NUCLEAR ROCKET DIVISION

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FINAL REPORT, CY 1969
SHIELDING CODE DEVELOPMENT PROGRAM
PROJECT 393

NERVA Program

Contract SNP-1

February 1970

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FINAL REPORT, CY 1969
SHIELDING CODE DEVELOPMENT PROGRAM
PROJECT 393, CONTRACT SNP-1

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ABSTRACT

This report describes work performed under Project 393 in the SNP-1 contract. This project covers work in the development of improved shielding and radiation analysis computer codes.

A new program, designated DASH, was developed to accept leakage angular flux data from the discrete ordinates code, DOT and serve as a bridging code as follows: This flux information can be used to trace particle histories in space and be used as source information for Monte Carlo calculations or other DOT calculations. Since DASH takes DOT output and puts it in Monte Carlo format, a very powerful tool is thus made available, wherein the DOT code can be used where it offers the best solution and Monte Carlo codes can be used where they perform best, without the requirement of starting out as a Monte Carlo analysis (e.g., from the fission events in a reactor problem).

A number of neutron cross-section handling codes were also developed. An investigation was made which shows some promise of incorporating importance biasing using the adjoint function as a basis for improving the efficiency of Monte Carlo calculations.

The geometry routine of the FASTER Monte Carlo code was incorporated into the FMC-G and FMC-N Monte Carlo codes and the QAD and GGG point kernel codes, to minimize the setup time required for use of more than one code for the same geometrical model.

ACKNOWLEDGEMENT

Under separate subcontracts, Radiation Research Associates (RRA) assisted in the preparation of the bridging codes and performed a large fraction of the work related to the neutron library programs. RRA also performed the brief evaluation of the adjoint function biasing. ART Research Corporation assisted in incorporating the FASTER geometry in the FMC Monte Carlo program.

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I. INTRODUCTION

To predict the radiation environment of the NERVA engine, associated space vehicles, and test facilities, it is necessary to accurately calculate the transport of leakage fluxes from the nuclear subsystem with flexibility and economy. This calculation could be performed best by Monte Carlo methods since configurations are complex with many void or low-density regions. Where densities are high (as within the pressure vessel), S_n discrete ordinates constitutes the best method of calculation for most applications. S_n methods are limited to descriptions in 1-D and 2-D. In 2-D, S_n may display "ray effects" wherein calculations carried along discrete angular paths may predict radiation levels erroneously in low-density regions. Monte Carlo methods do not suffer from this inherent limitation. On the other hand, in high-density regions, it may be found that Monte Carlo methods require excessively large computer running times to achieve reasonable statistical precision.

In some applications (especially parameter studies primarily involving low-density regions) point kernel methods furnish sufficient accuracy. At the same time, these methods normally can be used at a much lower computer cost than S_n and Monte Carlo methods.

In general, improvements in accuracy, flexibility, or economy of any of the three methods would result in expanded capabilities in NERVA shielding calculations. It was determined that the following improvement areas would impact most heavily on these capabilities.

A. BRIDGING CODES

To best use the capabilities of S_n and Monte Carlo methods, a means should be developed whereby a bridging between the two is accomplished. Where 2-D descriptions are adequate and material densities are relatively high, S_n should be employed. Where 3-D descriptions are necessary and where densities

are low, Monte Carlo should be used. Data sufficient to describe the angular flux leaking from one region should be changed to the source format of the code used to calculate transport through the other region.

B. NEUTRON LIBRARIES

A standard library of neutron cross sections (ENDF/B) is now available. The codes presently available antedate this standard compilation. Although existing libraries have been adequate, their incompatibility with standard tapes adopted by industry will greatly increase the effort required to maintain their currency. Machine procedures should be developed to convert existing ENDF/B data to the formats required by the codes and then prepare the appropriate libraries.

C. BIASING

The character of Monte Carlo is such that great economies can be effected by proper biasing. Importance-biasing, using the adjoint function, has the potential of being the optimum method, although it has been seen that complex biasing schemes sometimes are more costly to use than Monte Carlo with simpler schemes. Existing Monte Carlo codes use biasing schemes that are considerably simpler than importance biasing. It cannot be known a priori whether importance-biasing would provide greater or lesser economy for a particular application. As a first step in an investigation of importance-biasing for NERVA application, methods for implementing it within existing codes should be sought.

D. GEOMETRY SPECIFICATIONS

One of the most time-consuming tasks in creating data decks to run transport codes is specifying the configuration of the region under consideration. It is often necessary to specify this same configuration in a different format for each code, each requiring a comparable effort. Large savings in setup time could be accomplished if commonly used codes required identical specification formats. The FASTER code has an especially flexible and easy to use format which should be incorporated into other codes.

Work has been conducted in these areas throughout CY 1969. In many cases, the accrued improvements are now being routinely employed in NERVA radiation analysis. A discussion of the results of this work follows, including present and anticipated applications.

II. BRIDGING CODES

In preparing procedures for using leakage data from one code as source data for another, a new code was written. This code, DASH, is a single package with several input, output, and handling options. It accepts (r, z) DOT¹ leakage information as input, using end leakage, side leakage, or end and side leakage. Any angular quadrature set is acceptable.

Radial bridging interface surfaces are specified at any location. If they are specified at either end surface, DASH can be used to integrate the leakage angular fluxes. If they are specified radially outwards from the sides, above the top end, or below the bottom end, DASH can be used to calculate the fluxes that would be transported across a void to these surfaces. Unscattered components of the fluxes can be calculated by specifying absorber regions composed of combinations of disks and rings between the leakage and interface surfaces.

The basic relationships of the DASH code were originally derived to calculate fluxes on surfaces in a void, using leakage fluxes predicted by DOT. The void transport, in general, cannot be calculated directly by DOT since two-dimensional S_N calculations are susceptible to ray effects². These effects occur when the mathematical model places radiation along a particular quadrature ray that encounters insufficient scattering materials for redirection to one of the other allowed directions. The result is a spreading of radiation, not uniformly, but with peaks along the quadrature rays and valleys between them. Figure 1 is a model that was used to study this effect in a geometry similar to that encountered in NERVA problems.

A graphite cylinder, 120-cm high by 65-cm radius, was modeled. Within the graphite, fission-induced neutron and gamma sources were distributed. This cylinder was included in a larger model with a plane at one end on which radial flux distributions were desired.

Figure 1 - Geometry of Sample Problem

Since rays are not redirected after leaking from the graphite, ray effects can be expected to be observed in the flux distributions on the plane above. The angles allowed by the S_N quadrature solutions can be visualized by rays to the center of blocks of an igloo, the S_N order, N , being two times the number of layers of such blocks. With no ray near the axis, for such configurations, a relatively low-order solution would underpredict fluxes near the axis and overpredict where the first allowed ray predominates.

Fast neutron fluxes are shown in Figure 2, as predicted by DOT for $N = 4, 6, 8$ (12, 24, 40 angles, respectively). Ray effects are observed instead of the nearly flat flux expected from the physical considerations. While the S_8 fluxes appear best among these low-order results, they still appear insufficient.

If the grid describing the configuration is improved instead of approaching the physical values, the improved description shows the erroneous ray effects in greater detail. This is illustrated in Figure 3.

To view the effect of redistribution by interceding scattering materials, the void region around the graphite was filled with hydrogen gas of different densities. Thermal fluxes that result with scattering mean-free paths in hydrogen of 0.4, 4, and 40 are shown in Figure 4*. For 0.4 mean-free paths, some flattening occurs, but the ray effect is still seen. For 4 mean-free paths, the ray effect is not apparent. For 40 mean-free paths, the flux is reduced by the accompanying attenuation and scatter losses to the sides. However, a hint of the ray-effect shape is still observed, possibly because thermalization can occur in a few scatters in hydrogen, and some of the thermal flux will result from fast flux that has retained its ray-effect shape and penetrated deeply before thermalization.

It is possible to avoid ray effects as shown by using very high order quadratures or asymmetric quadratures which are high order only in the direction of interest³. These may have quite large computer time and storage requirements. Whereas relatively low order S_N solutions seem adequate in high scattering regions,

* The mean-free paths were given for epithermal neutrons since they have a nearly constant scattering cross section of about 20 barns. The cross section for slower neutrons is greater, giving mean-free paths of 1.5 to 2 times the epithermal mean-free paths, depending on the spectrum.

(480 CM ABOVE MODEL,
 S_4 , S_6 , S_8 DOT
 CALCULATIONS)

156 REGION IN
 GRAPHITE

NEUTRON FAST FLUX

Figure 2 - Neutron Fast Flux, S_4 , S_6 , S_8 Dot Calculations

(480 CM ABOVE MODEL,
CALCULATED BY S_6 DOT)

REGION GRIDS IN GRAPHITE:

— 42

- - - 156

- - - 624

NEUTRON FAST FLUX

Figure 3 - Neutron Fast Flux, S_6 Dot Calculations

(THROUGH 480 CM OF H_2
CALCULATED BY S_6 DOT)

H SCATTERING MEAN FREE
PATHS (EPITHERMAL):

- 0
- 0.4
- 4.0
- 40

Figure 4 - Thermal Neutron Flux, S_6 Dot Calculation

like the graphite cylinder, it seems wasteful to strain budgets and computer capabilities to trace radiation through void or low-scatter regions when Monte Carlo or point kernel methods can accomplish the task with little difficulty.

DASH calculates the void transport by ray tracing. The rays are chosen by random number sampling of radial or axial surface intervals, polar angle, and azimuthal angle. The limits are chosen to minimize the number of traces that have no chance of interception by a detector surface.

The calculation of radiation transport between surfaces is accomplished by a Monte Carlo approach. Leakage fluxes are sampled by random numbers applied to limits of surface r or z , of polar angle, and of azimuthal angle. The limits are chosen to minimize traces that have no chance of interception by a detector surface.

The value of the radiation current applied to any single sample trace depends on the angles chosen, the area of the leakage surface interval, the number of samples to be generated, and the angular quadrature leakage flux predicted by DOT. The sample flux relation to the angular quadrature leakage flux is controlled by a smoothing option. The flux for any trace may be taken as the same as that predicted by DOT for the quadrature in whose equivalent solid angle the trace falls. This amounts to the DASH procedure being one of extending solid angle histograms outward to intersect with the detector surfaces. Alternatively, if the angular quadrature description is symmetric, so that the direction cosines η and μ have the same limits, the fluxes may be smoothed by a set of least-squares fits to power series. For each energy group, the fluxes for each η level are summed and the quadrature fluxes normalized. These η -level fluxes are then summed for each space interval and the η -level fluxes normalized. Least-squares fits are then carried out for the different space intervals, for the η levels within each space interval, and for the μ sections within each η level. As a result, the angular flux is evaluated for each sample as the product of curve fits in r or z , η , and μ , as determined by the random numbers.

The resulting interpolation in three dimensions has proven to be a reasonable representation of the result that would be predicted by a much higher order of quadrature detail. The fluxes predicted by this procedure do not appear to change appreciably as the quadrature detail of the DOT source leakage is increased.

In Figure 5, fast and thermal neutron fluxes from DOT/DASH are compared with DOT extended model results. The DOT/DASH results are shown as falling within regions containing all values resulting from S4, S6, S8, DOT solutions and different model grids. Some statistical scatter, too, is inherent in the result.* Nothing resembling the DOT ray effects appear in the DOT/DASH results.

For comparison with other methods, DOT/DASH gamma fluxes at the 480-cm plane were calculated. In Figure 6 these results (also shown as a region in which the different orders and grids fall) are compared with FMC-G and QAD point kernel results for the same geometry and gamma sources. Also shown in Figure 6 is the DOT/DASH result in which the flux is uninterpolated, but is evaluated by applying the quadrature flux for the block of the igloo through which each trace passes. This is equivalent to projecting the blocks as angular flux histograms. As would be expected for a histogram, more structure results than is observed in the cases where fluxes are obtained from curve fits. The flux is underestimated slightly on the axis (but by a small percentage compared to the extended DOT under-estimation of decades).

If the detector intervals are chosen as the radial intervals of a second DOT problem, DASH can be made to sum the sample traces in the appropriate angular quadrature sets for each interval and produce magnetic tape records which can be used as boundary source data for a DOT problem.

The sample data generated by DASH is equivalent to the kind of data generated by Monte Carlo codes in sampling probability distribution tables. Thus, DASH can be employed to replace this part of a Monte Carlo code, using the DASH generated data directly.

* A DASH calculation of this type requires approximately 2 minutes of IBM 360/65 time for 5% standard deviation.

(480 CM ABOVE MODEL,
CALCULATED BY S_6 DOT
& S_6 DOT/DASH)

THERMAL FLUX
 < 0.4 eV
FAST FLUX
 > 1 MeV

NEUTRON FLUX

Figure 5 - Neutron Fluxes, S_6 Dot and S_6 Dot/Dash Calculations

(RELATIVE GAMMA FLUX
480 CM ABOVE MODEL)

- ENVELOPE OF INTERPOLATED DASH RESULTS FOR S_4, S_6, S_8
- UNINTERPOLATED DASH RESULTS, S_8
- ANALOG MONTE CARLO (FMC) RESULTS
- POINT KERNEL (QAD) RESULTS

RELATIVE PHOTON FLUX

Figure 6 - Comparison Results

If the space between leakage surfaces and detector surfaces is not a void, but contains insufficient scattering material to avoid ray effects, the radiation transport would be handled best by Monte Carlo. Monte Carlo codes are excessively long-running in dense regions. Where S_N codes suffer from ray effects because of inadequate resolution or insufficient redistribution by scattering, Monte Carlo codes are most efficient. Therefore, in problems where both high- and low-density regions exist, the two computational methods should be complementary.

DASH was extended to generate information on magnetic tape in the formats used by COHORT, FMC-G, AND FMC-N. The DASH coupling information flow is shown schematically in Figure 7. Data can be exchanged at any level since the flow of internal information in DASH is from the tabular form of discrete ordinates to the weighted particle form of Monte Carlo, then back to the discrete ordinates form. DOT can be used as a source of information at the first level and to accept data at the third level, making possible a DOT/DASH/DOT coupling scheme. Monte Carlo codes can accept data at the second level, making possible DOT/DASH/Monte Carlo coupling schemes. When the need arises, more complicated schemes can be devised using successive couplings, such as DOT/DASH/DOT/DASH/Monte Carlo.

Figure 7 - Dash Coupling Information Flow

Since DOT geometry descriptions are two-dimensional, DASH extends this to three dimensions using azimuthal symmetry when generating data to be used in a DOT/DASH/Monte Carlo coupling.

DASH was used for several coupled code calculations on the NERVA system in the second half of the contract year. In each case, DOT was used to analyze the pressure vessel and reactor assembly (PVARA) and leakage fluxes interfaced with DASH at the pressure vessel surface. Couplings to DOT, COHORT*, FMC-N, and FMC-G were then made to calculate disk shield heating, dose rates to payloads and test facilities, and secondary gamma strengths in engine components.

Figure 8 shows a cutaway model of the engine test compartment at the Nuclear Rocket Development Station. Gamma and neutron leakage from the pressure vessel of a flight-engine reactor were calculated by DOT. These were coupled by DASH to COHORT. Flux and dose levels were calculated at several locations inside the facility shield by COHORT.

In Figure 9, a problem incorporating DOT/DASH/DOT coupling is illustrated. DASH was used to calculate the neutron and gamma radiation transported from the pressure-vessel surface, through a void, to a disk shield above the reactor. Records were stored on magnetic tape in tabular discrete-ordinates form. These were then used as source input for a DOT analysis of the shield. DOT provided radiation heating data for the shield and tapes for DASH calculation of transport to the bottom of the propellant tank.

At the propellant tank, gamma tapes were produced containing data in the formats used by COHORT AND FMC-G. The tank geometry is shown in Figure 10. Using COHORT, gamma levels were calculated at tank top and in a simple Apollo-type spacecraft located near tank top for several different liquid hydrogen

* COHORT was made operational on the Aerojet-General IBM 360/65 during CY 1969 by Radiation Research Associates personnel.

Figure 8 - Model for Radiation Analysis of Engine Test Compartment

Figure 9 - Model for Disk Shield Radiation Analysis

Figure 10 - Model for Calculation of Radiation Levels from Reactor at Top of Propellant Tank

levels. Later calculations with FMC-G produced tapes of FMC-G source data at tank top. With these tapes, FMC-G could be restarted with various spacecraft configurations. This coupling scheme allowed use of the code best suited for each region, insuring the best combination of accuracy and economy. Additionally, it allowed the flexibility and economy of changing spacecraft models without repeating propellant tank and reactor analyses and of changing propellant levels without repeating the reactor analysis.

A coupling scheme was used to calculate nozzle secondary source strengths, as illustrated in Figure 11. In this case, DOT-calculated neutron angular fluxes at the pressure vessel surface were used by DASH to produce a COHORT source tape at the surface, with no void transport. COHORT was then used to calculate neutron fluxes in the nozzle materials. Secondary gamma strengths were calculated by using the appropriate (n,γ) absorption and inelastic scattering cross-sections.

In the study using FMC-G to calculate gamma transport through the propellant tank, the tape of source data at the bottom of the propellant tank was used with several FMC-G runs, each with a different liquid hydrogen level in the tank, to produce tank-top data for mission profile. In each FMC-G case, a tape was produced containing FMC source data at the tank top. These tapes can be used again for longer tanks and/or various payloads. This offers a Monte Carlo solution without returning to the sources in the engine and repeating the profile analyses for each tank-top change. It has been estimated that the code coupling method used in developing the Monte Carlo data for PVARA radiation was able to accomplish the task in $1/8$ to $1/6$ of the computer time that would have been required using pure Monte Carlo. In a single Monte Carlo run, for a single liquid hydrogen level, 8 to 10 hours of IBM 360/65 time would have been necessary to obtain equivalent data. Using coupling techniques, radiation transport in the PVARA was accomplished in 40 minutes, providing surface leakage fluxes. These fluxes were then processed by DASH in the FMC input format in 10 minutes. For each liquid hydrogen level, then, an FMC run of 60 to 80 minutes was necessary. For 5 liquid levels, a total of 40 to 50

Figure 11 - Model for Calculation of Secondary Gamma Sources in Nozzle

hours would be necessary for pure Monte Carlo, whereas the coupled code method has required only 6 to 7 hours of computer time.

Thus, approximately \$20,000 in computing time is saved in computing tank top dose for a typical mission profile. This has been applied in CY 1969 with a realization of the original investment of approximately \$30,000 in coupling codes virtually obtained with a single propulsion module analysis savings of \$20,000. By the completion of the first quarter of CY 1970, the costs of the SRT funding in CY 1969 will have been realized as savings in CY 1969 and 1970 production applications.

Two papers have been presented at ANS meetings discussing DASH and the code coupling technique. The first, "Leakage Tracing from Boundaries of Low Order S_N Solutions"⁴ discussed the basis of the DASH code, sampling S_N data, smoothing, and void transport. The second, "Coupled Discrete Ordinates - Monte Carlo Technique and Application to NERVA"⁵, discussed the information flow, code coupling, and the several analyses to which the method has been applied.

The experience with code coupling in CY 1969 and the success obtained have suggested a number of extensions which may be developed as well. Prominent among them are: (1) a generalization of the detector geometry to allow other than radial intervals on planes; (2) a coupling using Monte Carlo data to begin the coupling process (begun in CY 1969); and (3) neutron energy interface coupling in which only those Monte Carlo histories which have been degraded to below a preset energy will be coupled to S_N for analysis of thermalization.

DASH and the necessary technical description and utilization instructions are being prepared for transmittal to the Radiation Shielding Information Center, Oak Ridge, Tennessee. The first transmittal is expected to take place early in 1970 and will contain all options produced in CY 1969 plus a few of the later improvements which will have been tested at the time of the mailing.

A copy of the DASH Technical Report is included as Appendix A.

III. NEUTRON LIBRARIES

A standard library of neutron cross-sections is becoming available for use in the industry. This library (ENDF/B⁶), a part of the ENDF (Evaluated Nuclear Data File), is a magnetic-tape storage for evaluated nuclear data used in reactor design calculations.

The ENDF/B system is one phase of a larger plan for the automated processing of nuclear data. An ENDF/B tape contains evaluated point data and is intended to serve as direct input to multigroup and Monte Carlo preprocessing codes. It contains one complete set of data for each material. The data on the ENDF/B serve as a reference cross-section set to facilitate inter-laboratory comparisons, and provide small user groups with recommended data. Nuclear data other than that for neutron induced reactions required for reactor applications are not included at this time.

Currently, the energy range on the ENDF/B is from 0.001 ev, or below, to 1.5×10^7 ev, or above. All required data that is nonzero must be specified in some fashion over this range. Included in the requirements are smooth cross-sections (e.g., total, elastic, and fission), the number of neutrons per fission, secondary angular distributions, and secondary energy distributions. Although some data may be represented by parameters used in equations over certain energy intervals, the majority is in tabular form. A large amount of data must be prepared and processed in the generation of an ENDF/B tape.

There are two kinds of programs associated with ENDF/B: (1) those concerned with the data file per se; and (2) those which process the data for use in reactor calculations. There are four programs^{7,8} which maintain and manipulate the data file, and several codes which retrieve and process the file for later calculations. The four programs are:

1. CHECKER - to check the data on an ENDF/B BCD card image tape.
2. CRECT - to correct the data on an ENDF/B BCD card image tape.

3. DAMMET - to Delete, Alter Mode, and Merge ENDF/B tapes.
4. EDIT - edit the data on an ENDF/B tape.

The codes which retrieve data from the ENDF/B tape can be separated into two classes: (1) for use in discrete ordinates programs; and (2) for input to Monte Carlo codes. SUPERTOG⁹ and the SUPERTOG Data Retrieval Code (SNOOPY) draw from the ENDF/B in a format suitable for input to DOT¹ or ANISN¹⁰. Table 1 lists the codes for data retrieval and input to FMC-N and COHORT¹¹. These programs were written by Radiation Research Associates for the specific function as noted.

TABLE 1
MONTE CARLO DATA PREPARATION CODES

<u>FMC-N</u>	<u>COHORT</u>	<u>Data Type Handled</u>
CROS1	CROS2	Elastic, inelastic, fission, and total cross-sections.
SCAT1	SCAT2	Elastic scattering probability tables.
SPCT1	SPCT2	Inelastic neutron spectrum probability tables.

A. CHECKER

CHECKER is a code to check data on an ENDF/B tape in BCD card image form. The main purpose is to insure that the tape is properly structured and that all required fields are completed, rather than to check the physics of the data.

Since the ENDF/B input tape is in the form of BCD data images, the terms "tape" and "deck" are used interchangeably. The nomenclature used in this description and in the error messages printed by CHECKER follows that used in the ENDF/B manual.

B. CRECT

CRECT is a code to correct data on an ENDF/B tape in card image form. Records from tape LIBØ are transferred to memory, corrected if necessary, and then copied onto tape LIBN. Some or all of the material on the tape can be printed on the system output tape (NØUT). The system input tape (NIN) is also used.

C. DAMMET

DAMMET is a service routine to Delete, Alter Mode, and Merge ENDF/B Tapes. It is written in FORTRAN IV for a computer with 20K of available storage. The code requires three tapes plus the system input, output, and scratch (two required) tapes.

DAMMET does not compute or process ENDF/B data but simply transfers data from tape to tape. The logic is simple and straightforward. As a consequence, certain operations may be highly inefficient and involve excessive tape handling time. If available, discs should be used in place of the tapes, particularly the input tapes.

D. EDIT

EDIT is a service routine written in FORTRAN IV, Level H, for the Evaluated Nuclear Data File, Version B (ENDF/B), System. Using EDIT, selected portions of an ENDF/B magnetic tape can be punched on cards and/or printed.

E. SUPERTO

SUPERTO is a program to generate fine-group parameters and group-to-group scattering matrices using basic ENDF/B cross-section data. A calculation to generate resonance data which uses single-level Breit-Wigner resonance

parameters is included in the code. The energy group structure, the order of cross-section expansion, and the spectral weighting function are arbitrary and can be specified by the user. Data can be generated in forms for use in the GAM-I, GAM-II, ANISN, and DOT programs. Auxiliary programs are available for obtaining library tapes for XSDRN¹².

F. CROS1

The CROS1 code is written in FORTRAN IV for the IBM-360. The purpose of the code is to obtain neutron cross-sections from the ENDF/B data tapes for input into the FMC Monte Carlo procedure. The required cross-sections include: (1) elastic; (2) inelastic; (3) fission; and (4) total. They are taken from smooth cross-section data given in File 3 of the ENDF/B data tapes. Output is punched on cards in the proper format for direct input into FMC.

Since only smooth ENDF/B cross-section data is included, hand corrections are required for some elements to account for strong resonance peaks. For energies where strong resonances occur, the File 3 data usually contain abrupt discontinuities which are noted in the printout. Corrections should be made by inserting proper upper- and lower-bound cross-sections based on available data which effectively yield group averages that represent the resonance peaks. Such hand corrections are usually required for only a few energy groups in the lower ev range.

G. CROS2

The CROS2 code is written in FORTRAN IV for the IBM-360. The purpose of the code is to obtain neutron cross-sections from the ENDF/B data tapes for input into the COHORT Monte Carlo procedure. The cross-sections required for input into Library 4 of the H01, A01, and A02 routines of COHORT include: (1) total; (2) total scattering; and (3) elastic scattering. The cross-sections are taken from the smooth cross-section data given in File 3 of the ENDF/B tapes. Output is punched on cards for direct input into COHORT.

Since only smooth ENDF/B cross-section data are included, hand corrections are required for some elements to account for strong resonance peaks. For energies where strong resonances occur, the File 3 data usually contain abrupt discontinuities which are noted in the CROS2 printout. Corrections should be made for these energies by inserting point cross-sections on the basis of available data which effectively yield group averages that represent the resonance peaks. Such hand corrections are usually required for only a few energies in the lower ev range.

H. SCAT1

The SCAT1 code calculates elastic scattering probability tables from information given on the ENDF/B data tapes for input into FMC. The required FMC tables contain data in the form of cumulative probability distributions with corresponding scattering angle cosines for each material and each incident neutron energy group. SCAT1 is designed to produce the required probability tables from the ENDF/B tape data which may be in the form of tabulated probabilities or Legendre polynomial coefficients. The FMC data are punched on cards in the proper format for direct input into the code. SCAT1 is written in FORTRAN IV for the IBM-360 system.

I. SCAT2

The SCAT2 code is used to provide differential elastic scattering cross-section data suitable for input into the COHORT Monte Carlo procedure. The data required for input into Library 7 of the H01 and A01 codes of COHORT are in the form of cosines of the center-of-mass scattering angles for equal probability intervals. SCAT2 is designed to produce cosines for equal probability intervals from data on the ENDF/B data tapes. Elastic scattering data are in the form of tabulated probabilities or Legendre polynomial coefficients. Scattering angle cosines for 20 equal-probability intervals for each incident energy are punched on cards in the proper format for direct input into the COHORT codes. SCAT2 is written in FORTRAN IV for the IBM-360 system.

J. SPCT1

The SPCT1 code was written to provide inelastic neutron spectrum probability tables for input into the FMC Monte Carlo procedure. The probability tables for exciting discrete energy levels are obtained from the ENDF/B data tapes for the low incident neutron energies. At energies above those for which the discrete excitation levels are defined on the ENDF/B data tapes, the nuclear temperature as a function of incident neutron energy is given. In this incident energy range, the inelastic neutron spectrum is assumed to be a continuum which may be described by a Maxwellian distribution which is used to calculate excitation probabilities for pseudo-excitation levels that are distributed over the continuum. These pseudo-excitation levels are used to approximate the continuum.

The probability tables are punched on cards for direct input into FMC. SPCT1 is written in FORTRAN IV for the IBM-360.

K. SPCT2

The SPCT2 code was written to provide inelastic neutron spectrum probability tables for input in the Hol code of the COHORT procedure. Probability tables for exciting discrete energy levels are obtained directly from the ENDF/B data tapes for low incident energies. For energies above those defined by discrete excitation levels on the ENDF/B data tapes, the nuclear temperature is given as a function of incident energy. In this incident energy range, the inelastic neutron spectrum is assumed to be a continuum that is defined by a Maxwellian distribution which is used to calculate excitation probabilities for pseudo-excitation levels that are distributed over the continuum and used to approximate the continuum. The probability tables are punched on cards for direct input into H01. SPCT2 is written in FORTRAN IV for the IBM-360.

During the contract year, the Monte Carlo data preparation codes were used to generate cross-section data for hydrogen, chromium, iron, nickel, carbon, molybdenum, tungsten, gold, manganese, copper, niobium, oxygen, and boron-10.

IV. BIASING

Monte Carlo calculations are based upon the mathematical simulation of many individual particles, following them through all interactions from source to eventual loss from, or absorption within, the system. By summing the particles arriving at any location of interest and normalization to the real source strengths, the appropriate response at that location to the simulated source can be calculated. This approach can be termed analog Monte Carlo since it is essentially a mathematical analog to reality.

Unfortunately, a complete analog calculation is practical only in the simplest cases. If few of the original particles arrive at the region of interest because of a large source-to-detector distance or intervening shields, most of the computing time does not affect the results. To improve efficiency in Monte Carlo calculations, many techniques have been devised which seek to limit the consideration of ineffective radiation and accelerate the consideration of effective radiation by appropriate simplifying assumptions.

To a great degree, the application of efficiency improvement techniques (biasing) in Monte Carlo calculations is an art. Great judgement must be exercised in the choice of parameters to limit the error of simplifying assumptions and to avoid the exclusion of significant radiation. Usually, to maintain confidence in the results of a Monte Carlo calculation, these biasing techniques are used conservatively. As a result, the calculation is nearer to the analog case than is necessary, and more computer time is used than might have been needed with a more "educated" judgement.

Ideally, biasing would be optimized by considering any radiation source, direction, or energy in relation to its "importance." This importance, an adjoint function, is a measure of the relative contribution to detector response as measured by the adjoint flux. This flux can be obtained, essentially, by running the analysis backward. To determine the degree of

interaction between it and its surroundings, the detector is treated as if it were the source. Then using this information, those sources, directions, and energies which interact most strongly with the detector are treated in the manner most like reality. Those which interact weakly with the detector are treated in the most approximate manner, and those which interact negligibly are disregarded.

Of course, since any real analysis would probably consider several detectors simultaneously, no single optimum adjoint flux distribution could be determined. An even bigger difficulty in obtaining an optimization by this method is that the "reverse" problem that must be solved to obtain the adjoint flux is of the same order of difficulty and consumes as much computer time as the "forward" problem which calculates the desired final result.

Clearly, some middle ground is necessary. In any attempt to systematize biasing so that undue conservatism need not be employed, an approximation to the adjoint flux would be the best general guide. Such an approximation might be found by calculating the adjoint flux with a more approximate method or by a simpler model using the same method as the forward calculation.

During CY1969, Radiation Research Associates conducted an investigation to determine how an approximation to adjoint flux might be applied to FMC and COHORT at Aerojet-General. As a result of this study, it was recommended that adjoint biasing could result in significant gains in efficiency and that it would be more fruitfully applied to COHORT. Further, it appears that low-order approximations to the adjoint function can be used to evaluate parameters used in standard biasing techniques (e.g., exponential transformation).

Research Note RRA-N931, which discusses these points, is included as Appendix B.

It is anticipated that standard biasing techniques and application of adjoint biasing will be extended in CY1970 with implementation and testing of the methods applied to NERVA problems.

V. GEOMETRY SPECIFICATIONS

The geometry specification scheme used in the FASTER program¹³ was incorporated in Monte Carlo codes FMC-G and FMC-N^{14,15} at the A.R.T. Research Corporation.* This scheme, which is described below, has now been included in the Aerojet-General versions of point kernel codes QAD¹⁶ and GGG¹⁷.

Radiation analyses are often conducted with point kernel codes to obtain preliminary results for parameter studies. These may then be followed by studies using Monte Carlo (FMC) to arrive at more precise results over a limited range of parameters. In these cases, the common specification removes the necessity of repetitious modeling. When only a single method is used, a saving is still achieved, since the FASTER specification is generally more convenient to use than those specifications it replaced, and the initial setup time is thereby reduced.

The most important feature of the Monte Carlo method (in comparison with other transport calculation methods) is its applicability to complicated geometries. This feature is implemented in the FASTER program by utilizing the general quadratic surface equation. The numerical analysis presented below follows that of Reference¹⁸.

The general quadratic equation for a specified surface i is:

$$\begin{aligned} u_i(\vec{r}) = & a_{0,i} + a_{1,i}x + a_{2,i}y + a_{3,i}z \\ & + a_{4,i}x^2 + a_{5,i}y^2 + a_{6,i}z^2 \\ & + a_{7,i}xy + a_{8,i}yz + a_{9,i}zx \end{aligned}$$

where $a_{j,i}$, $j = 0, 1, 2, \dots, 9$ are constants,

$$\vec{r} = x\vec{i} + y\vec{j} + z\vec{k}$$

x, y, z are rectangular coordinates (cm), and

*Superscript numbers indicate references listed in Section VI.

i, j, k are unit vectors parallel to the x -, y -, and z - axes, respectively. The value of this equation, $u_i(\vec{r})$ is zero for points $\vec{r}$ on the surface.

These surfaces are described independently of the regions which define the material distributions to eliminate redundant input. Provision has been made in the FASTER program for recognizing more simple surfaces (e.g., planes, cones, elliptical cylinders, and ellipsoids). The equations for these surfaces are expanded by subroutine GEOMIN to obtain the coefficients of the general equation above.

A summary of the surfaces that can be handled by the FASTER geometry, further description of the numerical analysis, and input instructions for code users can be found in Reference 13.

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APPENDIX A

DASH NUCLEAR CODE, PROGRAM E16903

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APPENDIX A

DASH NUCLEAR CODE

Program E16903

I. TECHNICAL REPORT

A. Abstract

DASH is a FORTRAN IV program designed to process surface angular fluxes generated by the two-dimensional discrete ordinates code, DOT. Using angular fluxes stored on tape by DOT from a cylindrical geometry calculation, DASH calculates angular fluxes on arbitrary cylindrical geometry surfaces outside the DOT boundaries.

The calculation is carried out by a numerical integration of angular fluxes employing a single-event Monte Carlo routine. Particle traces are generated by random sampling of the S_n angular flux histograms or of power series fits to the S_n information. This employment of random sampling avoids the "ray effects" that would occur if DOT were extended to include void or pure absorber regions.

Since flux information internal to DASH has a Monte Carlo format and can be collected into the tables appropriate to an S_n calculation, DASH can be used as a coupling code. Source information can be input to DASH in either S_n or Monte Carlo format and either format can be output for use as source information for a following coupled code.

B. Problem to be Solved

The two dimensional discrete ordinates code, DOT⁽¹⁾, generates a tape on which are tabulated the angular fluxes in the boundary intervals. In order to obtain angular fluxes at a surface outside the boundary of the DOT problem, it is necessary to extend them to this surface in a way that does not reflect the limitations of the calculation, but adequately represents the physical case modelled. Extending radiation paths along the discrete quadrature angles from discrete points at the surface, ray effects⁽²⁾

would result, distributing the radiation at those places which could be "seen" by the relatively small number of paths. By choosing leakage positions and angles randomly, then applying the appropriate flux contributions to the resulting paths, the ray effects can be avoided. Simply extending the DOT geometry to include the external plane would also result in these ray effects unless the extended region contained several mean free paths of scattering material. The flux contribution for any path can be taken as that of the discrete path nearest it, or preferably, that resulting from an interpolation among the discrete paths around it.

An option should be included to account for a possible attenuating region in the region of the particle paths to account for small obstructions.

The angular fluxes obtained at the external plane can be summed to obtain the total fluxes, or a response to them, or can be used as boundary sources for a second DOT problem. Further, since Monte Carlo methods are used to trace fluxes between surfaces, input or output coupling with a Monte Carlo code is feasible.

C. Mathematical Formulation and Method of Solution

1. Vector Geometry

The geometry of a vector from an axial or radial interval I_1 of radius ρ_1 to a radial interval I_2 of radius ρ_2 is shown in Fig. 1.

Fig. 1. Geometry of vector between space intervals in cylindrical geometry.

η and μ are the direction cosines used to describe the quadrature angles in DOT. When I_1 is a radial interval, the normal distance between planes is d and when I_2 is an axial interval, the distance between the plane of I_2 and the plane of the vector origin is d' , where $d' > d$.

Looking in more detail at the geometry in Fig. 2, we can derive the radial position of any vector in the plane of I_2 in terms of η and μ or η and θ_2 .

Fig. 2. Angular description of vector.

$$\eta = \frac{z_1}{v} = \cos\theta_1, \quad \frac{\ell_1}{v} = \sin\theta_1$$

$$\mu = \frac{x_1}{v} = \frac{x_1}{\ell_1} \frac{\ell_1}{v} = \cos\theta_2 \sin\theta_1$$

$$\ell_1 = z_1 \tan \theta_1 = z_1 \frac{\sin \theta_1}{\cos \theta_1} = z_1 \frac{\sqrt{1-\eta^2}}{\eta} = z_1 \sqrt{\frac{1}{\eta^2} - 1}$$

Translating this vector to a second plane, the new radial position and quadrature description are as shown in Figure 3.

Fig. 3. Geometry of vector translation between planes.

It can be seen from Figure 3 that the radial position of the vector at plane 2 is given by ρ_2 , where

$$\rho_2^2 = (\rho_1 + l_1 \cos \theta_2)^2 + (l_1 \sin \theta_2)^2.$$

The angle θ_1 (and thus η) is maintained between planes, whereas θ_2' becomes the other describing angle, where

$$\cos \theta_2' = \frac{l_1^2 + \rho_2^2 - \rho_1^2}{2l_1\rho_2}$$

2. Discrete Angle Intervals

The quadrature angles are described by the direction cosines η and μ and each can be considered to be located by the intersection of two minor arcs on a unit sphere. A common set of quadrature angles for a

fourth order (S_4) calculation are shown in Figure 4. Only 4 of the octants are shown because the geometry is identical for + or - values of the third direction cosine, ξ , since $\xi^2 = 1 - \eta^2 - \mu^2$.

Each quadrature has a weight which can be visualized in Figure 4 as the fractional surface area of the hemisphere associated with a particular angle. Each surface area is bounded by a constant η latitude

Fig. 4. Symmetric S_4 quadratures on unit sphere.

and a constant θ_2 , giving the appearance of an "igloo" when the boundaries are marked on the surface of the sphere. In this instance, all of the weights are the same, thus resulting in all of the "blocks" of the igloo having the same surface area. Angles 1, 6, 9, and 14 of Figure 4 are necessary for solution of the quadrature problem, but have a zero weight associated with them.

3. Flux Integration

Angular fluxes are available from DOT for each quadrature angle from each radial or axial surface interval. Given a point or sequence of points within an interval from which a vector representing a particle path emerges, one could calculate the proper interval(s) to which a flux contribution is made on surface 2. If the vectors are simply the quadrature angles, it is likely that "ray effects" will result. That is, there may be regions in which a confluence of quadrature angles result in maxima and minima with no physical origin. In an extreme case, for distances between planes of the order of source dimensions or greater, there may be regions which cannot be connected to source regions by any quadrature angle vector, resulting in a null. These effects would be reduced by allowing vectors to emerge at any angle within the interval defined by the igloo section for that particular quadrature.* Using randomly chosen angles from random positions within the interval, each case can be tested for intersection with an interval of surface 2 and a contribution to the flux tabulated according to number of such vectors generated (number of histories), relative interval sizes, and the appropriate angular flux. Tables of flux for quadrature angles in the half-space containing surface 2 are then available for each surface interval in surface 2 and can be used as boundary sources for a second DOT problem. This analysis is repeated for each energy group.

The polar angle, θ_1 , may be chosen by sampling in θ_1 or $\eta = \cos\theta_1$. If sampled in θ_1 , biasing will occur such that greater detail will be observed near the $\theta_1=0$ (or $\eta = 1$) polar axis than near the equator. If

* This method would not remove ray effects that may have appeared in the DOT problem, but would avoid amplifying them or creating new ones in the region described by DASH.

sampled in η , detail will be uniform for all polar angles. If sampled in η , the flux at the k^{th} interval of surface 2 is given by

$$\phi_k = \sum_{i=1}^{NI} \sum_{n=1}^{NH} \frac{\phi_{in} \frac{A_i}{A_k} \left| \frac{\gamma_1}{\gamma_2} \right|_n \delta_{ikn}}{NH \frac{W_n}{WGEN}}$$

and if sampled in θ_1 , by

$$\phi_k = \sum_{i=1}^{NI} \sum_{n=1}^{NH} \frac{\phi_{in} \frac{A_i}{A_k} \left| \frac{\gamma_1}{\gamma_2} \right|_n \sin \theta_1 \delta_{ikn}}{NH \frac{W_n}{WLEVL2} \frac{\Delta \eta}{\cos^{-1} \eta_{\min}}}$$

If the n^{th} trace intersects the i^{th} leakage interval and k^{th} receiver interval, $\delta_{ikn} = 1$ and $= 0$ if not. ϕ_{in} is the angular flux of the n^{th} trace at the i^{th} interval. A_i and A_k are the areas of the leakage and receiver intervals, respectively. NI is the number of leakage intervals and NH is the number of histories traced per interval. W_n is the weight associated with the particular quadrature region in which the trace falls. $WGEN$ is the sum of weights for all regions in which histories are generated. $WLEVL2$ is the sum of weights on the level defined by a single quadrature polar cosine in which the trace falls. $\Delta \eta$ is the difference between the boundary cosines defining the level in which the trace falls. $\eta_{\min}$ is the value of η defining the boundary of polar angles considered. γ_1 and γ_2 are the cosines of the angles between the trace vector and normals to the interval surfaces.

The angular leakage flux ϕ_{in} is taken as either of two options: (a) the quadrature flux for the particular "block" of the igloo in which the generated path falls, or (b) a value resulting from a least-squares fit to the discrete leakage fluxes. If the first option is used, the leakage can be viewed as a histogram in the two independent quadrature cosines, with constant leakage flux within each angular region. Similarly, the same quadrature histogram is used throughout each space interval. If the second option is used, a series of least-squares fits will be performed in order to apply fluxes to the generated paths which are interpolated from among the one

spatial and two angular coordinates. The flux so obtained is of the form

$$\phi = \psi_R(r) \psi_E(\eta) \psi_M(\mu)$$

where ψ_R , ψ_E , and ψ_M are fits, respectively, to ϕ_R , ϕ_E , and ϕ_M with

$$\begin{aligned} \phi_R &= \sum_{\eta} \sum_{\mu} \phi(r, \eta, \mu) W(\eta, \mu), \\ \phi_E &= \frac{\sum_{\mu} \phi(r, \eta, \mu) W(\eta, \mu)}{\phi_R \sum_{\mu} W(\eta, \mu)} \quad \text{for each radial interval,} \end{aligned}$$

and

$$\phi_M = \frac{\phi(r, \eta, \mu)}{\phi_R \phi_E} \quad \text{for each } \eta \text{ level within each radial interval.}$$

The fits are performed using a power series

$$\phi(x) = a_1 + a_2 x + a_3 x^2 + a_4 x^3$$

where x represents the appropriate independent variable r , z , η , or μ .

4. Attenuation

For any material obstructing the radiation through which the radiation has a mean free path $1/\Sigma$, the reduction in flux due to attenuation would be

$$e^{-\Sigma \delta v}$$

where v is the length of the trace vector, and δ is the fraction of that vector length which passes through the material

so that

δv is the path length in the material.

The regions of attenuating material can be described as disks, rings, or cylinders by defining the inner and outer radii and the upper and lower axial locations. An off-axis cylinder can be approximated if the results of the DASH calculation are to be used in two dimensions only.

Azimuthal flux variations resulting from the cylinder cannot be calculated. The resulting fluxes in R,Z must represent an azimuthal average. The cylinder is approximated by a section of a ring with cross-sectional area equal to the cross sectional area of the cylinder. The transmitted fraction with such a ring section is

$$A_F = FA + (1-F)$$

where A is the transmitted fraction with the entire ring and

$$F = \frac{D^2}{4(R_2^2 - R_1^2)}$$

with D the diameter of the cylinder and R_1 and R_2 the inner and outer radial locations of the cylinder walls.

5. Statistics

Since the fluxes are determined by a summing of simulated particle paths, a statistical accuracy can be estimated. This can provide the basis for choice of a number of histories to be traced.

If n_i is the number of successful incidents in a radial interval I_2 from a particular interval I_1 and quadrature, the flux would be given by

$$\phi_2 = \frac{n_i}{N_i} C_i$$

where N_i histories are available as possible incidents and C_i is the appropriate coefficient giving the correct flux contribution from an incident of type i. Summing over I such types of incidents (to account for flux from all I_1 and/or quadratures),

$$\phi_2 = \sum_{i=1}^I \frac{n_i}{N_i} C_i$$

For different sets of random numbers, slightly different values of n_i , and thus of ϕ_2 , would result. The best value of n_i would be some average value $\bar{n}_i$ of a large number of measurements. Assuming a Poisson distribution of events, the probability of observing n_i from a possible N_i

events would be

$$P(n_i/N_i) = \frac{(f_i N_i)^{n_i}}{n_i!} e^{-f_i N_i}$$

where f_i is the fraction of successes for $N_i \rightarrow \infty$. Now

$$\overline{n_i} = \sum_{n_i=0}^{\infty} n_i P(n_i/N_i) = f_i N_i$$

This can be obtained only by taking an infinite number of histories.

An estimate of the uncertainty in the flux obtained after a finite number of histories is given by the standard deviation of ϕ_2 as calculated from the above expressions. This is given by

$$\sigma[\phi_2] = \{V[\phi_2]\}^{1/2}$$

where $V[\phi_2]$ is the variance of ϕ_2 .

$$V[\phi_2] = V\left[\sum_{i=1}^I \frac{n_i}{N_i} C_i\right] = \sum_{i=1}^I \left(\frac{C_i}{N_i}\right)^2 V[n_i]$$

Again assuming a Poisson distribution,

$$V[n_i] = \sum_{n_i=0}^{\infty} (n_i - \overline{n_i})^2 P(n_i/N_i) = \overline{n_i}$$

so that

$$V[\phi_2] = \sum_{i=1}^I \left(\frac{C_i}{N_i}\right)^2 \overline{n_i}$$

and

$$\sigma[\phi_2] = \left\{ \sum_{i=1}^I \left(\frac{C_i}{N_i}\right)^2 \overline{n_i} \right\}^{1/2}$$

As before, $\overline{n_i}$ cannot be determined in a finite number of histories, but where n_i can be used as an estimate of $\overline{n_i}$ in the calculation of ϕ_2 , it can be used also as an estimate in the calculation of $\sigma[\phi_2]$.

Therefore,

$$\phi_2 \approx \sum_{i=1}^I \frac{n_i}{N_i} C_i$$

and

$$\sigma[\phi_2] \approx \left\{ \sum_{i=1}^I \left(\frac{C_i}{N_i} \right)^2 n_i \right\}^{1/2}$$

D. Nomenclature

Symbols

A	Fraction of radiation transmitted through an attenuating material.
A _F	Fraction of radiation transmitted through a section of an attenuating material.
A _i	Area of leakage interval, cm ² .
A _k	Area of receiver interval, cm ² .
C _i	Coefficient giving flux contribution from fraction of histories striking an interval.
F	Fractional area of ring in a section approximating an off-center cylinder.
I ₁	Any radial or axial surface interval at which angular fluxes are available from DOT.
I ₂	Any radial surface interval at which DASH calculates angular flux, using DOT results.
N _i ,NH	Number of histories tested.
P(n _i /N _i)	Probability of n _i successes in N _i tries, Poisson distribution.
V	Variance.
W _n	Weight of quadrature in region of which trace n is generated.
WGEN	Sum of weights of all quadratures in whose regions histories are traced.
WLEVL2	Sum of weights of all quadratures in a given level.
a	Power series coefficients for least-squares fit.
d	Distance between planes of I ₁ radial intervals and I ₂ radial intervals.

Symbols

d'	Distance between plane containing point in I_1 axial interval and plane of I_2 radial intervals, cm.
f_i	Fraction of histories of type i that intersect I_2 .
ℓ_1	Projection on the XY plane of a vector displaced distances x_1 , y_1 , and z_1 along the X, Y, and Z coordinates, cm.
n_i	Number of histories of type i successfully reaching an interval.
v	Length of vector, cm.
x_i	Displacement of a vector along the X-axis, cm.
y_i	Displacement of a vector along the Y-axis, cm.
z_i	displacement of a vector along the Z-axis, cm.
γ_1	Cosine of the angle between the particle path vector and the normal to the surface of interval I_1 .
γ_2	Cosine of the angle between the particle path vector and the normal to the surface of interval I_2 .
δ_{ikn}	= 1 if trace vector n intersects both the i^{th} leakage interval and the k^{th} receiver interval, = 0 if not.
δ	Fraction of vector passing through obstructing material.
η	The cosine of the angle between the Z-axis and the particle path vector.
θ_1	The angle between the Z-axis and the particle path vector, radians.
θ_2	The angle between l_1 and ρ_1
θ'_2	The angle between l_1 and ρ_2
μ	The cosine of the angle between the X-axis and the particle path vector.
ξ	The cosine of the angle between the Y-axis and the particle path vector.
ρ_1	The radial position in interval I_1 (leakage plane) at which the particle path vector originates, cm.
ρ_2	The radial position at which the particle path vector intersects the receiver plane.
σ	Standard deviation.
ϕ_1	The angular flux in interval I_1 , particle-cm/unit wt-cm ³ -sec.

Symbols

ϕ_2	The angular flux in interval I_2 , particle-cm/unit wt-cm ³ -sec.
ϕ_{in}	Flux due to trace n from interval i .
ϕ_R, ϕ_E, ϕ_M	Functions fit to r , η , and μ , respectively, to interpolate angular fluxes.
ψ_R, ψ_E, ψ_M	Values of the separable flux functions calculated from the power series fits, resulting in interpolated flux values.
Σ	(1) Macroscopic cross-section (1/mean free path) for radiation through obstructing material, cm ⁻¹ , or (2) sign indicating summation of the following values.
$\Delta\eta$	Difference between values of η bounding a quadrature level.

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APPENDIX B

THE APPLICATION OF ADJOINT BIASING TO MONTE CARLO

By

M. B. Wells and J. D. Marshall

APPENDIX B

I. INTRODUCTION

Most radiation transport calculational methods do not lend themselves readily to problems which deal with complicated geometrical configurations. The noted exception to this is the Monte Carlo method. Because of this ability to treat complicated geometries, it appears that Monte Carlo should be applied to most transport calculations; however, application of the analog Monte Carlo method to transport problems where results are desired at several mean-free-path distances from the source regions can lead to unacceptable statistical results. This is obviously caused by an insufficient number of particles being transported to the region of interest. The brute force method of increasing the number of histories until the variance of the answer becomes acceptable is not feasible since the increase in computer time and subsequent increase in cost would be monumental. One means of improving answers obtained in deep-penetration calculations is the application of biasing or variance reduction techniques in the selection of randomly selected variables. The purpose of this note is to discuss how biasing functions or importance functions obtained from adjoint solutions of the transport equation for problems which have uncomplicated geometrical configurations may be applied to Monte Carlo calculations which include detail geometrical descriptions.

APPENDIX B

II. THE TRANSPORT EQUATION

The conservation equation for particle transport is given by the expression

$$X(P)dP = S(P)dP + \int dP' X(P') K(P' \rightarrow P) dP \quad (1)$$

where dP is a incremental volume in phase space about the point P and

- $X(P)dP$ = the expected number of particles from collisions or sources, which are leaving the volume element dP ,
- $S(P)dP$ = the expected number of particles which are created within the volume dP by extraneous sources,
- $K(P' \rightarrow P)dP$ = the expected number of particles which have collisions in dP and come from collisions which occurred at phase space position P' .

Particles which leave sources at positions P' are included in the $K(P' \rightarrow P)dP$ term and may be thought of as zeroth order collisions. Usually the term $K(P' \rightarrow P)$ is split into two multiplicative factors as follows:

$$\begin{aligned} K(P' \rightarrow P)dP &= K(E' \rightarrow E, \vec{r}' \rightarrow \vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) dE d\vec{r} d\vec{\Omega} \\ &= T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) dE d\vec{r} d\vec{\Omega} . \end{aligned} \quad (2)$$

The term $T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) d\vec{r}$ is the usual transport kernel and $C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})$ is the corresponding collision kernel. C may or may not be a function of the position vector $\vec{r}$ depending upon the variation of material or cross sections with respect to position. If cross sections are constant for all $\vec{r}$, then the $\vec{r}$ dependence of C is removed. Using T and C the transport equation may be rewritten as follows

$$\begin{aligned} X(\vec{r}, E, \vec{\Omega}) d\vec{r} dE d\vec{\Omega} &= S(\vec{r}, E, \vec{\Omega}) d\vec{r} dE d\vec{\Omega} + \\ \iiint d\vec{r}' dE' d\vec{\Omega}' X(\vec{r}', E', \vec{\Omega}') &T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) d\vec{r}' dE' d\vec{\Omega}' \end{aligned} \quad (3)$$

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If one wishes to obtain the quantity λ then

$$\lambda = \iiint F(\vec{r}, E, \vec{\Omega}) X(\vec{r}, E, \vec{\Omega}) d\vec{r} dE d\Omega \quad (4)$$

where λ may be referred to as an eigenvalue and $F(\vec{r}, E, \vec{\Omega})$ is the response function for λ . Depending on the form of $F(\vec{r}, E, \vec{\Omega})$, λ may be fluence, current, dose, energy fluence, or energy current. The integral for λ is usually obtained by the use of statistical estimation as part of the Monte Carlo calculation.

III. IMPORTANCE BIASING AND ADJOINT FORMULATION

If randomly chosen variables are selected using probability density functions other than those defined by S and K , then the selections are said to be biased. Equation (1) can be modified by multiplying the equation by a function $I(P)$ with a normalization constant α as follows:

$$\frac{X(P)I(P)}{\alpha} = \frac{S(P)I(P)}{\alpha} + \int \frac{X(P')I(P')}{\alpha} K(P' \rightarrow P) \frac{I(P)}{I(P')} dP' \quad (5)$$

where $\alpha = \int I(P) dP$.

The eigenvalue equation then becomes

$$\lambda = \int \frac{F(P)\alpha}{I(P)} \frac{X(P)I(P)}{\alpha} dP. \quad (6)$$

Equations (5) and (6) may then be rewritten as follows

$$\tilde{X}(P) = \tilde{S}(P) + \int \tilde{X}(P') \tilde{K}(P' \rightarrow P) dP' \quad (7)$$

and

$$\lambda = \int \tilde{F}(P) \tilde{X}(P) dP \quad (8)$$

Note that these are in the same form as the original equations.

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Application of the above transformation will be no better than use of the original equations unless the arbitrary function $I(P)$ is chosen such that it reduces the variance of λ for a given sample size. If a judicious choice of $I(P)$ is made such that particles will be transported to regions near points of interest, then the desired results will occur. The selection of parameters according to their importance in contributing to the desired answer, lends the name of "importance function" to $I(P)$.

One method of obtaining a function which is a reasonable choice for $I(P)$ is through the use of the adjoint formulation of the original problem. The adjoint formulation may be written as follows:

$$V(P)dP = F(P)dP + \int dP' K(P \rightarrow P') V(P')dP \quad (9)$$

and $\lambda = \int S(P)V(P)dP \quad (10)$

where λ is the same eigenvalue as obtained from equation (4). $V(P)dP$ may be interpreted as the expected contribution to λ of particles emerging from collisions in dP about P . Hence $V(P)$ should always be a reasonable choice of $I(P)$.

If equations (9) and (10) could be solved exactly, then there would be no need to pursue the problem further since the eigenvalue λ would be known. Since the same geometrical conditions exist for the application of these equations as exist for the application of equations (3) and (4), equations (9) and (10) cannot in general be applied to problems which contain complicated geometrical constraints. However, the adjoint equations could be applied to a simplified problem whose geometrical configuration has the same characteristics as that of a more complicated problem. Then the solution of the adjoint equation for the simplified geometry should yield a function which would be a good choice for the importance function to be used in the Monte Carlo calculation for the more complicated geometry.

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It must be noted that the importance function $I(\vec{r}, E, \vec{\Omega})$ is defined for a given value of the response function, which, in turn, fixes the spatial location for which λ is to be evaluated. If λ is to be evaluated at more than one spatial position, then it is highly unlikely that acceptable results would be obtained for those receiver positions for which the optimum importance function differed significantly from the importance function used in the Monte Carlo calculation.

To make use of the full adjoint it would be highly desirable to have a means of selecting collision sites and energies and directions of motion after collision. To do so means that one make use of the spatial, energy and direction parameters defined by the adjoint, $V(\vec{r}, E, \vec{\Omega})$.

Let us examine the function $\hat{K}(P' \rightarrow P)$ for the case of a three dimensional geometry. We have that

$$\begin{aligned} \hat{K}(P' \rightarrow P) &= T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) \times \\ &I(\vec{r}, E, \vec{\Omega}) / I(\vec{r}', E', \vec{\Omega}'). \end{aligned} \quad (11)$$

If we can evaluate the integral

$$\bar{\alpha}(\vec{r}', E', \vec{\Omega}') = \int T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) \frac{I(\vec{r}, E', \vec{\Omega}')}{I(\vec{r}', E', \vec{\Omega}')} d\vec{r} \quad (12)$$

then $\hat{K}(P' \rightarrow P)$ can be rewritten as

$$\begin{aligned} K(P' \rightarrow P) &= \left[\frac{T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) I(\vec{r}, E', \vec{\Omega}')}{\bar{\alpha}(\vec{r}', E', \vec{\Omega}') I(\vec{r}', E', \vec{\Omega}')} \right] \times \\ &\left[\frac{\bar{\alpha}(\vec{r}', E', \vec{\Omega}') C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) I(\vec{r}, E, \vec{\Omega})}{I(\vec{r}, E', \vec{\Omega}')} \right] \end{aligned} \quad (13)$$

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Thus, the collision site could be selected from $I(\vec{r}, E', \vec{\Omega}')$ which is dependent on the energy and direction after the previous collision and the energy and direction after collision can be selected from $I(\vec{r}, E, \vec{\Omega})$, which is dependent on the collision position, $\vec{r}$.

IV. EXAMPLES OF ADJOINT BIASING IN MONTE CARLO

There have been several studies undertaken to investigate the application of adjoint biasing in Monte Carlo calculations. Kalos (Ref. 1) applied an importance function estimated from the importance of the last and next-to-last flight contributions to a study of neutron transport in a one-dimensional slab of hydrogen. For the case of hydrogen, an analytical approximation of the energy dependence of the cross section is possible since it is a monotonically decreasing function of energy. An analytical expression for the probability of scattering through a given angle made it feasible for Kalos to incorporate the energy-angle correlation into the importance function. He was able to write the importance function as an analytic expression. Using this function to sample angles and distances to collisions, it was possible for Kalos to calculate the dose due to 8.1-Mev neutrons through 179 mean-free-paths of hydrogen.

Armstrong (Ref. 2) extended the ideas of Kalos to the case of gamma-ray transport in slabs of water and lead. The scattering cross section may be expressed analytically the Klein-Nishina formula, thus it was possible to include the energy-angle correlation. Armstrong found that an importance function based on the importance of last-flight gammas to the quantity of interest at the receiver resulted in gamma-ray transport calculations that were about 100 times more efficient than the use of a simple space-dependent exponential transform. When using the importance function he found that approximately an equal gain in efficiency was obtained with energy- and angle-dependent spatial biasing as was obtained with biasing only on the collision kernel.

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In both the work of Kalos and Armstrong it was possible to estimate the importance function by the use of simple physical models. These models, which are estimates of the adjoint, gave expressions for the importance function which were found to be reasonable importance functions. In most cases of three dimensional geometry it is not possible to develop simple models for estimating the adjoint. Therefore, one must resort to a numerical representation of the importance function.

Cain (Ref. 3) has used a one-dimensional discrete ordinance calculation to determine the adjoint for a simple geometrical model. The results were then used as importance functions in a three-dimensional Monte Carlo calculation. The initial problem was that of a monodirectional source normally incident on the centerline of a LiH SNAP-2 shield, which was surrounded by an iron and transformer oil collar. Since the computations were made to determine the fast-neutron dose behind the shield, the response function used in the adjoint calculation was the energy-dependent flux-to-dose conversion factors. Therefore, the source employed in the adjoint calculation was this response function which was placed in the most forward angular bin. Numerical values of the energy, angle, and spatial dependence of the importance function were obtained. The use of the one-dimensional S_n calculated adjoint solution as a step function in space importance function in the LiH shield problem resulted in a reduction in variance of a factor of 4 to 5 over that obtained using an empirically determined importance function.

In a later study Cain tried an importance function which was an analytical fit to the results of an adjoint calculation. The flexibility of an analytic function was found by Cain to be a great advantage in the application of adjoint biasing. With such an analytical fit he was able to obtain a calculation for the LiH shield that was a factor of 36 better than that obtained by trial and error biasing.

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V. AN APPROACH FOR USE OF ADJOINT IMPORTANCE FUNCTIONS IN AN EXISTING MONTE CARLO PROCEDURE

First let us assume that importance functions can be obtained from an adjoint solution of a similar but simpler geometry than the one to which the Monte Carlo method is to be applied. The results of such a calculation would yield numerical values for the importance function. The first question which must be answered is; in what form can these results be used in a Monte Carlo procedure? One approach would be to determine a function which closely represents the numerical values. A guide in determining the form of the analytical expressions may be obtained from a simple importance function model. One may estimate the importance by the value of the last and next to the last flight contributions to $V(P)$. In terms of the adjoint, this means an approximation of V by the first two terms of a Neumann series,

$$V(P) \simeq V^0(P) + V^1(P) \quad (14)$$

$$\text{where} \quad V^0(P) = F(P) \quad (15)$$

$$\text{and} \quad V^1(P) = \int K(P \rightarrow P') F(P) dP'. \quad (16)$$

The specific form of $V(P)$ depends on the particular problem. Physical conditions may provide the expected shape of the value function for which the magnitude may be obtained from the results of an adjoint calculation.

Another approach to using the adjoint solution as an importance function would be that of direct employment of the numerical values of the adjoint solution. To determine the adjoint for a three-dimensional problem, one would first make approximations in the geometry so that it could be represented by a one-dimensional geometry. The adjoint for the one-dimensional geometry could then be used to approximate the adjoint for the three-dimensional geometry. The three-dimensional geometry will then be divided into a number, j , of volumes, v . For each of these volumes the adjoint will be used to approximate the importance function $I(v_j, E_k, \vec{\Omega}_1)$, where the energy range is divided into K

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intervals, E_k , and the solid angle about v_j is divided into L intervals, $\vec{\Omega}_1$. The initial direction of particles leaving the source will be taken to be defined by the importance function for the volume v_j containing the source. If more than one volume contains the source, then the importance functions for those volumes will be used to select the volume from which a history is to be started. The importance functions at the source energy and direction selected for all of the volumes lying along a line from the source point in the direction $\vec{\Omega}$, selected for the initial direction of the history, will be used to form a cumulative distribution to determine the location of the collision point. Let us assume that the collision occurred in volume v_n . Then the importance function for that volume will be used to select an energy and direction after collision. Weights will be used to account for the bias introduced in the calculation. In a program such as COHORT, the weight, energy, and direction before collision, the type of collision, and the collision position could be stored on magnetic tape for use in an analysis procedure with which the eigenvalue λ can be computed.

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RECOMMENDATIONS

From the application of adjoint biasing, as illustrated by Kalos, Armstrong, and Cain to simple-geometry problems, it was seen that significant gains in the efficiency of a Monte Carlo calculation is possible. In implementing an "exact adjoint" biasing, this means that the biasing is for one detector location and a detector quantity specified by the response function $F(P)$. Such an implementation appears to be easier to accomplish in COHORT than in any other Monte Carlo procedure now in use at Aerojet-General. It is therefore recommended that the COHORT procedure be modified so as to include a systematic application of the adjoint in selecting collision sites, energies, and directions from the transport and scattering kernels of the integral transport equation. Such a modification would provide a tool that could be used to study the application of adjoint biasing to nuclear rocket transport problems in which transport is highly geometry dependent.

The V^0 approximation of the adjoint that has been used by Armstrong as an importance function closely resembles the exponential transform function. Although Armstrong found that implementation of the full importance function as given by the adjoint was about 100 times more efficient than use of a simple space dependent exponential transform, it would appear that use of the adjoint in determining the parameters to be used in the exponential transformation would be much more efficient than the trial and error method now used. Both COHORT and FMC provide options for using an exponential transform that is dependent on spatial position and direction of motion. A study of the application of the adjoint to determining optimum values of the exponential transform biasing parameter as used in COHORT and FMC is recommended.

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