

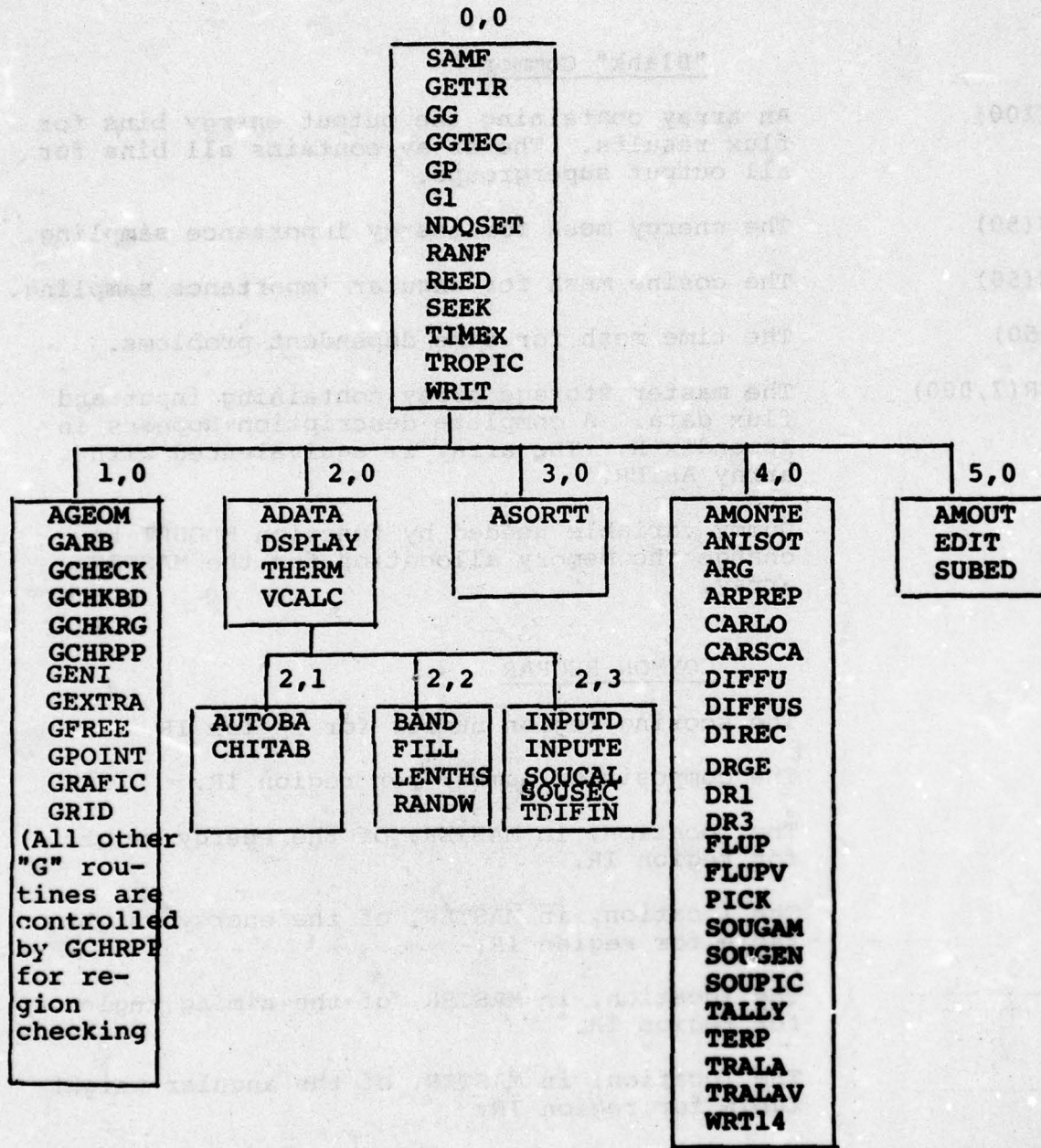
TABLE 3.1

Description of 14-Word Particle Descriptive Array

WORD(s)	NAME	Stored in Latent Table (Supergroup Option Only)	Stored on External Source Tape	Interactions Stored on Interaction/ Transmission Tape	Transmissions Stored on Interaction/ Transmission Tape
1-3	\overline{XB}	Cartesian Coordinates	Cartesian Coordinates	Cartesian Coordinates	Cartesian Coordinates
4-6	\overline{WB}	Direction of Particle from the Source or Coming out of Collision	Direction of Particle from the source	Direction of Precursor Primary Particle	Direction of Precursor Particle Entering Transmission Region
7	E	Energy of Particle	Energy of Particle	Energy of Precursor Primary Particle	Energy of Particle
8	IR	Region Number	Region Number	Region Number (Must Match Precursor Run)	Region Number (Must Match Precursor Run)
9	T	Time	Time	Time	Time
10	IDET	=100x KDLIV+IDLIV if J12345=1 =IDLIV if J12345=2,3 = detector no. if J12345=4,5	(same) ← →	=200000xKDLIV+SIGN (KDLIV)xIATWT Note: = IATWT for no detectors	= IDLIV if J12345=2 = detector no. if J12345=4,5
	F	Statistical Weight	Statistical Weight	Statistical Weight	Statistical Weight
	NHIST	History Number	History Number	Precursor Primary Particle History Number	Precursor Primary Particle History Number
	WC	= particle weight if J12345=1,2,3 = distance to detector if J12345=5 is ignored if J12345=4	Carry-Along Weight	Carry-Along Weight	= particle weight if J12345=2 = distance to detector if J12345=5 is ignored if J12345=4
	J12345	= 1 for source particle = 2 for particle coming out of elastic scattering = 3 for particle coming out of inelastic scattering = 4 for small-volume latent = 5 for point detector latent	1	10	= 2 for real track transmission = 4 for small-volume estimation transmission = 5 for point detector estimation transmission

3.3.3 Overlay Structure of SAM-F

The following is the overlay structure of SAM-F.



3.3.4 Glossary of Important Common Arrays

The following is a description of each variable in blank COMMON and in some of the more important labeled common arrays.

"Blank" Common

EQOUT(100)	An array containing the output energy bins for flux results. The array contains all bins for all output supergroups.
EWTAB(50)	The energy mesh for energy importance sampling.
ANGLE(50)	The cosine mesh for angular importance sampling.
TTAB(50)	The time mesh for time dependent problems.
MASTER(7,000)	The master storage array containing input and flux data. A complete description appears in Appendix H. The array is equivalenced with array ASTER.
KDUM	Dummy variable needed by function NDQSFT to change the memory allocation for the MASTER array.

COMMON REGPAR

ISC	The scoring region number for region IR.
NREG	The composition number for region IR.
IRW	The location, in MASTER, of the energy weight for region IR.
IEW	The location, in MASTER, of the energy weight table for region IR.
IAM	The location, in MASTER, of the aiming angle for region IR.
IANG	The location, in MASTER, of the angular weight table for region IR.

2.4.1.1 Geometry Input

Item 1 General Information (Format 5I5,E15.5,10A4)

- IGOPT = 0, Suppress both geometry checking and picture taking options
- = 1, Check for body and region description errors
- = 2, Make picture(s) of plane slice(s) through the geometry and/or check user-specified points
- = 3, Do both 1 and 2
- ISEC* Escape Region. (See also footnote 2.)
- IORPP* = 0, During geometry checking, suppress all printout except for region error messages.
- = 1, During geometry checking, provide buttressing surface (BSTB) and two and three body intersection (TBI) information, in addition to printout of IORPP=0.
- = 2, During geometry checking, provide equivalent ARB or BOX overlap (EBOXARBO) information, in addition to printout of IORPP=1
- = 3, During geometry checking, provide equivalent RPP overlap (ERPPO) information, in addition to printout of IORPP=2
- IPRINT = 0, Print out body and region data which follow
- = 1, Print out body and region data, the internal arrays in which they are stored, as well as additional information regarding ARB bodies.
- = 2, Suppress all geometry printout

* These items need be entered only if IGOPT=1 or 3. Otherwise, they may be left blank.

** The escape region is a special region which generally encloses all other regions. In ray-tracing part of the code, rays entering the escape region are terminated.

- = 0, no printout
- = 1, main debug printout option
- = 2, same as IDBG=1 plus much extra geometry tracking printout.
- = 3, same as IDBG=1 plus gamma ray production data printout.
- = 4, same as IDBG=2 plus gamma ray production data printout.

SCALE Scale Factor. Multiply all Combinatorial Geometry dimensions by this factor. (Default=1.0)

MA Title, 40 arbitrary Hollerith characters.

Item 3 Region Cards (Format 2X,A3,free field for rest of card)

Each region must be numbered and described by a logical combination of the bodies which make up that region. Use as many cards as necessary to describe each region and begin each region on a new card.

<u>Columns</u>	<u>Input</u>
1-2	Blank
3-5	Arbitrary non-blank Hollerith Data
6-80	Free field input describing the logical combination of bodies making up the region. All bodies specified are usually preceded by either the "+" or "-" operators. If no operator is given, the code will assume a "+". (For IBM [029] punched cards the "+" must not be explicitly given.) Insert OR operators if needed*, before the "+", "-" or blank operators*. Blanks may be freely left anywhere on the card, except in a body number where, for example, 1 2 (for body twelve) is interpreted as 1+2.

Use as many cards of the above type as needed to complete a region description, but leave Columns 1-6 blank on all continuation cards; do not split an operator and its corresponding body numbers onto more than one card.

The last region description card must be followed by a card containing an END in Columns 3, 4 and 5. This informs the code that all regions have been described.

*For SAM-F, the source region(s), see item 34, must precede sequentially any region which is described by the (OR) operator. For SAM-A, the detector region, (see Section 4.4.1), must precede sequentially any region which is described by the (OR) operator.

NOTE: If NUSE = 0, Omit Item 5

Item 5 Character Set (Format 46A1)

ATABLE(N), N=1,NUSE: The list of characters that are to be printed for each region. If NUSE>47, the character is Modulo (46) e.g., N=48 is the same as N=2.*

The standard default values of ATABLE are:

<u>Region Number</u>	<u>Character Printed</u>
1 through 9	1 through 9
10	0 (zero)
11	A
12	B
13	C
14	D
15	E
16	F
17	G
18	H
19	I
20	J
21	K
22	L
23	M
24	N
25	O
26	P
27	Q
28	R
29	S
30	T
31	U
32	V
33	W
34	X
35	Y
36	Z
37	+
38	-
39	*
40	/
41	(
42)
43	=
44	.
45	,
46	(blank)
>47	Modulo (46)

* Unless NBRK of Item 4 is >0. Then the character is Modulo (NUSE-1).

3.4.1.2 Cross Section Input

Item 11 Option and Title Card (Format 3I3,3X,2(2X,L1),A2,15A4)

IODT - Cross section energy banding option

= 0, do energy banding of cross sections

= 1, energy banding previously done; output must be available on logical unit 10.

IBEDT- band edit option (applicable only if IODT=0)

= 0, do not display energy banded cross section arrays

= 1, do display energy banded cross section arrays

NBAND- number of energy bands in which the cross sections are to be processed. Use NBAND=0 for automatic banding or for banding previously done and available as Tape 10. During tracking, the cross sections in only one band are in the computer at any one time. (NBAND<49.) Do not use automatic banding procedure for secondary gamma ray problems*.

SSDR1= F, no debug printout from subroutine DR1

= T, debug printout from subroutine DR1

SSDR3= F, no debug printout from subroutine DR3

= T, debug printout from subroutine DR3

NAME = Title; any 62 arbitrary Hollerith characters

* This restriction will eventually be lifted.

NOTE: If NBAND=0, omit Item 12.

Item 12 Cross Section Band Limits (Format 5E15.6)

Enter the energy limits (in ev) of each band starting with the highest energy and proceeding to the lowest energy. There must be NBAND+1 entries, using as many cards as necessary. The energy bands must exceed the energy range from EHIGH to ECUT (see Item 21 below).

NOTE: If IODT (of Item 11)=1, omit Items 13,14 and 15.

Item 13 Composition Identification (Format 2I10)

NCOMP - total number of compositions in the problem.

NNDQ - Maximum size of a band + storage arrays (<NDQ).
Default option: NNDQ = NDQ

NOTE: Repeat Items 14 and 15 for each (NCOMP) composition.

Item 14 Number of Elements (Format I10)

NE - number of nuclides in present composition (<10).

NOTE: Repeat Item 15 for each (NE) nuclide in present composition.

Item 15 Element Card (Format 10X,I10,E15.6)

ID - an integer which identifies the nuclide (5 decimal digits ZZAAA)

ZZ = atomic number

AAA = truncated atomic weight for a nuclide

= 000 for a naturally occurring mixture of isotopes

CONC - atomic concentration of nuclide in this composition in units of 10^{24} atoms/cm³.*

* Calculate by multiplying weight density in material (grams/cm³) by $\frac{.6023}{A}$, where A = non-truncated atomic weight and .6023 = Avogadro's Number in units of 10^{24} atoms/gm. For a vacuum description, use a vanishingly small, but nonzero, concentration, for example, 1.E-10.

Item 21 Cutoff Information (Format 4E14.5)

ECUT Low energy cutoff (ev). Tracking of a particle is terminated if its energy degrades below ECUT. However, for the thermal option (see next entry) the particle is not terminated but is restored, in energy, to ETHERM. ECUT must be greater than the lowest energy for which cross sections are available.

ETHERM Thermal energy (ev), if a thermal group is required. For no thermal treatment, leave this entry blank. For thermal treatment, set ETHERM slightly above ECUT.

IMPORTANT NOTE: If IODT (item 11) equals 0, then NBAND must also equal 0 on item 11 in order to use this option.

FZ Generally, $.01 < FZ < .10$. (See discussion Section 3.2.10). At MAGI, FZ = .05 is usually used.

EHIGH High energy cutoff (ev). This must be less than the highest energy for which cross sections are available.

Item 22 Output Energy Bins (Format 5E14.5)*

These cards give the boundaries of the output energy bins (ev) used for the flux edit. There should be five entries per card with a total of (NOUT+1) entries. The energies should be listed from high to low. The first and last entries should be negative. Any number of negative intermediate energies may also be used, and these negative energies define the output supergroup structure (see Section 3.2.3). Note: EHIGH and ECUT must be within the output energy bins.

* The complete energy hierarchy for SAM-F is given in Appendix E.

Item 33 Source Specifications (Format 4110)

- NSR** Number of different source regions in the problem.
If NSR=0, an external source or a previously generated transmission tape (tape 15) is used and no further source input is required after this card. Skip to Item 40.
If NSR<0, a previously generated interaction tape (TAPE 15) and a gamma ray production data tape (TAPE 12) are supplied. Skip to Item 40. For NSR<0, |NSR| is an upper limit on the number of secondary gamma rays which can be generated.
- IFLAG** Number of energies used in Item 35 to define the source spectrum. If IFLAG=1, a monoenergetic source will be used. If IFLAG=0, a built-in Cranberg fission spectrum will be used for a neutron problem. (IFLAG_≤150).
- ISW** If ISW=0, fluxes will normalize to one source particle. If ISW=1, fluxes will be normalized to the total source power as given in the next card.
- ISWW** For external source (NSR=0) only. ISWW=0 means distributed source (must be isotropic). ISWW≠0 means monodirectional source - usage is the same as for ISO, as described below in Item 34. If a transmission tape is used, ISWW is irrelevant. In case NSR<0, ISWW is automatically set =0.

NOTE: Enter Items 34-38 Only if NSR>0

Item 34 Source Regions (Formats I10,E20.8,I10)

One card is required for each source region with a total of NSR such cards

ISR* Geometrical region number

P Total power in the region (source particles per unit volume x total volume).

ISO** If ISO=0, the source will be emitted isotropically (direction may be biased, however. See Item 29).

If ISO=+1, the source will be monodirectional, with the direction specified on Item 38. No uncollided estimates are allowable for point detectors with ISO \neq 0.

If ISO=-1, the source will be monodirectional and the code will not try to score uncollided estimates for small-volume detectors.***

* Sources can be generated only in regions consisting of single bodies. The body must be a sphere, right circular cylinder, box, or rectangular parallelepiped. Also, the source regions must be lower in order than any region described with the "OR" Combinatorial Geometry operator.

** ISO must be the same for all source regions.

*** For certain geometries, involving small-volume detectors, no monodirectional uncollided rays can intercept the small-volume detectors. Setting ISO=-1, will save computer time, by instructing the code not to try to score uncollided fluxes. Under these conditions, ISO=+1 is not incorrect, it is merely inefficient.

Each element encountered on the EDT is identified even if a particular element is not used in the problem. Thus, if an element not on the tape is specified a complete list of all elements on the tape is printed and the program will terminate.

The total length of each band is printed out and if requested, a printout of the energy banded cross section arrays will also be provided.

Monte Carlo Data

The Monte Carlo printed output data are basically a repeat of the input data.

Intermediate Results

All the parameters of the first few source particles are printed out. In number, this is the smaller of either two aggregates or 50 lines of printout. The program will also print for each statistical aggregate the following items:

Number of completed histories

Number of collisions

Number of time cutoffs and energy degrades

Number of absorptions

Number of escapes (Each estimate times particle weight)

Total energy deposition (Including by scattering, absorption and escape events.) Also, energy of particle killed

by time cutoff or energy degrade is included)

Number of deaths (Including losses due to escapes, absorptions, time cutoffs and energy degrades. Each estimate times particle weight).

The number of transmissions and interactions recorded on tape 14.

Last random number sequencer. (See Section 3.2.18)

preset nor internally calculated, see input Item 41, then the region and small volume detector answers must be divided by the region volume. For point detectors this is never necessary.)

For each flux answer a statistical percentage error is given. (The description of the flux and statistical percentage error calculation is given as Appendix I.) Following the last energy bin the energy-integrated results are presented for each response set. This is, for each set, the sum over all energy bins of the flux in the energy bin, times the energy width of the bin, times the appropriate value of the response function set in the bin.

3.4.3 Tape and Disk File Assignments

The following are the file (magnetic tapes or disk) assignments of SAM-F. Those assignments which correspond to the use of various options, are so labeled. File numbers refer to FORTRAN logical numbers. All files used are in the binary mode except for file 8 which is BCD mode and contains 80 column card images.

File 8 (Option)

This is used as a scratch working file when automatic banding is performed. It is also used as the sorted interaction tape for secondary gamma ray problems.

File 9

A temporary storage disk file used by the BAND subroutine. Subsequently, the file is also used for temporary storage of particle latents in the PICK routine, where it is referred to, and equivalenced to, file 18.

File 10

The organized data file (ODT). The file contains cross section data for a given problem. The structure of file 10 is given in Appendix C. File 10 may be saved for future runs.

File 11 (Option - may be omitted if File 10 from a previous run is saved.)

The element data tape (EDT). The file contains a library (SAM-X Output) of available elements. Subroutine BAND uses this tape to get the data for a given problem. BAND and its subsidiary routines are the only routines using this file. The organization of the EDT is given in Appendix A for neutrons and B for gamma rays.

File 12 (Option)

The file contains secondary gamma ray production data. (SAM-X Output).

File 13 (Option)

This file contains the organized secondary gamma ray production data. It is derived from file 12.

File 14 (Option)

The interaction/transmission file. All interactions and transmissions are written on this file for use in subsequent problems.

File 15 (Option)

An external source file. The file may also be the interaction/transmission file (File 14) from a previous run, if it is being used as a supplier of new source particles.

File 16

The statistical aggregate tape. The AMONTE routine uses this file to record each completed aggregate. The edit routines then process the file to obtain the final flux, and flux-functional results. Tape must be saved for restart option.

File 17

A temporary storage file for latents. The tape is used by the PICK routine.

File 18

See File 9.

In addition, Files 5 and 6 are the standard input and output media, respectively. File 7 has been reserved for possible future (or ad hoc) use as the standard punch medium.

3.5 Variable Core Size Requirement for the SAM-F Program

At the present time, the standard version of SAM-F loads at 120,000 - 130,000 octal locations on a CDC 6600 machine; the exact amount depending on the given computer facility. This required core allocation can be reduced or increased under certain conditions:

(1) The MASTER array holds the cross section band data as well as the output scores in the appropriate bins. The size of the MASTER array, presently 7,000, is set in the blank COMMON statement in SAMF (Main Routine). This dimensioned size is referred to as "NDQ". The user may be able to reduce this value even further. (Do not reduce NDQ below 4000.) On the other hand, the user may wish to increase NDQ to increase the output scoring bin capability (see Section 3.6) or to accommodate an unusually large bloc of gamma ray production data for a given nuclide.

Note that the number of cross section bands and thus the amount of internal tape reading and writing increases with decreasing values of NDQ. The user will have to strike his own balance. At MAGI, NDQ=7,000 to 10,000 is usually used.

(2) ISIGP array in BAND is presently set to 6630. This dimensioned size is referred to as "NDD". The user may wish to reduce NDD or upon bombing with error message 1205 may have to increase NDD.

(3) The FPD and MA arrays are used in the geometry routines to store body and region data, respectively. At the current dimensioned values (4000 each), about 400 bodies and 200 regions can be treated by the code. The user may wish to reduce these arrays.

primary overlays. ^{*} AMONTE can be reduced, and thus SAM-F reduced, under the following conditions:

- (a) if no point detectors are required, it is not necessary to load ARG, ARPREP, FLUP and TRALA.
- (b) if no small-volume detectors are required, it is not necessary to load FLUPV and TRALAV.
- (c) if the thermal diffusion option is not required, it is not necessary to load DIFFU, DIFFUS and TDIFIN.
- (d) for primary gamma ray problems it is not necessary to load ANISOT.

3.6 Limitations Upon Size of Output Scoring Arrays

The size of the MASTER array may have to be adjusted (see Section 3.5) to accommodate desired output scoring array requirements. In addition to individual array limitations given in the Monte Carlo Input (Section 3.4.1.3), the following limitations upon NDQ must be observed:

$$(a) \quad NDQ > 2 \left[(MAX) (NT) (NUMSC + NDET) \right] + NUMSC$$

where MAX = maximum number of energy bins
in any supergroup

NT = number of time bins

NDET = number of detectors

NUMSC = number of scoring regions

$$(b) \quad NDQ > LEGEOM + (MAX) (NT) (NUMSC + NDET) + 12NRMAX$$

$$\begin{aligned} &+ NRWL + (NEWL) (NEW) + 3NAIML + (NUMANL) (NUMANG) \\ &+ 2LFOG + 4NSR + (JSPEC) (NSE+1) \\ &+ (NUMANL+1) (NSA) + 3 \end{aligned}$$

where LEGEOM = storage allocated for cross sections
(printed out)

NRMAX = number of regions

NRWL = number of distinct region weights

NEWL, NEW = number of energy importance sampling
energy bins and weight sets, respectively

* Sometimes Overlay ASORTT is the largest overlay. ASORTT can be replaced by a dummy program if a secondary gamma ray problem is not being run.

TABLE 3.3
ERROR STOP MESSAGES

<u>STOP NUMBER</u>	<u>ROUTINE</u>	<u>OVERLAY</u>	<u>MEANING</u>
1	SAMF	0,0	Execution went to completion.
11	GG	0,0	ITYPE error. (ITYPE<1 or ITYPE>10)
21	G1	0,0	Region not found.
25	SEEK	0,0	Vector out of range.
31	TROPIC	0,0	Error in generating random cosine by the rejection technique.
1001	GENI	1,0	ITYPE error. (ITYPE<1 or ITYPE>10)
1003	GCHKRG	1,0	Too much data to continue geometry checking.
1005	GFREE	1,0	Limit of DO loop exceeded.
1007			Limit of DO loop exceeded.
1011	THERM	2,0	Cumulative input data too great.
1101	AUTOBA	2,1	Too many pointers for element data.
1103	AUTOBA	2,1	Cross section upper energy is below upper energy of problem.
1105	AUTOBA	2,1	Anisotropic continuum inelastic data given. Coding not presently available to treat this option.

<u>STOP NUMBER</u>	<u>ROUTINE</u>	<u>OVERLAY</u>	<u>MEANING</u>
1107	AUTOBA	2,1	Cross section lower energy is is above lower energy of problem.
1111	AUTOBA	2,1	Elemental data is missing.
1113	AUTOBA	2,1	Index mismatch. Memory probably clobbered.
1121	CHITAB	2,1	Error in order of energies for chi-tables.
1123	CHITAB	2,1	Index mismatch. Memory probably clobbered.
1201	BAND	2,2	Too many composition elements.
1203	BAND	2,2	End of data tape reached.
1205	BAND	2,2	Element has too many pointers to be processed.
1207	BAND	2,2	Error in processing continuum inelastic scattering.
1211	BAND	2,2	Band of data is too large
1221	FILL	2,2	Error in processing energy tables.
1231	LENTHS	2,2	Index #2 for E1<EBH
1233	LENTHS	2,2	Index =1 for E>EBLX
1401	INPUTD	2,3	Negative region found for a detector.
1403	INPUTD	2,3	No room for input data.

Either a point or a volume detector may be used. In the case of a volume detector, only spheres, cylinders, rectangular parallelepipeds or boxes are presently allowed.

(e) Region and energy dependent importance sampling.

The adjoint transport and post collision energy selections are biased towards the gamma ray source, according to an input set of importance values.

(f) Angular Biasing at the Detector.

When calculation of adjoint currents at a scoring surface is desired, angular biasing of initial tracks at the detector about a specified axis is allowed by means of specified angular weights.

This allows aiming toward a surface or surfaces of interest.

A step by step description of the calculation flow is now given:

1. Read all input data (cross sections, gamma production data, geometry, importance sampling data, detector response data).

If adjoint currents are desired proceed immediately to Step 4.

2. For a primary gamma ray problem read in a single source particle from the source tape and proceed to Step 4. For a secondary gamma ray problem read the neutron interaction data for a single interaction. During the previous SAM-F neutron problem all gamma ray producing interactions (absorptions and inelastics) were written on an interaction tape. For each interaction the following data was written on tape.

X(3)	neutron collision position
W(3)	direction cosines before scatter (not presently used by SAM-A because the existing coding assumes the secondary gammas are generated isotropically)*
E	neutron energy before the interaction
IR	region in which collision occurred (not used by SAM-A)
T	time of flight of the neutron

* It is anticipated that this restriction will be eliminated in the near future.

4.3.4.2 Implementation of the Biasing Procedure for Unspecified Source Points

The choice of the direction imparted to a ray starting at the detector is done on the basis of a biased angular distribution. A biasing axis is chosen on input. A set of polar cosines about the biasing axis is also specified. The direction of a ray is then determined on the basis of a biased density distribution that is read in as input and the proper weighting of the history is maintained.

4.3.5 Description of Subroutine DOSEDT

The DOSEDT routine prints the detector responses (i.e., flux, dose, etc.) as functions of energy and time using the energy mesh of the detector response. The routine is called, from the main program, once for each time bin and also for the time integrated results. For each time bin, the collided, uncollided and total results, as functions of energy, are printed out with associated deviations. The energy integrated results are also printed out.

Note that all answers are normalized to one primary particle history and are also divided by the appropriate value of Δt and ΔE . Thus the results are on a per primary source particle per unit time (sec) and per unit energy (ev) basis.

4.3.6 Description of Subroutine EDIT

The EDIT subroutine prints the track length scores if $NG < 2$ (or the adjoint current scores for $NG = 2$) and associated deviations as functions of energy and region azimuthal angle and cosine of the polar angle. The energy mesh used is EOUT (or ESOR) as described in Section 4.2.5. All answers are normalized to one primary source particle and divided by the appropriate value of ΔE . This subroutine is the same as that used in SAM-F except that no additional response function calculation is provided, since the detector particle energies are selected directly from the normalized response function.

4.3.7 Description of Subroutine ENDET

This routine is called from the main program to select the initial detector energy. The initial energy is chosen from the detector response function supplied as input.

Item 2 - Number of Elements (Format I10)

NE - number of nuclides in present composition

Repeat Item 3 for each (NE) nuclide in present composition.

Item 3 - Element Card (Format 10X,I10,E15.6)

ID - an integer which identifies the nuclide (5 decimal digits ZZAAA)

ZZ = atomic number

AAA = truncated atomic weight for a nuclide

= 000 for a naturally occurring mixture of isotopes

CONC - atomic concentration of nuclide in this composition in units of 10^{24} atoms/cm³. *

Item 4 - Geometry Input

(a) Display option and title ** (Format I10,A2,17A4)

IPRINT = 0, print out body and region data which follow

= 1, print out body and region data as well as the internal arrays in which they are stored

= 3, suppress all geometry printout

(b) Body and Region cards are the same as used by SAM-F and are described in Section 3.4.1.1 (Items 2 and 3).

Item 5 - General Parameters (Format 3I10,9I5)

NSTART = Maximum running time in seconds ***

NSTOP = Total number of primary particle histories ****

NSTAT = Number of primary histories per statistical group

NRMAX = Number of geometric regions (<200)

NG = 0, neutron interaction tape supplied for source

= 1, external gamma ray source tape supplied

= 2, adjoint currents (time-independent) scored in energy and angle bins for tracks leaving scoring region surfaces abutting the escape region.

* Calculate by multiplying weight density in material (grams/cm³) by $\frac{.6023}{A}$ where A=non-truncated atomic weight (gms) and .6023 is Avogadro's Number times 10^{24} .

** At present geometry checking is not available utilizing SAM-A. Checking of geometry data should be done with SAM-F utilizing the geometry cards of Section 3.4.1.1 (Items 1-10)

*** Upon completion of each statistical aggregate the code estimates the total (real) running time at the end of two additional aggregates. If this time exceeds NSTART (seconds) no new aggregates will be started and control is switched to the edit routines.

**** Refers to primary neutron histories for secondary gamma ray problems.

Item 5 - Continued

MT = Number of time bins (≤ 25); for no time dependence use MT=0
(No time dependence is currently allowed for NG=2 option)

NOU^T = Number of output energy bins (≤ 25)

MRS = Number of scoring regions

NRWL = Number of distinct regions weights (≤ 100)

IESC = Escape region number

IBG = 0, no debug printout
= 1, debug printout

MUL = If NG=0, MUL is the number of times each neutron interaction
is to be used. (If a zero is entered, the code assumes
MUL=1)

Item 6 - Detector Parameters (Format 3E14.6,I4)

XD = Detector coordinates (x,y,z); (for point detector only)

IRDET= Detector region number* (use negative number for point
detector, or a positive number for volume detector)

Item 7 - Output Gamma Energy Mesh (Format 5E14.5)

The mesh at which the track length scores will be tallied. Enter
NOU^T+1 numbers from high to low energy. Use as many cards as required.

Item 8 - Output Time Bin Mesh (Format 5E14.5)

Time mesh (seconds) at which detector scores will be tallied.
Enter MT+1 numbers from longest to shortest times. Omit this set if
MT=0.

Item 9 - Region Weights (Format 5I4.6)

Enter the NRWL region weights to be used in the problem. The
weights need not be entered monotonically by value but their order
determines the region weight numbers (i.e., entry one is weight #1,
etc.).

* The volume detector must be a region restricted to a single body.
Either a sphere, right circular cylinder, box, or rectangular
parallelepiped is allowed. Furthermore, no regions employing the
(OR) operator, see Section 3.2.1.1, may sequentially precede this
detector region.

NOTE: Enter Items 17-24 only
if NG=2 (See Item 5)

Item 17 - Scoring Parameters (Format 3I10)

MWSR - Number of polar angle cosine bins ≤ 34

MSOR - Number of scoring energy bins ≤ 34

MASR - Number of equally spaced azimuthal bins ≤ 34

Item 18 - Scoring Polar Angle Cosines (5E14.5)

Polar cosine mesh. Enter MWSR+1 cosines, in descending order, from +1. to -1.

Item 19 - Scoring Energies (5E14.5)

Scoring energy mesh (ev). Enter MSOR+1 numbers, in descending order.

Item 20 - Scoring Axis Direction Cosines (3E14.5)

Specification of direction cosines of the axis for polar cosine mesh as specified in Item 18. Enter x,y,z direction cosines in order.

Item 21 - Biasing Axis Direction Cosines (3E14.5)

Specification of aiming axis about which is specified a polar cosine mesh for biased selection of the direction out of the detector (Item 23). Enter x,y,z direction cosines in order.

Item 22 - Number of Biasing Polar Cosines Bins (I10)

Enter number, NB, of such bins. ≤ 20

Item 23 - Biasing Polar Cosine Mesh Points (5E14.6)

Enter NB+1 cosines, in descending order, from +1. to -1.

Item 24 - Biasing Polar Cosine Direction Weights (5E14.6)

Enter NB weights.

4.4.2 Description of Output

The SAM-A output falls into the following general categories (in the order in which they are printed).

- a. Cross section and composition information,
- b. Geometry information,
- c. Problem input data,
- d. End of aggregate tally,
- e. Track length or adjoint current scores,
- f. Gamma ray collision tally,
- g. Detector edit. (NG=2)

After the final aggregate the total Monte Carlo running time is printed.

e. Track Length or Adjoint Current Scores

NG< 2 - For each region designated as a scoring region, (input parameter), the track length scores as function of the track length energy mesh (also input) will be printed. The displayed results have been divided by ΔE and by the number of primary histories. This edit is time-integrated and is, in general, the same as used for track length scores in the SAM-F program. Note that the answers are not divided by the region volumes.

In addition to the energy dependent scores, the energy integrated scores are also given for each region.

NG=2

For a single azimuthal bin and a single scoring region the adjoint current computed from the track length scores are given as functions of the track length energy mesh and the cosine of the polar angle. Both energy dependent and energy integrated scores are given. The adjoint current printout is given for each scoring region. When more than one azimuthal bin is given the adjoint current is printed out only for the first bin in order to shorten the otherwise voluminous output.

f. Gamma Ray Collision Edit

The number of gamma ray collisions in each geometric region, (as a function of energy, using the track length energy mesh), is printed. Region numbers are given across the page and energy bin bounds are given down the page.

g. Detector Response Edit (NG< 2)

The detector response edit give the uncollided, collided and total detector responses as functions of energy and time. The results are scored in bins using the energy mesh for the response function data

and the input-specified time mesh. The units of the response correspond to the detector response function supplied as input. Hence, if the input response function was flux-to-dose conversion factors, the final results are doses. If a unity response function was supplied, the results are number fluxes. If the average energy of a scoring energy bin was entered, the results are energy fluxes, etc.

Each time bin is edited separately and the energy integrated response is given for each time bin. In addition, a time-integrated response is given after the time-dependent results for each time bin have been printed.

4.4.3 Tape and Disk File Assignments

The following are the file (magnetic tapes or disk) assignments of SAM-A. File numbers refer to FORTRAN logical numbers.

File 7 (Option)

The gamma ray production cross section file.

File 11

The gamma ray cross section tape.

File 14

If $NG < 2$ it is the neutron interaction tape or the primary gamma source tape. When $NG=2$ the adjoint currents are written on tape in the form of BCD records.

In addition, Files 5 and 6 are the standard input and output media, respectively.

When $NG=2$ the interactions or gamma ray sources are written on the tape in blocks of 35 particles per record with the following write statement.

```
WRITE(14) ((B(I,J),I=1,14),J=1,35)
```

Thus, each column of "B" is a 14 word particle record.

The format of each 14 word particle record on File 14 is shown below.

Letting $\omega = \cos\theta$, the law of cosines yields:

$$p^2 = p_1^2 + p_2^2 - 2p_1p_2\omega \quad (G.2)$$

Rearranging equation (G.2) and squaring both sides

$$4\omega^2 p_1^2 p_2^2 = p_1^4 + p_2^4 + 2p_1^2 p_2^2 + p^4 - 2p^2(p_1^2 + p_2^2) \quad (G.3)$$

Substituting equations (G.1a,b,c) into equation (G.3) yields, after canceling common terms and rearranging

$$a_1 E_2^2 + a_2 E_2 + a_3 = 0 \quad (G.4)$$

where the coefficients of the quadratic equation are given by

$$a_1 = 4(1-\omega^2)E_1^2 + (A+1)^2 r^2 + 4(1-\omega^2+A)rE_1 \quad (G.5a)$$

$$a_2 = 4(1-\omega^2-A)rE_1^2 + 2(1-A^2-2\omega^2)r^2 E_1 \quad (G.5b)$$

$$a_3 = (A-1)^2 r^2 E_1^2 \quad (G.5c)$$

Letting $T = E_2/E_1$:

$$T = \frac{4(\omega^2+A-1)rE_1 + 2(2\omega^2+A^2-1)r^2 + 4r\omega(E_1+r)\sqrt{\omega^2-1+A^2}}{2(A+1)^2 r^2 + 8(1-\omega^2)E_1^2 + 8(1-\omega^2+A)rE_1} \quad (G.6)$$

where we have retained the root which yields $T=1$ for $\omega=1$ (recall that the additional root was introduced by squaring equation (G.2)).

$$B_{kl} \geq \sqrt{\left(1 - \frac{R_k^2}{|X-X_k|^2}\right) \left(1 - \frac{R_l^2}{|X-X_l|^2}\right)} - \frac{R_k R_l}{|X-X_k| |X-X_l|}$$

the COT is satisfied, and an MDC exists.

Although references to "sphere overlaps" (see algorithm (O-2)) and "multiple intersections" (see algorithm (O-3)) also imply the existence of an "angle" MDC, these tests comprise a sub-set of the COT. Finally, only a sphere overlap is a significant MDC for position reselection.

4.3 Resolution of an MDC

An MDC may be resolved by Russian roulette, in which one ("live") detector is chosen for sampling purposes. The implication of this selection depends on the particular stage of the particle history at which it occurs.

4.3.1 Position Checking (Source)

After the selection of a source position at the start of a history, the resolution of an MDC is recorded by the appropriate setting of the live detector "position flag", KDLIV. The relevant algorithms are best summarized by a logical flow chart (Figure 0-2).

4.3.4 Interpretation of KDLIV

As a result of positron checking, both for a source and a collision, the setting of KDLIV has the following implications:

- (a) The case $KDLIV > 0$ implies that there was no MDC.
- (b) For $KDLIV \neq 0$, detector number ($-KDLIV$) is used for sampling purposes, and a special weight adjustment allows bounded estimation for all detectors. This weight adjustment is given by

$$b_n = \frac{1}{\sum_{m=1}^n b_m}$$

where

$$k = |KDLIV|$$

$$b_n = \max(1, R_m^2 / |X - X_m|^2)$$

- (c) The value of KDLIV influences the direction checking preceding angle reselection, as described in Section 4.3.2 above.

REFERENCE FOR APPENDIX O

1. H.A. Steinberg and M.H. Kalos, Nuc. Sci. and Eng., 44, 406-412 (1971).
2. H. A. Steinberg, Bounded Estimation of Flux-at-a-Point for One or More Detectors, ANL-NEACRP Meeting of a Monte Carlo Study Group, Argonne National Lab., July 1974.

APPENDIX P

Combinatorial Geometry Example Employing

All Allowed Body Types

The data sheets which follow, provide the complete input description for Combinatorial Geometry Example #5, as shown in Section 3.2.1.3.

FOR PIN STATEMENT

IDENTIFICATION

SPECIAL INSTRUCTIONS

card code = 026
029

0 : ZERO 1 : ONE 2 : TWO
β : ALPHA 0 I : ALPHA 1 Z : ALPHA 2

STATEMENT NO.	0	1	2	3	4	5	6	7	8	9	
0	0	0	0	1	EXAMPLE EMPLOYING ALL ALLOWED BODY TYPES						
RPP	1	-12	12	-12	12	-16	18	0	0	0	
DφX	2	-11	-11	-12	20	0	0	0	0	0	
TRC	3	0	0	0	0	0	0	0	0	0	
REC	4	0	0	13	0	0	0	0	0	0	
ARB	5	-6	-5	12	-5	-5	2	0	0	0	
	5	5	-5	1	5	-5	12	0	0	0	
	5	5	5	1	5	5	12	0	0	0	
	-6	5	5	12	-5	5	2	0	0	0	
RAW	2341	3564	0765	2170	1467	3205	0	0	0	0	
	6	-5	1	0	0	0	1	0	0	0	
RCC	10	0	0	0	0	10	0	0	0	0	
	7	-8.5	0	-9	0	0	5	0	0	0	
	1.5	0	0	0	0	0	0	0	0	0	
ELL	8	8	0	-9.3	8	0	-5.7	0	0	0	
	4	0	0	0	0	0	0	0	0	0	
SPH	9	-8.5	0	-11.5	2	0	0	0	0	0	

(continued on next page)

STATEMENT NO.	FORTRAN STATEMENT				IDENTIFICATION			
	0 - ZERO	1 - ONE	2 - TWO	SPECIAL INSTRUCTIONS				
	β - ALPHA 0	I - ALPHA I	Z - ALPHA Z	card code = 026				
1	10	-1.	0.	-1.	1.5	0.	1.	
2		0.	0.	1.	0.	0.	0.	
3		1.	0.75	2.				
4	END							
5	1	-2						
6	2	-3	-4	-5	-6	-7	-8	-9
7	DR	3	-5	-6	-100R	4		
8	4	-6						
9	7	-9						
10	8							
11	9	-2	-7					
12	7	9						
13	10							
14	END							

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